

Hybrid dimensional Darcy flow in fractured porous medium and parallel implementation in code ComPASS

Feng Xing^{1,2,3}

joint work with

Konstantin Brenner^{1,2}, Simon Lopez³, Roland Masson^{1,2}

- (1) *Laboratoire J.A. Dieudonné, Université de Nice*
- (2) *Team COFFEE, INRIA Sophia Antipolis*
- (3) *Institut BRGM*



Goal: develop a parallel prototype to test promising numerical methods on realistic cases

Brief history

0. CEMRACS 2012: heat equation as a toy problem.
E. Dalissier, C. Guichard, P. Havé, R. Masson, C. Yang.
1. Two phase flow in porous media: work on the linear solvers (FVCA 7).
R. Eymard, C. Guichard, R. Masson.
2. Tracer model on a fractured porous media.
R. Masson, F. Xing

Goal: develop a parallel prototype to test promising numerical methods on realistic cases

Main specifications

- Parallel programming with MPI using Fortran 2003
- General meshes (polyhedral cells, possibly non planar faces)



- Adapted to Finite Volume schemes with d.o.f. at nodes, cells, faces and 'usual' compact stencil
- Connected with scientific computing libraries: METIS, PETSc, Trilinos, VTK

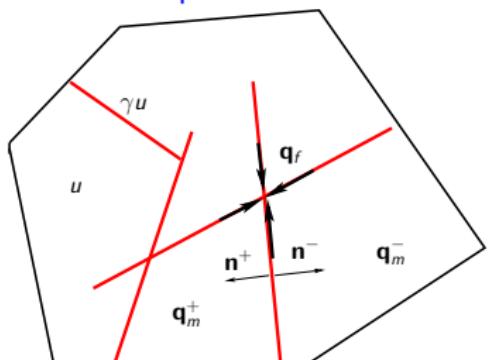
Outline

- Tracer problem on discrete fracture network
- Vertex-centered discretisation (VAG)
- Implementation in code ComPASS
- Numerical results

Tracer problem on a Discrete Fracture Network (DFN)

Hybrid dimensional models for DFN [Alboin-Jaffré-Roberts-Serres 2002]
 $d_f \ll \text{diam}(\Omega)$ continuous pressure u on $\bar{\Omega}$ $\dim(\Gamma) = \dim(\Omega) - 1$

1. Pression equation


$$\left\{ \begin{array}{ll} \text{div}(\mathbf{q}_m) = 0 & \text{on } \Omega \setminus \bar{\Gamma} \\ \text{div}_\tau(\mathbf{q}_f) + [\![\mathbf{q}_m \cdot \mathbf{n}]\!] = 0 & \text{on } \Gamma \\ \mathbf{q}_m = -\Lambda_m \nabla u & \text{on } \Omega \setminus \bar{\Gamma} \\ \mathbf{q}_f = -d_f \Lambda_f \nabla_\tau \gamma u & \text{on } \Gamma \end{array} \right.$$

with the jump $[\![\mathbf{q}_m \cdot \mathbf{n}]\!] = \mathbf{q}_m^+ \cdot \mathbf{n}^+ + \mathbf{q}_m^- \cdot \mathbf{n}^-$

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2. Tracer equation

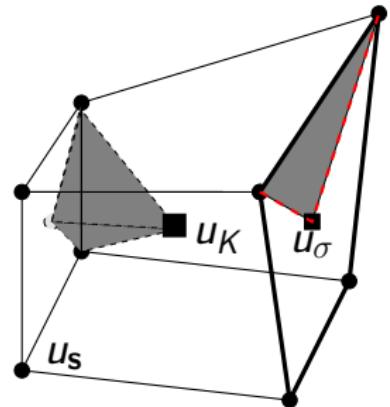
$$\left\{ \begin{array}{ll} \partial_t c_m + \text{div}(c_m \mathbf{q}_m) = 0 & \text{on } \Omega \setminus \bar{\Gamma} \\ \partial_t (d_f c_f) + \text{div}_\tau(c_f \mathbf{q}_f) + [\![c_m \mathbf{q}_m \cdot \mathbf{n}]\!] = 0 & \text{on } \Gamma \\ c_m^+ = c_f & \text{on } \{x \in \Gamma \mid \mathbf{q}_m^+ \cdot \mathbf{n}^+ > 0\} \\ c_m^- = c_f & \text{on } \{x \in \Gamma \mid \mathbf{q}_m^- \cdot \mathbf{n}^- > 0\} \end{array} \right.$$

