Space-Time Domain Decomposition Methods for Transport Problems in Porous Media

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OUTLINE

Outline

Objective: to formulate numerical methods for flow and transport in heterogeneous porous media

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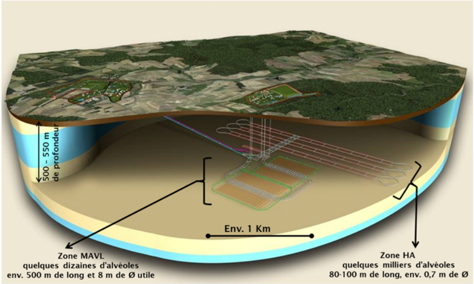
Examples of heterogeneous media:

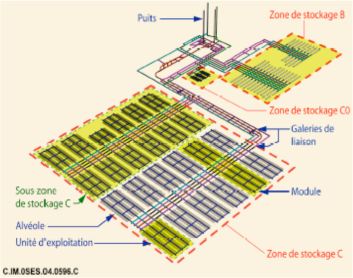
- porous media around underground nuclear waste deposit sites

Heterogeneities mean difficulties for simulation

Deep underground repository

(High-level waste)





A repository 2km $\times$ 2km

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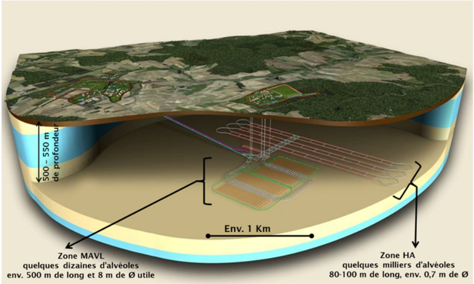

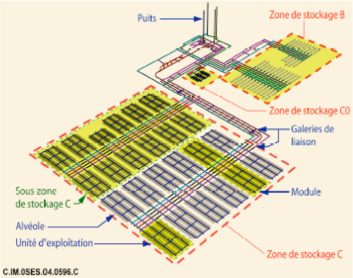

A repository 2km $\times$ 2km

- Different materials $\rightarrow$ strong heterogeneity, different time scales.
- Large differences in spatial scales.
- Long-term computations.

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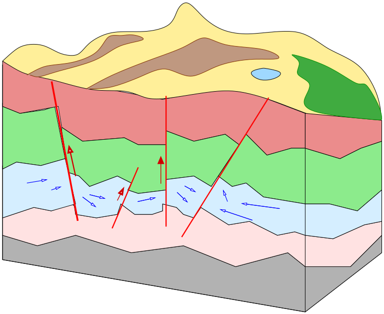
Examples of heterogeneous media:

- porous media around underground nuclear waste deposit sites
- porous media with fractures

Difficulty for modeling flow in media with fractures



A problem requiring multi-scale modelling

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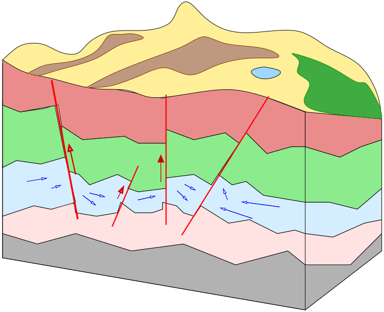

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- Fractures represent heterogeneities in porous media
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  - May be of much lower permeability so that they act as a barrier

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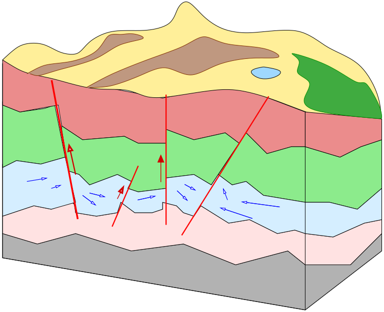

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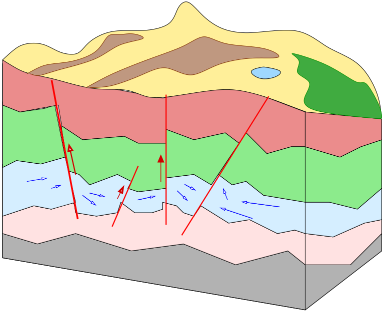

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Different types of models for flow in fractures

- double continuum models.
- discrete fracture networks (DFN's) (no exchange with surrounding matrix rock)
- reduced fracture models (with exchange with matrix rock)

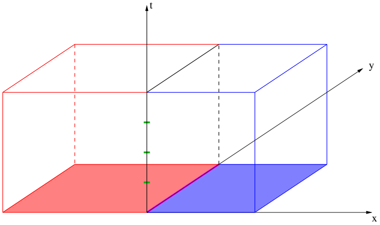
Objective here: to formulate methods for subdomain time-stepping

More specifically:

- develop and compare two different space-time (global in time) domain decomposition methods for the linear transport problem in mixed formulation.
- extend these methods to the case of a domain with a discrete fracture
- extend these method to two phase flow models, with discontinuous capillary pressure (in progress)

Domain decomposition (DD) methods

Domain decomposition in space



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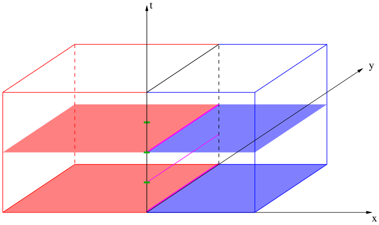

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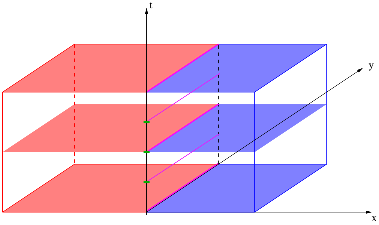

- Discretize in time and apply DD algorithm at each time step:
  - ▶ Solve stationary problems in the subdomains
  - ▶ Exchange information through the interface
- Use the same time step on the whole domain.

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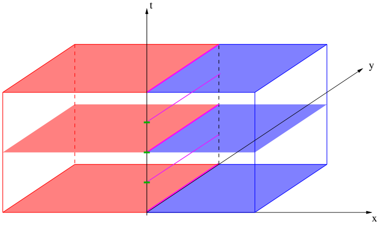
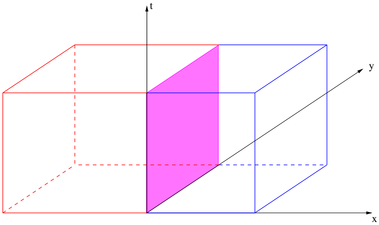


Space-time domain decomposition



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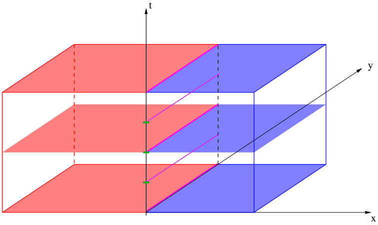

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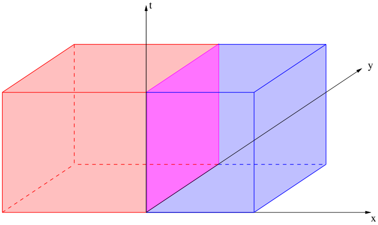

- Solve time-dependent problems in the subdomains
- Exchange information through the space-time interface
- Enable local discretizations both in space and in time

  $\longrightarrow$ local time stepping

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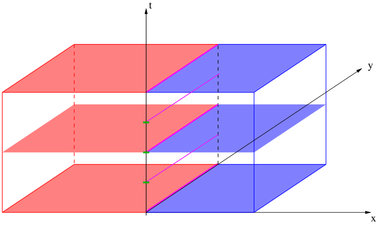

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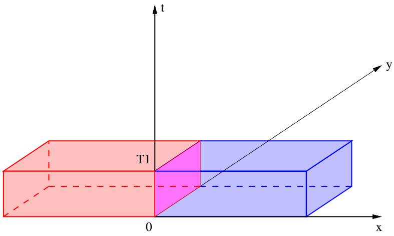
Space-time DD with Time windows



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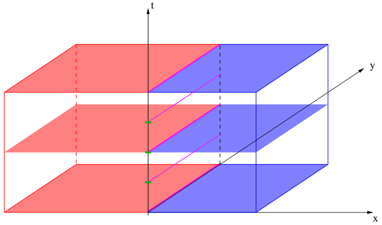

