Space–time domain decomposition methods for linear and non–linear diffusion problems

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Outline

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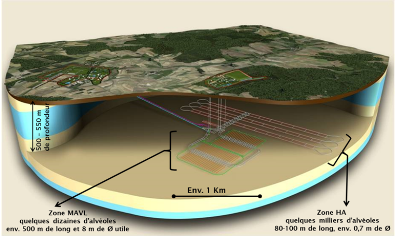
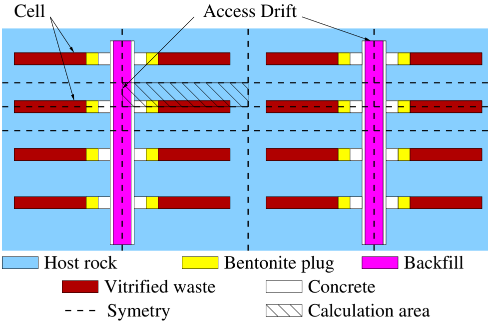
Simulation of the transport of radionuclides around a repository



Far-field simulation



Near-field simulation

Challenges

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

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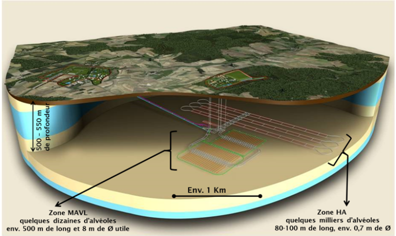

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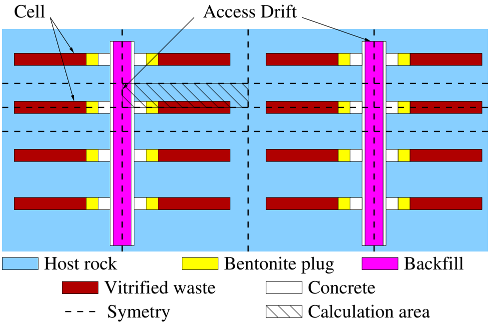

Near-field simulation

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⇒ Domain Decomposition methods
Global in Time

Model problem: Simplified model for two–phase immiscible flow

- Fractional flow (global pressure), with Kirchoff transformation
- Neglect advection (focus on capillary trapping) : decouple pressure from saturation, Enchery et al. (06), Cances (08)

Simplified system: Nonlinear (degenerate) diffusion equation

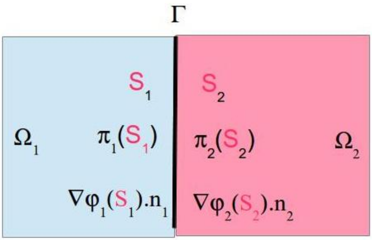
$$\omega \partial_t S - \Delta \phi(S) = 0 \quad \text{in } \Omega \times [0, T]$$

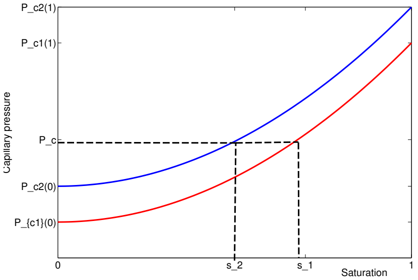
$$\phi(S) = \int_0^S \lambda(u) \pi'(u) \, du$$

- ω porosity
- λ mobility
- S_α water saturation
- π capillary pressure (increasing)

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

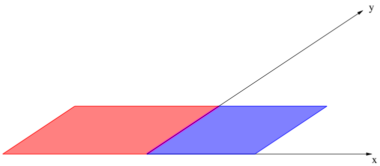
Continuity of capillary pressure $\pi_1(S_1) = \pi_2(S_2)$ on Γ

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)

Space–time domain decomposition

Domain decomposition in space



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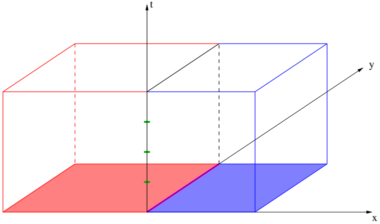