VAG discretization for a tracer problem on a Discrete Fracture Network (DFN)

* Discrete Unknowns *

$$u_{\mathcal{D}} = (u_K, u_\sigma, u_s, K \in \mathcal{M}, \sigma \in \mathcal{F}_\Gamma, s \in \mathcal{V})$$

\mathcal{M} : cells, \mathcal{F}_Γ : fracture faces, \mathcal{V} : vertex



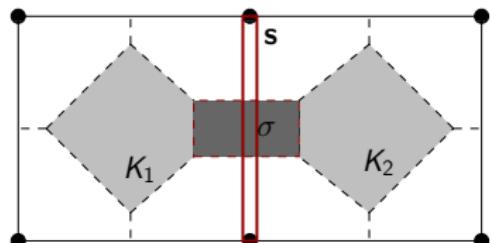
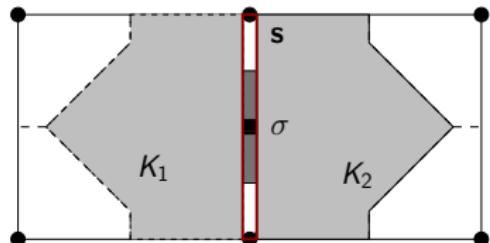
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* Volume redistribution *

$$\omega_K, K \in \mathcal{M}, \quad \omega_\sigma, \sigma \in \mathcal{F}_\Gamma, \quad \omega_s, s \in \mathcal{V}$$

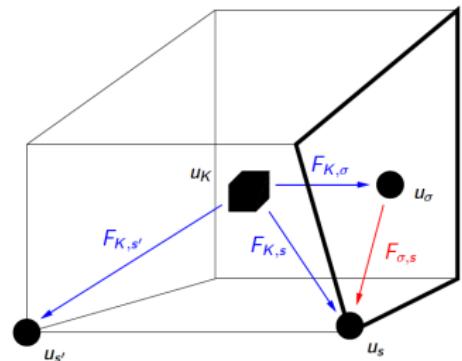


mixing of rocktype
⇒ non accurate results

★ Fluxes ★

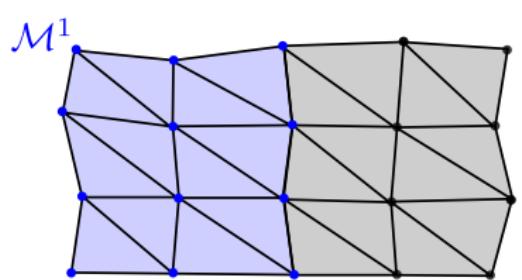
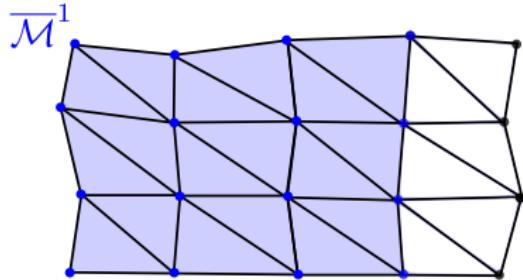
In the matrix : The fluxes $F_{K,s}(u_D)$, $F_{K,\sigma}(u_D)$ are computed from all the nodes and the fracture faces connected to K .

In the fracture : The fluxes $F_{\sigma,s}(u_D)$ are computed from all the nodes connected to σ .



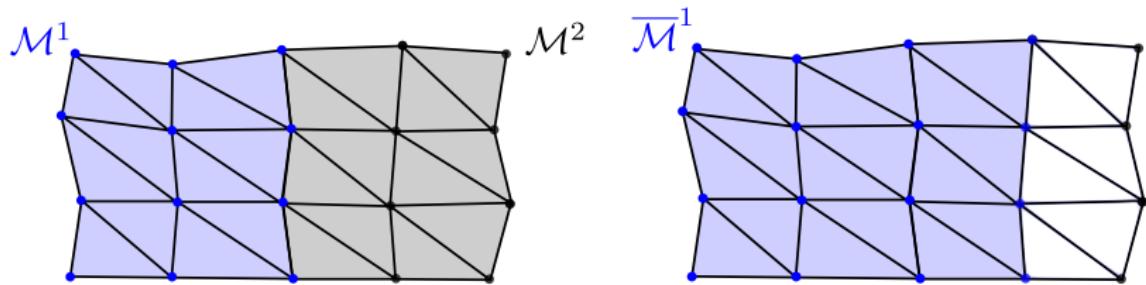
Mesh decomposition

- Mesh decomposition by METIS: \mathcal{M}^1 and \mathcal{M}^2
- One layer ghost cells: $\overline{\mathcal{M}}^1$ and $\overline{\mathcal{M}}^2$


$$\mathcal{M}^2$$


Mesh decomposition

- Mesh decomposition by METIS: \mathcal{M}^1 and \mathcal{M}^2
- One layer ghost cells: $\overline{\mathcal{M}}^1$ and $\overline{\mathcal{M}}^2$

