Space-time domain decomposition methods for mixed formulations for flow and transport in porous media

Caroline Japhet
Co-authors: Thi-Thao-Phuong Hoang, Jérôme Jaffré, Michel Kern and Jean E. Roberts

Université Paris 13 & INRIA Paris-Rocquencourt
work supported by Andra

Journée DDM - parallélisation, jeudi 11 juin 2015
Objective: to formulate numerical methods for flow and transport in heterogeneous porous media

Examples of heterogeneous 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 × 2km
Heterogeneities mean difficulties for simulation

Deep underground repository
(High-level waste)

Different materials → strong heterogeneity, different time scales.

Large differences in spatial scales.

Long-term computations.

A repository 2km × 2km
Introduction

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
- porous media with fractures
Difficulty for modeling flow in media with fractures

A problem requiring multi-scale modelling
Difficulty for modeling flow in media with fractures

A problem requiring multi-scale modelling

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

Fracture width much smaller than any reasonable parameter of spatial discretization.
Difficulty for modeling flow in media with fractures

A problem requiring multi-scale modelling

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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)
Introduction

Objective here: to formulate methods for subdomain time-stepping

More specifically:

- to develop and compare two different space-time (global in time) domain decomposition methods for the linear transport problem in mixed formulation.

- to extend these methods to the case of a domain with a discrete fracture
Domain decomposition (DD) methods

Domain decomposition in space

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

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
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- Exchange information through the space-time interface
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  \[\rightarrow\text{local time stepping}\]
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Space-time domain decomposition

- Solve time-dependent problems in the subdomains
- Exchange information through the space-time interface
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  → local time stepping

Space-time DD with Time windows

- 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.
Domain decomposition (DD) methods

Space-time domain decomposition

- Solve *time-dependent* problems in the subdomains
- Exchange information through the *space-time interface*
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  \[\rightarrow\] local time stepping

Space-time DD with Time windows

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Objectives of the work

Space-time domain decomposition methods with mixed formulations
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Space-time domain decomposition methods with mixed formulations

- **Global-in-time preconditioned Schur (GTP Schur):** using the Steklov-Poincaré operator
  - *Elliptic problems:* Agoshkov (87), Widlund (87), Destuynder-Roux (88), Bjørstad-Brækhus-Hvidsten (90), Quarteroni-Valli (91);
  - *Neumann-Neumann preconditioners:* Pasciak (88), Bourgat-Glowinski-Le Tallec-Vidrascu (89), De Roeck-Le Tallec (91);
  - *Balancing domain decomposition:* Mandel (93), Mandel-Brezina (96).

- **Parabolic problems:** Dryja (91), Gastaldi (94).

→ Time-dependent Steklov-Poincaré operators + mixed methods
Objectives of the work

**Space-time domain decomposition methods with mixed formulations**

- **Global-in-time preconditioned Schur (GTP Schur): using the Steklov-Poincaré operator**
  - *Elliptic problems*: Agoshkov (87), Widlund (87), Destuynder-Roux (88), Bjørstad-Brækhus-Hvidsten (90), Quarteroni-Valli (91);
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  - *Balancing domain decomposition*: Mandel (93), Mandel-Brezina (96).

- **Global-in-time optimized Schwarz (GTO Schwarz): using optimized Schwarz waveform relaxation (OSWR)**
  - *Optimized Schwarz methods*: CJ (98), CJ-Nataf-Rogier (01), Gander (06).
  - *OSWR methods*: Gander-Halpern-Nataf (99), Martin (05), Bennequin-Gander-Halpern (09)
  - *Non-conforming time grids (FEM or FVM)*: Gander-Halpern-Nataf (03), Gander-Halpern-Kern (07), Blayo-Halpern-CJ (07), Halpern-CJ-Szeftel (10), Haeblerlein (11), Hoang (13), Berthe (13).