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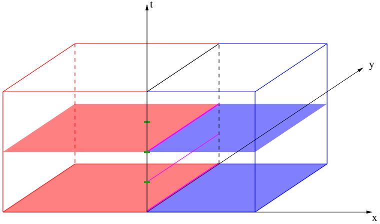

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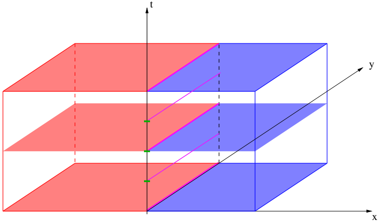
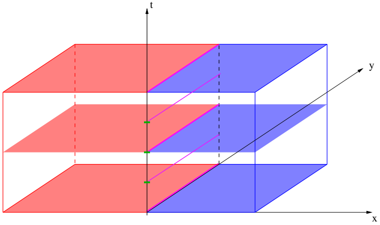


- Discretize in time and apply DD algorithm at each time step:
  - ▶ Solve stationary problems in the subdomains
  - ▶ Exchange information through the interface
- Use the same time step on the whole domain.

Space–time domain decomposition

Domain decomposition in space



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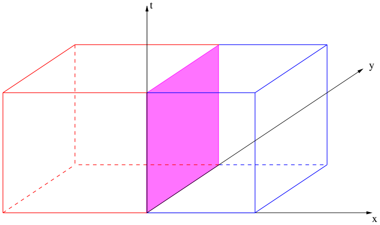

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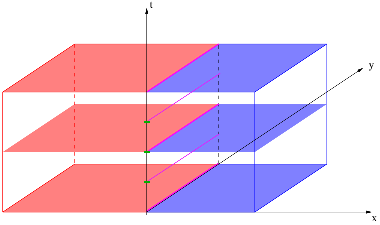

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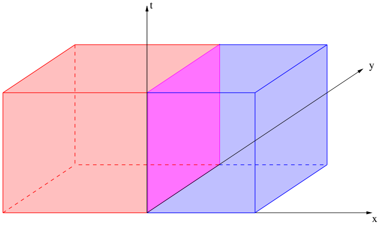

- Solve time-dependent problems in the subdomains
- Exchange information through the space-time interface
- Enable local discretizations both in space and in time
- Minimize number of communication between subdoains

$\longrightarrow$ local time stepping

Outline

Linear diffusion problem

- Time-dependent diffusion equation + homogeneous Dirichlet BC & IC $c(\cdot,0) = c_0$.

$$\omega \partial_t c + \text{div}\left(-\mathbf{D}\nabla c\right) = f \quad \text{in } \Omega \times (0,T),$$

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- Equivalent multi-domain formulation obtained by solving subproblems

$$\begin{aligned} \omega\partial_t c_i + \operatorname{div}(-\mathbf{D}\nabla c_i) &= f && \text{in } \Omega_i \times (0,T) \\ c_i &= 0 && \text{on } \partial\Omega_i \cap \partial\Omega \times (0,T) \qquad \text{for } i = 1,2, \\ c_i(\cdot,0) &= c_0 && \text{in } \Omega_i, \end{aligned}$$

with transmission conditions on space–time interface

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

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- Equivalent Robin TCs on $\Gamma\times[0,T]$. For $\beta_1, \beta_2 > 0$:

$$\begin{aligned} -\nabla c_1\cdot\mathbf{n}_1 + \beta_1 c_1 &= -\nabla c_2\cdot\mathbf{n}_1 + \beta_1 c_2 \\ -\nabla c_2\cdot\mathbf{n}_2 + \beta_2 c_2 &= -\nabla c_1\cdot\mathbf{n}_2 + \beta_2 c_1 \end{aligned}$$