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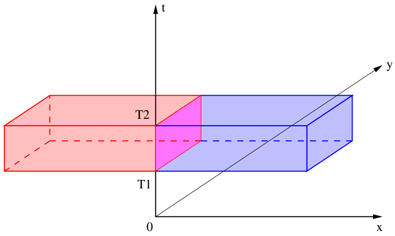

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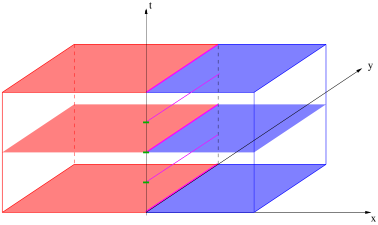

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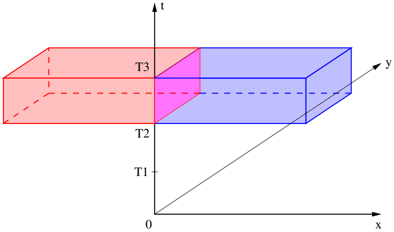

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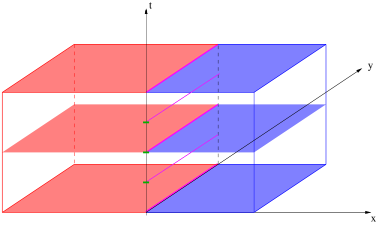

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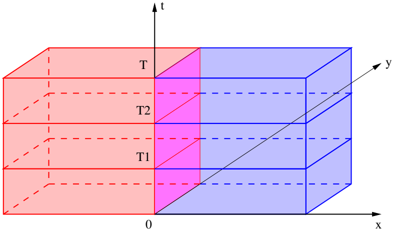

- Perform few iterations per window
- Use different space-time grids in each window
- Use the solution in the previous window to calculate a “good” initial guess on the interface.

Outline

Model problem

Transport of a contaminant in a porous medium under the effect of diffusion, written in mixed form:

$$
\begin{aligned}
\mathcal{L}(c,\mathbf{r}) := \phi\partial_t c + \operatorname{div}\mathbf{r} &= f && \text{in } \Omega\times(0,T),\\
\mathcal{M}(c,\mathbf{r}) := \mathbf{D}^{-1}\mathbf{r} + \nabla c &= 0 && \text{in } \Omega\times(0,T),\\
c &= 0 && \text{on } \partial\Omega\times(0,T),\\
c(\cdot,0) &= c_0 && \text{in } \Omega,
\end{aligned}
$$

- c concentration of a contaminant dissolved in a fluid, $\mathbf{r}$ diffusive flux.
- ϕ porosity; $\mathbf{D}$ symmetric, positive definite, time-independent diffusion tensor.

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Existence and uniqueness

If $\mathbf{D}\in \boldsymbol{L}^{\infty}(\Omega)$, $f\in L^2(0,T;L^2(\Omega))$ and $c_0\in H_0^1(\Omega)$ then problem above has a unique weak solution

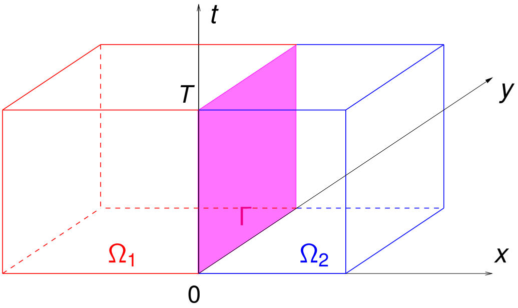
$$(c,\mathbf{r})\in\ H^1(0,T;L^2(\Omega))\times\left(L^2(0,T;H(\operatorname{div},\Omega))\cap L^\infty(0,T;\boldsymbol{L}^2(\Omega))\right).$$

Moreover, if $\mathbf{D}\in\boldsymbol{W}^{1,\infty}(\Omega)$, $f\in H^1(0,T;L^2(\Omega))$ and $c_0\in H^2(\Omega)\cap H_0^1(\Omega)$, then

$$(c,\mathbf{r})\in\ W^{1,\infty}(0,T;L^2(\Omega))\times\left(L^\infty(0,T;H(\operatorname{div},\Omega))\cap H^1(0,T;\boldsymbol{L}^2(\Omega))\right).$$

Proof. Galerkin's method and a priori estimates.

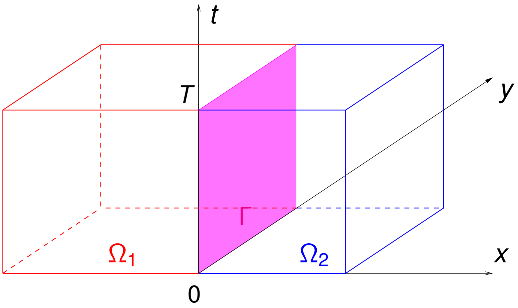
Multi-domain problem



Equivalent multi-domain problem:

$$\begin{aligned}
\mathcal{L}(c_1,\mathbf{r}_1) &= f, && \text{on } \Omega_1 \times (0,T), \\
\mathcal{M}(c_1,\mathbf{r}_1) &= 0, && \text{on } \Omega_1 \times (0,T), \\
c_1(\cdot,0) &= c_0, && \text{in } \Omega_1,
\end{aligned}
\qquad
\begin{aligned}
\mathcal{L}(c_2,\mathbf{r}_2) &= f, && \text{on } \Omega_2 \times (0,T), \\
\mathcal{M}(c_2,\mathbf{r}_2) &= 0, && \text{on } \Omega_2 \times (0,T), \\
c_2(\cdot,0) &= c_0, && \text{in } \Omega_2,
\end{aligned}$$

Multi-domain problem



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together with the transmission conditions on the **space-time interface**

$$\left. \begin{aligned} c_1 &= c_2 \\ \mathbf{r}_1 \cdot \mathbf{n}_1 + \mathbf{r}_2 \cdot \mathbf{n}_2 &= 0 \end{aligned} \right. \quad \text{on } \Gamma \times (0, T).$$

An overview

Different (equivalent) transmission conditions (TCs)

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$\Downarrow$

GTP Schur

- Physical TCs
+ N-N preconditioner

GTO Schwarz

More general TCs with optimized parameters
$\rightarrow$ accelerate the convergence rate.

- Robin TCs
- Ventcell TCs

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Substructuring technique: **Space-time interface problem**

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Iterative solvers (GMRES, Richardson iteration)

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T.T.P. Hoang, J. Jaffré, C. Japhet, M.K, and J. E. Roberts. Space-time domain decomposition methods for diffusion problems in mixed formulations. SIAM J. Numer. Anal., 51(6):3532–3559, 2013.

Time-dependent Steklov-Poincaré operator

- Dirichlet-to-Neumann operators, for $i = 1, 2$:

$$\mathcal{S}_i^{DtN} : (\lambda, f, c_0) \longmapsto (\mathbf{r}_i \cdot \mathbf{n}_i)_{|\Gamma} \,,$$

where $(c_i, \mathbf{r}_i)\,,\ i = 1, 2$, is the solution of

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- Space-time interface problem:

$$\begin{aligned} \mathcal{S}_1^{DtN}(\lambda, f, c_0) &+ \mathcal{S}_2^{DtN}(\lambda, f, c_0) = 0, \\ &\Updownarrow \\ \sum_{i=1}^{2} \mathcal{S}_i^{DtN}(\lambda, 0, 0) &= \sum_{i=1}^{2} \mathcal{S}_i^{DtN}(0, f, c_0), \\ &\Updownarrow \\ \mathcal{S}\lambda &= \chi, \quad \text{on } \Gamma \times (0, T). \end{aligned}$$

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- Neumann-Neumann preconditioner with weights:

$$\left(\sigma_1 \mathcal{S}_1^{NtD} + \sigma_2 \mathcal{S}_2^{NtD}\right) \mathcal{S}\lambda = \widehat{\chi}, \quad \text{on } \Gamma \times (0, T),$$

where $\sigma_i : \Gamma \times (0, T) \to [0, 1]$ such that $\sigma_1 + \sigma_2 = 1$.

