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

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Work supported by Andra & ANR Dedales

Journées MoMaS – Multiphasiques

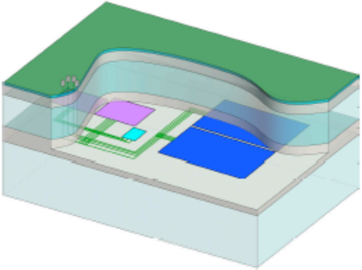
LJAD – Université de Nice   October 2015

Outline

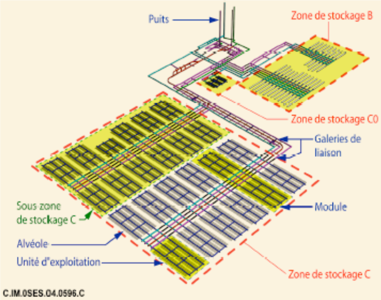
Outline

Geological repository for nuclear waste

Waste package 1.3m × Ø0.43m



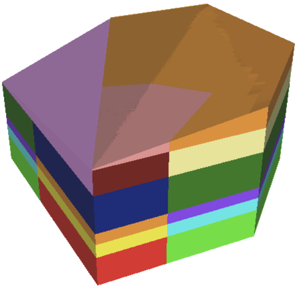
Geological formation 20km × 20km × 500m



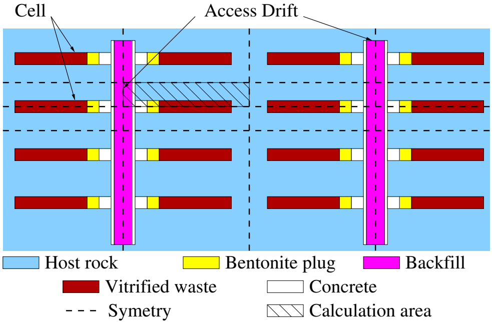
A repository 2km × 2km

ANDRA

Simulation of the transport of radionuclides around a repository



Far-field simulation



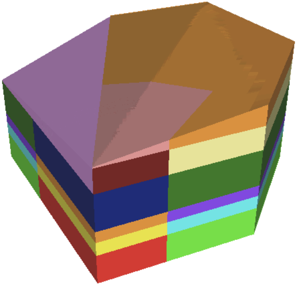
Near-field simulation

Challenges

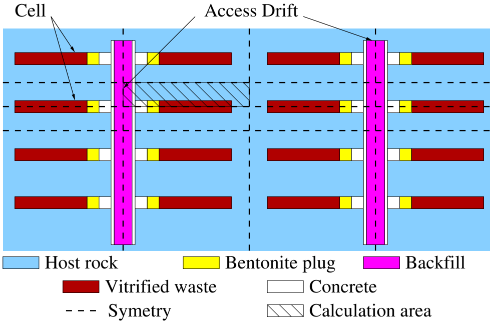
- Different materials $\rightarrow$ strong heterogeneity, different time scales.
- Large differences in spatial scales.
- Long-term computations.

$\rightarrow$ How to simulate efficiently & accurately?

Simulation of the transport of radionuclides around a repository



Far-field simulation



Near-field simulation

Challenges

- Different materials $\rightarrow$ strong heterogeneity, different time scales.
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$\rightarrow$ How to simulate efficiently & accurately?

$\Rightarrow$ Domain Decomposition methods
Global in Time

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

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

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

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

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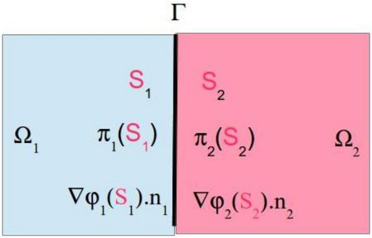
Simplified system: neglect advection

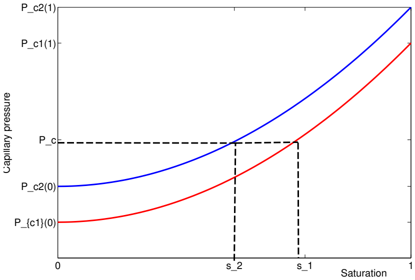
$$\omega \partial_t S - \Delta\phi(S) = 0 \quad \text{in } \Omega \times [0, T]$$

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

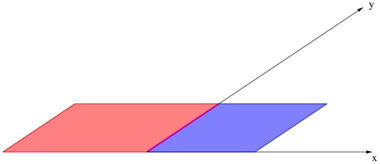
Continuity of capillary pressure $\pi_1(S_1) = \pi_2(S_2)$ on Γ

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).

