Virtual Element Methods for subsurface flow and transport simulations in fractured media

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Virtual Element Methods III
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Discrete fracture network and flow model:

- 3D network of intersecting fractures in the rock matrix
- Fractures are represented as planar polygons
- Rock matrix is considered impervious: the flow only occurs in the fractures
- Flow modeled by Darcy law in the fractures
- Flux balance and hydraulic head continuity imposed across fracture intersections (traces)

No changes on the given DFN geometry stochastically generated (position, orientation, size, shape) → uncertainty quantification

Complex domain: difficulties in good quality mesh generation
find $H \in H_D^1(F')$ such that:

$$(K \nabla H, \nabla v) = (q, v)$$

$$+ \langle G_N, v|_{\Gamma_N} \rangle_{H^{-\frac{1}{2}}(\Gamma_N), H^{\frac{1}{2}}(\Gamma_N)}, \forall v \in V = H_{0,D}^1(F')$$

- $H$ is the hydraulic head on the fracture $F'$;
- $K$ is the fracture transmissivity tensor: a symmetric and uniformly positive definite tensor depending on the hydrological properties and thickness of the real fracture (Boussinesq model: $K = e^3 \frac{\rho g}{12\nu}$);
- $\frac{\partial H}{\partial \hat{n}} = \hat{n}^t K \nabla H = G_N$ is the outward co-normal derivative of the hydraulic head and $\hat{n}$ the unit outward vector normal to the boundary $\Gamma_N$. 
Coupled fracture formulation

For each trace $S \in \mathcal{S}$ on the fracture $F_i \ i = 1, \ldots, N$, let us denote by

$$U^S_i := \left[ \frac{\partial H_i}{\partial \hat{v}_S^i} \right]_S \quad U^S_i \in \mathcal{U}^S \subseteq \mathcal{H}^{-\frac{1}{2}}(S)$$

the flux entering in the fracture through the trace $S$, and $U_i \in \mathcal{U}^{S_i}$ the tuple of fluxes $U^S_i \ \forall S \in \mathcal{S}_i$.
Solving $\forall i \in I$ the problem: find $H_i \in H^1_D(F_i)$ and $U_i \in S_i$ such that:

$$(K_i \nabla H_i, \nabla v) = (q, v) + \langle U_i, v|_{S_i} \rangle u^S_i, u^{S_i}$$. 

$$+ \langle G_{iN}, v|_{\Gamma_{iN}} \rangle \mathbf{H}_{-\frac{1}{2}}(\Gamma_{iN}), \mathbf{H}_{\frac{1}{2}}(\Gamma_{iN}), \forall v \in V_i = H^1_{0,D}(F_i)$$ 

with additional conditions

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

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

provides the hydraulic head $H \in V = H^1_D(\Omega)$.

- $H_i$ 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 function.
Virtual Element Method allows meshes with

- **Polygonal elements** with a different number of edges,
- elements with **aligned edges**: **hanging nodes** straightforwardly managed,
- we can easily obtain **polygonal partially or totally conforming meshes** on DFNs starting from **independent triangular meshes** on the fractures.

- **We need a lot of information on the traces** → conforming meshes are useful.

Totally/Partially conforming meshes

**Figure:** Totally conforming triangular mesh: *Conforming VEM*


**Figure:** Partially conforming triangular mesh: *Mortar VEM*

The space discretization: VEM

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 segment-trace is prolonged up to the opposite mesh edge.

3. Elements cut by prolonged segment-traces are then split into new “sub-elements”, which become elements in their own right. Convex polygons are obtained.
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Mesh smoothing

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

Figure: Mesh generation
Mesh smoothing

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

Figure: Mesh generation
Mesh smoothing

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

Figure: Mesh modifications
Once we have obtained a partially conforming mesh a simple step forward allows us to obtain a globally conforming mesh simply adding to the elements of each fracture with an edge on the trace the nodes on the trace of the twin fracture:

Partially conforming mesh \( \rightarrow \) Totally conforming mesh.
Figure: Final globally conforming VEM mesh
Let us define the space of “continuous” test functions

\[ V = \{ v : v|_{F_i} \in H^1_{0,D}(F_i), \forall i = 1, \ldots, N, \gamma_S(v|_{F_i}) = \gamma_S(v|_{F_j}), \forall S \in S_i, i, j = I_S \} , \]

find \( H_i \in H^1_D(F_i), \forall i = 1, \ldots, N, \) such that \( \forall v \in V: \)

\[
\sum_{i=1}^{N} \int_{F_i} K_i \nabla H_i \nabla v|_{F_i} dF_i = \sum_{i=1}^{N} \left[ \int_{F_i} q_i v|_{F_i} dF_i + \langle G_i,N,v|_{\Gamma N_i} \rangle_{H^{-\frac{1}{2}}(\Gamma N_i),H^{\frac{1}{2}}(\Gamma N_i)} \right],
\]

\[
\gamma_T(H_i) = \gamma_T(H_j), \quad \forall S \in S, \{i, j\} = \mathcal{T}(S).
\]
\[
\begin{bmatrix}
K & L^T \\
L & 0
\end{bmatrix}
\begin{bmatrix}
h \\
\lambda
\end{bmatrix} =
\begin{bmatrix}
f \\
0
\end{bmatrix}.
\]

\[
K =
\begin{pmatrix}
K_1 & 0 & \cdots & 0 \\
0 & K_2 & \cdots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
0 & \cdots & \cdots & K_N
\end{pmatrix}
, 

f =
\begin{pmatrix}
f_1 \\
\vdots \\
f_N
\end{pmatrix}
, 

h =
\begin{pmatrix}
h_1 \\
\vdots \\
h_N
\end{pmatrix}
, 

L =
\begin{pmatrix}
L_1 \\
\vdots \\
L_{n_{dof_t}}
\end{pmatrix}.
\]

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

The multiplier \( \lambda_t \) penalizes the jump \( h_{dof_j} - h_{dof_i} \).
27 Fractures

Figure: Spatial distribution of fractures for a DFN with 27 fractures
Figure: DFN 27: Trace very close to an edge. Smoothing can prevent these situations
Figure: DFN 27, F3: Critical situations and orthogonal polynomials
Orthogonal basis

\[ p^{k-1} = Q^{k-1} m^{k-1}, \text{ s.t. } p^k H^{k-1} = \int_E p^{k-1} \left( p^{k-1} \right)^T d\Omega = I^{k-1} \]

\[ p^{k/k-1} = m^{k/k-1} - \left( \int_E m^{k/k-1} \left( p^{k-1} \right)^T d\Omega \right) p^{k-1} \]

\[ = m^{k/k-1} - \left( \int_E m^{k/k-1} \left( m^{k-1} \right)^T d\Omega \right) m^{k-1} \]

\[ = \left[ -m H^{k,k-1} I^{k/k-1} \right] m^k. \]

\[ p^{k/k-1} = Q^{k/k-1} m^k, \text{ s.t. } p^{k/k-1} H^{k,k-1} = I^{k/k-1} \]

\[ p^k = Q^k m^k, \text{ with } Q^k = \begin{bmatrix} Q^{k-1} & O^{k-1,k} \\ Q^{k/k-1} & O^{k/k-1,k} \end{bmatrix} \]
<table>
<thead>
<tr>
<th>order</th>
<th>minimum aspect ratio</th>
<th>m polygons</th>
<th>ill-conditioned polygons ($&gt;10^{10}$)</th>
<th>badly shaped polygons</th>
<th>both causes</th>
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<tr>
<td>5</td>
<td>150</td>
<td>4256</td>
<td>124</td>
<td>66</td>
<td>9</td>
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<tr>
<td>5</td>
<td>50</td>
<td>4177</td>
<td>115</td>
<td>145</td>
<td>18</td>
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<tr>
<td>5</td>
<td>10</td>
<td>3775</td>
<td>60</td>
<td>547</td>
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<tr>
<td>6</td>
<td>150</td>
<td>3193</td>
<td>1187</td>
<td>43</td>
<td>32</td>
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<tr>
<td>6</td>
<td>50</td>
<td>3143</td>
<td>1149</td>
<td>93</td>
<td>70</td>
</tr>
<tr>
<td>6</td>
<td>10</td>
<td>2888</td>
<td>947</td>
<td>348</td>
<td>272</td>
</tr>
</tbody>
</table>

Table: DFN 27. Number of polygons where orthogonal polynomials were used and the motivations for their use.
Figure: DFN 27, F4: Critical situations and orthogonal polynomials

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Figure: DFN 27, Condition number of local projectors, order 6
Figure: Spatial distribution of fractures for a DFN with 130 fractures

- up to 24 traces in a fracture,
- minimum angle $= 0.41^\circ$,
- $\text{TraceLength}_{\text{Max}} / \text{TraceLength}_{\text{Min}} \approx 4.5E3$. 
Figure: DFN 130: Detail of two traces meeting at a very small angle
Figure: DFN 130: Comparison of results for problematic situations