→ Time-dependent Steklov-Poincaré operators + mixed methods

→ Extension to mixed FEM: Robin and Ventcell transmission conditions
OUTLINE

1. Introduction

2. Pure diffusion problems
   - Multi-domain mixed formulations
   - Nonconforming discretizations in time

3. Advection-diffusion problems
   - Operator splitting
   - Numerical results

4. Extension to reduced fracture models
Transport of a contaminant in a porous medium under the effect of diffusion, written in mixed form:

\[
\begin{align*}
\mathcal{L}(c, r) &:= \phi \frac{\partial c}{\partial t} + \text{div } r = f \quad \text{in } \Omega \times (0, T), \\
\mathcal{M}(c, r) &:= D^{-1}r + \nabla c = 0 \quad \text{in } \Omega \times (0, T), \\
\quad c &= 0 \quad \text{on } \partial \Omega \times (0, T), \\
\quad c(\cdot, 0) &= c_0 \quad \text{in } \Omega,
\end{align*}
\]

- $c$ concentration of a contaminant dissolved in a fluid, $r$ diffusive flux.
- $\phi$ porosity; $D$ symmetric, positive definite, time-independent diffusion tensor.
Multi-domain problem

Equivalent multi-domain problem:

\[
\begin{align*}
\mathcal{L}(c_1, r_1) &= f, & \text{on } \Omega_1 \times (0, T), \\
\mathcal{M}(c_1, r_1) &= 0, & \text{on } \Omega_1 \times (0, T), \\
c_1(\cdot, 0) &= c_0, & \text{in } \Omega_1,
\end{align*}
\]

\[
\begin{align*}
\mathcal{L}(c_2, r_2) &= f, & \text{on } \Omega_2 \times (0, T), \\
\mathcal{M}(c_2, r_2) &= 0, & \text{on } \Omega_2 \times (0, T), \\
c_2(\cdot, 0) &= c_0, & \text{in } \Omega_2,
\end{align*}
\]
Multi-domain problem

Equivalent multi-domain problem:

\[ \mathcal{L}(c_1, r_1) = f, \quad \text{on } \Omega_1 \times (0, T), \]
\[ M(c_1, r_1) = 0, \quad \text{on } \Omega_1 \times (0, T), \]
\[ c_1(\cdot, 0) = c_0, \quad \text{in } \Omega_1, \]
\[ \mathcal{L}(c_2, r_2) = f, \quad \text{on } \Omega_2 \times (0, T), \]
\[ M(c_2, r_2) = 0, \quad \text{on } \Omega_2 \times (0, T), \]
\[ c_2(\cdot, 0) = c_0, \quad \text{in } \Omega_2, \]

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

\[ c_1 = c_2 \quad \text{on } \Gamma \times (0, T). \]
\[ r_1 \cdot n_1 + r_2 \cdot n_2 = 0 \quad \text{on } \Gamma \times (0, T). \]
An overview

Different (equivalent) transmission conditions (TC’s)

GTP Schur
- Physical TC’s
- + N-N preconditioner

GTO Schwarz
- More general TC’s with optimized parameters
  $\rightarrow$ accelerate the convergence rate.

- Robin TC’s
- Ventcell TC’s
An overview

Different (equivalent) transmission conditions (TC’s)

↓

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

Different (equivalent) transmission conditions (TC’s)

\[\Downarrow\]

GTP Schur
- Physical TC’s
+ N-N preconditioner

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\[\Downarrow\]

Physical TC’s
Ventcell TC’s

Substructuring technique: \textit{Space-time interface problem}

\[\Downarrow\]

Iterative solvers (GMRES, Richardson iteration)
Time-dependent Steklov-Poincaré operator

