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(Article begins on next page)

Refinement strategies for polygonal meshes applied to adaptive VEM discretization.[☆]

Stefano Berrone^{a,b,*}, Andrea Borio^{a,b}, Alessandro D’Auria^{a,b}

^a*Dipartimento di Scienze Matematiche, Politecnico di Torino
Corso Duca degli Abruzzi 24, Torino, 10129, Italy*

^b*Member of the INdAM research group GNCS*

Abstract

In the discretization of differential problems on complex geometrical domains, discretization methods based on polygonal and polyhedral elements are powerful tools. Adaptive mesh refinement for such kind of problems is very useful as well and states new issues, here tackled, concerning good quality mesh elements and reliability of the simulations. In this paper we propose several new polygonal refinement strategies and numerically investigate the quality of the meshes generated by an adaptive mesh refinement process, as well as optimal rates of convergence with respect to the number of degrees of freedom. Among the several possible problems in which these strategies can be applied, here we have considered a geometrically complex geophysical problem as test problem that naturally yields to a polygonal mesh and tackled it by the Virtual Element Method. All the adaptive strategies here proposed, but the “Trace Direction strategy”, can be applied to any problem for which a polygonal element method can be useful and any numerical method based on polygonal elements and can generate good quality isotropic mesh elements.

Keywords: Mesh adaptivity, Polygonal mesh refinement, Virtual Element Method, Simulations in complex geometries, A posteriori error estimates
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*Corresponding author

Email addresses: stefano.berrone@polito.it (Stefano Berrone),
andrea.borio@polito.it (Andrea Borio), alessandro.dauria@polito.it (Alessandro D’Auria)

1. Introduction

In last years, a growing interest has arisen for the development of numerical methods for the solution of partial differential equations using general polygonal meshes. These methods are well suited for handling domains featuring geometrical complexities that can yield situations where the generation of good quality conforming triangular meshes can be particularly expensive or even unfeasible. On the other hand, the use of polygonal and polyhedral elements in conjunction with adaptive mesh refinement states new problems. In this paper we investigate several refinement strategies for polygonal meshes.

As model problem to test the different refinement strategies we consider the simulation of flow in a fractured medium. When fractures are represented as intersecting planar polygons, this problem naturally yields to polygonal meshes as first step of mesh generation (computation of the sub-fractures) and in this context the proposed refinement strategies can be part of the mesh production process and not only of the mesh refinement process, more details are provided in Section 4. Nevertheless we want to stress that the proposed refinement strategies can be applied to any problem for which a polygonal mesh can be valuable.

Flow simulation in underground fractured media is a key aspect in many applications such as aquifers monitoring, nuclear waste disposal, CO_2 geological storage or control of contaminant dispersion in the subsoil. In those situations where the rock matrix can be considered perfectly impervious, the Discrete Fracture Network (DFN) model is often used, representing fractures as planar polygons randomly intersected in the 3D space [1, 2, 3, 4]. These kind of domains usually present many geometrical challenges, in particular when a conforming mesh is required, for example in order to apply standard finite element approaches. To circumvent these difficulties, many approaches have been devised, relying on domain decomposition techniques [5, 6], or devising particular meshing strategies [7, 8, 9, 10], or using extensions of the finite element method [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]. In [22, 23], a PDE-constrained optimization approach was devised, enabling for the use of completely non-conforming meshes, where finite element, extended finite element [24] or virtual element spaces [25] can be used. Here we follow the approach based on the Virtual Element Method (VEM) [26, 27, 28, 29] first introduced for DFN flow simulations in [25] and extended in [30, 31, 32].

The huge cost of large scale simulations on the scale of a geological basin raises the issue of efficiency. Moreover, due to the large uncertainty in geometrical configurations and hydrogeological parameters a stochastic approach is advisable yielding to the need of many simulations. Beside efficiency, reliability of these simulations is of crucial importance being connected with risk analysis of human activities. Efficiency and reliability strongly affect the application of uncertainty quantification techniques for the estimation of relevant quantities of interest [33, 34]. For these reasons adaptivity plays a key role both on the side of reliability and efficiency.

Although we focus on the simulation of flow in DFN using VEM, the refinement strategies explored here are suitable for any kind of method relying

on polygonal meshes, except for the so-called “Trace Direction” refinement, that is particularly suited for DFN problems taking into account the behaviour of the solution approaching the traces. The approach here followed is based on isotropic *a posteriori* error estimates and aims at generating good quality isotropic polygonal elements. Anisotropic estimates and mesh refinement strategies are currently under investigation in [35]. Other *a posteriori* error estimates and mesh refinement strategies can be found in [36, 37, 38]. In [37], *a posteriori* error estimates are applied to curved virtual elements, in [36] and [38] hp virtual elements are considered, the *a posteriori* error estimate in [38] being based on equilibrated fluxes.

In Section 2 we introduce the DFN model used to test the refinement strategies and define some useful notations. In Section 3 we introduce its Virtual Element discretization, we define the error estimators and state the *a posteriori* error estimate. In Section 4 we show an algorithm to generate a globally conforming polygonal mesh for DFNs. This algorithm can be also applied to generate conforming polygonal mesh for 2D domains with embedded 1D subdomains. In Section 5 we describe the adaptive algorithm, and some polygonal refinement strategies that preserve the global conformity of the mesh. In Section 6 we validate their application to some test cases with known solution, and, in Section 7, we analyse some results on a more realistic DFN. In Section 8 we draw conclusions concerning the refinement strategies and the quality of the meshes that are produced.

2. Discrete Fracture Networks

Let us consider a set of open convex planar polygonal fractures $F_i \subset \mathbb{R}^3$ with $i = 1, \dots, N$, with boundary ∂F . A DFN is $\Omega = \bigcup_i F_i$, with boundary $\partial\Omega$. Even though the fractures are planar, their orientations in space are arbitrary, such that Ω is a 3D set. The set $\Gamma_D \subset \partial\Omega$ is where Dirichlet boundary conditions are imposed, and we assume $\Gamma_D \neq \emptyset$, whereas $\Gamma_N = \partial\Omega \setminus \Gamma_D$, is the portion of the boundary with Neumann boundary conditions. Dirichlet and Neumann boundary conditions are prescribed by the functions $h^D \in H^{\frac{1}{2}}(\Gamma_D)$ and $g^N \in H^{-\frac{1}{2}}(\Gamma_N)$ on the Dirichlet and Neumann part of the boundary, respectively. We further set $\Gamma_{iD} = \Gamma_D \cap \partial F_i$, $\Gamma_{iN} = \Gamma_N \cap \partial F_i$, and $h_i^D = h^D|_{\Gamma_{iD}}$ and $g_i^N = g^N|_{\Gamma_{iN}}$. The set \mathcal{S} collects all the traces, i.e. the intersections between fractures, and each trace $S \in \mathcal{S}$ is given by the intersection of exactly two fractures, $S = \bar{F}_i \cap \bar{F}_j$, such that there is a one to one relationship between a trace S and a couple of fracture indices $\{i, j\} = \mathcal{I}(S)$. We will also denote by \mathcal{S}_i the set of traces belonging to fracture F_i .

Subsurface flow is governed by the gradient of the hydraulic head $H = \mathcal{P} + \zeta$, where $\mathcal{P} = p/(\varrho g)$ is the pressure head, p is the fluid pressure, g is the gravitational acceleration constant, ϱ is the fluid density and ζ is the elevation.

We define the following functional spaces:

$$\begin{aligned} V_i &= \mathbf{H}_0^1(F_i) = \left\{ v \in \mathbf{H}^1(F_i) : v|_{\Gamma_{iD}} = 0 \right\}, \\ V_i^D &= \mathbf{H}_D^1(F_i) = \left\{ v \in \mathbf{H}^1(F_i) : v|_{\Gamma_{iD}} = h_i^D \right\}, \end{aligned}$$

and

$$\begin{aligned} V &= \left\{ v : v|_{F_i} \in V_i, \forall i=1, \dots, N, \gamma_S(v|_{F_i}) = \gamma_S(v|_{F_j}), \forall S \in \mathcal{S}_i, \{i, j\} = \mathcal{I}(S) \right\}, \\ V^D &= \left\{ v : v|_{F_i} \in V_i^D, \forall i=1, \dots, N, \gamma_S(v|_{F_i}) = \gamma_S(v|_{F_j}), \forall S \in \mathcal{S}_i, \{i, j\} = \mathcal{I}(S) \right\}, \end{aligned}$$

where γ_S is the trace operator onto S . In order to formulate the DFN flow problem, let $a_i : V_i^D \times V_i \rightarrow \mathbb{R}$ be defined as

$$a_i(w, v) = (\mathcal{K}_i \nabla(w|_{F_i}), \nabla(v|_{F_i}))_{F_i} \quad \forall w \in V_i^D, v \in V,$$

where \mathcal{K}_i is the fracture transmissivity tensor, that we assume to be constant on each fracture. Let us denote by $H \in V^D$ the hydraulic head on the DFN and by $H_i \in V_i^D$ its restriction to the fracture F_i and by $v \in V$ the test functions. Assuming the hydraulic head modelled by the Darcy law, the whole problem on the DFN is: find $H \in V^D$ such that $\forall v \in V$

$$\sum_{i=1}^N a_i(H_i, v) = \sum_{i=1}^N (f_i, v)_{F_i} + \left\langle g_i^N, v|_{\Gamma_{Ni}} \right\rangle_{\mathbf{H}^{-\frac{1}{2}}(\Gamma_{Ni}), \mathbf{H}^{\frac{1}{2}}(\Gamma_{Ni})}. \quad (1)$$

3. Virtual Element discretization

In this section we describe the Virtual Element discretization of equation (1) assuming a globally conforming polygonal mesh is given on the DFN. A globally conforming mesh is a polygonal mesh on each fractures such that polygon edges match exactly at traces.