Space–time domain decomposition

Domain decomposition in space



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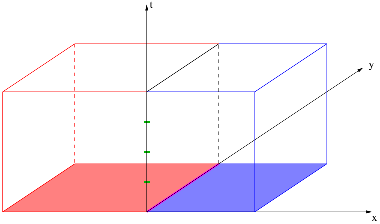

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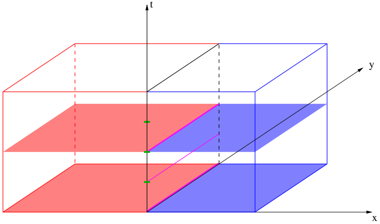

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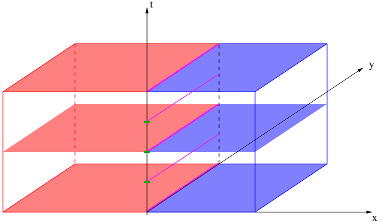
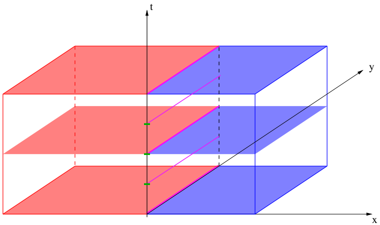


- Discretize in time and apply DD algorithm at each time step:
  - ▶ Solve stationary problems in the subdomains
  - ▶ Exchange information through the interface
- Use the same time step on the whole domain.

Space–time domain decomposition

Domain decomposition in space



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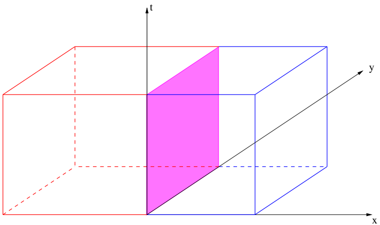

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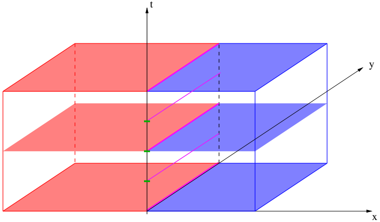

- Discretize in time and apply DD algorithm at each time step:
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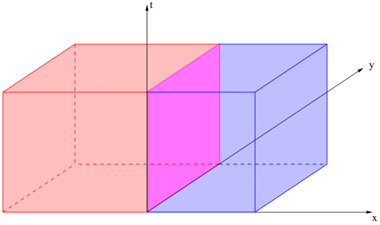
- Use the same time step on the whole domain.

Space-time domain decomposition



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

  ⟶ local time stepping

Outline

Diffusion Problem in a mixed formulation

- Time-dependent diffusion equation

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

+ homogeneous Dirichlet BC & IC $c(\cdot,0) = c_0$.

- $0 < \omega \in L^\infty(\Omega)$, $\mathbf{D} = \mathbf{D}(x) \in W^{1,\infty}(\Omega)$ symmetric, positive definite.
- Mixed variational formulation

$$\begin{aligned} \frac{d}{dt}(\omega c,\mu) + (\operatorname{div}\mathbf{r},\mu) &= (f,\mu), && \forall\mu\in L^2(\Omega),\\ -(\operatorname{div}\mathbf{v},c) + (\mathbf{D}^{-1}\mathbf{r},\mathbf{v}) &= 0, && \forall\mathbf{v}\in H(\operatorname{div},\Omega),\\ IC. \end{aligned} \tag{MVF}$$

