

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

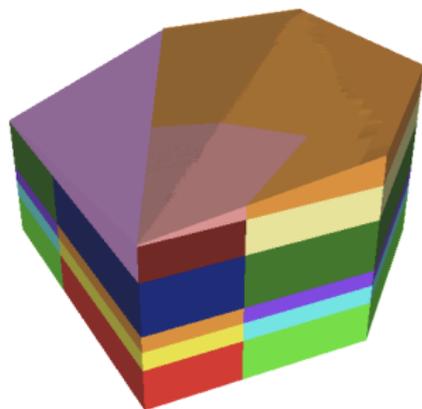
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Maison de la Simulation

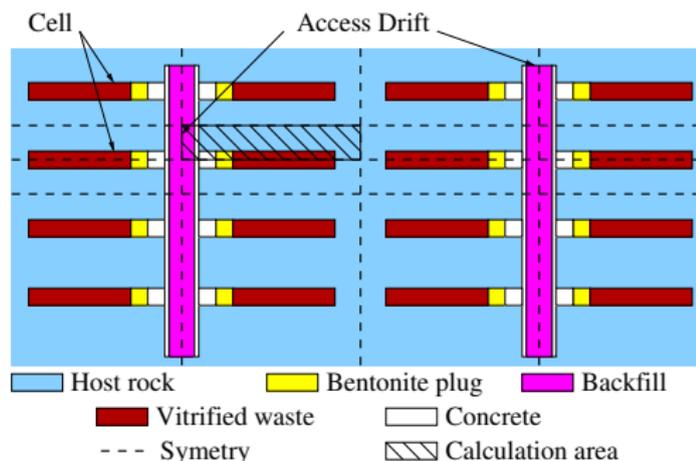
Computer and Computational Sciences at Exascale
Andra, April 24, 2013



Simulation of the transport of radionuclides around a repository



Far-field simulation



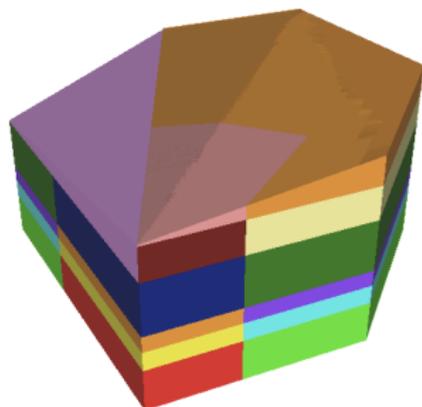
Near-field simulation

Challenges

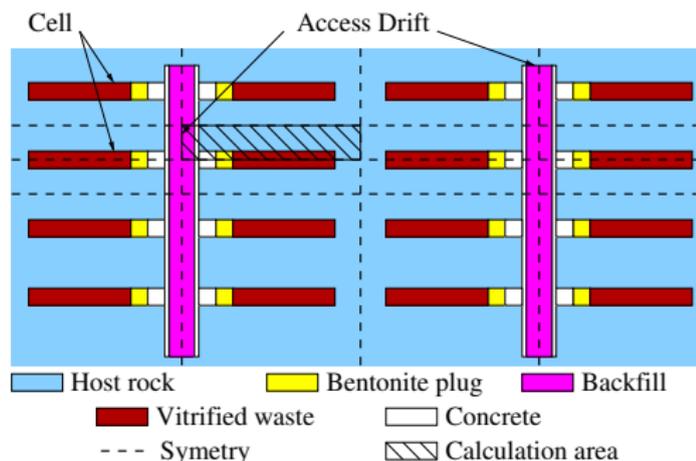
- ▶ Different materials → strong heterogeneity, **different time scales**.
- ▶ Large differences in spatial scales.
- ▶ Long-term computations.

