A family of methods for DFN flow simulations with non-conforming meshes

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joint work with
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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

DFN are stochastically generated starting from probabilistic distributions of density, dimension, position, orientation, aspect ratio, hydro-geological properties.

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 traces and denoted by $S, S \in \mathcal{S}$.
- Each trace is shared by exactly two fractures: $S = \bar{F}_i \cap \bar{F}_j$, and $I_S = \{i,j\}$. 
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:

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

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

- $H_i$ is the hydraulic head on the fracture $F_i$;
- $K_i$ is the fracture transmissivity tensor: a symmetric and uniformly positive definite tensor, it takes into account the variations in thickness;
- $\frac{\partial H_i}{\partial \nu_i} = \hat{n}_i^t K_i \nabla H_i = G_{iN}$ is the incoming flux trough $\Gamma_{iN}$, it is the outward co-normal derivative of the hydraulic head and $\hat{n}_i$ the unit outward vector normal to the boundary $\Gamma_{iN}$. 
Let $\partial \Omega = \Gamma_N \cup \Gamma_D$ with $\Gamma_N \cap \Gamma_D = \emptyset$ and $\Gamma_D \neq \emptyset$.

Find $H \in H_D^1(\Omega)$ such that:

$$\langle K \nabla H, \nabla v \rangle = \langle q, v \rangle + \langle G_N, v|_{\Gamma_N} \rangle_{H^{-\frac{1}{2}}(\Gamma_N), H^{\frac{1}{2}}(\Gamma_N)}, \quad \forall v \in H^1_{0,D}(\Omega)$$

provides the hydraulic head $H \in H_D^1(\Omega)$, “continuity” at traces required for trial and test functions (required also for the discrete subspaces).

In the following $\left[ \frac{\partial H_i}{\partial \nu^i_S} \right]_S$ denotes the jump of the co-normal derivative along the unique normal $\hat{n}^i_S$ fixed 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 $F_i$. "continuity" at traces required for trial and test functions (required also for the discrete subspaces).
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 $U_i^S \forall S \in \mathcal{S}_i$. 

Stefano Berrone
Let us set \( \partial F_i = \Gamma_{iN} \cup \Gamma_{iD} \) with \( \Gamma_{iN} \cap \Gamma_{iD} = \emptyset \) and \( \Gamma_{iD} \neq \emptyset \) (for ease of exposition).

Solving \( \forall i \in I \) the problem: find \( H_i \in H^1_D(F_i) \) and \( U_i \in S_i \) such that:

\[
(K_i \nabla H_i, \nabla v) = (q_i, v) + \langle U_i, v|_{S_i} \rangle_{U^S_i, U^S_i} + J(U) \nonumber
\]

\[
+ \langle G_{iN}, v|_{\Gamma_{iN}} \rangle_{H^{-\frac{1}{2}}(\Gamma_{iN}), H^{\frac{1}{2}}(\Gamma_{iN})}, \quad \forall v \in V_i = H^1_0, D(F_i) \nonumber
\]

with additional conditions

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

\[
U^S_i + U^S_j = 0, \quad \text{for } i, j \in I_S, \forall S \in S \nonumber
\]

provides the hydraulic head \( H \in V = H^1_D(\Omega) \).
Totally/Partially conforming meshes

Figure : Totally conforming mesh

Figure : Partially conforming mesh
non-conforming meshes: \textbf{120} fractures, \textbf{256} traces DFN

\textbf{Figure}: Non-conforming mesh on a 120 fracture DFN
PDE constrained optimization approach

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

$$H^1(S) \subseteq \mathcal{H}^S(= U^S), \quad \forall S \in \mathcal{S}, \quad \mathcal{H}^S_i = \prod_{s \in S_i} \mathcal{H}^S, \quad \mathcal{H} = \prod_{i \in I} \mathcal{H}^S_i.$$

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

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

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:

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

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

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

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

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

\[
(K_i \nabla H_i, \nabla v) + \alpha \left( H_i|_{S_i}, v|_{S_i} \right)_{S_i} = (q_i, v) + \langle U_i, v|_{S_i} \rangle_{\mathcal{U}^S_i, \mathcal{U}^S_i'} + \langle G_iN, v|_{\Gamma_iN} \rangle_{H^{-\frac{1}{2}}(\Gamma_iN), H^{\frac{1}{2}}(\Gamma_iN)'}, \ \forall v \in V_i = H^1_{0,D}(F_i)
\]
Definition of the discrete problem