Let \mathcal{T}_δ be a globally conforming polygonal mesh of Ω fulfilling the regularity requirements needed by the Virtual Element method [28], $E \in \mathcal{T}_\delta$ be any polygon of this tessellation. Let $\mathbb{P}_k(E)$ be the space of polynomials of degree $\leq k$ defined on E . To define the discrete functional space on E , we introduce the \mathbf{H}^1 -orthogonal projector $\Pi_{k,E}^\nabla : \mathbf{H}^1(E) \rightarrow \mathbb{P}_k(E)$ such that

$$(\nabla(v - \Pi_{k,E}^\nabla v), \nabla p)_E = 0, \forall p \in \mathbb{P}_k(E)$$

and

$$\begin{cases} \left(\Pi_{k,E}^\nabla v, 1 \right)_{\partial E} = (v, 1)_{\partial E} & \text{if } k = 1, \\ \left(\Pi_{k,E}^\nabla v, 1 \right)_E = (v, 1)_E & \text{if } k \geq 2. \end{cases}$$

The Virtual Element space of order $k \in \mathbb{N}$ on E is defined as

$$V_\delta^E = \{v \in \mathbf{H}^1(E) : \Delta v \in \mathbb{P}_k(E), v \in \mathbb{P}_k(e) \forall e \subset \partial E, \gamma^{\partial E}(v) \in C^0(\partial E), \\ (v, p)_E = (\Pi_{k,E}^\nabla v, p)_E \forall p \in \mathbb{P}_k(E) / \mathbb{P}_{k-2}(E)\},$$

where $\mathbb{P}_k(E) / \mathbb{P}_{k-2}(E)$ denotes the subspace of $\mathbb{P}_k(E)$ containing polynomials that are $L^2(E)$ -orthogonal to $\mathbb{P}_{k-2}(E)$. Furthermore, let us denote by $\mathcal{T}_{\delta,i}$ the restriction of \mathcal{T}_δ to fracture F_i . The Virtual Element space on $\mathcal{T}_{\delta,i}$ is

$$V_{\delta,i} = \{v \in C^0(F_i) : v \in V_\delta^E \forall E \in \mathcal{T}_{\delta,i}\}.$$

Since \mathcal{T}_δ is globally conforming, we can define the global discrete spaces as

$$V_\delta = \{v \in V : v|_{F_i} \in V_{\delta,i}\}, \quad V_\delta^D = \{v \in V^D : v|_{F_i} \in V_{\delta,i}\}.$$

A function in the above space is uniquely identified by the following set of degrees of freedom:

1. the values at the vertices of the polygons;
2. if $k \geq 2$, for each edge e of the mesh, the value of v at $k-1$ internal points of e ;
3. if $k \geq 2$, for each $E \in \mathcal{T}_\delta$, the scaled moments $\frac{1}{|E|} (v, m_\alpha)_E$ for all the scaled monomials m_α , with $\alpha = (\alpha_1, \alpha_2)$, $|\alpha| = \alpha_1 + \alpha_2 \leq k-2$, such that

$$\forall (x, y) \in E, \quad m_\alpha(x, y) := \frac{(x - x_E)^{\alpha_1} (y - y_E)^{\alpha_2}}{h_E^{\alpha_1 + \alpha_2}},$$

being (x_E, y_E) the centroid of the cell and h_E its diameter.

For any element $E \in \mathcal{T}_\delta$, given a function $v_\delta \in V_\delta^E$, it can be seen [26, 39] that the values of its degrees of freedom are uniquely defined by its $L^2(E)$ -orthogonal projection on $\mathbb{P}_{k-1}(E)$, denoted by $\Pi_{k-1,E}^0 v_\delta$, and the orthogonal projection of its gradient on $\mathbb{P}_{k-1}(E) \times \mathbb{P}_{k-1}(E)$, denoted by $\Pi_{k-1,E}^0 \nabla v_\delta$. A basis of the local VEM space is defined implicitly as the set of functions that are Lagrangian with respect to the degrees of freedom.

To discretize (1) by the Virtual Element method we suppose to know, for each $E \in \mathcal{T}_{\delta,i}$, $i = 1, \dots, N$, a bilinear form $S : V_\delta^E \times V_\delta^E \rightarrow \mathbb{R}$ such that, $\forall v_\delta \in V_\delta^E \cap \ker \Pi_{k,E}^\nabla$,

$$\exists c_*, c^* > 0 : c_* (\mathcal{K}_i \nabla v_\delta, \nabla v_\delta)_E \leq S^E(v_\delta, v_\delta) \leq c^* (\mathcal{K}_i \nabla v_\delta, \nabla v_\delta)_E.$$

With the above assumption, we define, for each $E \in \mathcal{T}_{\delta,i}$, $i = 1, \dots, N$, the bilinear form $a_\delta^E : V_\delta^E \times V_\delta^E \rightarrow \mathbb{R}$ such that, $\forall u_\delta, v_\delta \in V_\delta$,

$$a_\delta^E(u_\delta, v_\delta) = (\mathcal{K}_i \Pi_{k-1}^0 \nabla u_\delta, \Pi_{k-1}^0 \nabla v_\delta)_E + \mathcal{K}_i S^E((I - \Pi_k^\nabla) u_\delta, (I - \Pi_k^\nabla) v_\delta),$$

and the global bilinear form $a_\delta : V_\delta^D \times V_\delta \rightarrow \mathbb{R}$ such that

$$a_\delta(u_\delta, v_\delta) = \sum_{i=1}^N \sum_{E \in \mathcal{T}_{\delta,i}} a_\delta^E(u_\delta|_{F_i}, v_\delta|_{F_i}).$$

Finally, the Virtual Element discretization of (1) is: find $H_\delta \in V_\delta^D$ such that, $\forall v_\delta \in V_\delta$

$$a_\delta(H_\delta, v_\delta) = \sum_{i=1}^N \sum_{E \in \mathcal{T}_{\delta,i}} (f_i, \Pi_{k-1,E}^0(v|_{F_i}))_E + \langle g_i^N, v|_{\Gamma_{N_i}} \rangle_{H^{-\frac{1}{2}}(\Gamma_{N_i}), H^{\frac{1}{2}}(\Gamma_{N_i})}.$$

We remark that the continuity conditions are automatically satisfied by the definition of the functional space and the degrees of freedom, viable because \mathcal{T}_δ is a globally conforming mesh.

In [32], a residual a posteriori estimator was derived for the Poisson problem proving the equivalence between the estimator and the error with respect to a suitable polynomial projection of the VEM solution. The extension of this estimate to the case of a globally conforming discretization of the Laplace problem on a DFN is quite straightforward. Let us define the following error measure:

$$|||v||| = \sup_{w \in V} \frac{\sum_{i=1}^N a_i(v_i, w)}{\left(\sum_{i=1}^N \|\sqrt{\mathcal{K}} \nabla w\|_{F_i}^2 \right)^{\frac{1}{2}}},$$

then, we denote $H_\delta^\pi = \Pi_k^\nabla(H_\delta)$ and define

$$\begin{aligned} est_\delta^2 &= \sum_{i=1}^N \left(\sum_{E \in \mathcal{T}_{\delta,i}} \frac{h_E^2}{\mathcal{K}_i} \|\Pi_{k-1}^0 f + \mathcal{K}_i \Delta H_{\delta i}^\pi\|_E^2 + \sum_{e \in \mathcal{E}_{\delta,i}^{\text{int}}} \frac{h_e}{\mathcal{K}_i} \left\| \left[\mathcal{K}_i \frac{\partial H_{\delta i}^\pi}{\partial \mathbf{n}} \right]_e \right\|_e^2 + \right. \\ &\quad \left. + \sum_{e \in \mathcal{E}_{\delta,i}^N} \frac{h_e}{\mathcal{K}_i} \left\| \left[\mathcal{K}_i \frac{\partial H_{\delta i}^\pi}{\partial \mathbf{n}} \right]_e - g_i^N \right\|_e^2 + \sum_{E \in \mathcal{T}_\delta} \frac{h_E^2}{\mathcal{K}_i} \|f - \Pi_{k-1}^0 f\|_E^2 \right) \\ &\quad + \sum_{\substack{S \in \mathcal{S}: \\ \mathcal{I}(S) = \{i,j\}}} \left(\sum_{e \in \mathcal{E}_{\delta,S}} \frac{h_e}{\min\{\mathcal{K}_i, \mathcal{K}_j\}} \left\| \left[\mathcal{K}_i \frac{\partial H_{\delta i}^\pi}{\partial \mathbf{n}} \right]_e + \left[\mathcal{K}_j \frac{\partial H_{\delta j}^\pi}{\partial \mathbf{n}} \right]_e \right\|_e^2 \right), \end{aligned}$$

where $\forall i = 1, \dots, N$, $\mathcal{E}_{\delta,i}^{\text{int}}$ is the set of edges of $\mathcal{T}_{\delta,i}$ such that, $\forall e \in \mathcal{E}_{\delta,i}^{\text{int}}$, $e \cap S = \emptyset$ $\forall S \in \mathcal{S}_i$ and $e \cap \Gamma_{N_i} = \emptyset$, $\mathcal{E}_{\delta,i}^N$ is the set of edges e of $\mathcal{T}_{\delta,i}$ such that $e \cap \Gamma_i^N \neq \emptyset$ and $\forall S \in \mathcal{S}$, $\mathcal{E}_{\delta,S}$ is the set of edges e of \mathcal{T}_δ such that $e \cap S \neq \emptyset$. Then, there exist two constants $c, C > 0$ independent of δ such that

$$c \cdot est_\delta \leq |||H - H_\delta^\pi||| \leq C \cdot est_\delta. \quad (2)$$

In view of an adaptive approach, we define, for each cell E , a local estimator $est_{\delta,E}$, such that the estimators defined on the edges are split among neighbouring cells according to their areas.