GTO Schwarz: Robin transmission conditions

- Equivalent Robin TCs on $\Gamma \times (0, T)$: for $\alpha_1, \ \alpha_2 > 0$

$$
\begin{aligned}
-\mathbf{r}_1 \cdot \mathbf{n}_1 + \alpha_1 c_1 &= -\mathbf{r}_2 \cdot \mathbf{n}_1 + \alpha_1 c_2, \\
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- Robin-to-Robin operators, for $i = 1, 2$ and $j = 3 - i$:

$$\mathcal{S}_i^{RtR} : (\xi_i, f, c_0) \longmapsto \left(-\mathbf{r}_i \cdot \mathbf{n}_j + \alpha_j c_i\right)_{|\Gamma},$$

where $(c_i, \mathbf{r}_i)$, $i = 1, 2$, is the solution of

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- Space-time interface problem with two Lagrange multipliers:

$$\begin{aligned} \xi_1 &= \mathcal{S}_2^{RtR}(\xi_2, f, c_0), \\ \xi_2 &= \mathcal{S}_1^{RtR}(\xi_1, f, c_0), \end{aligned} \quad \text{on } \Gamma \times (0, T),$$

or equivalently,

$$\mathcal{S}_R \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \chi_R, \quad \text{on } \Gamma \times (0, T).$$

OSWR algorithm with Robin TCs

OSWR iterative algorithm: at the k^{th} iteration, for $i = 1, 2$ and $j = (3 - i)$

$$\begin{aligned} \phi_i \partial_t c_i^k + \operatorname{div} \mathbf{r}_i^k &= f \ \text{ in } \Omega_i \times (0, T) \\ \mathbf{D}_i^{-1} \mathbf{r}_i^k + \nabla c_i^k &= 0 \ \text{ in } \Omega_i \times (0, T) \\ -\mathbf{r}_i^k \cdot \mathbf{n}_i + \alpha_i c_i^k &= -\mathbf{r}_j^{k-1} \cdot \mathbf{n}_i + \alpha_i c_j^{k-1} \text{ on } \Gamma \times (0, T), \end{aligned}$$

for given initial guess $g_i = \left(-\mathbf{r}_i^0 \cdot \mathbf{n}_i + \alpha_i c_i^0 \right), \ i = 1, 2.$

OSWR algorithm with Robin TCs

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\mathbf{D}_i^{-1} \mathbf{r}_i^k + \nabla c_i^k &= 0 \text{ in } \Omega_i \times (0, T) \\
-\mathbf{r}_i^k \cdot \mathbf{n}_i + \alpha_i c_i^k &= -\mathbf{r}_j^{k-1} \cdot \mathbf{n}_i + \alpha_i c_j^{k-1} \text{ on } \Gamma \times (0, T),
\end{aligned}$$

for given initial guess $g_i = \left(-\mathbf{r}_i^0 \cdot \mathbf{n}_i + \alpha_i c_i^0\right), \ i = 1, 2.$

Theorem (Convergence of OSWR algorithm in mixed formulation)

If the algorithm above is initialized by $(g_i) \in H^1\left(0, T; L^2(\Gamma)\right)$ for $i = 1, 2$, then

- a sequence of iterates $\left(c_i^k, \mathbf{r}_i^k\right) \in H^1\left(0, T; L^2(\Omega_i)\right) \times L^2(0, T; \mathcal{H}(\operatorname{div}, \Omega_i))$ is well-defined
- $\displaystyle\sum_{i=1}^{2} \left(\| c_i^k - c_{|\Omega_i} \|_{H^1(0,T;L^2(\Omega_i))} + \| \mathbf{r}_i^k - \mathbf{r}_{|\Omega_i} \|^2_{L^2(0,T;\mathcal{H}(\operatorname{div},\Omega_i))} \right) \xrightarrow{k \to \infty} 0.$

where $\mathcal{H}(\operatorname{div}, \Omega_i) := \left\{ \mathbf{v} \in H(\operatorname{div}, \Omega_i) : (\mathbf{v} \cdot \mathbf{n}_i)_{|\Gamma} \in L^2(\Gamma) \right\}.$

Remark. The proof is carried out for the multiple subdomain case.

GTO Schwarz: Ventcell transmission conditions

With sufficient regularity $\rightarrow$ equivalent Ventcell transmission conditions

GTO Schwarz: Ventcell transmission conditions

With sufficient regularity $\rightarrow$ equivalent Ventcell transmission conditions

- In primal form: on $\Gamma \times (0, T)$:

$$-\mathbf{r}_1 \cdot \mathbf{n}_1 + \alpha_1 c_1 + \qquad = -\mathbf{r}_2 \cdot \mathbf{n}_1 + \alpha_1 c_2 +$$

$$-\mathbf{r}_2 \cdot \mathbf{n}_2 + \alpha_2 c_2 + \qquad = -\mathbf{r}_1 \cdot \mathbf{n}_2 + \alpha_2 c_1 +$$

GTO Schwarz: Ventcell transmission conditions

With sufficient regularity $\rightarrow$ equivalent Ventcell transmission conditions

- In primal form: on $\Gamma \times (0, T)$:

$$
\begin{aligned}
-\mathbf{r}_1 \cdot \mathbf{n}_1 + \alpha_1 c_1 + \beta_1 \left(\phi_2 \partial_t c_1 + \mathrm{div}_\tau \left(-\mathbf{D}_{2,\Gamma} \nabla_\tau c_1\right)\right) &= -\mathbf{r}_2 \cdot \mathbf{n}_1 + \alpha_1 c_2 + \\
&\quad \beta_1 \left(\phi_2 \partial_t c_2 + \mathrm{div}_\tau \left(-\mathbf{D}_{2,\Gamma} \nabla_\tau c_2\right)\right), \\
-\mathbf{r}_2 \cdot \mathbf{n}_2 + \alpha_2 c_2 + \beta_2 \left(\phi_1 \partial_t c_2 + \mathrm{div}_\tau \left(-\mathbf{D}_{1,\Gamma} \nabla_\tau c_2\right)\right) &= -\mathbf{r}_1 \cdot \mathbf{n}_2 + \alpha_2 c_1 + \\
&\quad \beta_2 \left(\phi_1 \partial_t c_1 + \mathrm{div}_\tau \left(-\mathbf{D}_{1,\Gamma} \nabla_\tau c_1\right)\right).
\end{aligned}
$$

$\longrightarrow$ α_i, β_i: positive constants to be optimized to accelerate convergence rate.

GTO Schwarz: Ventcell transmission conditions

With sufficient regularity $\rightarrow$ equivalent Ventcell transmission conditions

- In primal form: on $\Gamma \times (0, T)$:

$$\begin{aligned}
-\mathbf{r}_1 \cdot \mathbf{n}_1 + \alpha_1 c_1 + \beta_1 \left(\phi_2 \partial_t c_1 + \mathrm{div}_\tau \left(-\mathbf{D}_{2,\Gamma} \nabla_\tau c_1\right)\right) &= -\mathbf{r}_2 \cdot \mathbf{n}_1 + \alpha_1 c_2 + \\
&\quad \beta_1 \left(\phi_2 \partial_t c_2 + \mathrm{div}_\tau \left(-\mathbf{D}_{2,\Gamma} \nabla_\tau c_2\right)\right), \\
-\mathbf{r}_2 \cdot \mathbf{n}_2 + \alpha_2 c_2 + \beta_2 \left(\phi_1 \partial_t c_2 + \mathrm{div}_\tau \left(-\mathbf{D}_{1,\Gamma} \nabla_\tau c_2\right)\right) &= -\mathbf{r}_1 \cdot \mathbf{n}_2 + \alpha_2 c_1 + \\
&\quad \beta_2 \left(\phi_1 \partial_t c_1 + \mathrm{div}_\tau \left(-\mathbf{D}_{1,\Gamma} \nabla_\tau c_1\right)\right).
\end{aligned}$$

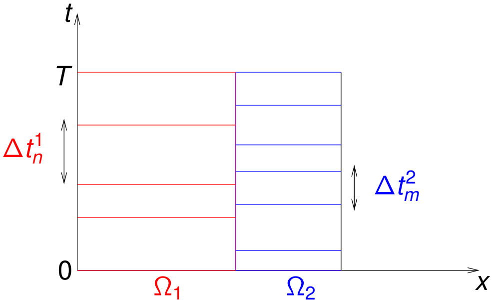
$\longrightarrow$ α_i, β_i: positive constants to be optimized to accelerate convergence rate.