→ **How to simulate efficiently & accurately?**

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Challenges

- ▶ Different materials → strong heterogeneity, **different time scales**.
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⇒ **Domain Decomposition methods**
Global in Time

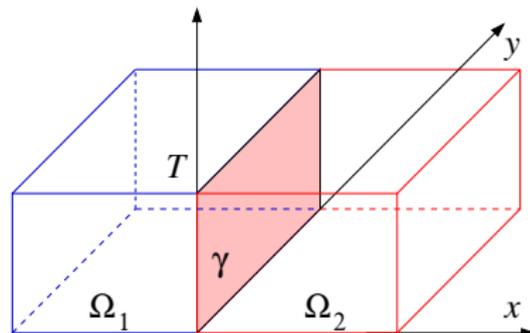
→ **How to simulate efficiently & accurately?**

Multi-domain mixed formulation for transport equation

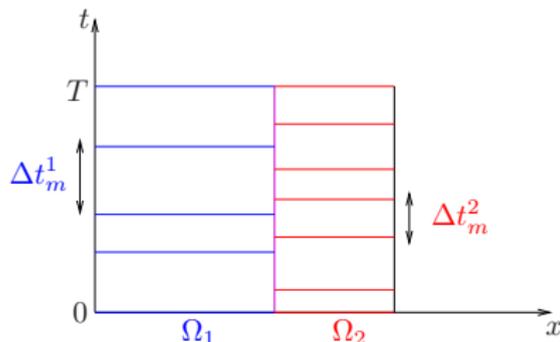
$$\begin{aligned}\omega \partial_t \mathbf{c} + \operatorname{div}(\mathbf{u} \mathbf{c} - \mathbf{r}) &= f, & \text{in } \Omega \times (0, T), \\ \mathbf{D}^{-1} \mathbf{r} + \nabla \mathbf{c} &= 0, & \text{in } \Omega \times (0, T) + \text{BCs, IC,}\end{aligned}$$

Decomposition
non-overlapping
domains.

into sub-



Different time steps for different subdomains



L^2 projections from piecewise constant functions on \mathcal{T}_i onto piecewise constant functions on \mathcal{T}_j

The Steklov-Poincaré interface equation

Natural transmission conditions

$$c_1 = c_2 \quad \text{on } \gamma \times (0, T),$$
$$(\mathbf{u}_1 \cdot \mathbf{n}_1 c_1 + \mathbf{r}_1 \cdot \mathbf{n}_1) + (\mathbf{u}_2 \cdot \mathbf{n}_2 c_2 + \mathbf{r}_2 \cdot \mathbf{n}_2) = 0$$

- ▶ Use **Dirichlet data** on the interface

$$c_i = \lambda \quad \text{on } \gamma \times (0, T), \text{ for } i = 1, 2,$$

and solve subdomain problem:

$$(\lambda, f, c_0) \mapsto (c_i(\lambda, f, c_0), \mathbf{r}_i(\lambda, f, c_0)).$$

- ▶ Transmission conditions reduced to flux equality:

$$\mathcal{S}\lambda \equiv \mathbf{r}_1(\lambda, f, c_0) \cdot \mathbf{n}_1 + \mathbf{r}_2(\lambda, f, c_0) \cdot \mathbf{n}_2 = 0, \quad \text{on } \gamma \times (0, T),$$

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

- ▶ Solved iteratively (e.g., with GMRES).

- ▶ Apply **Neumann-Neumann preconditioner** with weights

Optimized Schwarz Waveform Relaxation (OSWR) method

- ▶ Equivalent Robin transmission conditions on $\gamma \times (0, T)$:

$$-(\mathbf{u}_1 \cdot \mathbf{n}_1 c_1 + \mathbf{r}_1 \cdot \mathbf{n}_1) + \alpha_{1,2} c_1 = -(\mathbf{u}_2 \cdot \mathbf{n}_1 c_2 + \mathbf{r}_2 \cdot \mathbf{n}_1) + \alpha_{1,2} c_2$$

$$-(\mathbf{u}_2 \cdot \mathbf{n}_2 c_2 + \mathbf{r}_2 \cdot \mathbf{n}_2) + \alpha_{2,1} c_2 = -(\mathbf{u}_1 \cdot \mathbf{n}_2 c_1 + \mathbf{r}_1 \cdot \mathbf{n}_2) + \alpha_{2,1} c_1$$

- ▶ Use **Robin data** on the interface

$$-(\mathbf{u}_j \cdot \mathbf{n}_j c_j + \mathbf{r}_j \cdot \mathbf{n}_j) + \alpha_{j,j} c_j = \xi_j \text{ on } \gamma \times (0, T),$$

and solve subdomain problem with

$$\mathcal{R}_j : (\xi_j, f, c_0) \mapsto (c_j(\xi_j, f, c_0), \mathbf{r}_j(\xi_j, f, c_0)).$$

- ▶ **Interface problem**: global in space and time with **2 interface concentrations**

$$\mathcal{S}_R \left(\begin{array}{c} \xi_1 \\ \xi_2 \end{array} \right) = \chi_R \quad \text{on } \gamma \times (0, T).$$

- ▶ Solve iteratively (Jacobi = OSWR, GMRES, etc.).