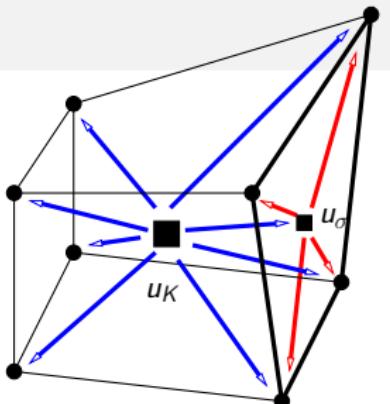


- Vertex: \mathcal{V}^1 and \mathcal{V}^2
- Vertex with ghost: $\overline{\mathcal{V}}^1$ and $\overline{\mathcal{V}}^2$
- Fracture faces: \mathcal{F}^1 and \mathcal{F}^2
- Fracture faces with ghost: $\overline{\mathcal{F}}^1$ and $\overline{\mathcal{F}}^2$

VAG discretization of the pressure equation

On each processor p , the unknowns are:

$$\bar{u}_{\mathcal{D}}^p = (u_K, u_\sigma, u_s, K \in \overline{\mathcal{M}}^p, \sigma \in \overline{\mathcal{F}}_\Gamma^p, s \in \overline{\mathcal{V}}^p)$$



On each processor p , the equations are:

$$\left\{ \begin{array}{l} \sum_{\nu \in \mathcal{V}_K \cup (\mathcal{F}_K \cap \mathcal{F}_\Gamma)} F_{K,\nu}(u_{\mathcal{D}}) = 0, \quad K \in \overline{\mathcal{M}}^p \\ \sum_{s \in \mathcal{V}_\sigma} F_{\sigma,s}(u_{\mathcal{D}}) + \sum_{K \in \mathcal{M}_\sigma} -F_{K,\sigma}(u_{\mathcal{D}}) = 0, \quad \sigma \in \mathcal{F}_\Gamma^p \\ \sum_{K \in \mathcal{M}_s} -F_{K,s}(u_{\mathcal{D}}) + \sum_{\sigma \in \mathcal{F}_{\Gamma,s}} -F_{\sigma,s}(u_{\mathcal{D}}) = 0, \quad s \in \mathcal{V}^p \setminus dof_{Dir} \\ u_s = u_{Dir}, \quad s \in dof_{Dir} \end{array} \right.$$

VAG discretization of the concentration equation, Upwind scheme

On each processor p , at each time step $n \rightarrow n + 1$, the unknowns are:

$$\bar{c}_{\mathcal{D}}^{p,\{n+1\}} = (c_K^{n+1}, c_\sigma^{n+1}, c_s^{n+1}, K \in \overline{\mathcal{M}}^p, \sigma \in \overline{\mathcal{F}}_\Gamma^p, s \in \overline{\mathcal{V}}^p)$$

On each processor p , the equations are:

$$\left\{ \begin{array}{l} |\omega_K| \frac{c_K^{n+1} - c_K^n}{\Delta t} + \sum_{\nu \in \mathcal{V}_K \cup (\mathcal{F}_K \cap \mathcal{F}_\Gamma)} H_{K,\nu}(c_{\mathcal{D}}^n) = 0, \quad K \in \mathcal{M}^p \\ |\omega_\sigma| \frac{c_\sigma^{n+1} - c_\sigma^n}{\Delta t} + \sum_{s \in \mathcal{V}_\mathcal{F}} H_{\sigma,s}(c_{\mathcal{D}}^n) - \sum_{K \in \mathcal{M}_\sigma} H_{K,\sigma}(c_{\mathcal{D}}^n) = 0, \quad \sigma \in \mathcal{F}_\Gamma^p \\ |\omega_s| \frac{c_s^{n+1} - c_s^n}{\Delta t} - \sum_{K \in \mathcal{M}_s} H_{K,s}(c_{\mathcal{D}}^n) - \sum_{\sigma \in \mathcal{F}_{\Gamma,s}} H_{\sigma,s}(c_{\mathcal{D}}^n) = 0, \quad s \in \mathcal{V}^p \setminus dof_{Dir} \\ c_s = c_{Dir}, \quad s \in dof_{Dir} \end{array} \right.$$