- Dirichlet-to-Neumann operators, for $i = 1, 2$: $S_{i}^{DtN} : (\lambda, f, c_0) \mapsto (r_i \cdot n_i)|_{\Gamma}$,

where $(c_i, r_i), \ i = 1, 2$, is the solution of

\begin{align*}
\mathcal{L}(c_i, r_i) &= f, \quad \text{on } \Omega_i \times (0, T), \\
\mathcal{M}(c_i, r_i) &= 0, \quad \text{on } \Omega_i \times (0, T), \\
c_i &= \lambda, \quad \text{on } \Gamma \times (0, T), \\
c_i(\cdot, 0) &= c_0, \quad \text{in } \Omega_i.
\end{align*}
Time-dependent Steklov-Poincaré operator

- Dirichlet-to-Neumann operators, for $i = 1, 2$:
  
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  $\mathcal{L}(c_i, r_i) = f, \quad \text{on } \Omega_i \times (0, T),$
  
  $\mathcal{M}(c_i, r_i) = 0, \quad \text{on } \Omega_i \times (0, T),$
  
  $c_i = \lambda, \quad \text{on } \Gamma \times (0, T),$
  
  $c_i(\cdot, 0) = c_0, \quad \text{in } \Omega_i.$

- Space-time interface problem:

  $$S^\text{DtN}_1(\lambda, f, c_0) + S^\text{DtN}_2(\lambda, f, c_0) = 0,$$
Time-dependent Steklov-Poincaré operator

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  \[
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  \mathcal{L}(c_i, r_i) &= f, & \text{on } & \Omega_i \times (0, T), \\
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  c_i &= \lambda, & \text{on } & \Gamma \times (0, T), \\
  c_i(\cdot, 0) &= c_0, & \text{in } & \Omega_i.
  \end{align*}
  \]

- Space-time interface problem:
  \[
  S_{1}^{DtN}(\lambda, f, c_0) + S_{2}^{DtN}(\lambda, f, c_0) = 0, \\
  - \sum_{i=1}^{2} S_{i}^{DtN}(\lambda, 0, 0) = \sum_{i=1}^{2} S_{i}^{DtN}(0, f, c_0), \\
  S\lambda = \chi, \text{ on } \Gamma \times (0, T).
  \]
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  S_{1}^{DtN}(\lambda, f, c_0) + S_{2}^{DtN}(\lambda, f, c_0) = 0,
  \]
  \[
  \begin{align*}
  &- \sum_{i=1}^{2} S_{i}^{DtN}(\lambda, 0, 0) = \sum_{i=1}^{2} S_{i}^{DtN}(0, f, c_0), \\
  \implies & S\lambda = \chi, \quad \text{on } \Gamma \times (0, T).
  \end{align*}
  \]

- Neumann-Neumann preconditioner with weights:
  \[
  \left(\sigma_1 S_{1}^{NtD} + \sigma_2 S_{2}^{NtD}\right) S\lambda = \hat{\chi}, \quad \text{on } \Gamma \times (0, T),
  \]
  where \( \sigma_i : \Gamma \times (0, T) \rightarrow [0, 1] \) such that \( \sigma_1 + \sigma_2 = 1 \).
GTO Schwarz: Robin transmission conditions

- Equivalent Robin TC’s on $\Gamma \times (0, T)$: for $\alpha_1, \alpha_2 > 0$

\[
-r_1 \cdot n_1 + \alpha_1 c_1 = -r_2 \cdot n_1 + \alpha_1 c_2,
\]
\[
-r_2 \cdot n_2 + \alpha_2 c_2 = -r_1 \cdot n_2 + \alpha_2 c_1,
\]
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  \[-r_1 \cdot n_1 + \alpha_1 c_1 = -r_2 \cdot n_1 + \alpha_1 c_2,\]
  \[-r_2 \cdot n_2 + \alpha_2 c_2 = -r_1 \cdot n_2 + \alpha_2 c_1,\]