Diffusion Problem in a mixed formulation

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$$\begin{aligned} \tfrac{d}{dt}(\omega c, \mu) + (\operatorname{div} \mathbf{r}, \mu) &= (f, \mu), && \forall \mu \in L^2(\Omega), \\ -(\operatorname{div} \mathbf{v}, c) + (\mathbf{D}^{-1}\mathbf{r}, \mathbf{v}) &= 0, && \forall \mathbf{v} \in H(\operatorname{div}, \Omega), \\ IC. & \end{aligned} \tag{MVF}$$

Theorem 1 (Well-posedness for homogeneous Dirichlet BCs)

If $f \in L^2(0,T; L^2(\Omega))$ and $c_0 \in H_0^1(\Omega)$ then (MVF) has a unique solution

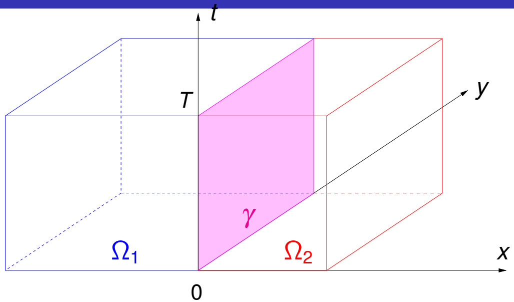
$$(c, \mathbf{r}) \in H^1(0,T; L^2(\Omega)) \times \left(L^2(0,T; H(\operatorname{div}, \Omega)) \cap L^\infty(0,T; L^2(\Omega))\right).$$

Moreover, if $f \in H^1(0,T; L^2(\Omega))$ and $c_0 \in H^2(\Omega) \cap H_0^1(\Omega)$ then

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

Multi-domain mixed formulation

Decomposition into non-overlapping subdomains.



Equivalent multi-domain formulation obtained by solving subproblems

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

with transmission conditions on space–time interface

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

Time dependent Steklov – Poincaré operators

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

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

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

$$\begin{aligned} \mathbf{D}_i^{-1}\mathbf{r}_i + \nabla c_i &= 0 && \text{in } \Omega_i \times (0, T) \\ \omega_i \partial_t c_i + \text{div } (\mathbf{r}_i) &= f && \text{in } \Omega_i \times (0, T) \\ c_i &= \lambda && \text{on } \Gamma \times (0, T) \end{aligned}$$

- Space – time interface problem

$$\mathscr{S}_1^{\text{DtN}}(\lambda, f, c_o) + \mathscr{S}_2^{\text{DtN}}(\lambda, f, c_0) = 0 \Longleftrightarrow \mathscr{S}\lambda = \chi, \text{ on } \Gamma \times [0, T]$$

- Solve with GMRES, preconditioned with Neumann – Neumann

Schwarz waveform relation: Robin transmission conditions

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

$$-\mathbf{r}_1 \cdot \mathbf{n}_1 + \beta_1 c_1 = -\mathbf{r}_2 \cdot \mathbf{n}_1 + \beta_1 c_2$$
$$-\mathbf{r}_2 \cdot \mathbf{n}_2 + \beta_2 c_2 = -\mathbf{r}_1 \cdot \mathbf{n}_2 + \beta_2 c_1$$

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

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

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

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

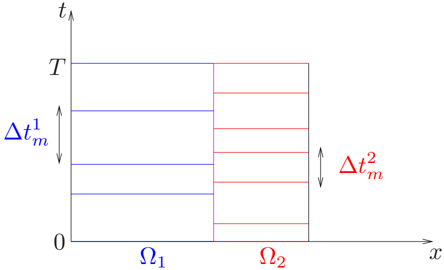
$$\begin{aligned} \mathbf{D}_i^{-1}\mathbf{r}_i + \nabla c_i &= 0 && \text{in } \Omega_i \times (0,T) \\ \omega_i \partial_t c_i + \operatorname{div}(\mathbf{r}_i) &= f && \text{in } \Omega_i \times (0,T) \\ -\mathbf{r}_i \cdot \mathbf{n}_i + \beta_i c_i &= \xi_i && \text{on } \Gamma \times (0,T) \end{aligned}$$