- In mixed form: introduce Lagrange multipliers on the interface, $c_{i,\Gamma}$ and $\mathbf{r}_{\Gamma,i}$, for $i = 1, 2$,

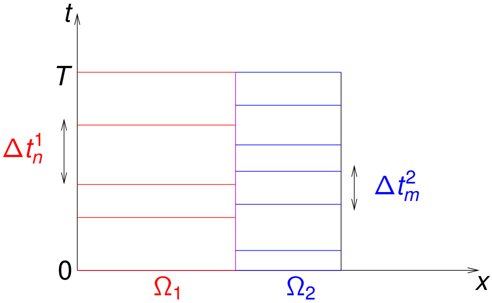
$$\begin{aligned}
-\mathbf{r}_i \cdot \mathbf{n}_i + \alpha_i c_{i,\Gamma} + \beta_i \left(\phi_j \partial_t c_{i,\Gamma} + \mathrm{div}_\tau\, \mathbf{r}_{\Gamma,i}\right) &= -\mathbf{r}_j \cdot \mathbf{n}_i + \alpha_i c_{j,\Gamma} + \\
&\quad \beta_i \left(\phi_j \partial_t c_{j,\Gamma} + \mathrm{div}_\tau \left(\mathbf{D}_{j,\Gamma} \mathbf{D}_{i,\Gamma}^{-1} \mathbf{r}_{\Gamma,j}\right)\right), \\
\mathbf{D}_{j,\Gamma}^{-1}\, \mathbf{r}_{\Gamma,i} + \nabla_\tau c_{i,\Gamma} &= 0.
\end{aligned}$$

  - $c_{i,\Gamma}$: pressure trace on Γ.
  - $\mathbf{r}_{\Gamma,i} := -\mathbf{D}_{j,\Gamma} \nabla_\tau c_{i,\Gamma}$: NOT the tangential trace of $\mathbf{r}_i$ on $\Gamma \times (0, T)$.

Nonconforming discretizations in time



Nonconforming discretizations in time



- Time discretization: non-conforming time grids $\mathcal{T}_1, \mathcal{T}_2$; discontinuous Galerkin with piecewise polynomials of degree 0.
- Projections: Π_{ji} is an L^2 projection from piecewise constant functions on $\mathcal{T}_i$ onto piecewise constant functions on $\mathcal{T}_j$.
  Ex:
$$(\Pi_{21}(\lambda_1))^m = \frac{1}{\mid J_m^2 \mid} \sum_{n=1}^{M_1} \int_{J_n^1 \cap J_m^2} \lambda_1, \text{ for } m = 1, \cdots, M_2.$$

Semi-discrete transmission conditions with nonconforming time grids

- For GTP Schur method: take $\lambda = \left(\lambda^1, \cdots, \lambda^{M_1}\right)$ piecewise constant on $J_n^1 = \left(t_1^n, t_1^{n+1}\right)$, for $n = 0, \cdots, M_1 - 1$.
  - Continuity of concentration: $c_1 = \Pi_{11}(\lambda)$ and $c_2 = \Pi_{21}(\lambda)$.
  - Conservation of the flux over each time subinterval

$$\int_{J_n^1}\int_\Gamma \left(\Pi_{11}(\mathbf{r}_1 \cdot \mathbf{n}_1) + \Pi_{12}(\mathbf{r}_2 \cdot \mathbf{n}_2)\right) dt = 0, \text{ for } n = 0, \cdots, M_1 - 1.$$

Semi-discrete transmission conditions with nonconforming time grids

- For GTP Schur method: take $\lambda = \left(\lambda^1, \cdots, \lambda^{M_1}\right)$ piecewise constant on $J_n^1 = \left(t_1^n, t_1^{n+1}\right)$, for $n = 0, \cdots, M_1 - 1$.
  - Continuity of concentration: $c_1 = \Pi_{11}(\lambda)$ and $c_2 = \Pi_{21}(\lambda)$.
  - Conservation of the flux over each time subinterval

$$\int_{J_n^1} \int_\Gamma \left(\Pi_{11}(\mathbf{r}_1 \cdot \mathbf{n}_1) + \Pi_{12}(\mathbf{r}_2 \cdot \mathbf{n}_2)\right) dt = 0, \text{ for } n = 0, \cdots, M_1 - 1.$$

- For GTO Schwarz method: conservation of the two Robin (Ventcell) conditions across the interface over each time subinterval

$$\int_{J_n^1} \int_\Gamma \left[(-\mathbf{r}_1 \cdot \mathbf{n}_1 + \alpha_1 c_1) - \Pi_{12}(-\mathbf{r}_2 \cdot \mathbf{n}_1 + \alpha_1 c_2)\right] dt = 0, \ \forall n = 0, \cdots, M_1 - 1,$$

$$\int_{J_m^2} \int_\Gamma \left[(-\mathbf{r}_2 \cdot \mathbf{n}_2 + \alpha_2 c_2) - \Pi_{21}(-\mathbf{r}_1 \cdot \mathbf{n}_2 + \alpha_2 c_1)\right] dt = 0, \ \forall m = 0, \cdots, M_2 - 1.$$

$\rightarrow$ Convergence of semi-discrete, nonconforming in time, OSWR algorithm

Outline

Extension to advection-diffusion problems

Linear advection-diffusion equation:

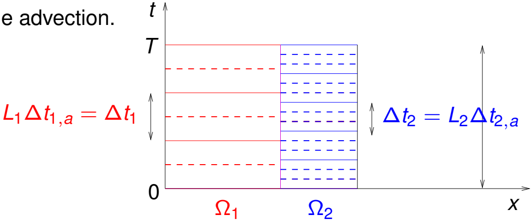
$$\begin{aligned} \phi\partial_t c + \operatorname{div}(\mathbf{u}c) + \operatorname{div}\mathbf{r} &= f && \text{in } \Omega \times (0,T), \\ \nabla c + \mathbf{D}^{-1}\mathbf{r} &= 0 && \text{in } \Omega \times (0,T), \\ c &= 0 && \text{on } \partial\Omega \times (0,T), \\ c(\cdot,0) &= c_0 && \text{in } \Omega. \end{aligned}$$

Operator splitting

- Advection eq.: explicit Euler + upwind, cell-centered finite volumes.
- Diffusion eq.: implicit Euler + mixed finite elements.

$\Rightarrow$ CFL condition: sub-time steps for the advection.

$$T = N_1 \Delta t_1 = N_2 \Delta t_2$$



Discrete interface problems

- **GTP Schur method**:

$$\widetilde{\mathcal{S}}_h \begin{pmatrix} \lambda_a \\ \lambda \end{pmatrix} = \widetilde{\chi}_h, \quad \text{on } \Gamma \times (0, T).$$

$\Longrightarrow$ Generalized Neumann-Neumann preconditioner

- **GTO Schwarz method with Robin TCs**:

$$\widetilde{\mathcal{S}}_{R,h} \begin{pmatrix} \lambda_a \\ \xi_1 \\ \xi_2 \end{pmatrix} = \widetilde{\chi}_{R,h}, \quad \text{on } \Gamma \times (0, T).$$

$\Longrightarrow$ Optimized Robin parameters for the diffusion eq. only

$\neq$ fully implicit scheme.

Remark. $\lambda_a \in \Lambda_h^{N \times L}$ while $\lambda, \xi_1, \xi_2 \in \Lambda_h^N$.

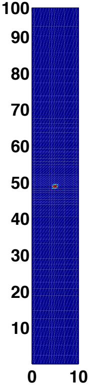
T.T.P. Hoang, J. Jaffré, C. Japhet, M.K., and J. E. Roberts. Proc. Mamern 2015, in preparation.