- Robin-to-Robin operators, for $i = 1, 2$ and $j = 3 - i$:
  \[S_{i}^{RtR} : (\xi_i, f, c_0) \mapsto (-r_i \cdot n_j + \alpha_j c_i) |_{\Gamma},\]

where $(c_i, r_i), \ i = 1, 2,$ is the solution of

\[
\begin{align*}
\mathcal{L}(c_i, r_i) &= f, \quad \text{on } \Omega_i \times (0, T), \\
\mathcal{M}(c_i, r_i) &= 0, \quad \text{on } \Omega_i \times (0, T), \\
-r_i \cdot n_i + \alpha_i c_i &= \xi_i, \quad \text{on } \Gamma \times (0, T), \\
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  where $(c_i, r_i), \ i = 1, 2$, is the solution of
  
  $$\mathcal{L}(c_i, r_i) = f, \quad \text{on } \Omega_i \times (0, T),$$
  $$\mathcal{M}(c_i, r_i) = 0, \quad \text{on } \Omega_i \times (0, T),$$
  $$-r_i \cdot n_i + \alpha_i c_i = \xi_i, \quad \text{on } \Gamma \times (0, T),$$
  $$c_i(\cdot, 0) = c_0, \quad \text{in } \Omega_i.$$  

- Space-time interface problem with two Lagrange multipliers:
  
  $$\xi_1 = S_2^{\text{RtR}}(\xi_2, f, c_0), \quad \text{on } \Gamma \times (0, T),$$
  $$\xi_2 = S_1^{\text{RtR}}(\xi_1, f, c_0),$$
  
  or equivalently,
  
  $$S_R \left( \begin{array}{c}
  \xi_1 \\
  \xi_2 
  \end{array} \right) = \chi_R, \quad \text{on } \Gamma \times (0, T).$$
GTO Schwarz: Ventcell transmission conditions

With sufficient regularity → equivalent Ventcell transmission conditions

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

\[
-\alpha_i c_i, \beta_i: \text{positive constants to be optimized to accelerate convergence rate.}
\]

In mixed form: introduce Lagrange multipliers on the interface, \( c_i, \Gamma \) and \( \tau_{\Gamma,i} \), for \( i = 1, 2 \):

\[
-\tau_i \cdot n_i + \alpha_i c_i, \Gamma + \beta_i (\varphi_j \partial_t c_i, \Gamma + \text{div} \tau_{\Gamma,i}) = -\tau_j \cdot n_i + \alpha_i c_j, \Gamma + \beta_i (\varphi_j \partial_t c_j, \Gamma + \text{div} \tau_{\Gamma,j}) - \text{div} \tau_{\Gamma,j} f_i, \Gamma = 0.
\]

\( c_i, \Gamma \): concentration trace on \( \Gamma \).

\( \tau_{\Gamma,i} \): NOT the tangential trace of \( \tau_i \) on \( \Gamma \times (0, T) \).
GTO Schwarz: Ventcell transmission conditions

With sufficient regularity $\rightarrow$ equivalent Ventcell transmission conditions

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

  $-r_1 \cdot n_1 + \alpha_1 c_1 + \quad = \quad -r_2 \cdot n_1 + \alpha_1 c_2 +$

  $-r_2 \cdot n_2 + \alpha_2 c_2 + \quad = \quad -r_1 \cdot n_2 + \alpha_2 c_1 +$
GTO Schwarz: Ventcell transmission conditions

With sufficient regularity → equivalent Ventcell transmission conditions

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

$$-\mathbf{r}_1 \cdot \mathbf{n}_1 + \alpha_1 c_1 + \beta_1 \left( \phi_2 \partial_t c_1 + \text{div}_\tau (-\mathbf{D}_2, \Gamma \nabla_\tau c_1) \right) = -\mathbf{r}_2 \cdot \mathbf{n}_1 + \alpha_1 c_2 + \beta_1 \left( \phi_2 \partial_t c_2 + \text{div}_\tau (-\mathbf{D}_2, \Gamma \nabla_\tau c_2) \right),$$

$$-\mathbf{r}_2 \cdot \mathbf{n}_2 + \alpha_2 c_2 + \beta_2 \left( \phi_1 \partial_t c_2 + \text{div}_\tau (-\mathbf{D}_1, \Gamma \nabla_\tau c_2) \right) = -\mathbf{r}_1 \cdot \mathbf{n}_2 + \alpha_2 c_1 + \beta_2 \left( \phi_1 \partial_t c_1 + \text{div}_\tau (-\mathbf{D}_1, \Gamma \nabla_\tau c_1) \right).$$