- 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 or GMRES

Nonconforming discretization in time

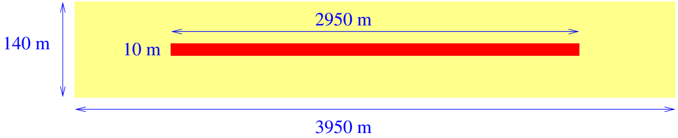


Information on one time grid at the interface is passed to the other time grid at the interface using L2-projections

$\rightarrow$ use an optimal projection algorithm, Gander-Japhet-Maday-Nataf (2005)

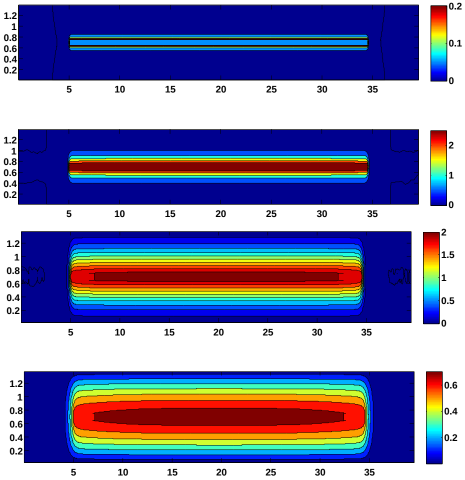
T. T. P. Hoang, J. Jaffré, C. Japhet, M. K., J.E. Roberts, Space-time domain decomposition methods for diffusion problems in mixed formulations. SIAM J. Numer. Anal., 51(6):3532–3559, 2013.

A test case (Andra)



- Porosity $\omega = 0.05$ in the clay layer (in yellow) and $\omega = 0.2$ in the repository (in red).
- Permeability $d = 5\,10^{-12}$ m^2/s in the clay layer and $d = 2\,10^{-9}$ m^2/s in the repository.
- Source term $f = 0$ in the clay layer, and $f = \begin{cases} 10^{-5} & \text{for } t \leq 10^5 \\ 0 & \text{for } t > 10^5 \end{cases}$ in the repository.
- Decomposition: 9 rectangular subdomains. Non-uniform spatial mesh $\Delta x = 1/300$.
- Non-conforming time grids: $\Delta t = 2000$ (years) in the repository and $\Delta t = 10000$ (years) in the clay layer.
- 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)

Snapshots of Solution



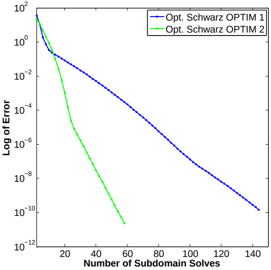
Snapshots of multi-domain solution at 2000 years, 10^5 years, $2\,10^5$ years and 1 million years respectively.

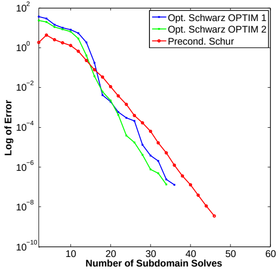
Note. Color bars change.

Convergence History for Short/Long Time Interval

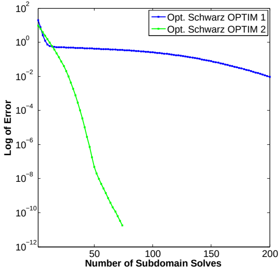
Error in concentration

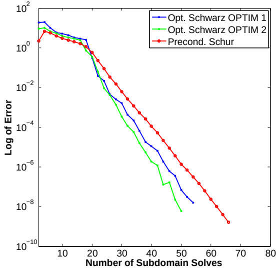
$T = 2\,10^5$ years





$T = 10^6$ years





Jacobi

GMRES

Extension to advection – diffusion

- Splitting method: different time steps for advection and diffusion
- Steklov – Poincaré method