(a) Order 1

(b) Order 3

(c) Order 4

(d) Order 4, orthogonal polynomials
Orthogonalization error $\| PH^{k-1} - I^{k-1} \|_\infty$

**Figure**: DFN 130: Orthogonalization error $\| PH^{k-1} - I^{k-1} \|_\infty$
Table: DFN 130. Counts of the elements with large orthogonalization error and maximum orthogonalization error for different orders.
Partially conforming approach: Mortar method

We may use a partially conforming mesh applying the Mortar method, imposing the head continuity at traces in a weak sense.

Recall the local problems: $\forall i = 1, \ldots, N$, $\forall v_i \in V_i$

$$a_i(H_i, v_i) = (q_i, v_i) + \sum_{S \in S_i} \langle U^S_i, v_i|_{S_i} \rangle_{H^{-1/2}(S), H^{1/2}(S)} + B.C.$$

$$U^S_i + U^S_j = 0, \quad [H]_S = 0 \quad \forall S = F_i \cap F_j$$

On each trace $S \in \mathcal{S}$ we define:

$$b_S(v, \psi_S) = \langle \psi_S, [v]_S \rangle_{H^{-1/2}(S), H^{1/2}(S)}, \quad v \in V_i \times V_j,$$

$$\Lambda_S = U^S_i = -U^S_j, \quad i \text{ smallest index of fractures generating } S.$$  

- impose $b_S(\psi_S, H) = 0 \forall S \in \mathcal{S}, \forall \psi_S \in H^{-1/2}(S)$
- set
  $$b_S(\Lambda_S, v_k) = (-1)^{k=i} \langle \Lambda_S, [v_k]_S \rangle_{H^{-1/2}(S), H^{1/2}(S)}, \quad k = i, j.$$
Summing up over the whole network:

\[ V = \prod_{i=1,\ldots,N} V_i, \quad M = \prod_{S \in \mathcal{S}} M_S = \prod_{S \in \mathcal{S}} H^{-1/2}(S) \]

\[ a(H, v) = \sum_{i=1}^{N} a_i(H_i, v_i), \quad b(\psi, v) = \sum_{S \in \mathcal{S}} b_S(\psi_S, v) \]

Global problem:

\[
\begin{cases}
    a(H, v) + b(\Lambda, v) = (q, v) + \langle H^N, v \rangle & \forall v \in V \\
    b(\psi, H) = 0 & \forall \psi \in M
\end{cases}
\]

\[
\begin{cases}
    a_\delta(H_\delta, v) + b_\delta(\Lambda_\delta, v) = (q_\delta, v)_\delta + (H_\delta^N, v)_{\Gamma N} & \forall v \in V_\delta \\
    b_\delta(\psi, H_\delta) = 0 & \forall \psi \in M_\delta = \prod_{S} M_{\delta, S}
\end{cases}
\]

\[ V_\delta = \text{VEM space of order } k, \text{ for several values of } k \]

\[ M_{\delta, S} = \text{three different Mortar bases } \mathcal{M}_0, \mathcal{M}_1, \mathcal{M}_2 \]
Numerical results - Convergence

Figure: Benchmark problem P2: spatial distribution of fractures
\[
\begin{align*}
(Err_{L^2}^\Lambda)^2 &= \sum_{S \in S} \sum_{e \subset S} \| \Lambda - \Lambda_\delta \|^2_e, \\
(Err_{H^{-1/2}}^\Lambda)^2 &= \sum_{S \in S} \sum_{e \subset S} |e| \| \Lambda - \Lambda_\delta \|^2_e. 
\end{align*}
\]

<table>
<thead>
<tr>
<th>VEM order</th>
<th>Mortar basis</th>
<th>$L^2$ Norm</th>
<th>$H^1$ Norm</th>
<th>$L^2$ Norm</th>
<th>$H^{-1/2}$ Norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\mathcal{M}_0$</td>
<td>1.00 (1)</td>
<td>0.50 (0.5)</td>
<td>1.19</td>
<td>1.79</td>
</tr>
<tr>
<td>1</td>
<td>$\mathcal{M}_1$</td>
<td>1.00 (1)</td>
<td>0.50 (0.5)</td>
<td>1.26</td>
<td>1.87</td>
</tr>
<tr>
<td>2</td>
<td>$\mathcal{M}_0$</td>
<td>1.38 (1.5)</td>
<td>0.91 (1)</td>
<td>0.98</td>
<td>1.54</td>
</tr>
<tr>
<td>2</td>
<td>$\mathcal{M}_1$</td>
<td>1.50 (1.5)</td>
<td>1.01 (1)</td>
<td>1.54</td>
<td>2.05</td>
</tr>
<tr>
<td>2</td>
<td>$\mathcal{M}_2$</td>
<td>1.51 (1.5)</td>
<td>1.01 (1)</td>
<td>2.45</td>
<td>3.02</td>
</tr>
</tbody>
</table>