β_1, β_2 numerical parameters, can be optimized to improve convergence rate

Schwarz waveform relation: Robin transmission conditions

- Robin to Robin operators, for $i = 1, 2,\ j = 3 - i$:

$$\mathscr{S}_i^{\mathrm{RtR}} : (\xi_i, f, c_0) \to (\nabla c_i \cdot \mathbf{n}_j + \beta_j c_i)_{|\Gamma}$$

where c_i ($i = 1, 2$) solution of

$$\begin{aligned} \omega \partial_t c_i + \operatorname{div}(-\mathbf{D} \nabla c_i) &= f && \text{in } \Omega_i \times (0, T) \\ -\nabla c_i \cdot \mathbf{n}_i + \beta_i c_i &= \xi_i && \text{on } \Gamma \times (0, T) \end{aligned}$$

Space – time interface problem with two Lagrange multipliers

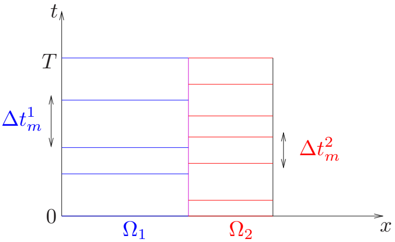
$$\begin{aligned} \xi_1 &= S_1^{\mathrm{RtR}}(\xi_2, f, c_0) \\ \xi_2 &= S_2^{\mathrm{RtR}}(\xi_1, f, c_0) \end{aligned} \quad \text{on } \Gamma \times [0, T] \quad \text{or } S_R \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \kappa_R$$

Solve with Richardson (original SWR) or GMRES

Need to solve subdomain problem with Robin BC

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

Nonconforming discretization in time



Information on one time grid at the interface is passed to the other time grid at the interface using optimal L2-projections (Gander-Japhet-Maday-Nataf (2005))

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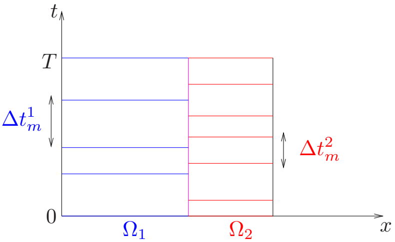

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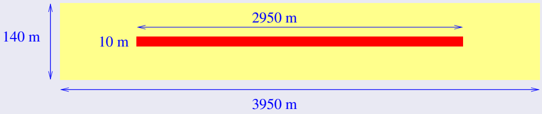
Application (Andra)



- Permeability $d = 5\,10^{-12}$ m^2/s in the clay layer and $d = 2\,10^{-9}$ m^2/s in the repository.
- Non-conforming time grids: $\Delta t = 2000$ (years) in the repository and $\Delta t = 10000$ (years) in the clay layer.

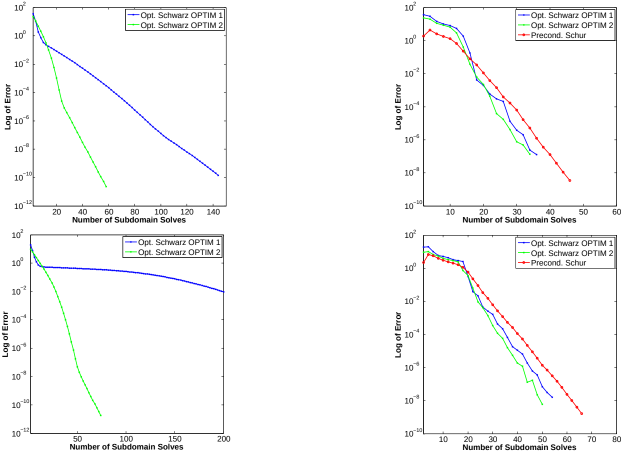
Convergence History for Short/Long Time Interval

2 optimization techniques (discontinuous coefficients) for computing parameters $\alpha_{i,j}$:

- Opt. 1: 2 half-space Fourier analysis.
- Opt. 2: taking into account the length of the domains Halpern-Japhet-Omnes (DD20, 11)

$T = 2\,10^5$ years

$T = 10^6$ years



Jacobi GMRES

Outline

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

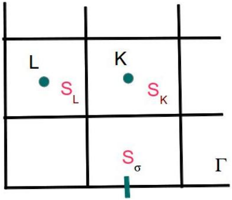
$$\omega\partial_t S_i^{k+1} - \Delta\phi_i(S_i^{k+1}) = 0 \quad \text{in } \Omega_i \times [0, T]$$
$$\nabla\phi_i(S_i^{k+1}).n_i + \beta_i\pi_i(S_i^{k+1}) = -\nabla\phi_j(S_j^k).n_j + \beta_i\pi_j(S_j^k) \quad \text{on } \Gamma \times [0, T],$$

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

Basic ingredient: subdomain solver with Robin bc.