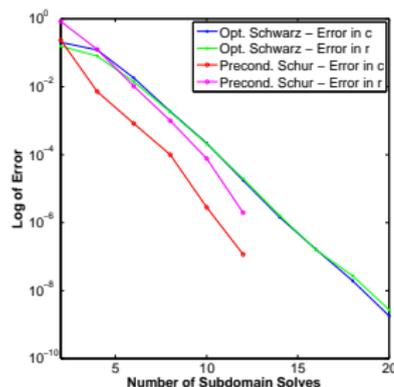
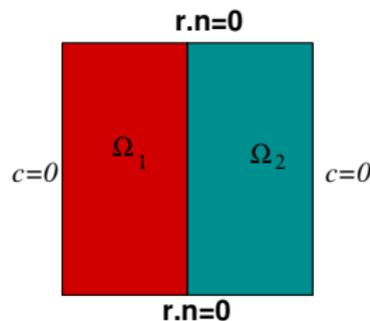
Test case 1: diffusion, 2 subdomains, varying contrast

- ▶ Matching meshes in space

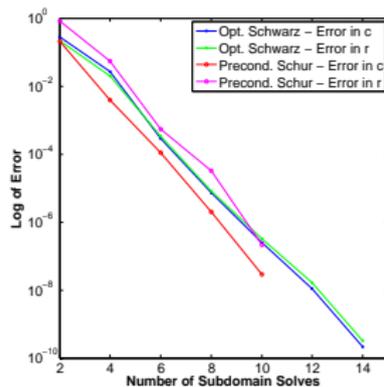
$$\Delta x = 1/200.$$

- ▶ **Non-conforming time grids**

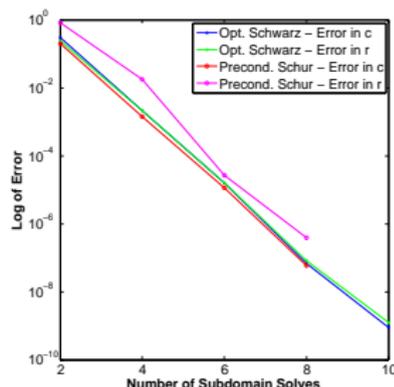
Contrast	d_1	$1/\Delta t_1$	$1/\Delta t_2$
10	0.02	150	200
100	0.002	50	200
1000	0.0002	20	200



Contrast = 10

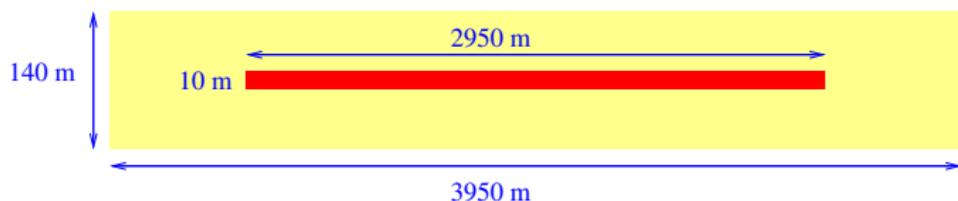


Contrast = 100

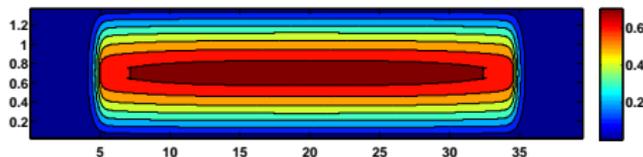


Contrast = 1000

Test case 2 (ANDRA) - Data



- ▶ Porosity $\omega = 0.05$ in clay layer and $\omega = 0.2$ in repository.
- ▶ Diffusion $d = 5 \cdot 10^{-12}$ m²/s in clay, $d = 2 \cdot 10^{-9}$ m²/s in repository.
- ▶ Source term $f = 0$ in clay, and $f = \begin{cases} 10^{-5} & \text{if } t \leq 10^5 \\ 0 & \text{if } t > 10^5 \end{cases}$ in repository.
- ▶ 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.