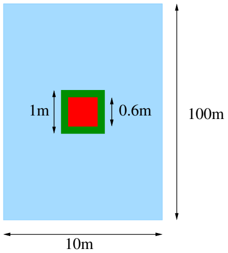
Test case 2: A near-field simulation (project PAMINA*)

* Performance Assessment Methodologies IN Application to Guide the Development of the Safety Case

Parameters of the simulation

Material	Permeability ($m.s^{-1}$)	Porosity	Diffusion ($m^2.\ s^{-1}$)
Host rock	10^{-13}	0.06	$6\,10^{-13}$
EDZ	$5\,10^{-11}$	0.2	$2\,10^{-11}$
Vitrified waste	10^{-8}	0.1	10^{-11}





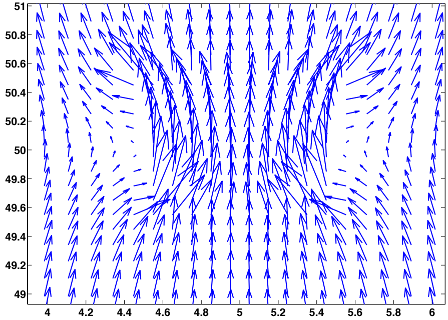
Advection field: Darcy flow

$$\begin{aligned} \text{div}\,\mathbf{u} &= 0 && \text{in } \Omega, \\ \mathbf{u} &= -\mathbf{K}\nabla p && \text{in } \Omega. \end{aligned}$$

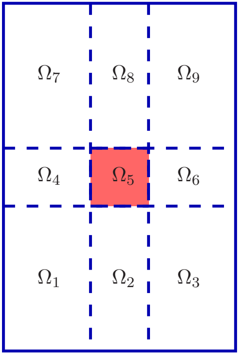
BCs:

Homogeneous Neumann at $x = 0$ and $x = 10$,

Dirichlet conditions with $p = 100$ Pa at $y = 0$ and $p = 0$ at $y = 100$.



Transport problem: time windows and decomposition



- Final time: $T_f = 2\,10^{11}$s ($\approx$ 20000 years)
  $\longrightarrow$ 200 time windows with size $T = 10^9$s.
- Decomposition into 9 subdomains.
- Nonconforming time grids:
  - Diffusion step:

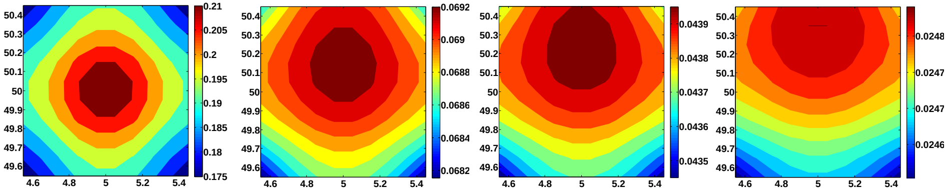
$$\begin{aligned} \Delta t_i &= T/500, \quad i = 5, \\ \Delta t_i &= T/100, \quad i \neq 5. \end{aligned}$$

  - Diffusion-dominated: $\mathrm{Pe}_L \leq 0.0513$
    $\longrightarrow \Delta t_{a,i} = \Delta t_i$.

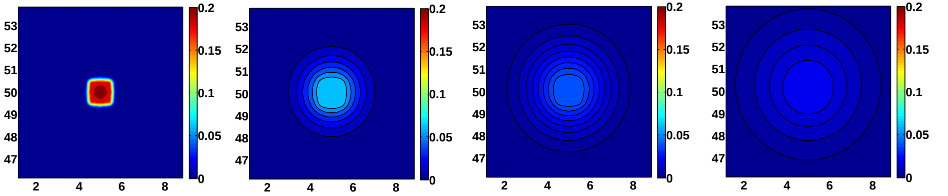
- Non-uniform mesh in space: uniform mesh in the repository (10 by 10), then progressively coarser with a factor of 1.05.

Evolution of concentration field

100 years | 5000 years | 10000 years | 20000 years

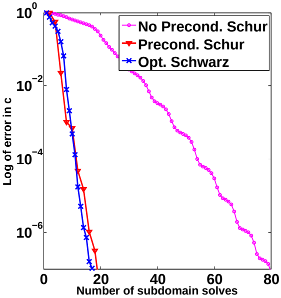


In the repository

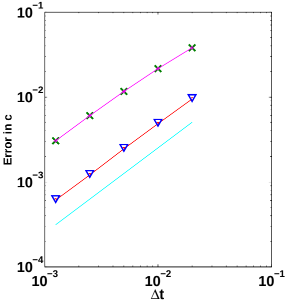


In the host rock

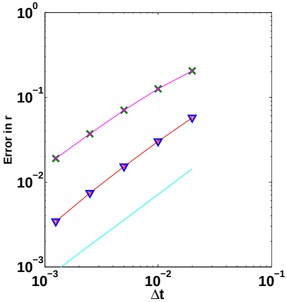
Performance of one time window



Convergence with GMRES



Error in c with nonconforming time grids.

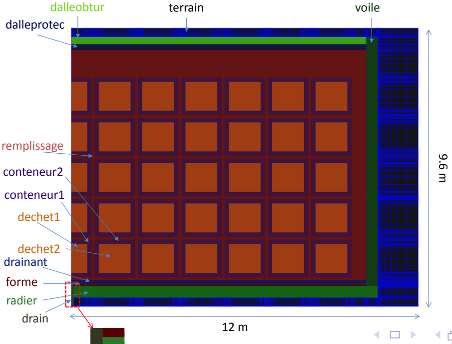


Error in $\mathbf{r}$ with nonconforming time grids.

- Time grid 1: $\Delta t_i = T/500, \forall i$
- Time grid 2: $\Delta t_5 = T/500$, $\Delta t_i = T/100$, $i \neq 5$
- Time grid 3: $\Delta t_5 = T/100$, $\Delta t_i = T/500$, $i \neq 5$
- Time grid 4: $\Delta t_i = T/100, \forall i$

A subsurface waste storage simulation

Zone	Hydraulic conductivity K (m/year)	Porosity ϕ	Molecular diffusion d_m (m^2/year)
terrain	94608	0.30	1
dalleprotec/dalleobtur	$3.1536\,10^{-3}$	0.20	$1.58\,10^{-3}$
voile	$3.1536\,10^{-3}$	0.20	$1.58\,10^{-3}$
remplissage	5045.76	0.30	$5.36\,10^{-2}$
conteneur1/conteneur2	$3.1536\,10^{-4}$	0.12	$4.47\,10^{-4}$
dechet1/dechet2	$3.1536\,10^{-4}$	0.30	$1.37\,10^{-3}$
radier	$3.1536\,10^{-4}$	0.15	$6.31\,10^{-5}$
drainant	94608	0.30	$5.36\,10^{-2}$

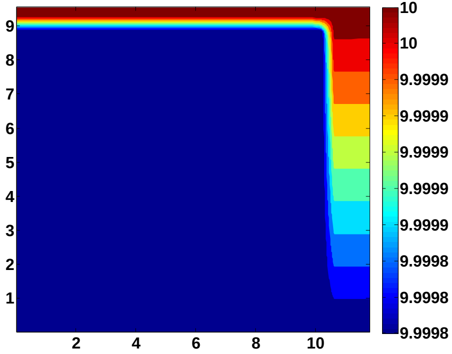


Darcy flow

$$\begin{aligned} \text{div}\,\mathbf{u} &= 0 && \text{in } \Omega, \\ \mathbf{u} &= -\mathbf{K}\nabla h && \text{in } \Omega. \end{aligned}$$

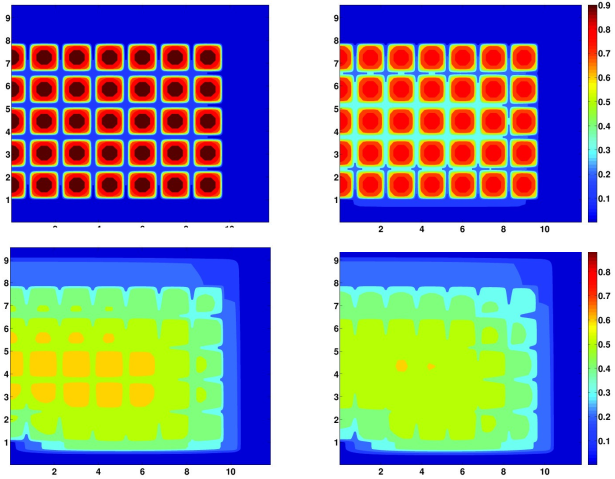
BCs:
Homogeneous Neumann at $x = 0$ and $x = 12$m,

Dirichlet conditions with $h = 9.998$m at $y = 0$ and $h = 10$m at $y = 9.6$m.