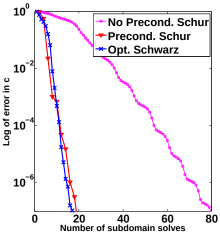
$$\tilde{\mathscr{S}}_h \begin{pmatrix} \lambda_a \\ \lambda \end{pmatrix} = \tilde{\chi}_h \quad \text{on } \Gamma \times [0, T]$$

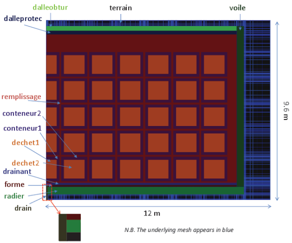
  Generalized Neumann – Neumann preconditioner
- Schwarz WR with Robin TC

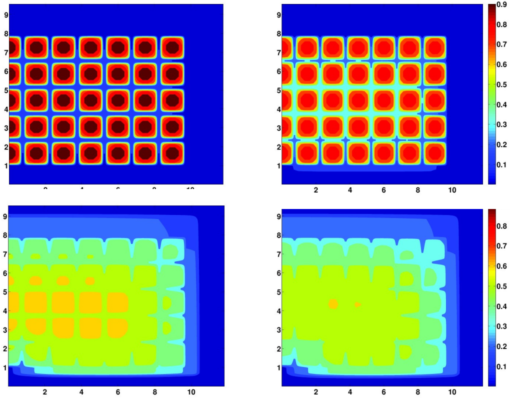
$$\tilde{\mathscr{S}}_{R,h} \begin{pmatrix} \lambda_a \\ \xi_1 \\ \xi_2 \end{pmatrix} = \tilde{\chi}_{R,h} \quad \text{on } \Gamma \times [0, T]$$

  Optimize Robin parameters for diffusion only, $\neq$ fully implicit method

Example: transport in a near–surface repository







Joint with C. Japhet, J. Roberts, PhD thesis of Ph. Hoang Thi Thao

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}, $i = 1, 2, j = 3 - i$

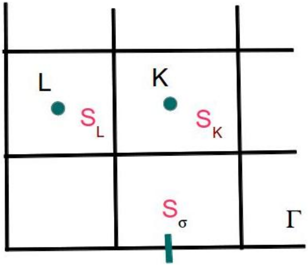
$$\omega\partial_t S_i^{k+1} - \Delta\phi_i(S_i^{k+1}) = 0 \qquad \text{in } \Omega_i \times [0, T]$$
$$\nabla\phi_i(S_i^{k+1}).n_i + \beta_i\pi_i(S_i^{k+1}) = -\nabla\phi_j(S_j^k).n_j + \beta_i\pi_j(S_j^k) \quad \text{on } \Gamma \times [0, T],$$

(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 $\mathscr{T}$, cells $K \in \mathscr{T}$, boundary faces $\sigma \subset \Gamma$.
Unknowns : cell values $(S_K)_{K \in \mathscr{T}}$, boundary face values $(S_\sigma)_{\sigma \in \mathscr{E}_\Gamma}$



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

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

Robin BC for boundary faces

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

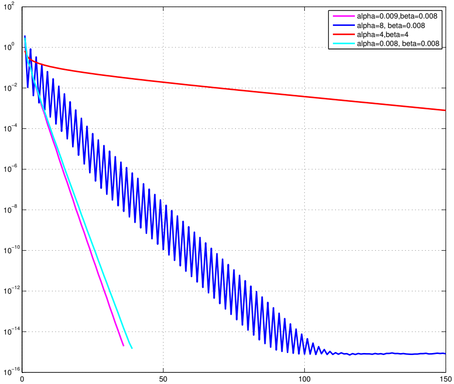
Implemented with Matlab Reservoir Simulation Toolbox (K. A. Lie et al. (14))
Solver with automatics differentiation : no explicit computation of Jacobian