with the following Explicit Upwind Two Point Fluxes:

$$H_{K,\nu}(c_{\mathcal{D}}^n) = c_K^n F_{K,\nu}(u_{\mathcal{D}})^+ + c_\nu^n F_{K,\nu}(u_{\mathcal{D}})^-$$

$$H_{\sigma,s}(c_{\mathcal{D}}^n) = c_\sigma^n F_{\sigma,s}(u_{\mathcal{D}})^+ + c_s^n F_{\sigma,s}(u_{\mathcal{D}})^-$$

VAG discretization of the concentration equation, MUSCL scheme

On each processor p , two steps for $n \rightarrow n + 1$:

A second order MUSCL type reconstruction

$$\bar{c}_{\mathcal{D}}^{p,*} = \{c_{K,\nu}^*, K \in \overline{\mathcal{M}}^p, \nu \in dof(K)\} \cup \{c_{\sigma,\nu}^*, \sigma \in \overline{\mathcal{F}}_{\Gamma}^p, \nu \in dof(\sigma)\}$$

Acceptable slopes:

$$\bar{I}_{\mathcal{D}}^{p,*} = (I_K^*, I_{\sigma}^*, I_s^*, K \in \overline{\mathcal{M}}^p, \sigma \in \overline{\mathcal{F}}_{\Gamma}^p, s \in \overline{\mathcal{V}}^p)$$

Compute

$$\begin{aligned} H_{K,\nu}(c_{\mathcal{D}}^{p,*}, \bar{I}_{\mathcal{D}}^{p,*}) &= (x_K^n + \mathcal{P}_{I_K^*}(c_{K,\nu}^* - c_K^n)) F_{K,\nu}(u_{\mathcal{D}})^+ \\ &\quad + (x_{\nu}^n + \mathcal{P}_{I_K^*}(c_{K,\nu}^* - c_K^n)) F_{K,\nu}(u_{\mathcal{D}})^- \end{aligned}$$

and

$$\begin{aligned} H_{\sigma,\nu}(c_{\mathcal{D}}^{p,*}, \bar{I}_{\mathcal{D}}^{p,*}) &= (x_{\sigma}^n + \mathcal{P}_{I_{\sigma}^*}(c_{\sigma,\nu}^* - c_{\sigma}^n)) F_{\sigma,\nu}(u_{\mathcal{D}})^+ \\ &\quad + (x_{\nu}^n + \mathcal{P}_{I_{\sigma}^*}(c_{\sigma,\nu}^* - c_{\sigma}^n)) F_{\sigma,\nu}(u_{\mathcal{D}})^- \end{aligned}$$

Outline of ComPASS implementation

0. Initialization

- Global to Local Mesh
- VAG scheme transmissivities

1. Pressure equation

- Assembling of non-square linear systems

$$\begin{pmatrix} A^p & B^p \\ C^p & D^p \end{pmatrix} \begin{pmatrix} U_{\bar{\mathcal{V}}^p \cup \bar{\mathcal{F}}_\Gamma^p} \\ U_{\bar{K}^p} \end{pmatrix} = RHS^p \quad A^p \in \mathbb{R}^{\mathcal{V}^p \cup \mathcal{F}_\Gamma^p} \otimes \mathbb{R}^{\bar{\mathcal{V}}^p \cup \bar{\mathcal{F}}_\Gamma^p} \quad C^p \in \mathbb{R}^{\bar{\mathcal{M}}^p} \otimes \mathbb{R}^{\bar{\mathcal{V}}^p \cup \bar{\mathcal{F}}_\Gamma^p}$$
$$B^p \in \mathbb{R}^{\mathcal{V}^p \cup \mathcal{F}_\Gamma^p} \otimes \mathbb{R}^{\bar{\mathcal{M}}^p} \quad D^p \in \mathbb{R}^{\bar{\mathcal{M}}^p} \otimes \mathbb{R}^{\bar{\mathcal{M}}^p}$$