**Table**: Benchmark problem: convergence rates with respect to $H_{dofs}$ and $\Lambda_{dofs}$ for several VEM orders and Mortar bases. The numbers in parentheses indicate the expected rates.
Figure: Test problem DFN134 (134 fractures): spatial distribution
Figure: DFN134 fractures, example of mesh and solution on a fracture. VEM with $k = 2$ and $\mathcal{M}_1$ mortar basis
Figure: DFN134 fractures, example of mesh and solution on a fracture. VEM with $k = 2$ and $M_1$ mortar basis
Advection dominated transport of a passive scalar

Figure: DFN

Figure: Hydraulic head

Figure: Darcy velocity field $\beta = -K \nabla h/e$
We start discretizing the steady convection diffusion equation in the convection dominated regime:

\[-\nabla \cdot (\nu \nabla c) + \beta \cdot \nabla c = f.\]

The problem formulation results in

\[B_{\text{supg},h} (u_h, v_h) = F_{\text{supg},h} (v_h) \quad \forall v_h \in V_h ,\]

Let us define the discrete bilinear form \( B_{\text{supg},h} : V_h \times V_h \to \mathbb{R} \) such that

\[B_{\text{supg},h} (w_h, v_h) := \left( \nu \Pi_{k-1}^0 \nabla w_h, \Pi_{k-1}^0 \nabla v_h \right) + \left( \beta \cdot \Pi_{k-1}^0 \nabla w_h, \Pi_k v_h \right) + \sum_{E \in T_h} \tau_E \left( -\nabla \cdot (\nu \Pi_{k-1}^0 \nabla w_h) + \beta \cdot \Pi_{k-1}^0 \nabla w_h , \beta \cdot \Pi_{k-1}^0 \nabla v_h \right)_E \]

\[+ \left( \nu_E + \tau_E \beta_E^2 \right) S^E \left( \left( I - \Pi_k \nabla \right) w_h, \left( I - \Pi_k \nabla \right) v_h \right) .\]

and the discrete linear operator \( F_{\text{supg},h} (v_h) : V_h \to \mathbb{R} \) such that

\[F_{\text{supg},h} (v_h) = \left( f, \Pi_{k-1}^0 v_h \right) + \sum_{E \in T_h} \tau_E \left( f, \beta \cdot \Pi_{k-1}^0 \nabla v_h \right)_E .\]
The stability parameter $\tau_E$ is classically defined, $\forall E \in \mathcal{T}_h$, by

$$
\tau_E := \begin{cases} 
\frac{h_E}{2\beta_E}, & \text{locally convection dominated regime}, \\
\frac{m_k^E h_E^2}{4\nu_E}, & \text{locally diffusion dominated regime}.
\end{cases}
$$

- L.P. Franca, S.L. Frey, T.J.R. Hughes,
SUPG stabilization, rate of convergence

**Figure**: Theoretical and numerical rates of convergence for VEM of order 1

**Figure**: Theoretical and numerical rates of convergence for VEM of order 3
Convection-Diffusion: no stabilization versus SUPG stabilization for very large Péclet numbers

Figure: Solution without stabilization

Figure: Solution with SUPG-like stabilization
DFN Geothermal application

Characteristic dimensions: 150 Fractures, 1000m depth, 1000m length, pumping pressure 30bar, rock temperature 50°C, water temperature 15°C.

