The Virtual Element Method for large scale Discrete Fracture Network simulations: fracture-independent mesh generation

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Discrete fracture network models for flow simulations:

- 3D network of intersecting fractures
- Fractures are represented as planar polygons
- Rock matrix is considered impervious - flow confined in the DFN
- Flow driven by hydraulic head gradients modeled by Darcy law in the fractures
- Flux balance and hydraulic head continuity imposed across trace intersections

Challenges:

- Complex domain: difficulties in good quality mesh generation
- $F_i \subset \mathbb{R}^3$, $i \in I$ is a generic fracture of the system.
- Fracture intersections are called \textit{traces} and denoted by $S$, $S \in S$.
- Each trace is shared by exactly two fractures: $S = \overline{F}_i \cap \overline{F}_j$, and $I_S = \{i, j\}$.
- $S_i$ is the set of traces on fracture $F_i$ while $S$ denotes the set of all the traces.
Single fracture model

Let $\partial F_i = \Gamma_{iN} \cup \Gamma_{iD}$ with $\Gamma_{iN} \cap \Gamma_{iD} = \emptyset$ and $\Gamma_{iD} \neq \emptyset$. Find $H_i \in H^1_D(F_i)$ such that:

$$
(K_i \nabla H_i, \nabla v) = (q_i, v) + \langle G_{iN}, v|_{\Gamma_{iN}} \rangle_{H^{-\frac{1}{2}}(\Gamma_{iN}), H^{\frac{1}{2}}(\Gamma_{iN})}, \forall v \in H^1_{0,D}(F_i)
$$

provides the hydraulic head $H_i \in H^1_D(F_i)$.

- $H_i$ is the hydraulic head on the fracture $F_i$, $H$ is the hydraulic head on $\Omega$;
- $K_i$ is the fracture transmissivity tensor: a symmetric and uniformly positive definite tensor;
- $\frac{\partial H_i}{\partial \tilde{n}_i} = \hat{n}_i^t K_i \nabla H_i = G_{iN}$ is the outward co-normal derivative of the hydraulic head and $\hat{n}_i$ the unit outward vector normal to the boundary $\Gamma_{iN}$.

In the following $\left[ \frac{\partial H_i}{\partial \tilde{n}_S^i} \right]_S$ denotes the jump of the co-normal derivative along a fixed normal $\hat{n}^i_S$ for the trace $S$ on the fracture $F_i$, this jump is independent of the orientation of $\hat{n}^i_S$ and is the net (incoming) flux provided by the trace $S$ to the fracture $F_i$. 

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Full fracture formulation

For each trace $S \in \mathcal{S}$ on the fracture $F_i$, let us denote by

$$U_i^S := \left[ \frac{\partial H_i}{\partial \nu_i^S} \right]_S , \quad U_i^S \in \mathcal{U}^S \subseteq H^{-\frac{1}{2}}(S)$$

the flux entering in the fracture through the trace, and $U_i \in \mathcal{U}^{S_i}$ the tuple of fluxes $U_i^S \forall S \in \mathcal{S}_i$.

Let us set $\partial F_i = \Gamma_iN \cup \Gamma_iD$ with $\Gamma_iN \cap \Gamma_iD = \emptyset$ and $\Gamma_iD \neq \emptyset$.

Solving $\forall i \in I$ the problem: find $H_i \in H^1_D(F_i)$ and $U_i \in \mathcal{S}_i$ such that:

$$(K_i \nabla H_i, \nabla v) = (q_i, v) + \langle U_i, v|_{S_i} \rangle_{\mathcal{U}^{S_i}, \mathcal{U}^{S_i}'} + J(U) + \langle G_iN, v|_{\Gamma_iN} \rangle_{H^{-\frac{1}{2}}(\Gamma_iN), H^{\frac{1}{2}}(\Gamma_iN)}, \forall v \in V_i = H^1_{0,D}(F_i)$$

with additional conditions

$$H_i|_S - H_j|_S = 0, \quad \text{for } i, j \in I_S, \forall S \in \mathcal{S},$$

$$U_i^S + U_j^S = 0, \quad \text{for } i, j \in I_S, \forall S \in \mathcal{S},$$

provides the hydraulic head $H \in V = H^1_D(\Omega)$. 
Instead of solving the differential problems on the fractures coupled by the corresponding matching conditions we look for the solution as the minimum of a PDE constrained quadratic optimal control problem, the variable $U$ being the control variable.