Hydraulic head field

Concentration field after 500 years



Outline

Model problem: Two–phase immiscible flow

Mathematical model

$$\partial_t (\omega \rho_\alpha S_\alpha) + \mathrm{div}(\rho_\alpha u_\alpha) = q_\alpha \quad \text{mass conservation}$$

$$u_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} K (\nabla p_\alpha - \rho_\alpha \nabla g) \quad \text{Darcy's law}$$

$$S_n + S_w = 1$$

$$p_n - p_w = \pi(S_w) \quad \text{capillary pressure}$$

Phase $\alpha = w$ water, n gas or oil. $\pi(S_w)$ increasing function on $[0, 1]$ (extend coninuously to $\mathbf{R}$).

- ω porosity
- S_α phase saturation
- u_α phase velocity
- $k_{r\alpha}$ relative permeability
- K permeability
- p_α: phase pressure
- ρ_α phase density
- μ_α viscosity

Simplified model

Enchery et al. (06), Cances (08), Brenner et al. (13), no gravity

1. Global pressure (Chavent) $P_g(S) = p_w + \int_0^S \frac{k_{rn}(u)/\mu_n}{\frac{k_{rn}(u)}{\mu_n} + \frac{k_{rw}(u)}{\mu_w}} \pi'(u)\, du,$
2. Kirchhoff transformation : $\phi(S) = \int_0^S K \frac{k_{rn}(u) k_{rw}(u)}{\mu_n k_{rw}(u) + \mu_w k_{rn}(u)} \pi'(u)\, du.$

Simplified model

Enchery et al. (06), Cances (08), Brenner et al. (13), no gravity

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2. Kirchhoff transformation : $\phi(S) = \int_0^S K \frac{k_{rn}(u)k_{rw}(u)}{\mu_n k_{rw}(u) + \mu_w k_{rn}(u)} \pi'(u)\, du.$

Transformed system : $f(S) = \frac{\mu_w k_{rn}(S)}{\mu_w k_{rn}(s) + \mu_n k_{rw}(S)}, \lambda(S) = \frac{k_{rn}(S)}{\mu_n} + \frac{k_{rw}(S)}{\mu_w}.$

$$\begin{cases} \omega \partial_t S + \mathrm{div}\,(f(S) q_T) - \Delta \phi(S) = 0 \\ \mathrm{div}\, q_T = 0, \quad q_T = -K\lambda(S)\,\mathrm{grad}\, P_g \end{cases} \quad \text{in } \Omega \times [0, T]$$

Simplified model

Enchery et al. (06), Cances (08), Brenner et al. (13), no gravity

1. Global pressure (Chavent) $P_g(S) = p_w + \int_0^S \frac{k_{rn}(u)/\mu_n}{\frac{k_{rn}(u)}{\mu_n} + \frac{k_{rw}(u)}{\mu_w}} \pi'(u)\, du,$
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Transformed system : $f(S) = \frac{\mu_w k_{rn}(S)}{\mu_w k_{rn}(s) + \mu_n k_{rw}(S)}$, $\lambda(S) = \frac{k_{rn}(S)}{\mu_n} + \frac{k_{rw}(S)}{\mu_w}$.

$$\begin{cases} \omega \partial_t S + \operatorname{div}\left(f(S) q_T\right) - \Delta\phi(S) = 0 \\ \operatorname{div} q_T = 0, \quad q_T = -K\lambda(S) \operatorname{grad} P_g \end{cases} \quad \text{in } \Omega \times [0, T]$$

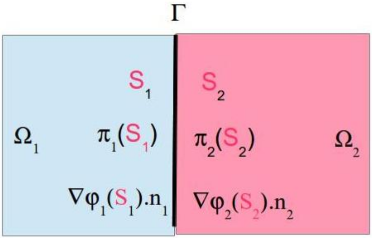
Simplified system: neglect advection

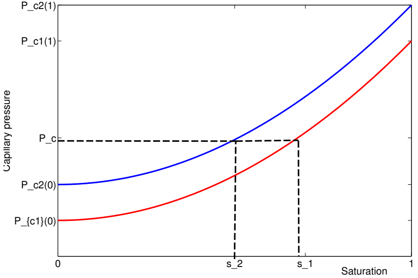
$$\omega \partial_t S - \Delta\phi(S) = 0 \quad \text{in } \Omega \times [0, T]$$

Nonlinear (degenerate) diffusion equation

Discontinuous capillary pressure: transmission conditions

Two subdomains $\bar{\Omega} = \bar{\Omega}_1 \cup \bar{\Omega}_2$, $\Omega_1 \cap \Omega_2 = \emptyset$. $\Gamma = \bar{\Omega}_1 \cap \bar{\Omega}_2$





Transmission conditions on the interface

Continuity of capillary pressure $\pi_1(S_1) = \pi_2(S_2)$ on Γ

Continuity of the flux $\nabla\phi_1(S_1).n_1 = \nabla\phi_2(S_2).n_2$ on Γ

Chavent – Jaffré (86), Enchéry et al. (06), Cances (08), Ern et al (10), Brenner et al. (13).

Non-linear Schwarz algorithm

Robin transmission conditions

$$\nabla\phi_1(S_1).n_1 + \beta_1\pi_1(S_1) = -\nabla\phi_2(S_2).n_2 + \beta_1\pi_2(S_2)$$
$$\nabla\phi_2(S_2).n_2 + \beta_2\pi_2(S_2) = -\nabla\phi_1(S_1).n_1 + \beta_2\pi_1(S_1)$$

Schwarz algorithm

Given S_i^0, iterate for $k = 0, \ldots$
Solve for S_i^{k+1}, $i = 1, 2, j = 3 - i$

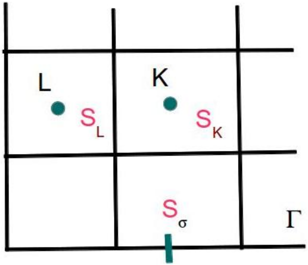
$$\omega\partial_t S_i^{k+1} - \Delta\phi_i(S_i^{k+1}) = 0 \qquad \text{in } \Omega_i \times [0, T]$$
$$\nabla\phi_i(S_i^{k+1}).n_i + \beta_i\pi_i(S_i^{k+1}) = -\nabla\phi_j(S_j^k).n_j + \beta_i\pi_j(S_j^k) \quad \text{on } \Gamma \times [0, T],$$

(β_1, β_2) are free parameters chosen to accelerate convergence

Basic ingredient: subdomain solver with Robin bc.

Finite volume scheme (1)

Extension to Robin bc of cell centered FV scheme by Enchéry et al. (06).
Triangulation $\mathcal{T}$, cells $K \in \mathcal{T}$, boundary faces $\sigma \subset \Gamma$.
Unknowns : cell values $(S_K)_{K\in\mathcal{T}}$, boundary face values $(S_\sigma)_{\sigma\in\mathcal{E}_\Gamma}$



Notations: $K|L$ = edge between K and L, $\tau_{K|L} = \dfrac{m(K|L)}{\bar{K}_{K|L}}$ (eg harmonic average).