- Schur complement system $(A^p - B^p(D^p)^{-1}C^p)U_{\bar{\mathcal{V}}^p \cup \bar{\mathcal{F}}_\Gamma^p} = \widetilde{RHS}^p$
- Resolution by PETSc (Trilinos) $\Rightarrow U_{\mathcal{V}^p \cup \mathcal{F}_\Gamma^p}$
- Synchronization $\Rightarrow U_{\bar{\mathcal{V}}^p \cup \bar{\mathcal{F}}_\Gamma^p}$
- Schur complement $\Rightarrow U_{\bar{K}^p}$

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- Schur complement $\Rightarrow U_{\bar{K}^p}$

3. CFL condition $\Rightarrow \Delta t$

4. Time loop for concentration equation

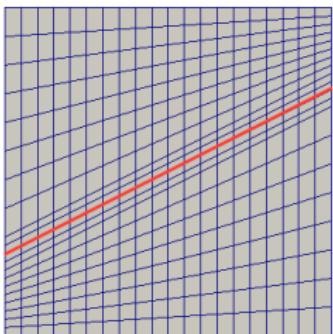
- Explicit scheme: $c_D^{n+1} \leftarrow \bar{c}_D^n$
- Synchronization: $\bar{c}_D^{n+1} \leftarrow c_D^{n+1}$

2D analytical example - Test case presentation

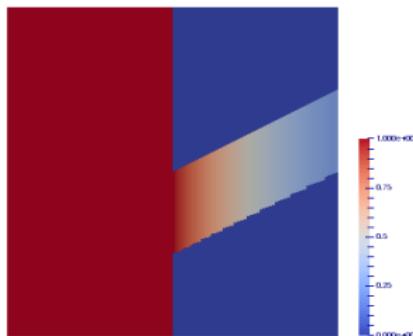
Geometry : 1 planar fracture, $\Omega = (0, 1)^2$

Test case configuration

- Isotropic media, $\Lambda_f = 20 \Lambda_m$, $d_f = 0.01$
- 1d linear pressure
- Initial concentration $c = 0$
- Injection at the left side $c = 1$



Example mesh



exact solution for c at $t = 0.5$

Analytical solution : discrete errors on the solution

2D analytical example - Discrete concentration - mesh $1600 \times 1 \times 1600$

2D analytical example - Discrete errors on the concentration c

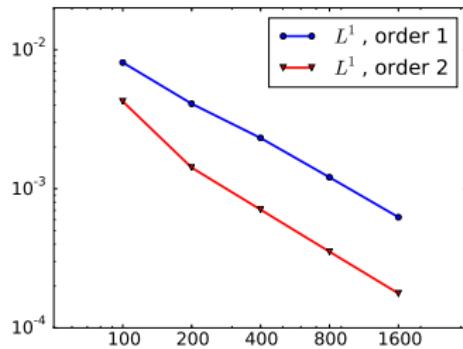
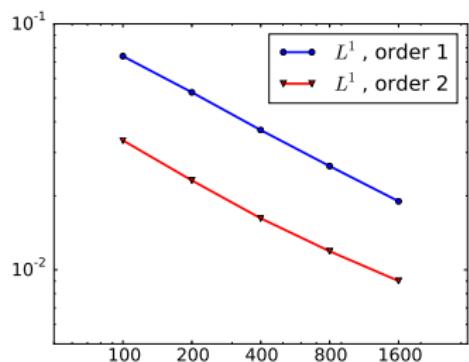


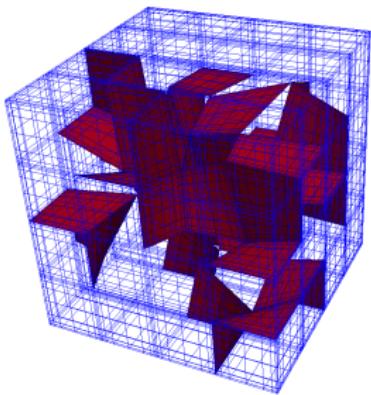
Figure: Errors in the matrix domain (left) and in the fracture (right).

3D fracture network with hexahedral mesh

Geometry : 3D network of fractures of $\Omega = (0, 1)^3$ with hexahedral meshes

Test case configuration

- Isotropic media, $\Lambda_f = 20 \Lambda_m$, $d_f = 0.01$
- non linear pressure
- Initial concentration $c = 0$
- Injection at the bottom side $c = 1$



3D fracture network - Discrete concentration - 128^3 cells

3D fracture network with hexahedral mesh

N_p	2	4	8	16	32	64	128	256	512
GMRES + Boomer AMG	15	15	15	15	15	16	15	15	15
GMRES + Aggregation AMG	65	70	98	95	59	86	65	91	54
GMRES + ILU(0)	751	707	655	644	648	634	633	624	613
GMRES + ILU(1)									> 1000
GMRES + ILU(2)									> 1000
BiCGSTAB + Boomer AMG	9	9	9	9	9	10	9	9	10
BiCGSTAB + ILU(0)	508	476	484	503	473	513	491	487	484
BiCGSTAB + ILU(1)									> 1000
BiCGSTAB + ILU(2)									> 1000

Table: Number of iterations vs. number of MPI processes with hexahedral mesh.