4. DFN Minimal mesh construction

In this section we introduce the strategy used for the construction of the initial coarse polygonal mesh on the DFNs. This mesh is obtained by the construction of convex polygons representing sub-fractures, i.e. portion of fractures

not crossed by traces that can have traces or portion of traces only on the boundary. Given a fracture and the set of its traces there exist many partitions of the fracture in sub-fractures with a different number of sub-fractures and different quality of the produced elements. The construction of the minimal mesh is a complex trade off between the number of the elements and the quality of the produced elements. In our approach we aim at limiting the number of elements. Improvement of the mesh quality is transferred to a following suitable refining strategy.

The approach we follow is an iterative splitting of the leaves of a tree structure. We start from the original fracture that is the root cell of the structure, then we select a trace and we split the given cell along the trace or along a segment overlapped to the trace extending the trace contained in the cell up to the edges/points of the cell producing two children.

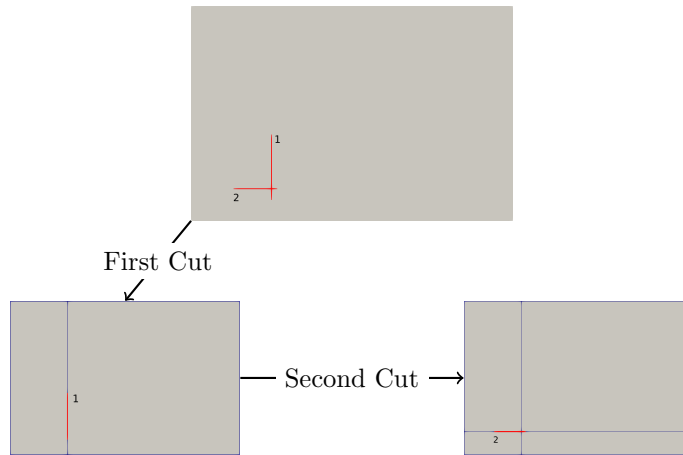


Figure 1: Minimal mesh generation on a fracture with two traces

Then we proceed iteratively choosing a new trace and cutting the leaves of the tree with the selected trace, exclusively in the case the trace is intersecting the internal part of the cell. At each iteration each cell can be split in two children cells or can be modified in a unique child cell that is the same polygon with one of the edges split in two aligned sub-edges in order to guarantee conformity of the global mesh. The algorithm is sketched in Algorithm 1. In Figure 1 we show the generation of a minimal polygonal mesh on a fracture with two traces. In this simple example two cuts to generate a polygonal mesh conforming to the traces are required. With the first cut we split the fracture along the vertical segment overlapped to the vertical trace, and with the second cut we split the two generated polygons (the two leaves of the current tree) along the segments overlapped to the horizontal trace. In Figure 2 we show the tree structure resulting from the first cut (level one) and the second cut (level

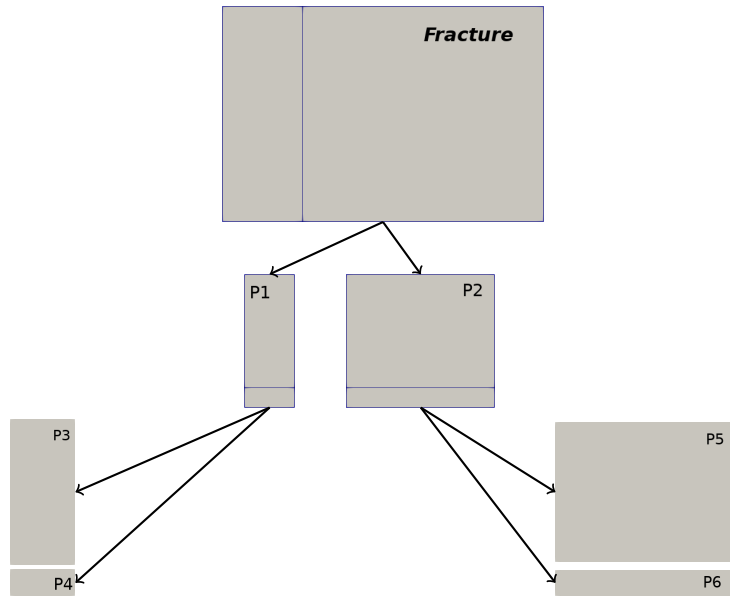


Figure 2: Second Cut

two). Each node in the tree structure represents a cell (or a temporary cell), the leaves represent the cells in the final mesh. The process starts setting the fracture as the root node of the tree (Fracture label in Figure 2). Taken the first trace, the intersections between the fracture cell and the segment generated by the trace one are computed. The intersection generates two cells, P1 and P2, that are inserted in the tree structure as children nodes of the root. Then we consider the second trace, all the leaves cells crossed by the trace are found (in this case both the level-one cells) and the intersections are computed. The intersections between the segment passing through the trace two and the cell P1 generates the cells P3 and P4, and the cell P2 generates the cells P5 and P6. The cells P3 and P4 and the cells P5 and P6 are inserted as children nodes of P1 and P2, respectively.

After the cut, all the leaves cells are updated adding the tips of the traces as vertices, introducing aligned edges and generating the minimal polygonal mesh on the fracture conforming to the traces.

In order to control the number of cells produced by the algorithm we cut the current cells with a suitable order of traces. We start considering the traces that cross the fracture intersecting two boundary edges of the fracture. Then we continue considering the remaining traces from the longest to the shortest. Considering the traces in this order usually yields to a smaller number of cells.

Algorithm 1 Minimal mesh

Given a fracture and the set of traces create a tree structure with the fracture as root cell

- 1: **for** All the traces **do**
 - 2: **for** All the leaves cells of the tree **do**
 - 3: Compute the intersection of the trace with the cell
 - 4: **if** There is an intersection with the internal part of the cell **then**
 - 5: Split the cell in two children cells
 - 6: **end if**
 - 7: Update the neighbouring cell with the new edges
 - 8: **end for**
 - 9: **end for**
-

5. Refinement and Marking algorithms

In this section we briefly introduce the algorithms used for marking the cells with largest estimators to be refined in order to reduce the discretization error and the different algorithms tested for the refinement of polygonal cells. This refinement step is part of the usual refinement process SOLVE-ESTIMATE-MARK-REFINE [40].

5.1. Marking Strategy

The marking strategy (see Algorithm 2) of the cells to be refined is simply based on the selection of all the cells with the largest error estimators. We mark the cells starting from those with largest estimators $est_{\delta,E}^2$ up to when the cumulative error estimator $est_{\delta,\mathcal{T}_{\delta,mark}}^2$ of the marked cells is a given ratio C of the total error estimator $est_{\delta,\mathcal{T}_{\delta}}^2 = \sum_{E \in \mathcal{T}_{\delta}} est_{\delta,E}^2$. In this algorithm we accept the sorting cost for the estimator vector [40] in order to maximally contain the refinement iterations that, in practical applications to large scale DFN simulations, can be quite expensive in the last refinement steps.

5.2. Refinement algorithms

In this section we introduce four different refinement algorithms used for cutting marked convex cells in two convex sub-cells. All the algorithms are based on a similar approach and differ for the choice of the cutting direction. The common approach is described in the Algorithm 3 and the four different approaches differ for the Step 3 of Algorithm 3.