Finite volume scheme (2)

Interior equation

$$m(K)\frac{S_K^{n+1} - S_K^n}{\delta t} + \sum_{L \in \mathcal{N}(K)} \tau_{K|L} \left(\phi(S_K^{n+1}) - \phi(S_L^{n+1}) \right) + \sum_{\sigma \in \mathcal{E}_\Gamma \cap \mathcal{E}_K} \tau_{K,\sigma} \left(\phi(S_K^{n+1}) - \phi(S_\sigma^{n+1}) \right) = 0, \quad K \in \mathcal{T}.$$

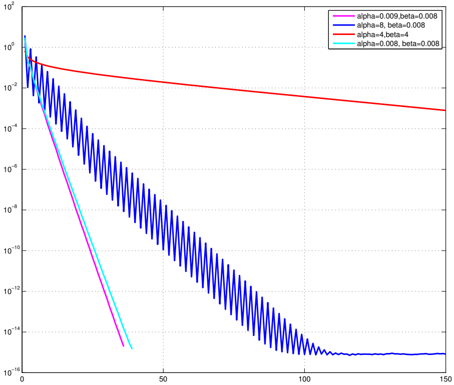
Robin BC for boundary faces

$$-\tau_{K,\sigma} \left(\phi(S_K^{n+1}) - \phi(S_\sigma^{n+1}) \right) + \beta m(\sigma) \pi(S_\sigma^{n+1}) = g_\sigma, \quad \sigma \in \mathcal{E}_\Gamma$$

Implemented with Matlab Reservoir Simulation Toolbox (K. A. Lie et al. (14))
Solver with automatics differentiation : no explicit computation of Jacobian

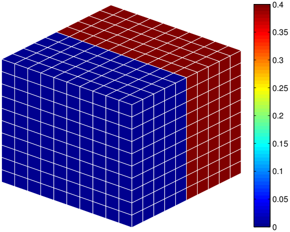
Numerical example

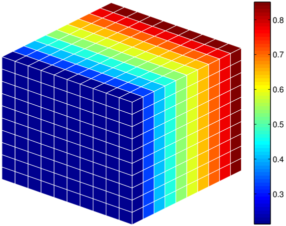
Homogeneous medium, $\Omega_1 = (0, 100)^3$, $\Omega_2 = (100, 200) \times (0, 100)^2$.
Mobilities $\lambda_0(S) = S$, $S \in [0, 1]$,
Capillary pressure $\pi(S) = 5S^2$, $S \in [0, 1]$

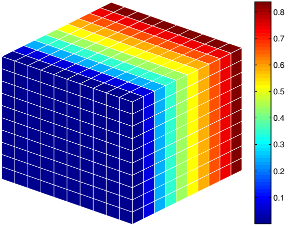


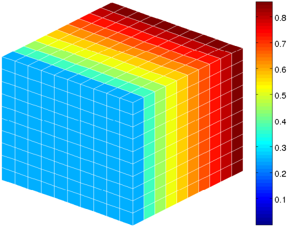
Convergence history for various parameters

Evolution of the concentration





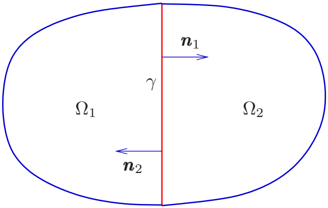




Outline

A reduced model: interface-fracture

Alboin-Jaffré-Roberts-Serres (2002)
Martin-Jaffré-Roberts (2005)
Knabner-Roberts (2014) (Forchheimer flow)



In this work: assume that $\mathbf{D}/\delta$ large
$\Rightarrow$ concentration continuity across the fracture
In the subdomains

$$
\left.
\begin{aligned}
\phi_i \partial_t c_i + \operatorname{div} \mathbf{r}_i &= f_i && \text{in } \Omega_i \times (0,T), \\
\mathbf{r}_i &= -\mathbf{D}_i \nabla c_i && \text{in } \Omega_i \times (0,T), \\
c_i &= 0 && \text{on } \partial\Omega_i \cap \partial\Omega \times (0,T), \\
c_i &= c_\gamma && \text{on } \gamma \times (0,T), \\
c_i(\cdot, 0) &= c_{0,i} && \text{in } \Omega_i,
\end{aligned}
\right.
\qquad \text{for } i = 1,2,
$$

A reduced model: interface-fracture

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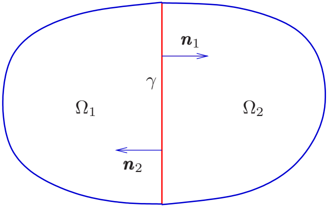

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c_i &= 0 && \text{on } \partial\Omega_i \cap \partial\Omega \times (0,T), \qquad \text{for } i = 1,2, \\
c_i &= c_\gamma && \text{on } \gamma \times (0,T), \\
c_i(\cdot,0) &= c_{0,i} && \text{in } \Omega_i,
\end{aligned}$$

and in the fracture

$$\begin{aligned}
\phi_\gamma \partial_t c_\gamma + \operatorname{div}_\tau \mathbf{r}_\gamma &= f_\gamma + \left(\mathbf{r}_1 \cdot \mathbf{n}_{1|\gamma} + \mathbf{r}_2 \cdot \mathbf{n}_{2|\gamma}\right) && \text{in } \gamma \times (0,T), \\
\mathbf{r}_\gamma &= -\mathbf{D}_\gamma \delta \nabla_\tau c_\gamma && \text{in } \gamma \times (0,T), \\
c_\gamma &= 0 && \text{on } \partial\gamma \times (0,T), \\
c_\gamma(\cdot,0) &= c_{0,\gamma} && \text{in } \gamma.
\end{aligned}$$

$\Rightarrow$ Communication between the fracture and the rock matrix.

Formulation as an interface problem (GTP Schur)

- The same (as with simple DD) Dirichlet-to-Neumann operators, for $i = 1, 2$:

$$\mathcal{S}_i^{DtN} : (\lambda, f, c_0) \longmapsto (\mathbf{r}_i \cdot \mathbf{n}_i)_{|\Gamma} \,,$$

  where $(c_i, \mathbf{r}_i)\,,\ i = 1, 2$, is the solution of

$$\begin{aligned} \mathcal{L}(c_i, \mathbf{r}_i) &= f, && \text{in } \Omega_i \times (0, T), \\ \mathcal{M}(c_i, \mathbf{r}_i) &= 0, && \text{in } \Omega_i \times (0, T), \\ c_i &= \lambda, && \text{on } \gamma \times (0, T), \\ c_i(\cdot, 0) &= c_0, && \text{in } \Omega_i. \end{aligned}$$

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- Different space-time interface problem: instead of

$$-\sum_{i=1}^{2} \mathcal{S}_i^{DtN}(\lambda, 0, 0) = \sum_{i=1}^{2} \mathcal{S}_i^{DtN}(0, f, c_0),$$

$$\Updownarrow$$

$$\mathcal{S}\lambda = \chi, \quad \text{on } \gamma \times (0, T).$$

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- Different space-time interface problem:

$$\begin{aligned} \mathcal{L}_\gamma(\lambda, \mathbf{r}_\gamma) + \mathcal{S}\lambda &= \chi + f_\gamma, && \text{in } \gamma \times (0, T), \\ \mathcal{M}_\gamma(\lambda, \mathbf{r}_\gamma) &= 0 && \text{in } \gamma \times (0, T), \\ \lambda(\cdot, 0) &= c_{0,\gamma}, && \text{in } \gamma. \end{aligned}$$

Formulation as an interface problem (GTP Schur)

- The same (as with simple DD) Dirichlet-to-Neumann operators, for $i = 1,2$:

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  - a Neumann-Neumann preconditionner with weights

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- Two possible preconditionners:
  - a Neumann-Neumann preconditionner with weights
  - a local preconditioner (coming from the observation that the interface problem is dominated by the 2nd order operator, Amir, MK, Martin, Robert, Arima 06)

Transmission conditions for a GTO Schwarz method

Taking a linear combination of the transmission conditions for the GTP Schur method we obtain:

$$\begin{aligned} -\mathbf{r}_1 \cdot \mathbf{n}_1 + \alpha_1 c_{1,\gamma} + \phi_\gamma \partial_t c_{i,\gamma} + \mathrm{div}_\tau\, \mathbf{r}_{\gamma,1} &= -\mathbf{r}_2 \cdot \mathbf{n}_1 + \alpha_1 c_{2,\gamma} + f_\gamma \\ \mathbf{r}_{\gamma,1} &= -\mathbf{D}_\gamma \delta \nabla_\tau c_{1,\gamma} \end{aligned}$$

$$\begin{aligned} -\mathbf{r}_2 \cdot \mathbf{n}_2 + \alpha_2 c_{2,\gamma} + \phi_\gamma \partial_t c_{2,\gamma} + \mathrm{div}_\tau\, \mathbf{r}_{\gamma,2} &= -\mathbf{r}_1 \cdot \mathbf{n}_2 + \alpha_2 c_{1,\gamma} + f_\gamma \\ \mathbf{r}_{\gamma,2} &= -\mathbf{D}_\gamma \delta \nabla_\tau c_{2,\gamma} \end{aligned}$$