Mesh: 2.1×10^6 cells, 2.1×10^6 vertexes and 5.2×10^4 fractures faces

3D fracture network with hexahedral mesh - strong scaling

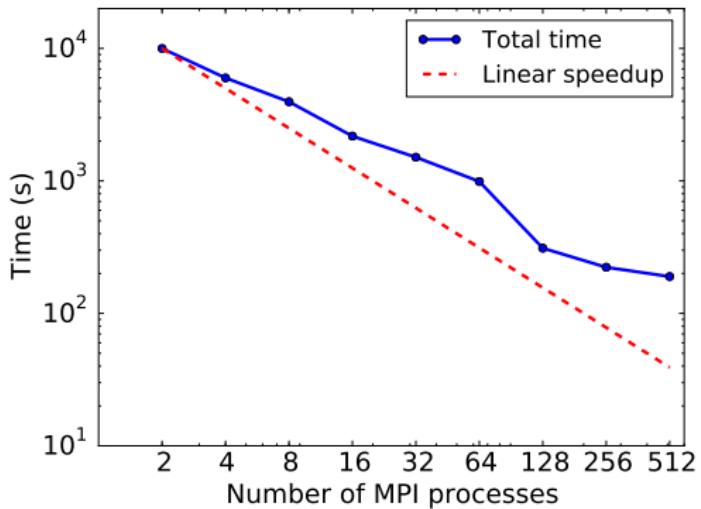


Figure: Total computation times vs. number of MPI processes with hexahedral mesh.

Mesh: $128^3 \Rightarrow : 2.1 \times 10^6$ cells, 2.1×10^6 vertexes and 5.2×10^4 fractures faces

cluster Cicada: <http://calculs.unice.fr/> - 72 Cpu nodes: 16 cores (2 Intel Sandy Bridge E5-2670), 64 GB, GCC 4.9.1, OpenMPI 1.8.2, 1 core/MPI

3D fracture network with hexahedral mesh

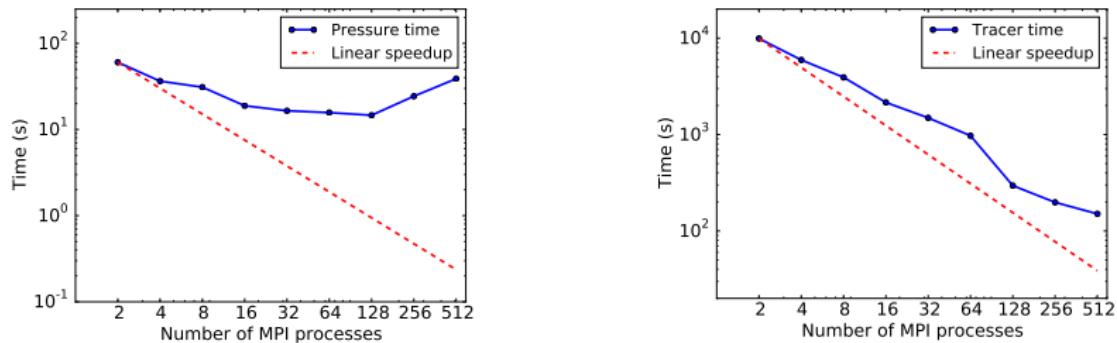


Figure: Computation times for pressure (left) and computation times for tracer (right) vs. number of MPI processes with hexahedral mesh.