In the following we compare four different refinement options for choosing the cutting direction denoted Maximum Momentum (MaxMom), Trace Direction (TrDir), Maximum Number of Points (MaxPnt) and Maximum Edge (MaxEdg). At the Step 8 of the Algorithm 3 we accept to slightly modify the chosen cutting direction in order to avoid the proliferation of edges and vertices of the new cells and consequently of VEM degrees of freedom that do not efficiently increase the

Algorithm 2 Cells marking algorithm

Given a convex polygon

- 1: Compute the cell error estimators $est_{\delta,E}^2$ and save them in a vector $Vest_{\delta}^2$.
 - 2: Compute the total error estimator $est_{\delta,\mathcal{T}_{\delta}}^2$
 - 3: Sort the cell estimators vector $Vest_{\delta}^2$
 - 4: Choose a constant $0 < C < 1$
 - 5: $i = 0$
 - 6: $est_{\delta,\mathcal{T}_{\delta,mark}}^2 = est_{\delta,\mathcal{T}_{\delta,mark}}^2 + Vest_{\delta}^2(i)$
 - 7: **repeat**
 - 8: $i++$
 - 9: $est_{\delta,\mathcal{T}_{\delta,mark}}^2 = est_{\delta,\mathcal{T}_{\delta,mark}}^2 + Vest_{\delta}^2(i)$
 - 10: **until** $est_{\delta,\mathcal{T}_{\delta,mark}}^2 \leq C * est_{\delta,\mathcal{T}_{\delta}}^2$
 - 11: Mark the cells corresponding to the first i positions of $Vest_{\delta}^2$
-

Algorithm 3 Refinement algorithm for convex polygons

Given a convex polygon

- 1: Check aspect ratio (AR)
 - 2: Compute the centroid \mathbf{X}_c
 - 3: Choose the cutting direction
 - 4: Build a straight line passing from the centroid with the chosen direction
 - 5: Choose the collapsing tolerance CollapseToll
 - 6: **for** Each edges of the cell **do**
 - 7: **if** There is an intersection **then**
 - 8: **if** The intersection point is near to the begin/end point of the edge according to the chosen tolerance CollapseToll **then**
 - 9: Change the cutting direction and set the intersection point as the begin/end point of the edge
 - 10: **else**
 - 11: The intersection point will be a new point in the mesh
 - 12: **end if**
 - 13: **end if**
 - 14: **end for**
 - 15: Create the two children cells
 - 16: Update the neighbourhood
-

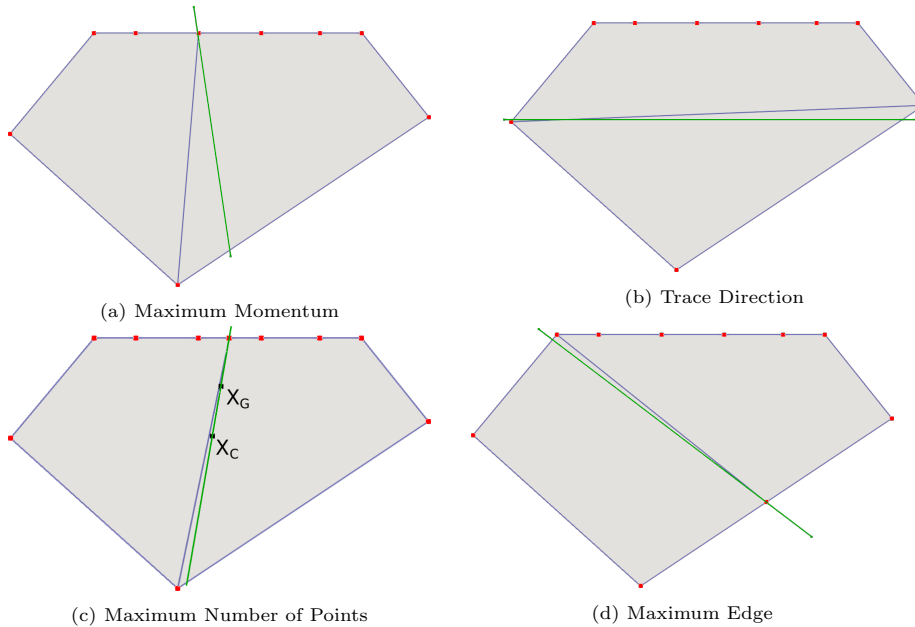


Figure 3: Different strategies for the selection of the cutting direction.

quality of the solution and to avoid the generation of very small edges that may induce stability problems [29, 41].

We collapse the points given by the intersection of the cutting direction with an edge to existing vertices of the cell when the distance of the intersection from the closest vertex are smaller than the tolerance `CollapseToll` multiplied by the length of the edge intersected.

For some of the proposed cutting directions we switch from the selected refinement criterion to the Maximum Momentum criterion in order to avoid the generation of cells with a huge aspect ratio (AR) defined as the ratio between the longest distance between the centroid and the vertices and the smallest distance between the centroid and the edges. In order to avoid the generation of elements with a huge aspect ratio, we define a fixed value denoted by `MaxAR` and if the aspect ratio of the cell to cut is larger than `MaxAR`, the cutting criterion is always `MaxMom`.

5.2.1. Maximum Momentum (*MaxMom*)

This cutting strategy of marked cells is based on the choice of cutting direction that is orthogonal to the direction of the eigenvector associated to the smallest eigenvalue of the inertia tensor of the cell (Figure 3a).

5.2.2. Trace Direction (*TrDir*)

This cutting strategy is based on the choice as cutting direction of the direction parallel to a trace (if any), see Figure 3c, where we have assumed that

the edge with several aligned points belongs to the trace. The rationale of this approach is related to the known property of the solution to the considered problem that displays strong gradient components in the direction orthogonal to the traces. If a cell intersects more than one trace we switch to MaxMom criterion.

5.2.3. Maximum Number of Points (*MaxPnt*)

This cutting strategy is based on the choice as cutting direction of the direction of the vector connecting the centroid of the cell X_C to the center of mass of the vertices X_G , see Figure 3c. This vector points towards the region of the marked cell with the highest density of vertices and should split the cell balancing the vertices of the two new subcells. In this strategy it is mandatory to define the option MaxNP, to set how many points the cells can have. This strategy switches to the MaxMom strategy in two cases: the first when the number of points of the cell to cut is less than MaxNP, the second when the centroid and the center of mass have a distance under a fixed tolerance. We remark that this refinement strategy can be considered as a simple improvement of the MaxMom strategy being the refinement strategy different only for the cells with a large number of cells and considering that when the number of vertices of the cell is larger than MaxNP this refinement strategy aims at dropping the number of vertices of the two produced cells under MaxNP.

5.2.4. Maximum Edge (*MaxEdg*)

This cutting strategy is based on the choice as cutting direction of the direction that splits the longest edge of the cell in the middle, see Figure 3d, where the longest edge is the right-bottom edge. If a cell displays aligned edges, these are considered as one unique edge.

6. Numerical Results: optimality and effectivity index

In order to validate our refinement algorithm we test it on two simple DFNs for which an exact solution is known. We consider two DFNs with two and three fractures, labelled as Problem 1 and Problem 2, respectively.

This first set of tests aims at validating the equivalence relation stated in (2) between the error and the error estimator. We have tested this equivalence relation on the meshes produced during the adaptive process although this property holds true on any sufficiently refined mesh. We apply our adaptive algorithm and compare at each refinement iteration the error and the error estimator computing the *effectivity index*

$$\varepsilon = \frac{err}{est_\delta}$$

in order to verify that it is independent of the mesh size obtained by adaptive refinements. See [32] for the same analysis performed on uniformly refined meshes.

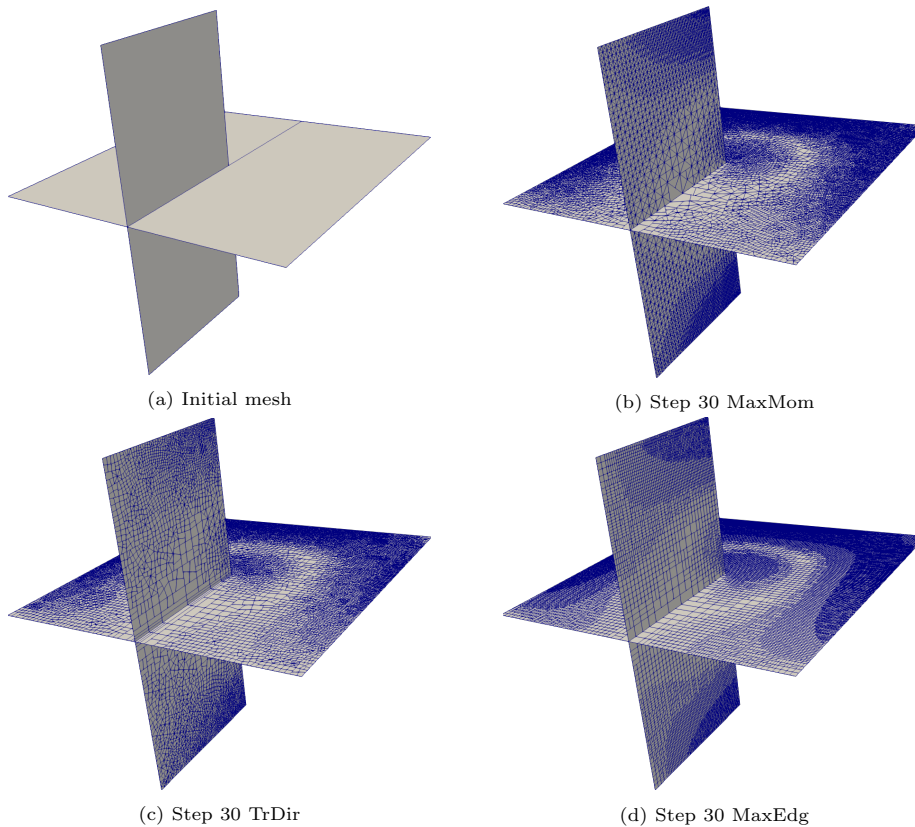


Figure 4: Problem 1: DFN with meshes at refining step 30.