Let us define the “observation” spaces

$$H^{1/2}(S) \subseteq \mathcal{H}^S, \ \forall S \in S,$$

$$\mathcal{H}^{S_i} = \prod_{S \in S_i} \mathcal{H}^S,$$

$$\mathcal{H} = \prod_{i \in I} \mathcal{H}^{S_i}.$$

Let us define the differentiable functional $J : \mathcal{U} \rightarrow \mathbb{R}$ as

$$J(U) = \sum_{S \in S} \left( \| H_i(U_i) |_S - H_j(U_j) |_S \|^2_{\mathcal{H}^S} + \| U_i^S + U_j^S \|^2_{\mathcal{U}^S} \right)$$

We look for the control variable $U$ providing the minimum of the functional $J(U)$ constrained by the equation for $H_i$ on each fracture.
PDE constrained optimization approach

In order to remove the requirement of having a non-empty portion of Dirichlet boundary on each fracture it is necessary to modify the definition of the control variables on each trace as follows:

\[
U_i^S = \left[ \frac{\partial H_i}{\partial \nu_i^S} \right]_S + \alpha H_i|_S \quad U_i^S \in U^S = H^{-\frac{1}{2}}(S), \forall S \in \mathcal{S}
\]

where \( \alpha \) is a strictly positive scalar parameter. The definition of the functional is modified accordingly as:

\[
J(U) = \sum_{S \in \mathcal{S}} \left( \|H_i(U_i)|_S - H_j(U_j)|_S\|^2_H^S + \mathcal{F}(K_i, K_j)\|U_i^S + U_j^S - \alpha (H_i(U_i)|_S - H_j(U_j)|_S)\|^2_U^S \right)
\]

The constraint equation on each fracture \( \forall i \in I \) becomes:

find \( H_i \in H_D^1(F_i) \) such that:

\[
(K_i \nabla H_i, \nabla v) + \alpha \left( H_i|_{S_i}, v|_{S_i} \right)_{S_i} = (q_i, v) + \langle U_i, v|_{S_i} \rangle_{U^S_i, U^S_{i'}} + \langle G_{iN}, v|_{\Gamma_{iN}} \rangle_{H^{-\frac{1}{2}}(\Gamma_{iN}), H^\frac{1}{2}(\Gamma_{iN})}, \forall v \in V_i = H^1_{0,D}(F_i)
\]
Totally/Partially conforming meshes

**Figure**: Totally conforming mesh

**Figure**: Partially conforming mesh
non-conforming meshes: 36 fractures, 65 traces DFN

Figure: Non-conforming mesh on a 36 fracture DFN
Let us introduce a triangulation on each fracture, completely **independent of the triangulation on the intersecting fractures**. Let us further define starting from this triangulation an element-like discretization $h$ for $H$.

Let us introduce a discretization $u$ for the control variable $U$, **on the traces of each fracture independently**.

Let us choose $U^S = H^S = L^2(S)$ for the discrete norms.

With arbitrary triangulations **the minimum of the functional is not null**.

The minimization of the functional can be performed by the conjugate gradient method.
Main advantages of the proposed method

- The gradient method makes the optimization approach to DFN simulations nearly **inherently parallel**:
  - exchange of very small amount of data between processes;
  - each process only exchanges data with a limited number of other known processes;
  - resolution of small linear systems independently performed.

- The optimization approach is **independent of the discretization approach used on each fracture**.
Circumventing mesh generation problems, different discretizations

The triangulation for the discrete solution is fully independent on each fracture and on each trace.