$\alpha_i, \beta_i$: positive constants to be optimized to accelerate convergence rate.
GTO Schwarz: Ventcell transmission conditions

With sufficient regularity → equivalent Ventcell transmission conditions

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

  \[-r_1 \cdot n_1 + \alpha_1 c_1 + \beta_1 (\phi_2 \partial_t c_1 + \text{div}_\tau (-D_{2,\Gamma} \nabla \tau c_1)) = -r_2 \cdot n_1 + \alpha_1 c_2 + \beta_1 (\phi_2 \partial_t c_2 + \text{div}_\tau (-D_{2,\Gamma} \nabla \tau c_2)), \]

  \[-r_2 \cdot n_2 + \alpha_2 c_2 + \beta_2 (\phi_1 \partial_t c_2 + \text{div}_\tau (-D_{1,\Gamma} \nabla \tau c_2)) = -r_1 \cdot n_2 + \alpha_2 c_1 + \beta_2 (\phi_1 \partial_t c_1 + \text{div}_\tau (-D_{1,\Gamma} \nabla \tau c_1)). \]

  $\rightarrow \alpha_i, \ \beta_i$: positive constants to be optimized to accelerate convergence rate.

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

  \[-r_i \cdot n_i + \alpha_i c_{i,\Gamma} + \beta_i (\phi_j \partial_t c_{i,\Gamma} + \text{div}_\tau r_{\Gamma,i}) = -r_j \cdot n_i + \alpha_i c_{j,\Gamma} + \beta_i (\phi_j \partial_t c_{j,\Gamma} + \text{div}_\tau \left(D_{j,\Gamma} D_{i,\Gamma}^{-1} r_{\Gamma,j}\right)), \]

  \[D_{j,\Gamma}^{-1} r_{\Gamma,i} + \nabla \tau c_{i,\Gamma} = 0. \]

  $c_{i,\Gamma}$: concentration trace on $\Gamma$.

  $r_{\Gamma,i} := -D_{j,\Gamma} \nabla \tau c_{i,\Gamma}$: NOT the tangential trace of $r_i$ on $\Gamma \times (0, T)$. 

Caroline Japhet (Paris13)  
Space-time DD & porous media  
Journée DDM - parallélisation  
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Nonconforming discretizations in time

Information on one time grid at the interface is passed to the other time grid at the interface using $L_2$-projections. Use an optimal projection algorithm, Gander-Japhet-Maday-Nataf (2005).


Nonconforming discretizations in time

Information on one time grid at the interface is passed to the other time grid at the interface using $L^2$-projections.

Information on one time grid at the interface is passed to the other time grid at the interface using $L^2$-projections.


Extension to advection-diffusion problems

Linear advection-diffusion equation:

\[ \phi \frac{\partial c}{\partial t} + \text{div}(uc) + \text{div} r = f \quad \text{in } \Omega \times (0, T), \]
\[ \nabla c + D^{-1}r = 0 \quad \text{in } \Omega \times (0, T), \]
\[ c = 0 \quad \text{on } \partial \Omega \times (0, T), \]
\[ c(\cdot, 0) = c_0 \quad \text{in } \Omega. \]

Operator splitting

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

⇒ 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:**
  \[
  \tilde{S}_h \left( \begin{array}{c}
  \lambda a \\
  \lambda
  \end{array} \right) = \tilde{\chi}_h , \quad \text{on} \ \Gamma \times (0, T).
  \]

  \[\Rightarrow\] Generalized Neumann-Neumann preconditioner

- **GTO Schwarz method with Robin TCs:**
  \[
  \tilde{S}_{R,h} \left( \begin{array}{c}
  \lambda a \\
  \xi_1 \\
  \xi_2
  \end{array} \right) = \tilde{\chi}_{R,h} , \quad \text{on} \ \Gamma \times (0, T).
  \]

  \[\Rightarrow\] Optimized Robin parameters for the diffusion eq. only \\
  \[\neq\] fully implicit scheme.