As stopping criterion for the adaptive process, we require the following condition on the estimated relative error:

$$\frac{est_\delta}{\left(\sum_{i=1}^N \|\sqrt{\mathcal{K}_i} \nabla \Pi_k^\nabla H_{\delta_i}\|_{F_i}^2\right)^{\frac{1}{2}}} \leq 0.05. \quad (3)$$

All the simulations here presented are performed with the following methods and parameters: VEM orders from 1 to 4, Preconditioned Conjugate Gradient as linear solver with relative stopping residual $1.0e - 15$, the preconditioner being an incomplete Cholesky factorization implemented as described in [42], CollapseToll = 0.2, MaxAR = 10, MaxNP = 12 and C = 0.50.

6.1. Problem 1

The geometry and the parameters of this test problem are described in detail in [43, Section 5.1]. The DFN is composed by two fractures that are planar

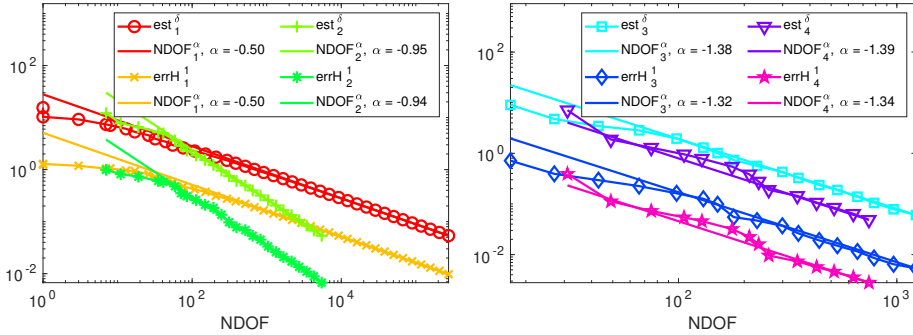


Figure 5: Problem 1: Rates of convergence (α) for error and estimator with MaxMom refinement.

TypeRef	Order 1	Order 2	Order 3	Order 4
MaxMom	$\alpha = -0.50$	$\alpha = -0.95$	$\alpha = -1.38$	$\alpha = -1.39$
	$\alpha_{err} = -0.50$	$\alpha_{err} = -0.94$	$\alpha_{err} = -1.32$	$\alpha_{err} = -1.34$
TrDir	$\alpha = -0.49$	$\alpha = -0.93$	$\alpha = -1.67$	$\alpha = -1.56$
	$\alpha_{err} = -0.50$	$\alpha_{err} = -0.92$	$\alpha_{err} = -1.63$	$\alpha_{err} = -1.30$
MaxEdg	$\alpha = -0.50$	$\alpha = -0.93$	$\alpha = -1.37$	$\alpha = -1.55$
	$\alpha_{err} = -0.50$	$\alpha_{err} = -0.93$	$\alpha_{err} = -1.41$	$\alpha_{err} = -1.38$

Table 1: Problem 1: Rates of convergence for the estimator (α) and the error (α_{err}) with refinement criteria MaxMom, TrDir and MaxEdg.

rectangles defined as

$$F_1 = (-1, 1) \times (-1, 1) \times \{0\}; \quad F_2 = (-1, 0) \times \{0\} \times (-1, 1).$$

Thus, the only trace of the DFN is $\Gamma_1 = (-1, 0) \times \{0\} \times \{0\}$. The differential model is set up by choosing the following exact solutions:

$$h_1(x, y, z) = (x^2 - 1)(y^2 - 1)(x^2 + y^2) \cos\left(\frac{1}{2} \arctan 2(x, y)\right),$$

$$h_2(x, y, z) = -(z^2 - 1)(x^2 - 1)(x^2 + z^2) \cos\left(\frac{1}{2} \arctan 2(z, x)\right),$$

where $\arctan 2(x, y)$ is the four-quadrant inverse tangent, that is the arctan of y/x in $[-\pi, \pi]$. The transmissivity of both fractures is set to 1.

In Figure 4 we report some of the meshes generated during the refinement process. We remark that in this test problem the presence of a known forcing function on the fractures induces a refinement in the whole domain, this will not be the same for the flow simulations in which the rock matrix surrounding the DFNs is considered impervious (Section 7).

In Figure 5 we report the convergence behaviour of the error (errH^1) and of the error estimator (est_s) and the final rates of convergence α with respect to the

Step	# Cells	NDOF	ε	PCG-It
1	4	1	0.0064	1
5	16	8	0.0221	5
10	58	44	0.0318	12
15	232	208	0.0326	23
20	958	910	0.0345	43
25	3997	3901	0.0343	88
30	16696	16214	0.0337	181
35	69827	67074	0.0334	370
39	219297	207112	0.0333	662
40	291581	274982	0.0332	777

Table 2: Problem 1: MaxMom refinement Order 1.

Step	# Cells	NDOF	ε	PCG-It
1	4	1	0.0064	1
5	14	5	0.0130	1
10	46	34	0.0441	12
15	167	147	0.0364	21
20	672	712	0.0356	46
25	2760	3232	0.0377	94
30	11528	13848	0.0357	188
35	48362	57738	0.0353	378
39	152185	178922	0.0349	695
40	202798	237727	0.0347	846

Table 3: Problem 1: TrDir refinement Order 1.

Step	# Cells	NDOF	ε	PCG-It
1	4	1	0.0064	1
5	16	7	0.0271	3
10	58	43	0.0347	12
15	239	223	0.0381	21
20	974	1007	0.0382	47
25	4101	4420	0.0382	100
30	17254	18980	0.0380	205
35	72401	80561	0.0386	414
37	128831	139214	0.0385	545

Table 4: Problem 1: MaxEdg refinement Order 1.

total number of degrees of freedom (NDOF): $est_\delta \sim (NDOF)^\alpha$, computed on the basis of the last five refinement iterations, considering the strategy MaxMom criterion. We can clearly appreciate a parallel behaviour of error and error estimator as well as the almost optimal asymptotic rate of convergence very close to -0.5 and -1 for the VEM orders 1 and 2, respectively. For higher VEM orders the sub-optimal rates of convergence are due to the bounded Besov regularity of the solution around the internal trace-tip. In Table 1 we report the rates of convergence for the estimator and for the error obtained by the refinement strategies MaxMom, TrDir and MaxEdg. For this problem we do not report results for the MaxPnt criterion that is always the MaxMom criterion being the number of vertices of the cells always smaller than MaxNP.

In Tables 2, 3 and 4 we report the most significant quantities to describe the refinement process for the MaxMom, TrDir and MaxEdge strategies: NCell is the total number of cells on the DFN, NDOF is the total numbers of degrees of freedom, ε is the effectivity index, PCG-It is the number of conjugate gradient iterations performed. For all the strategies, we highlight the relatively small variations of ε with respect to the large variations of number of cells and degrees of freedom, after the first iterations corresponding to very small number of NDOF. We also remark the weak growing of PCG-It with respect to the growing of NDOF. Observing the results concerning the number of degrees of freedom and the number of cells as well as the PCG iterations, the MaxEdg produces a lower NDOF and thus a lower PCG-It.

6.2. Problem 2

TypeRef	Order 1	Order 2	Order 3	Order 4
MaxMom	$\alpha = -0.48$	$\alpha = -0.93$	$\alpha = -1.22$	$\alpha = -1.49$
	$\alpha_{err} = -0.49$	$\alpha_{err} = -0.95$	$\alpha_{err} = -1.23$	$\alpha_{err} = -1.52$
TrDir	$\alpha = -0.49$	$\alpha = -0.95$	$\alpha = -1.14$	$\alpha = -1.49$
	$\alpha_{err} = -0.49$	$\alpha_{err} = -0.92$	$\alpha_{err} = -1.20$	$\alpha_{err} = -1.52$
MaxEdg	$\alpha = -0.49$	$\alpha = -0.92$	$\alpha = -1.32$	$\alpha = -1.47$
	$\alpha_{err} = -0.47$	$\alpha_{err} = -0.94$	$\alpha_{err} = -1.35$	$\alpha_{err} = -1.68$

Table 5: Problem 2: Rates of convergence for the estimator (α) and the error (α_{err}) with refinement criteria MaxMom, TrDir and MaxEdg.