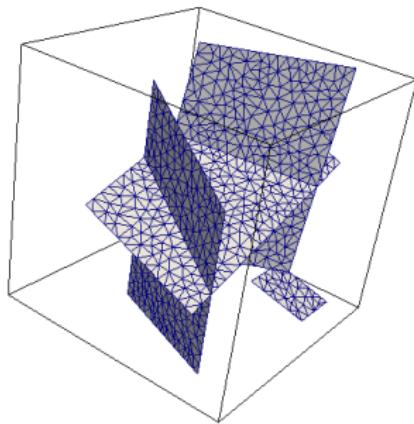
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3D fracture network with tetrahedral mesh

Geometry : 3D network of fractures of $\Omega = (0, 1)^3$ with tetrahedral meshes

Test case configuration

- Isotropic media, $\Lambda_f = 20 \Lambda_m$, $d_f = 0.01$
- non linear pressure
- Initial concentration $c = 0$
- Injection at the bottom side $c = 1$



3D fracture network with tetrahedral mesh

N_p	2	4	8	16	32	64	128	256	512
GMRES + Boomer AMG	11	12	12	12	12	12	12	12	12
GMRES + ILU(0)	-	725	717	682	667	656	644	629	612
GMRES + ILU(1)	> 1000								
GMRES + ILU(2)	154	153	152	151	149	147	144	142	140
BiCGSTAB + Boomer AMG	8	7	8	8	8	8	8	8	8
BiCGSTAB + ILU(0)	565	513	527	544	535	483	489	483	473
BiCGSTAB + ILU(1)	374	367	432	404	317	382	348	307	271
BiCGSTAB + ILU(2)	104	105	101	103	98	106	97	93	103

Table: Number of iterations vs. number of MPI processes with tetrahedral mesh.

Mesh: 6.2×10^6 cells, 9.7×10^5 vertexes and 7.1×10^4 fracture faces

3D fracture network with tetrahedral mesh - strong scaling

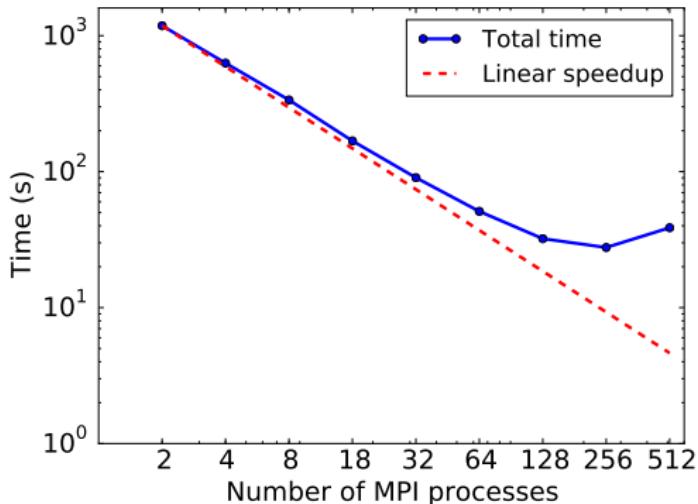


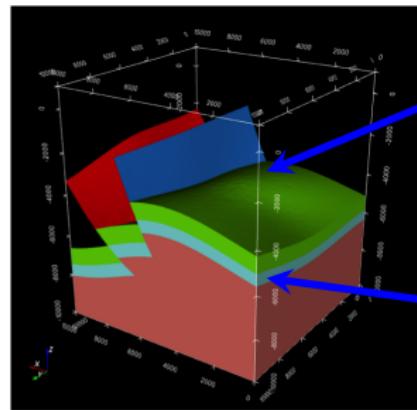
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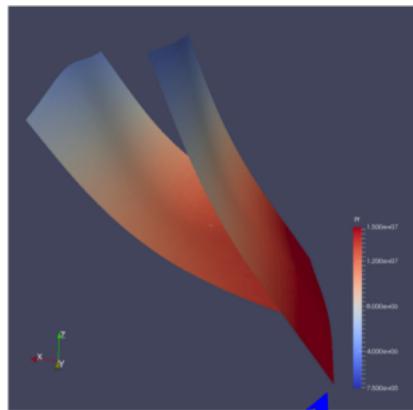
Geology simulation

A real case from S. Lopez (BRGM)