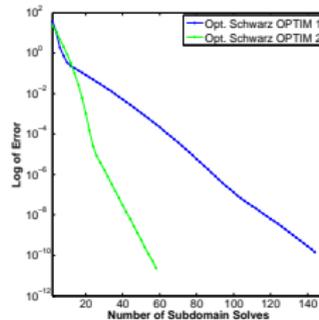
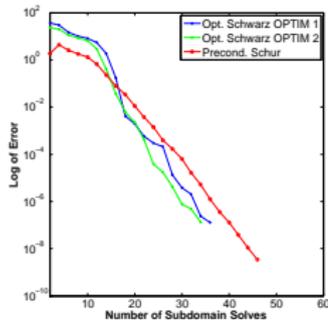
Snapshots of multi-domain solution at 1 million years

Convergence History for Short/Long Time Interval - Error in concentration

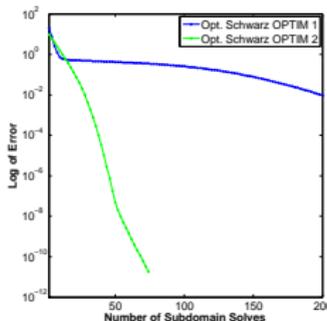
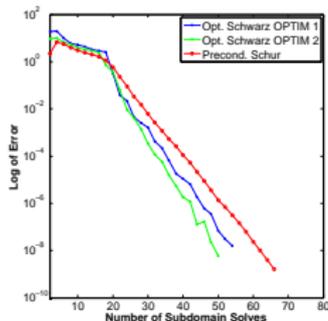
2 optimization techniques for computing parameters $\alpha_{i,j}$:

- ▶ **Opt. 1:** 2 half-space Fourier analysis.
- ▶ **Opt. 2:** taking into account the length of the domains

$T = 2 \cdot 10^5$ years



$T = 10^6$ years

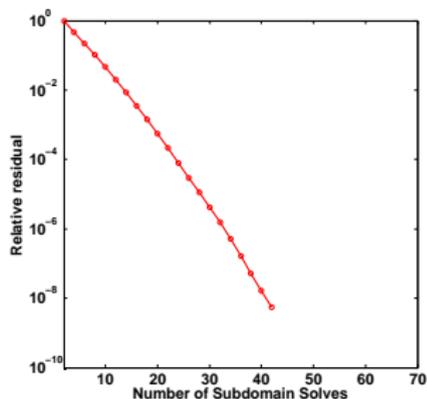
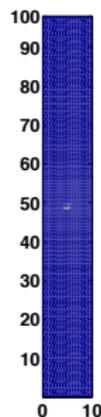


GMRES

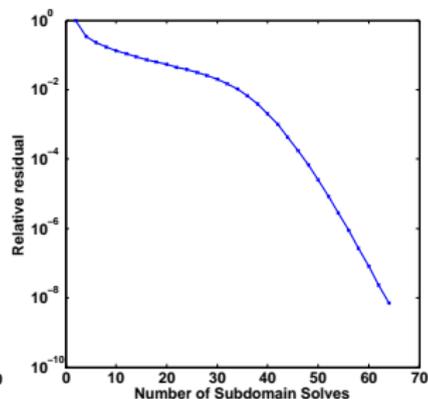
Jacobi

Near-field simulation with advection (CEA)

Material	Dims. (m)	Perm. ($\text{m}\cdot\text{s}^{-1}$)	Porosity	Diff. ($\text{m}^2\cdot\text{s}^{-1}$)
Host rock	10×100	10^{-13}	0.06	$6 \cdot 10^{-13}$
Repository	1×1	10^{-8}	0.1	10^{-11}



Precond. Schur



OSWR

Conclusion

Summary

- ▶ Diffusion problems
 - ▶ Two global-in-time methods: time-dependent Schur and OSWR.
 - ▶ Well-posedness of local problems in mixed form.
 - ▶ Performance of two methods for non-conforming time grids.
- ▶ Advection-Diffusion problems:
 - ▶ Formulation of interface problems with operator splitting.
 - ▶ Preliminary numerical results

Work in progress

- ▶ Fractures.
- ▶ Order 2 (Ventcel) transmission conditions.
- ▶ Non-matching grids in space.

T.T.P. Hoang, J. Jaffré, C. Japhet, MK and J.E. Roberts, **Space-Time Domain Decomposition Methods for Diffusion Problems in Mixed Formulations**, submitted to SINUM, hal-00803796