The geometry and the parameters of this test problem are described in detail in [30, Section 6.1]. The DFN is composed by three fractures and three traces, defined as

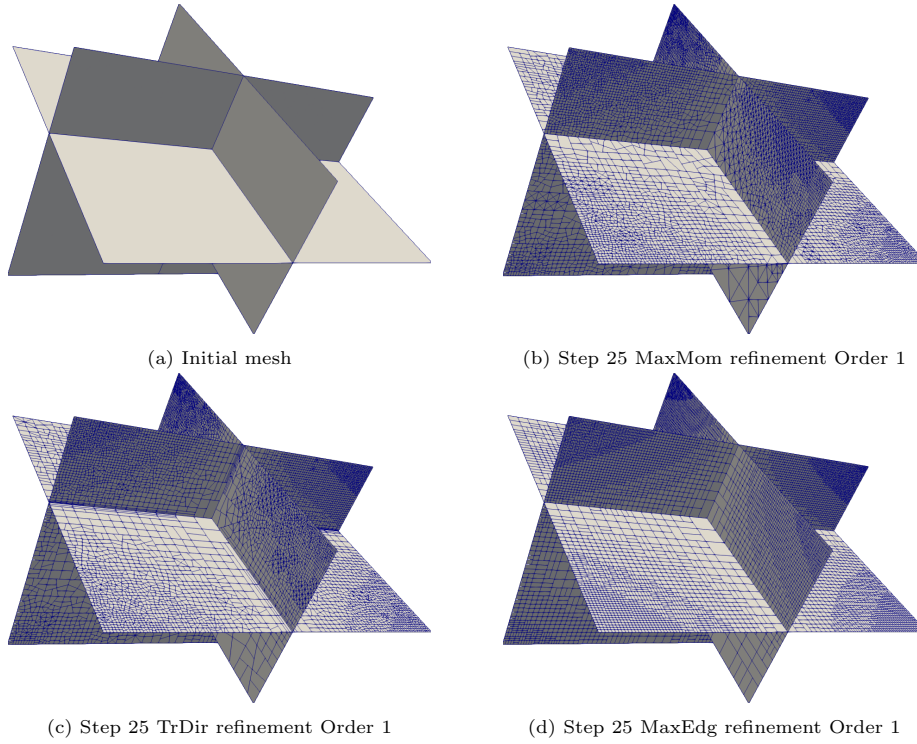


Figure 6: Problem 2: DFN with meshes at refining step 25

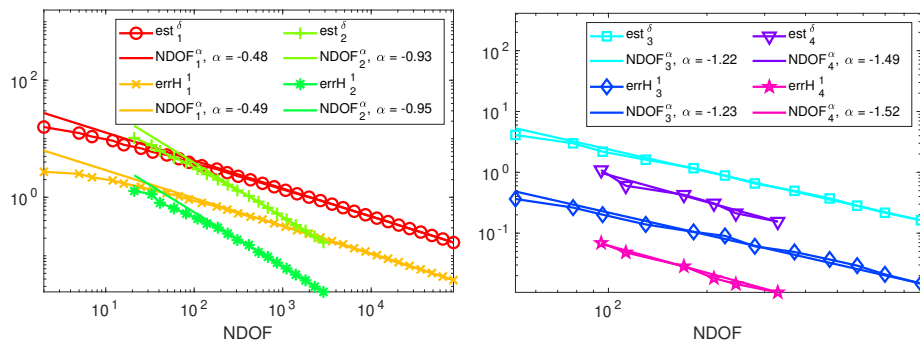


Figure 7: Problem 2: Rates of convergence (α) for error and estimator with MaxMom refinement.

Step	# Cells	NDOF	ε	PCG-It
1	12	2	0.0296	1
5	30	16	0.0472	6
10	114	87	0.0541	13
15	455	432	0.0552	25
20	1875	1979	0.0557	55
25	7752	8622	0.0552	114
30	32221	36261	0.0531	234
32	57076	64484	0.0520	309

Table 6: Problem 2: MaxMom refinement Order 1.

Step	# Cells	NDOF	ε	PCG-It
1	12	2	0.0296	1
5	30	16	0.0441	5
10	113	92	0.0500	13
15	433	428	0.0531	32
20	1741	1933	0.0596	77
25	7047	8221	0.0581	152
30	28933	34475	0.0574	411
33	67557	80552	0.0562	542

Table 7: Problem 2: TrDir refinement Order 1.

Step	# Cells	NDOF	ε	PCG-It
1	12	2	0.0296	1
5	30	16	0.0476	6
10	113	89	0.0555	12
15	450	418	0.0578	24
20	1847	1885	0.0614	55
25	7737	8203	0.0636	114
30	32385	34978	0.0679	243
31	43231	47014	0.0681	286

Table 8: Problem 2: MaxEdg refinement Order 1.

$$\begin{array}{l}
F_1 = \left(-1, \frac{1}{2}\right) \times (-1, 1) \times \{0\}, \\
F_2 = (-1, 0) \times \{0\} \times (-1, 1), \\
F_3 = \left\{\frac{1}{2}\right\} \times (-1, 1) \times (-1, 1),
\end{array}
\left|
\begin{array}{l}
\Gamma_1 = F_1 \cap F_2 = \left(-1, \frac{1}{2}\right) \times \{0\} \times \{0\}, \\
\Gamma_2 = F_1 \cap F_3 = (-1, 0) \times \{0\} \times (-1, 1), \\
\Gamma_3 = F_2 \cap F_3 = \left\{-\frac{1}{2}\right\} \times \{0\} \times (-1, 1).
\end{array}
\right.$$

The chosen exact solution is defined on each fracture as follows:

$$\begin{aligned}
h_1(x, y, z) &= -\frac{1}{10} \left(x + \frac{1}{2}\right) (8xy(x^2 + y^2) \arctan 2(y, x) + x^3), \\
h_2(x, y, z) &= -\frac{1}{10} \left(x + \frac{1}{2}\right) x^3 (1 - 8\pi |z|), \\
h_3(x, y, z) &= y(y - 1)(y + 1)(z - 1)z,
\end{aligned}$$

and all fractures have transmissivities set to 1.

In Figure 6, we report some of the meshes generated by the refinement process. Similarly to the previous test, a refinement is induced also far from traces due to the presence of a non-null forcing term.

In Figure 7 we report the rates of convergence (α) of the error and of the error estimator considering the strategy MaxMom. The rates of convergence for the strategies MaxMom, TrDir and MaxEdg are shown in the Table 5. The convergence rates are computed on the basis of the last five refinement iterations: again we can remark a very good agreement between the error and the estimator. The sub-optimal rates of convergence with higher VEM orders is still due to the bounded regularity of the solution.

In Tables 6-8 we report the same quantities reported in Tables 2-4 in order to describe the refinement process. We observe again that the effectivity index is almost independent of the meshsize since, as the mesh starts to have a sufficient number of DOFs, it displays small variations. As previously observed for Problem 1, the MaxEdg strategy produces a lower NDOF and thus a lower PCG-It.

7. Numerical Results on a realistic DFN

In this section we discuss the results obtained by the four presented refinement strategies when applied to more realistic DFNs. The geometry of the considered DFNs is fixed and is composed by 86 fractures and 159 traces, with a maximum number of traces per fracture equal to 11 and a mean value of traces per fracture equal to 1.85, see Figure 8. Working with this DFN we can easily produce several polygonal elements with a different number of edges, as well as, aligned edges. Moreover, the starting coarse mesh is commonly a poor quality mesh. All these configurations can be considered a good and challenging test

for the reliability and robustness of proposed approaches. The analysis for the quality of the elements generated by the algorithm can provide quite general results that can be extended to many different contexts.

We consider two test cases where the transmissivities of the fractures are sampled from two log-normal distributions having standard deviations equal to 10 and 10^4 , respectively. These two problems are tagged with the labels DFN86E01 and DFN86E04.

The problems considered have no forcing terms, and the flux is driven by the presence of two Dirichlet boundary conditions (10 on the boundaries at $x = 0$ and 0 at the boundaries at $x = 1000$), whereas homogeneous Neumann boundary conditions are imposed on all the other boundaries.

In the following analysis we display the convergence rates of the error estimate with respect to the number of degrees of freedom and we assess how the refinement strategies impact on the aspect ratio of the cells of a selected fracture (Fracture 72), and on the iterations of the preconditioned conjugate gradient method used to solve the linear system.

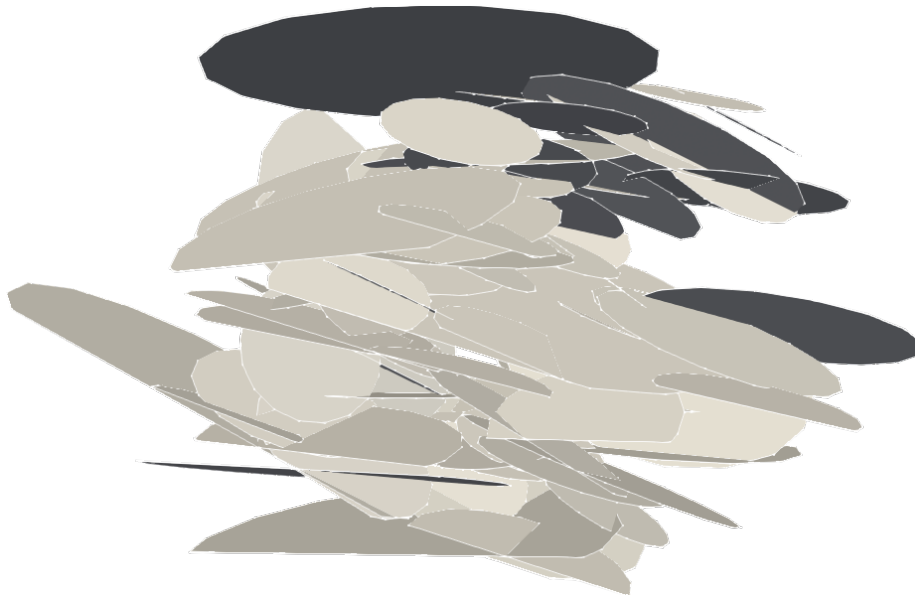


Figure 8: DFN with 86 fractures.