Finite volume scheme

Extension to Robin bc of cell centered FV scheme by Enchéry et al. (06).



Unknowns : cell values (S_K), boundary face values (S_σ)
$K|L =$ edge between K and L,
$\tau_{K|L} = \dfrac{m(K|L)}{\bar{K}_{K|L}}$ (eg harmonic average).

Interior equation

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

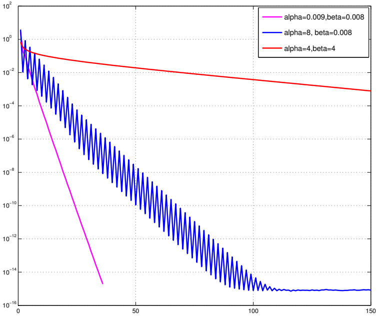
Robin BC for boundary faces

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

Numerical example

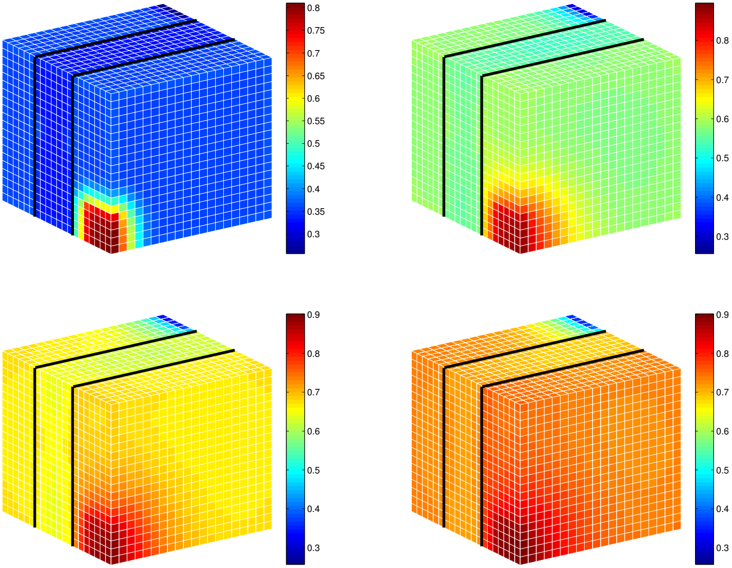
Implemented with Matlab Reservoir Simulation Toolbox (K. A. Lie et al. (14))
Solver with automatics differentiation : no explicit computation of Jacobian

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

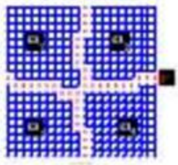
Three rock types: evolution of the concentrations

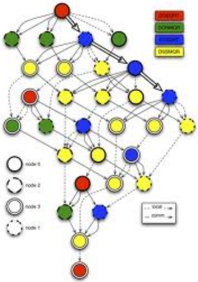


Towards two-level parallelism: hybrid solver

Dedales project (Serena (Inria), Hiepacs (Inria), Laga (Univ. Paris 13), Andra, MdlS)

- Solve subdomain problem with a parallel solver: Iterative solver (geometric DD, MPI parallelism) for the interface problem together with direct (algebraic, thread parallelism) within subdomains
- PaStiX direct linear solver (Inria Bordaux)
- Heterogeneous nodes: use scheduler (StarPU, Inria)
- Good coarse space ?
- Integration into Dune / DuMuX (with Dune-multidomaingrid ?)





Extensions – Coming attractions

- Convergence for Schwarz algorithm
- Advection–diffusion with splitting
- Use DD for fractured media (Ventcell BC, cf Hoang, Japhet, K. Roberts, to appear)

- Study influence of parameter β
- Find optimal parameter, compare
- Interface formulation 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)