Extended Finite Elements: catch the irregular behaviour of the solution across the traces improving accuracy;

Figure: Enrichment function away from trace tip

Figure: Tip enrichment function
The discrete problem

Figure: 3D view of DFN709 (left) and DFN1425 (right)

Figure: Zoom of angle distribution

Figure: Traces distances
Element-edges on traces → partially conforming mesh.

Mixing non overlapping polygons $E$ with straight edges and different number of edges.

For each element $E$, introduce the symmetric bilinear form

$$a^E_{i,\delta}(\phi, \varphi) = (K_i \nabla P^E\phi, \nabla P^E\varphi)_E + \alpha(\phi|_{S_{i} \cap \partial E}, \varphi|_{S_{i} \cap \partial E})_{S_{i} \cap \partial E} + S^E(\phi, \varphi).$$

$P^E : V_{i,\delta}|_E \mapsto \mathbb{P}_1(E)$ is the projection operator defined by

$$\begin{cases} (K_i \nabla P^E\phi, \nabla p)_E = (K_i \nabla \phi, \nabla p)_E \quad \forall p \in \mathbb{P}_1(E) \\ \sum_{k=1}^{n_E} P^E \phi(x_k) = \sum_{k=1}^{n_E} \phi(x_k) \end{cases}$$

$S^E : V_{i,\delta}|_E \times V_{i,\delta}|_E \mapsto \mathbb{R}$ is a stability functional.
Use flexibility of VEM in order to catch the behavior of the solution across the traces, allowing for a partially conforming mesh, but still maintaining an independent meshing process on each fracture.

1. Start from a given triangular mesh, built without taking into account trace positions or conformity requirements.

2. Whenever a trace intersects one element edge, a new node is created. New nodes are also created at trace tips. If the trace tip falls in the interior of an element, the trace is prolonged up to the opposite mesh edge.

3. Intersected elements are then split into two new “sub-elements”, which become elements in their own right. Convex polygons are obtained.
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The space discretization: VEM

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Mesh smoothing

Independent smoothing for each fracture to improve the quality of the mesh.

Figure: Left: VEM mesh without modification. Right: Same mesh after modifications.
6 fracture DFN with the VEM

Fracture size from $7m \times 7m$ to $4m \times 4m$, 6 traces

**Figure**: DFN: Solution and mesh
6 fracture DFN with the VEM

**Figure:** VEM: VEM elements on fracture 2

**Figure:** VEM: Solution on fracture 2
6 fracture DFN with the VEM

Figure: VEM: VEM elements on fracture 6

Figure: VEM: Solution on fracture 6
**Figure**: DFN36: Spatial distribution of fractures and the obtained solution for the hydraulic head.
The quality of the obtained solution can be evaluated in terms of two indicators, representing the mismatch errors in the continuity condition and in the flux balance condition on the traces per unit of trace length, defined respectively as:

\[
\Delta_{\text{cont}} = \frac{\sqrt{\sum_{m=1}^{M} \| h_i|_{S_m} - h_j|_{S_m} \|^2}}{\sum_{m=1}^{M} |S_m|},
\]

\[
\Delta_{\text{flux}} = \frac{\sqrt{\sum_{m=1}^{M} \| u_i^m + u_j^m - \alpha (h_i|_{S_m} + h_j|_{S_m}) \|^2}}{\sum_{m=1}^{M} |S_m|}.
\]
## DFN 36F

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DFNs with Conforming Virtual Element Method of several orders

Once we have obtained a partially conforming mesh a simple step forward allows us to obtain a globally conforming mesh simply adding all the nodes on each trace to both the meshes sharing that trace.

\[ V = \{ v : v|_{F_i} \in H^1_0, D(F_i), \forall i = 1, \ldots, N, \]
\[ \gamma_S(v|_{F_i}) = \gamma_S(v|_{F_j}), \forall S \in S_i, i, j = I_S \}, \]

\[
\int_{F_i} \mathcal{K}_i \nabla H_i \nabla v|_{F_i} dF_i = \int_{F_i} f_i v|_{F_i} dF_i + \langle G_N, v|_{\Gamma_{N_i}} \rangle_{H^{-\frac{1}{2}}(\Gamma_{N_i}), H^{\frac{1}{2}}(\Gamma_{N_i})},
\]
\[ \gamma_T(H_i) = \gamma_T(H_j), \forall T \in \mathcal{T}, \{i, j\} = \mathcal{I}(T). \]
Add to the elements of each fracture the nodes on the trace of the twin fracture: Partially conforming mesh $\rightarrow$ Totally conforming mesh.