Formulation as an interface problem (GTO Schwarz)

- We use Ventcell to Robin operators, for $i = 1, 2$:

$$\mathcal{S}_i^{VtR} : (\theta_i, f, c_0, f_\gamma, c_{0,\gamma}) \longmapsto \left(-\mathbf{r}_i \cdot \mathbf{n}_j + \alpha c_i\right)_{|\Gamma},$$

where $\left(c_i, \mathbf{r}_i, c_{i,\gamma}, r_{\gamma,i}\right)$, $i = 1, 2$, is the solution of

$$\begin{aligned}
\mathcal{L}(c_i, \mathbf{r}_i) &= f, && \text{in } \Omega_i \times (0,T),\\
\mathcal{M}(c_i, \mathbf{r}_i) &= 0, && \text{in } \Omega_i \times (0,T),\\
-\mathbf{r}_i \cdot \mathbf{n}_i + \alpha c_{i,\gamma} + \phi_\gamma \partial_t c_{i,\gamma} + \mathrm{div}_\tau \mathbf{r}_{\gamma,i} &= \theta_i && \text{on } \gamma \times (0,T),\\
\mathbf{r}_{\gamma,i} + \mathbf{D}_\gamma \delta \nabla_\tau c_{i,\gamma} &= 0, && \text{on } \gamma \times (0,T),\\
c_i(\cdot, 0) &= c_0, && \text{in } \Omega_i\\
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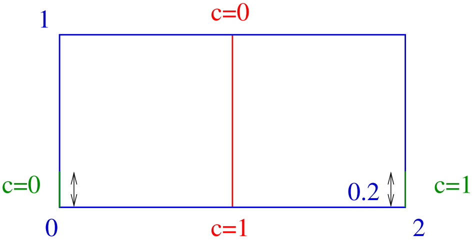
c_i(\cdot, 0) &= c_0, && \text{in } \Omega_i\\
c_{i,\gamma}(\cdot, 0) &= c_{0,\gamma}, && \text{in } \gamma.
\end{aligned}$$

- Space-time interface problem:

$$\begin{aligned}
\theta_1 &= \mathcal{S}_2^{VtR}(\theta_2, f, c_0, f_\gamma, c_{0,\gamma}) + f_\gamma, && \text{on } \gamma \times (0, T),\\
\theta_2 &= \mathcal{S}_1^{VtR}(\theta_1, f, c_0, f_\gamma, c_{0,\gamma}) + f_\gamma, && \text{on } \gamma \times (0, T).
\end{aligned}$$

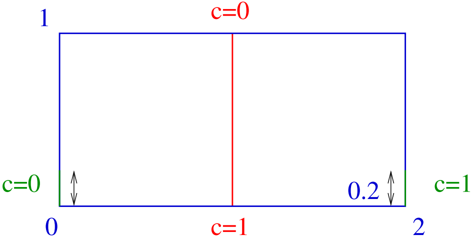
Numerical results



Geometry and boundary conditions.

- Isotropic coefficients: $\mathbf{D}_i = 1,\ i = 1, 2$, and $\mathbf{D}_\gamma = 1/\delta = 1000$.

Numerical results



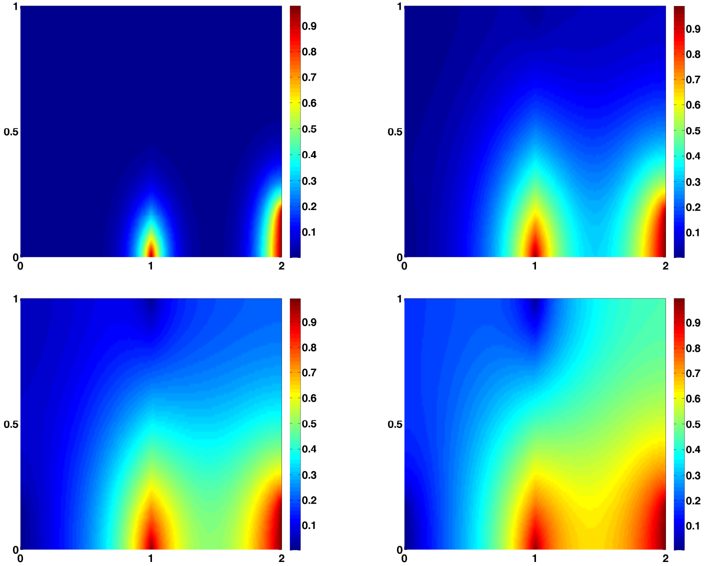
Geometry and boundary conditions.

- Isotropic coefficients: $\mathbf{D}_i = 1,\ i = 1, 2$, and $\mathbf{D}_\gamma = 1/\delta = 1000$.
- Zero source terms and initial condition.
- Spatial discretization: uniform rectangular mesh $h = 1/100$
  $\rightarrow$ mixed FE with the lowest-order Raviart-Thomas spaces.
- Time discretization (case 1): conforming grids $\Delta t_m = \Delta t_\gamma = T/300$ with $T = 0.5$.

Snapshots of solution - concentration field *c*

t=Δt

t=T/4

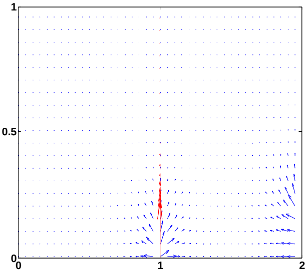


t=T/2

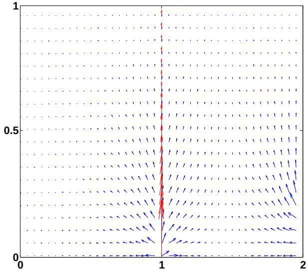
t=T

Snapshots of solution - diffusive flux **r**

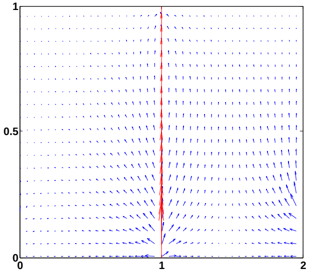
t=Δt



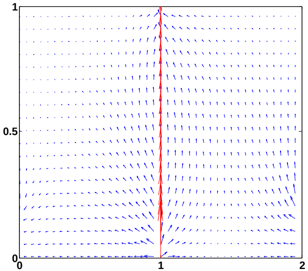
t=T/4



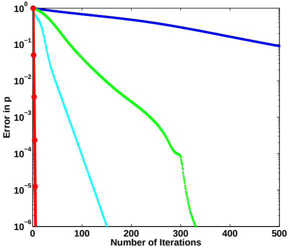
t=T/2



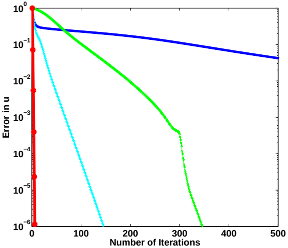
t=T



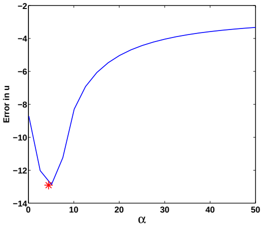
Convergence - GMRES



L^2 concentration errors (c)



L^2 flux errors ($\mathbf{r}$)



L^2 error versus α

- GT Schur with no preconditioner
- GTP Schur with local preconditioner
- GTP Schur with NN preconditioner
- GTO Schwarz method

T.T.P. Hoang, J. Jaffré, C. Japhet, M.K., and J. E. Roberts. Space-time Domain Decomposition and Mixed Formulation for reduced fracture models. SIAM J. Numer. Anal., to appear, 2016.

Conclusions – perspectives

- Space–time DD method with Robi TC for diffusion and advection–diffusion
- Extension to fractured media

- Convergence for GTP Schur (Gander et al. for homogeneous media)
- Convergence for fractured media

- Influence of Robin parameter β, find optimal parameter
- Study interface problem for non-linear case, Jacobi (SWR) vs Newton
- Extension to full two-phase model
- Convergence of Schwarz alg. for nonlinear case
- Large scale parallel solver (MdS)