MRST Code

```
grad = @(x)-C*x;
div  = @(x)C'*x;

vEq=@(p)   T .* grad(phi(p) - g*rho.*z) ;
pressureEq = @(p, p0, dt,p_rr) (1/dt) .* (p - p0) - div( vEq(p) ) +Arobin(p_rr);
robinEq =@(p,p_rr) ft(face_robin).*phi(p_rr)+beta.*pc(p_rr).*G.faces.areas(face_robin) ...
                  -ft(face_robin).*phi(p(Cellsonrobin));

[p_ad, p_rrad] = initVariablesADI(p_init, p_rrinit);

while t < totTime,
    t = t + dt;    p0  = double(p_ad);
    while (resNorm > tol) && (nit < maxits)
        % Create equations:
        eqs = cell([2, 1]);
        eqs{1} = pressureEq(p_ad, p0, dt,p_rrad);
        eqs{2} = robinEq(p_ad,p_rrad)-bc(step+1).value(1:length(face_robin));

        % Concatenate equations and solve:
        eq  = cat(eqs{:});
        J   = eq.jac{1};  % Jacobian
        res = eq.val;     % residual
        upd = -(J \ res); % Newton update

        % Update variables
        p_ad.val   = p_ad.val   + upd(pIx); p_rrad.val = p_rrad.val + upd(pRx);

        resNorm = norm(res); nit     = nit + 1;
    end
end
```

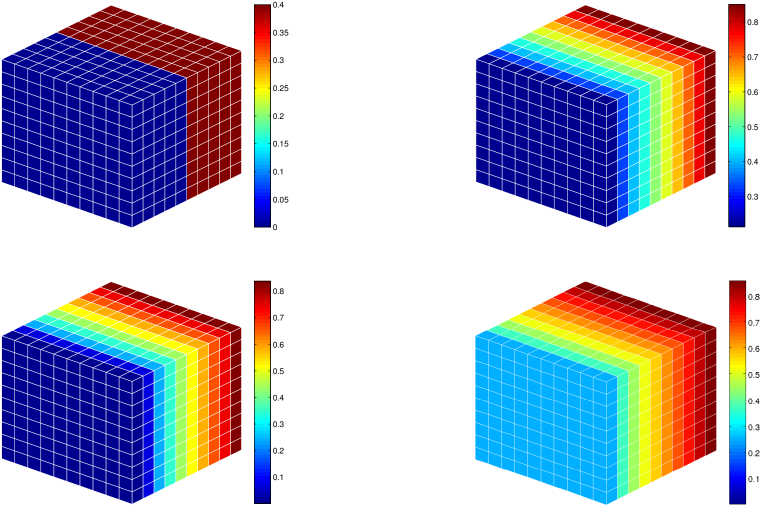
Numerical example

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



Formulation as interface problem

Local solver

$$S_i(g) = \left(\tau_{L,\sigma}\left(\phi(S_L^n) - \phi(S_{L,\sigma}^n)\right) + \beta_j m(\sigma)\pi(S_{L,\sigma}^n)\right)_{L\in\mathscr{T},\sigma\in\mathscr{E}_\Gamma}^{n=,0,\dots,N}$$

where $(S_L^n, S_{L,\sigma})_{L\in\mathscr{T},\sigma\in\mathscr{E}_\Gamma}^{n=,0,\dots,N}$ solves the local problem.

$$m(K)\frac{S_K^{n+1} - S_K^n}{\delta t} + \sum_{L\in\mathscr{N}(K)} \tau_{K|L}\left(\phi(S_K^{n+1}) - \phi(S_L^{n+1})\right)$$

$$+ \sum_{\sigma\in\mathscr{E}_\Gamma\cap\mathscr{E}_K} \tau_{K,\sigma}\left(\phi(S_K^{n+1}) - \phi(S_\sigma^{n+1})\right) = 0, \quad K\in\mathscr{T},$$

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

Multi-domain prolem is equivalent to

Find $(\Psi_{\sigma,1},\Psi_{\sigma,2})_{\sigma\in\mathscr{E}_\Gamma}^{n=0,\dots,N}$ such that $\begin{aligned}\Psi_{\sigma,2} &= S_1(\Psi_{\sigma,1})\\ \Psi_{\sigma,1} &= S_2(\Psi_{\sigma,2})\end{aligned}$

Extensions – Coming attractions

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

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