In Figures 9 and 10 we display the behaviour of the estimators with respect to the number of DOFs for the four refinement strategies considered and we report the slope of the estimator for each VEM order, for the two problems. We can observe that all the refinement strategies display an optimal asymptotic rate of convergence up to VEM order 2 (-0.5 for the VEM Order 1 and -1.0 for the VEM Order 2). For higher VEM orders the bounded regularity constraints the rates of convergence. The displayed behaviours suggest that the higher order VEM advisable for DFN flow simulations is $k = 2$. The trend of the

rate of convergence results similar even if the fluxes in the these two DFNs are completely different.

In Figure 11 we plot the behaviour of the ratio PCG-It/NDOF. After the initial noisy behaviour we can observe a decreasing asymptotical trend for all the considered refinement strategies. These plots highlight the advantages of a suitably refined mesh also on the performances of the linear solver.

In Figure 12 we report the minimal mesh on Fracture 72: this is the common initial mesh for all the refinement strategies and for both DFN86E01 and DFN86E04. In Figures 13 and 14 we display the meshes produced by all the considered refinement strategies. The TrDir strategy produces a stronger and sharper refinement along the traces. The switch from TrDir to MaxMom for elements with an aspect ratio over MaxAR prevents the generation of badly shaped elements parallel to the traces. The MaxPnt strategy produces a mesh quite similar to the mesh produced by MaxMom due to the fact that we have few cells with a number of vertices larger than MaxNP during the refinement process. In Figures 15 and 16 we report the minimum, the mean and the maximum aspect ratios of the cells on Fracture 72 along the refinement process. We remark that in all the strategies we use MaxMom strategy to refine the elements with large aspect ratio. The MaxMom and the MaxEdg strategies produce a decreasing mean aspect ratio, whereas TrDir and MaxPnt have a different behaviour. A slight difference from the two figures can be seen in the TrDir plots. The average AR grows in the DFN86E04 test case because the MaxMom strategy is less used due to the weaker refinement around the traces due to the different transmissivities on the intersecting fractures that justify a smaller flux (notice the more coarse mesh for DFN86E04 comparing Figures 13 and 14).

8. Conclusions

In this paper we propose several refinement algorithms for polygonal meshes, suitable for polygonal numerical methods such as Virtual Element methods (VEM), Discontinuous Galerkin methods, Hybrid High Order methods or Mimetic Finite Differences. The proposed strategies are based on selecting proper cutting directions, aimed at preserving the regularity of the resulting polygons and the quality of the resulting mesh. A suitable collapsing of intersection points is also discussed, in order to avoid the generation of too small new edges. A detailed discussion of the overall resulting mesh quality and corresponding rates of convergence is reported. An adaptive algorithm for the simulation of flow in Discrete Fracture Networks (DFN) using VEM is used to test the proposed refinement strategies in complex geometrical configurations. Such algorithm is based on the generation of a minimal mesh on the given DFN, that is refined using a residual based *a posteriori* error estimate to mark the cells to be refined and the proposed refining strategies to refine the mesh. Numerical results show the effectiveness and the robustness of the proposed refinement strategies, and confirm the viability of the approach. A comparison of the results provided by the four proposed refinement strategies on the test problems yields us to infer that all the methods behave correctly, improving the representation of

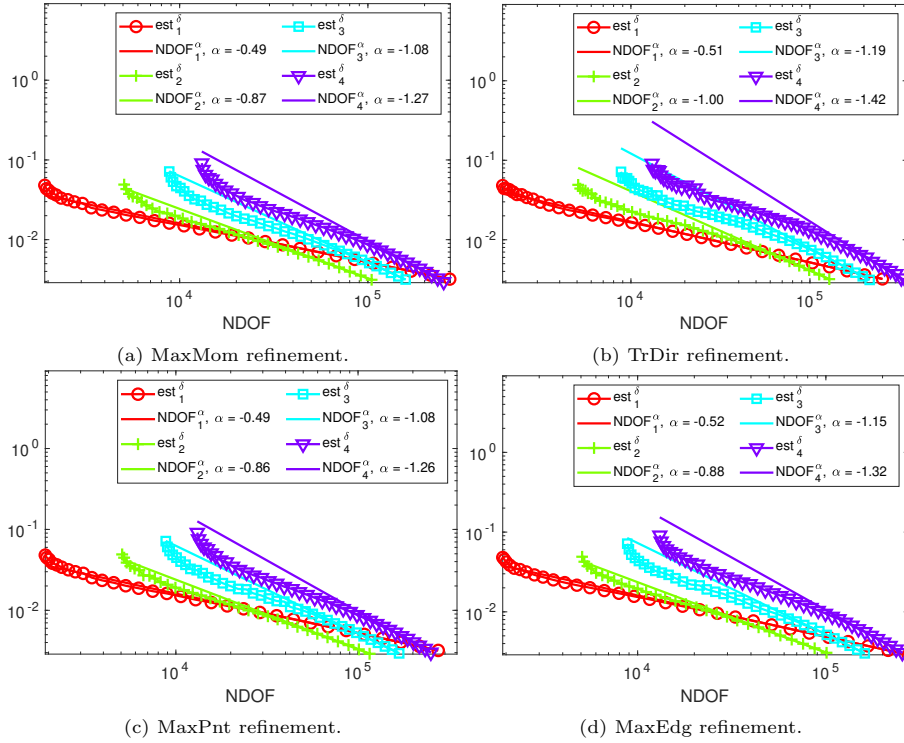


Figure 9: DFN86E01: Estimator vs. NDOF

the solution. From the mesh quality point of view, the MaxMom strategy and the MaxEdg strategy work better in reducing the aspect ratio of the elements, whereas MaxPnt and TrDir display sometimes some oscillations of the maximum aspect ratio. Moreover, the MaxMom strategy requires a lower computational cost and a less involved implementation, dealing with all the considered situations in a unified approach, in contrast to the MaxEdg that requires a slightly more complex implementation to deal with elements displaying aligned edges. On the other hand, when the mesh is composed mainly by simple polygons, the MaxEdg strategy performs slightly better, as can be seen in Problem 1 and 2.

Finally, an extension of the MaxMom refinement strategy has been applied to an anisotropic mesh refinement procedure in [35].

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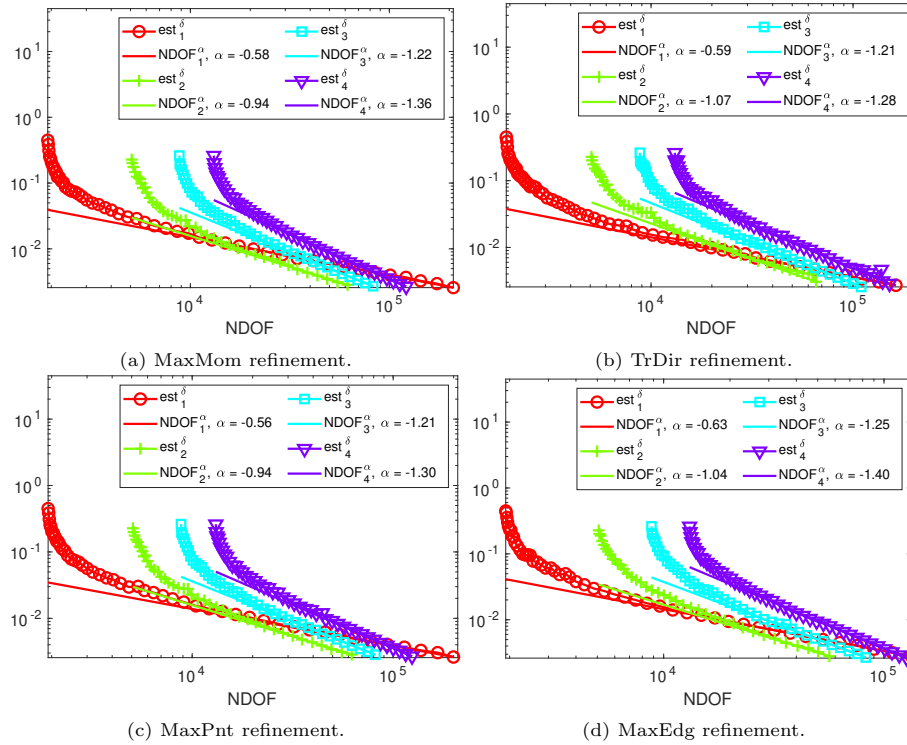