- Introduce a finite element triangulation on each fracture, completely independent of the triangulation on the intersecting fractures. Let us further define on this triangulation a finite element-like discretization $h$ for $H$.
- Introduce also 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 problem under consideration is therefore the equality constrained quadratic programming problem

\[
\begin{align*}
\min_{u,h} & \quad J(h, u) := \frac{1}{2} h^T G^h h - \alpha h^T Bu + \frac{1}{2} u^T G^u u \\
\text{s.t.} & \quad Ah - B u = q
\end{align*}
\]

- \( G^h \in \mathbb{R}^{NF \times NF} \), \( G^u \in \mathbb{R}^{NT \times NT} \) are symmetric positive semidefinite sparse matrices;
- \( B \in \mathbb{R}^{NF \times NT} \) is a sparse matrix;
- vectors \( h \in \mathbb{R}^{NF} \) and \( u \in \mathbb{R}^{NT} \) collect all DOFs for the hydraulic head on fractures and for the control variable on traces;
- matrix \( A \in \mathbb{R}^{NF \times NF} \) is the block diagonal (fracturewise) stiffness matrix;
- \( B \in \mathbb{R}^{NF \times NT} \) is a “block diagonal” sparse matrix;
- \( q \in \mathbb{R}^{NF} \) is a vector which accounts for possible source terms and boundary conditions.
The unconstrained problem

The first order optimality conditions for the constrained minimization problem are:

$$
\begin{pmatrix}
G^h & -\alpha B & A^T \\
-\alpha B^T & G^u & -B^T \\
A & -B & 0
\end{pmatrix}
\begin{pmatrix}
h \\
u \\
-p
\end{pmatrix} =
\begin{pmatrix}
0 \\
0 \\
q
\end{pmatrix}.
$$

Use the linear constraint to remove $h = A^{-1}(B u + q)$ from $J$:

$$
\hat{J}(u) = J(u, h(u)) = \frac{1}{2} u^T (B^T A^{-T} G^h A^{-1} B + G^u - \alpha B^T A^{-T} B - \alpha B^T A^{-1} B)u + q^T A^{-T} (G^h A^{-1} B - \alpha B) u = \frac{1}{2} u^T \hat{G} u + u^T \hat{q}.
$$

such that the minimum of the constrained problem is the same as the solution to the unconstrained problem: $\min \hat{J}(u)$

This is equivalent to solve the global linear system

$$
\nabla \hat{J}(u) = \hat{G} u + \hat{q} = 0.
$$
Proposition

Matrix $\hat{G} = \mathcal{B}^T A^{-T} G^h A^{-1} \mathcal{B} + G^u - \alpha \mathcal{B}^T A^{-T} B - \alpha B^T A^{-1} \mathcal{B}$ is symmetric positive definite.

Instead of solving the KKT system we solve the system $\hat{G} u = -\hat{q}$ with a PCG method performing the same operations.

Let us observe that, given a value to the control variables $u_i$, $\forall i \in I$ only LOCAL small independent s.p.d. linear systems on each fracture are solved in order to evaluate the gradient.

$$Ah = \mathcal{B} u + q,$$
$$A^T p = G^h h - \alpha Bu,$$
$$\nabla \hat{J}(u) = \hat{G} u + \hat{q} = \mathcal{B}^T p + G^u u - \alpha B^T h.$$
Main advantages of the proposed method

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

- the optimization approach is independent of the discretization approach used on the fractures.
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:** Tip enrichment function

**Figure:** Enrichment function away from trace tip
Size of fractures spans from $100\text{m} \times 100\text{m}$ to $50\text{m} \times 50\text{m}$, different aspect ratios;
Figure: 120F, Contour plot of the solution: detail
Numerical results

Meshes of $u_i^S$ and $u_j^S$ are given by the intersection of the independent triangulations on the twin-fractures $F_i$ and $F_j$ with the trace $S$, respectively (different independent coarse meshes for $u_i^S$ and $u_j^S$).