Figure: Wells and system of fractures
We start discretizing the unsteady reaction convection diffusion equation **in the convection dominated regime** on each fracture:

\[ e_i \rho c \frac{\partial u}{\partial t^*} - e_i \nabla^* \cdot (\lambda \nabla^* u) + e_i \rho c \beta^* \cdot \nabla^* u + \bar{h}u = \bar{h}u_r. \]

Fracture transmissivity and aperture

- \( K_i = 10^{-\alpha} \sqrt[4]{A_i} \frac{kg}{ms}, \)
- \( e_i = 2 \times 10^{-3} \sqrt{12A_i} m, \)

Fluid properties and surface heat transfer coefficient

- \( \rho = 1000 \frac{kg}{m^3}, \)
- \( c = 4186 \frac{J}{KgK}, \)
- \( \lambda = 0.6 \frac{W}{mK}, \)
- \( \bar{h} = 10 \frac{W}{m^2K}. \)

Characteristic dimensions:

- \( \bar{H} = 1000m, \)
- \( \bar{L} = 100m, \)
- \( \bar{e} = 10^{-3} m, \)
- \( \bar{U} = 1K, \)
- \( \bar{B} = 10^{-\alpha} \frac{\sqrt{LH}}{eL} = 10^{-\alpha} \frac{\bar{H}}{\bar{e} \sqrt{\bar{L}}}, \)
- \( \bar{T} = \frac{\bar{L}}{\bar{B}}, \)
Non-dimensional formulation:

\[
\frac{\partial u}{\partial t} - \nabla \cdot (\nu \nabla u) + \beta \cdot \nabla u + \gamma u = \gamma u_r.
\]

- \( \nu = \frac{L}{B \, e_i \rho c} \frac{1}{L^2} = 1.43 \, 10^{\alpha - 11} \frac{\bar{e}}{e_i} \),
- \( \beta = \frac{\beta^*}{B} \sim \mathcal{O}(1) \),
- \( \gamma = \frac{\bar{L}}{B \, e_i \rho c} = 2.39 \, 10^{\alpha - 6} \frac{\bar{L} \sqrt{\bar{L}}}{H} \frac{\bar{e}}{e_i} = 2.39 \, 10^{\alpha - 6} \frac{\bar{e}}{e_i} \)
\[
\frac{\partial u}{\partial t} - \nabla \cdot (\nu \nabla u) + \beta \cdot \nabla u + \gamma u = \gamma u_r.
\]

Let us define the discrete bilinear form \( B_{\text{supg},h} : V_h \times V_h \to \mathbb{R} \) such that

\[
B_{\text{supg},h} (w_h, v_h) := \left( \frac{\partial \Pi^0_{k-1} w_h}{\partial t}, \Pi^0_{k-1} \nabla v_h \right) + \left( \nu \Pi^0_{k-1} \nabla w_h, \Pi^0_{k-1} \nabla v_h \right)
+ \left( \beta \cdot \Pi^0_{k-1} \nabla w_h, \Pi^0_{k} v_h \right) + \gamma \left( \Pi^0_{k-1} w_h, \Pi^0_{k} v_h \right)
+ \sum_{E \in \mathcal{T}_h} \tau_E \left( \frac{\partial \Pi^0_{k-1} w_h}{\partial t} - \nabla \cdot (\nu \Pi^0_{k-1} \nabla w_h) + \beta \cdot \Pi^0_{k-1} \nabla w_h + \gamma \Pi^0_{k-1} w_h, \beta \cdot \Pi^0_{k-1} \nabla v_h \right)_E
+ (\nu_E + \tau_E \beta_E^2) S^E \left( \left( I - \Pi^\nabla_k \right) w_h, \left( I - \Pi^\nabla_k \right) v_h \right).
\]

and the discrete linear operator \( F_{\text{supg},h} (v_h) : V_h \to \mathbb{R} \) such that

\[
F_{\text{supg},h} (v_h) = \gamma (u_r, \Pi^0_k v_h) + \sum_{E \in \mathcal{T}_h} \tau_E \gamma (u_r, \Pi^0_{k-1} v_h)_E.
\]
The stability parameter $\tau_E$ is defined, $\forall E \in \mathcal{T}_h$, by

$$\tau_E := \frac{h_E}{2\beta_E} \min\{Pe_E, 1, Ka_E, Cour_E\}$$

$$Pe_E := m_k \frac{\beta_E h_E}{2\nu_E}, \quad Ka_E := C_\tau \frac{2\beta_E}{h_E \gamma_E}, \quad Cour_E := C_\tau \frac{2\beta_E \Delta t}{h_E}.$$ 

Let us take $\alpha = 7$:

$$Pe_E \sim 10^4 h_e, \quad Ka_E \sim 10 \frac{1}{h_E}, \quad Cour_E \sim \frac{\Delta t}{h_E}.$$
150 Fractures, steady solution

Figure: Steady solution
Figure: Temperature evolution in a DFN geothermal application ($\bar{h} = 0.1$ slightly doped)
Thank you!

References