Figure 10: DFN86E04: Estimator vs. NDOF

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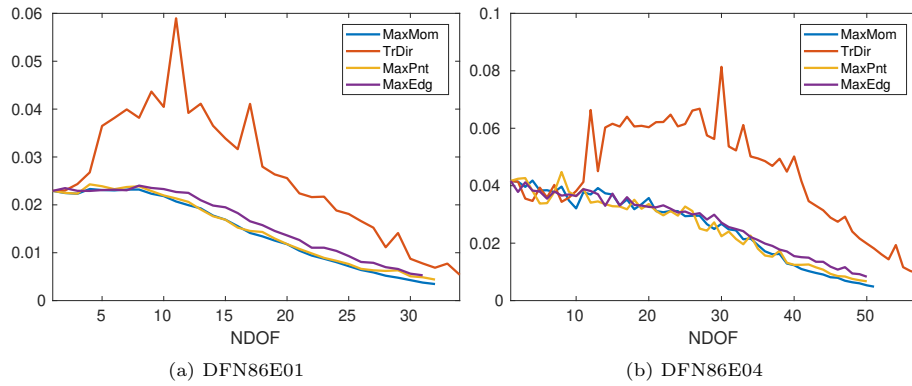


Figure 11: Ratio between PCG-It and NDOF

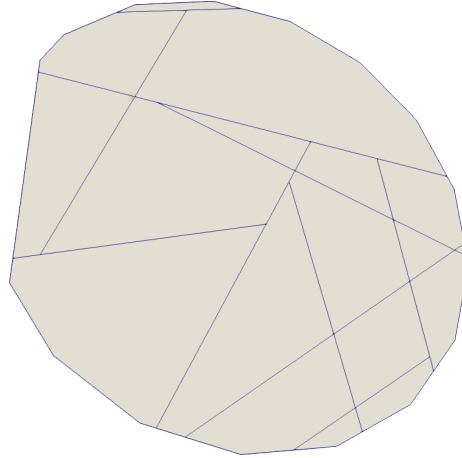


Figure 12: DFN86E01 - DFN86E04: initial mesh on Fracture 72.

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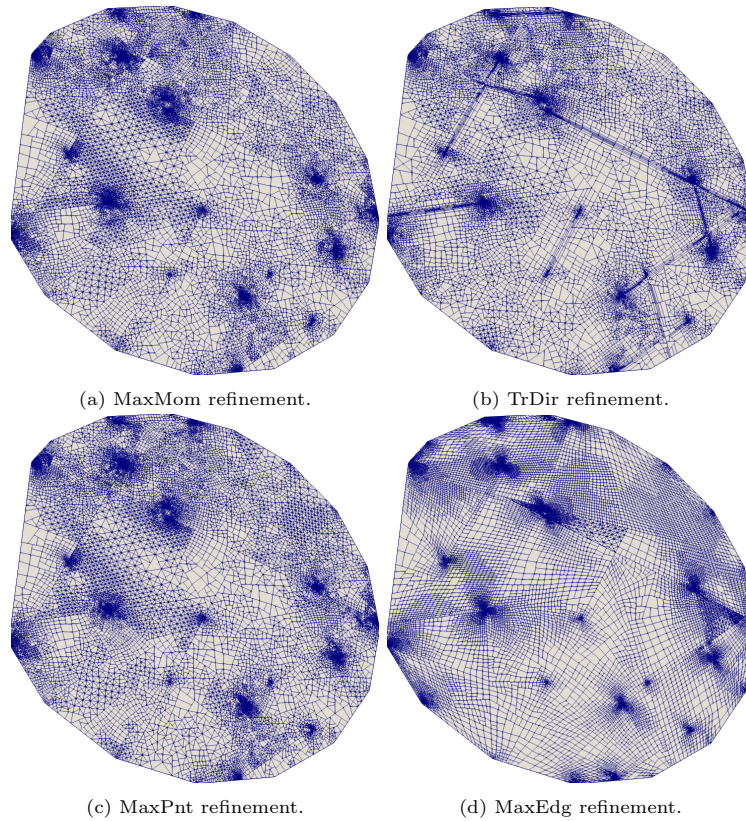


Figure 13: DFN86E01: final mesh on Fracture 72.

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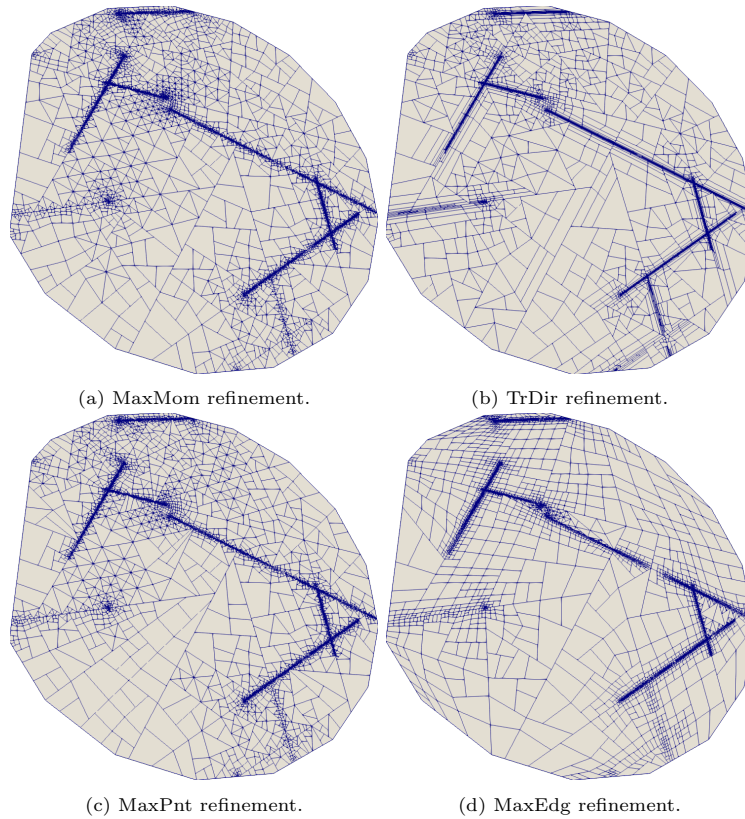


Figure 14: DFN86E04: final mesh on Fracture 72.

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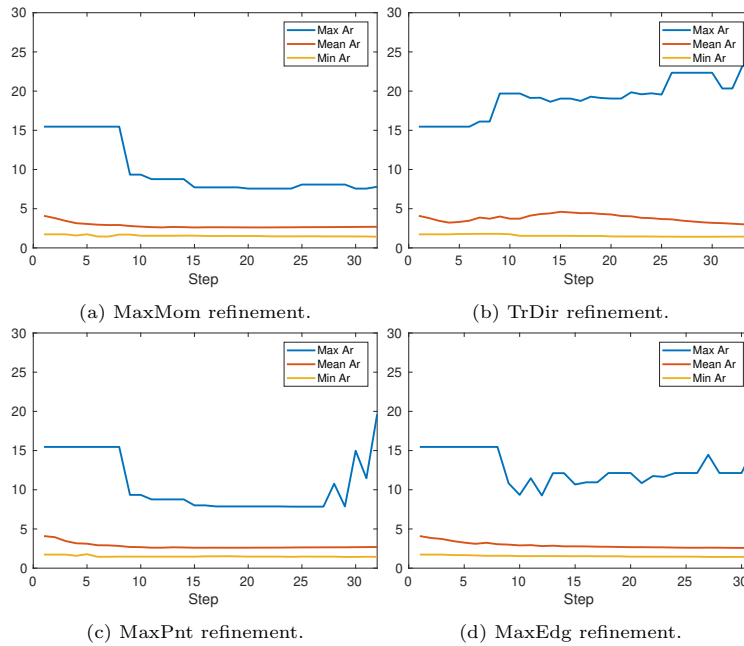


Figure 15: DFN86E01: aspect ratio statistics of the mesh on Fracture 72.

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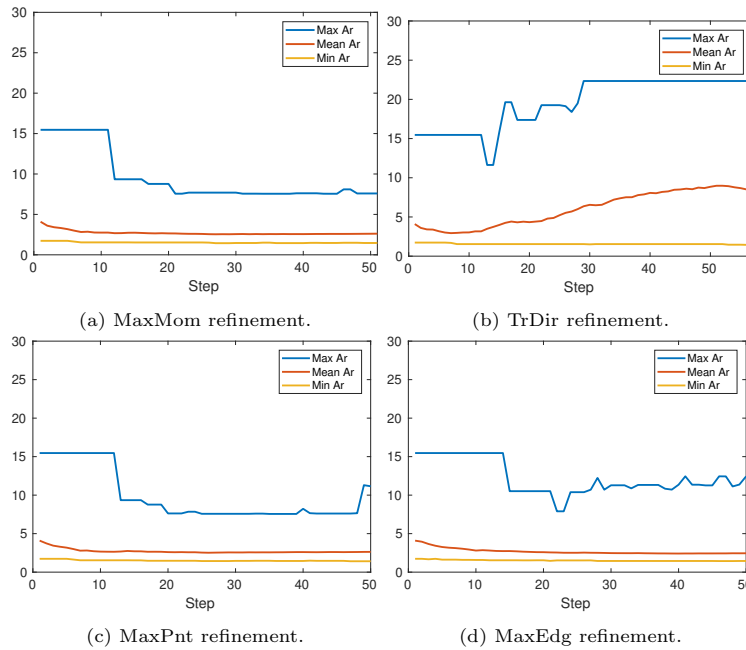


Figure 16: DFN86E04: aspect ratio statistics of the mesh on Fracture 72.

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