We have a source Fracture with non homogeneous Dirichlet boundary condition $H_D = 100$ and a Sink Fracture with $H_D = 0$.

\[
\bar{\Phi} = \frac{1}{2} \left( \sum_{i \in \mathcal{I}_{in}} \sum_{s_m \in S_i} \int_{s_m} (u_i^m - \alpha h_i|_{s_m}) - \sum_{i \in \mathcal{I}_{out}} \sum_{s_m \in S_i} \int_{s_m} (u_i^m - \alpha h_i|_{s_m}) \right),
\]

\[
\Delta_{cons} = \frac{\left| \sum_{i \in \mathcal{I}_{in} \cup \mathcal{I}_{out}} \sum_{s_m \in S_i} \int_{s_m} (u_i^m - \alpha h_i|_{s_m}) \right|}{\bar{\Phi}},
\]

\[
\Delta_{cont} = \sqrt{\sum_{m=1}^{M} \left\| h_i|_{s_m} - h_j|_{s_m} \right\|^2 \frac{h_{max} \sum_{m=1}^{M} |S_m|}{\bar{\Phi} \sum_{m=1}^{M} |S_m|}},
\]

\[
\Delta_{flux} = \sqrt{\sum_{m=1}^{M} \left\| u_i^m + u_j^m - \alpha (h_i|_{s_m} + h_j|_{s_m}) \right\|^2 \frac{\bar{\Phi} \sum_{m=1}^{M} |S_m|}{\bar{\Phi} \sum_{m=1}^{M} |S_m|}},
\]
Table: Results for DFN 120F with Induced Node for $u$. XFEM and standard FEM compared.

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Figure: 3D view of DFN 709 Fractures, 3939 Traces, Area: $376m^2 - 10^4m^2$

Figure: 3D view of DFN 1425 Fractures, 13086 Traces, Area: $3.2m^2 - 10^4m^2$
Figure: DFN709 and DFN1425. Left: distribution of angles between pairs of intersecting traces in the same fracture: $0.26^\circ - 90^\circ$; right: zoom of lower values.
Figure: DFN709 and DFN1425: distribution of trace lengths: $1.6\text{cm} - 260\text{m}$ (left) and of distances between couples of non-intersecting traces in the same fracture: $0.12\text{mm} - \sim 100\text{m}$ (right).
### Table: Relative residuals and flux conservation error $\Delta_{\text{cons}}$ through iterations

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Table: Hydraulic head mismatch $\Delta_{\text{head}}$ and flux unbalance $\Delta_{\text{flux}}$ through iterations

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Parallel preconditioner

Diagonal blocks of matrix $G''$ as preconditioner for the "virtual" matrix $\hat{G}$:

- Sparse and local preconditioner on the traces;
- Symmetric positive definite matrix.

### Table: Convergence behaviour DFN909

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<td>87902</td>
<td>24895</td>
<td>8.937e-7</td>
<td>3.825e-10</td>
<td>3.717e-5</td>
</tr>
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<td>42792</td>
<td>25259</td>
<td>5.213e-7</td>
<td>2.384e-10</td>
<td>4.895e-5</td>
</tr>
</tbody>
</table>
Figure: Master-Slave communication scheme
Figure: Point-to-Point communication scheme
### Speedup

$S_p = \frac{t_1}{t_p}$

### Efficiency

$E_p = \frac{S_p}{p}$

---

#### Table: Parallel efficiency [%] of the CG algorithm for DFN1425

<table>
<thead>
<tr>
<th>Slaves</th>
<th>$\delta = 0.5$</th>
<th>$\delta = 2$</th>
<th>$\delta = 7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI</td>
<td>3</td>
<td>97.03</td>
<td>96.05</td>
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<tr>
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<td>7</td>
<td>79.22</td>
<td>82.63</td>
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<td>15</td>
<td>62.70</td>
<td>65.82</td>
</tr>
<tr>
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<td>15</td>
<td>63.31</td>
<td>59.64</td>
</tr>
<tr>
<td></td>
<td>31</td>
<td>59.00</td>
<td>55.09</td>
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<tr>
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<td>63</td>
<td>28.64</td>
<td>26.50</td>
</tr>
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<td></td>
<td>127</td>
<td>31.89</td>
<td>29.66</td>
</tr>
<tr>
<td>MPI*</td>
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<td>63.31</td>
<td>59.64</td>
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<td>59.00</td>
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References