**Figure**: Final globally conforming VEM mesh
\[ K = \begin{pmatrix} K_1 & 0 & \cdots & 0 \\ 0 & K_2 & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & K_N \end{pmatrix}, \quad f = \begin{pmatrix} f_1 \\ \vdots \\ f_N \end{pmatrix}, \quad h = \begin{pmatrix} h_1 \\ \vdots \\ h_N \end{pmatrix}, \text{ and} \\
L = \begin{pmatrix} L_1 \\ \vdots \\ \vdots \\ L_{n_{dof}} \end{pmatrix}.\]

\[ L_t = \begin{pmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & -1 & 0 & \cdots & 0 \end{pmatrix} \]

\[ \begin{bmatrix} K & L^T \\ L & 0 \end{bmatrix} \begin{bmatrix} h \\ \lambda \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}. \]
Figure: Spatial distribution of fractures for benchmark problem 2
**Figure**: Convergence curves for benchmark problem 2 - Fracture 1
Figure: Solutions for benchmark problem 2 - Fracture 1 and trace 1
Figure: Spatial distribution of fractures for a DFN with 27 fractures.
Figure: Detail of two very close and almost parallel traces
Figure: Comparison of results for critical situations
Table : Net flux in source and sink fractures.

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<td>0.78</td>
<td><strong>10.21</strong></td>
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120 Fractures

Figure: Spatial distribution of fractures for a DFN with 120 fractures
Troublesome situations

(a) Mesh

(b) Detail

Figure: Detail of two very close and almost parallel traces
Figure: Comparison of results for critical situations
Once we have obtained a partially conforming mesh a simple step forward allows us to apply the Mortar method.

\[
\begin{cases}
a_i (h_\delta, v_\delta) + \sum_{S \in S_i} b_S ([v_\delta]_S, \lambda_\delta,S) = (f, v_\delta)_{F_i} & i = 1, \ldots, N, \\
b_S ([h_\delta]_S, \mu_\delta,S) = 0 & \forall S \in \mathcal{S}.
\end{cases}
\]

Figure: Spatial distribution of fractures for benchmark problem 2
Figure: Flux approximation

(a) $M_h^2$

(b) $M_h^4$

(c) $M_h^1$

(d) $M_h^3$
Figure: Flux approximation, $M_h^6$ basis
Thank you.

Bibliography:

Error computation: plots

\[
\begin{align*}
Err^{2}_{L^2} &= \sum_{E \in \mathcal{T}_\delta} \| H - \Pi_{E,k} h_E \|_{L^2(E)}^2, \\
Err^{2}_{H^1} &= \sum_{E \in \mathcal{T}_\delta} \| H - \Pi_{E,k} h_E \|_{H^1(E)}^2.
\end{align*}
\]

\[
\begin{align*}
ul_{left,e,i} &= \nabla \Pi_{E_{l},k} h_{E,i} \cdot n_{e,i}, \\
u_{right,e,i} &= \nabla \Pi_{E_{r},k} h_{E,i} \cdot n_{e,i}, \\
u_{e,i} &= ul_{left,e,i} - ur_{right,e,i}, \\
u_{T,i} &= \sum_{e \subset T} u_{e,i}.
\end{align*}
\]

The L2 error of the flux on the trace is then:

\[
ErrU^{2}_{L^2} = \| U_{T,i} - u_{T,i} \|_{L^2(T)}^2.
\]