**Remark.** \( \lambda_a \in \Lambda_h^{N \times L} \) while \( \lambda, \xi_1, \xi_2 \in \Lambda_h^N \).
A near-field simulation

Parameters of the simulation

<table>
<thead>
<tr>
<th>Material</th>
<th>Permeability (m.s(^{-1}))</th>
<th>Porosity</th>
<th>Diffusion (m(^2). s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Host rock</td>
<td>(10^{-13})</td>
<td>0.06</td>
<td>(6 \times 10^{-13})</td>
</tr>
<tr>
<td>EDZ</td>
<td>(5 \times 10^{-11})</td>
<td>0.2</td>
<td>(2 \times 10^{-11})</td>
</tr>
<tr>
<td>Vitrified waste</td>
<td>(10^{-8})</td>
<td>0.1</td>
<td>(10^{-11})</td>
</tr>
</tbody>
</table>
Advection-diffusion problems

Numerical results

Advection field: Darcy flow

\[
\begin{align*}
\text{div } u &= 0 \quad \text{in } \Omega, \\
u &= -K \nabla p \quad \text{in } \Omega.
\end{align*}
\]

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: $T_f = 2 \times 10^{11}$ s ($\approx 20000$ years)
  $\longrightarrow$ 200 time windows with size $T = 10^9$ s.
- Decomposition into 9 subdomains.
- Nonconforming time grids:
  - Diffusion step:
    \[
    \Delta t_i = \frac{T}{500}, \quad i = 5, \\
    \Delta t_i = \frac{T}{100}, \quad i \neq 5.
    \]
  - Diffusion-dominated: $\text{Pe}_L \leq 0.0513$
  $\longrightarrow \Delta t_{a,i} = \Delta t_i$.
- Non-uniform mesh in space: uniform mesh in the repository (10 by 10), then progressively coarser with a factor of 1.05.
Performance of one time window

Convergence with GMRES

Error in $c$ with nonconforming time grids.

Error in $r$ 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: $\Delta t_i = T/100, \forall i$
1. Introduction

2. Pure diffusion problems
   - Multi-domain mixed formulations
   - Nonconforming discretizations in time

3. Advection-diffusion problems
   - Operator splitting
   - Numerical results

4. Extension to reduced fracture models
A reduced model: interface-fracture

Martin-Jaffré-Roberts (2005)
Knabner-Roberts (2014) (Forchheimer flow)

In this work: assume that $D/\delta$ large
⇒ concentration continuity across the fracture

In the subdomains

$$
\begin{align*}
\phi_i \partial_t c_i + \text{div} \ r_i &= f_i \quad &\text{in } \Omega_i \times (0, T), \\
\ r_i &= -D_i \nabla c_i \quad &\text{in } \Omega_i \times (0, T), \\
\ c_i &= 0 \quad &\text{on } \partial \Omega_i \cap \partial \Omega \times (0, T), \quad \text{for } i = 1, 2, \\
\ c_i &= c_\gamma \quad &\text{on } \gamma \times (0, T), \\
\ c_i(\cdot, 0) &= c_{0,i} \quad &\text{in } \Omega_i,
\end{align*}
$$
A reduced model: interface-fracture

Martin-Jaffré-Roberts (2005)
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In this work: assume that $D/\delta$ large
⇒ concentration continuity across the fracture