caprock layer

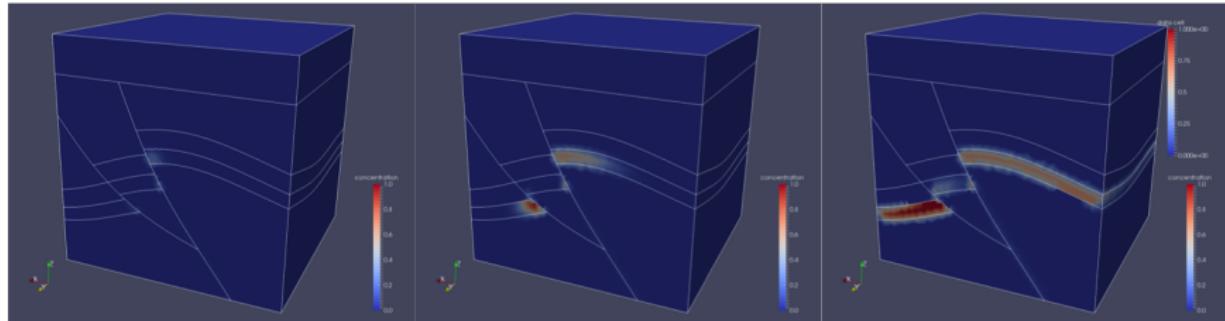
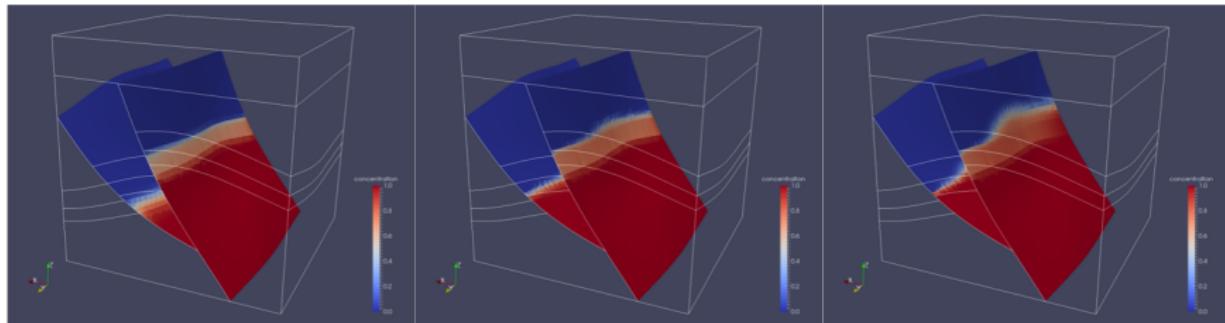
aquifer layer



tracer injection
along the fault

Geology simulation

A real case from S. Lopez (BRGM)



Ongoing works

- Multiphase compositional Darcy flux in fracture porous media
 - ◊ N_P phases, N_C components
 - ◊ Model is defined by a matrix of size $N_C \times N_P$
- Applications (S. Lopez at BRGM)
 - ◊ Real case studies, geothermal reservoir simulation in Guadeloupe
- Code
 - ◊ Optimization (OpenMP?)
 - ◊ User-friendly interface

Thanks

Thanks for your attention!

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"Centre de Calcul Interactif" hosted by University Nice Sophia Antipolis.



VAG discretization for a tracer problem on a Discrete Fracture Network (DFN)

* Discrete Unknowns *

$$u_{\mathcal{D}} = (u_K, u_\sigma, u_s, K \in \mathcal{M}, \sigma \in \mathcal{F}_\Gamma, s \in \mathcal{V})$$

* Discrete Operators *

In the matrix : $\forall K \in \mathcal{M}$

$$\Pi_{\mathcal{D}_m} u_{\mathcal{D}}(x) = \begin{cases} u_K & \text{for all } x \in \omega_K \\ u_s & \text{for all } x \in \omega_s \end{cases}$$

$$\nabla_{\mathcal{D}_m} u_{\mathcal{D}} = \nabla_{T_{K,\sigma,e}} u_{\mathcal{D}} , \quad \sigma \in \mathcal{F}_K , \quad e \in \mathcal{E}_\sigma$$

$T_{K,\sigma,e}$: tetrahedron joining cell center x_K to triangle $T_{\sigma,e}$

$$\forall \sigma \in \mathcal{F} \setminus \mathcal{F}_\Gamma \text{ interpolation of the face unknown } u_\sigma = \frac{\sum_{s \in \mathcal{V}_\sigma} u_s}{\text{card}(\mathcal{V}_\sigma)}$$

In the fracture : $\forall \sigma \in \mathcal{F}_\Gamma$

$$\Pi_{\mathcal{D}_f} u_{\mathcal{D}}(x) = \begin{cases} u_\sigma & \text{for all } x \in \omega_\sigma \\ u_s & \text{for all } x \in \omega_s \end{cases}$$

$$\nabla_{\mathcal{D}_f} u_{\mathcal{D}} = \nabla_{T_{\sigma,e}} u_{\mathcal{D}} , \quad e \in \mathcal{E}_\sigma$$

$T_{\sigma,e}$: triangle joining edge e to face center x_σ