In the subdomains

$$\phi_i \partial_t c_i + \text{div} \: r_i = f_i \quad \text{in } \Omega_i \times (0, T),$$
$$r_i = -D_i \nabla c_i \quad \text{in } \Omega_i \times (0, T),$$
$$c_i = 0 \quad \text{on } \partial \Omega_i \cap \partial \Omega \times (0, T), \quad \text{for } i = 1, 2,$$
$$c_i(\cdot, 0) = c_{0,i} \quad \text{in } \Omega_i,$$

and in the fracture

$$\phi_\gamma \partial_t c_\gamma + \text{div}_\tau r_\gamma = f_\gamma + (r_1 \cdot n_1|_\gamma + r_2 \cdot n_2|_\gamma) \quad \text{in } \gamma \times (0, T),$$
$$r_\gamma = -D_\gamma \delta \nabla c_\gamma \quad \text{in } \gamma \times (0, T),$$
$$c_\gamma = 0 \quad \text{on } \partial \gamma \times (0, T),$$
$$c_\gamma(\cdot, 0) = c_{0,\gamma} \quad \text{in } \gamma.$$

⇒ 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 \( i = 1, 2 \):

\[
S^\text{DtN}_i : (\lambda, f, c_0) \mapsto (r_i \cdot n_i)|_{\Gamma},
\]

where \((c_i, r_i), \ i = 1, 2,\) is the solution of

\[
\begin{align*}
\mathcal{L}(c_i, r_i) &= f, \quad \text{in } \Omega_i \times (0, T), \\
\mathcal{M}(c_i, r_i) &= 0, \quad \text{in } \Omega_i \times (0, T), \\
c_i &= \lambda, \quad \text{on } \gamma \times (0, T), \\
c_i(\cdot, 0) &= c_0, \quad \text{in } \Omega_i.
\end{align*}
\]
Formulation as an interface problem (GTP Schur)

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

$$S^\text{DtN}_i : (\lambda, f, c_0) \mapsto (r_i \cdot n_i)_{|\Gamma},$$

where $(c_i, r_i), \ i = 1, 2,$ is the solution of

$$\begin{align*}
L(c_i, r_i) &= f, \quad \text{in } \Omega_i \times (0, T), \\
M(c_i, r_i) &= 0, \quad \text{in } \Omega_i \times (0, T), \\
c_i &= \lambda, \quad \text{on } \gamma \times (0, T), \\
c_i(\cdot, 0) &= c_0, \quad \text{in } \Omega_i.
\end{align*}$$

Different space-time interface problem: instead of

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

$$\upharpoonright \quad S\lambda = \chi, \quad \text{on } \gamma \times (0, T).$$
The same (as with simple DD) Dirichlet-to-Neumann operators, for \( i = 1, 2 \):

\[
S_i^{DtN} : (\lambda, f, c_0) \mapsto (r_i \cdot n_i)|_{\Gamma},
\]

where \((c_i, r_i), i = 1, 2\), is the solution of

\[
\begin{align*}
\mathcal{L}(c_i, r_i) &= f, & \text{in } \Omega_i \times (0, T), \\
\mathcal{M}(c_i, r_i) &= 0, & \text{in } \Omega_i \times (0, T), \\
c_i &= \lambda, & \text{on } \gamma \times (0, T), \\
c_i(\cdot, 0) &= c_0, & \text{in } \Omega_i.
\end{align*}
\]

Different space-time interface problem:

\[
\begin{align*}
\mathcal{L}_\gamma(\lambda, r_\gamma) + S\lambda &= \chi + f_\gamma, & \text{in } \gamma \times (0, T), \\
\mathcal{M}_\gamma(\lambda, r_\gamma) &= 0, & \text{in } \gamma \times (0, T), \\
\lambda(\cdot, 0) &= c_{0,\gamma}, & \text{in } \gamma.
\end{align*}
\]
Formulation as an interface problem (GTP Schur)

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

\[
S^D_{\text{DtN}}: (\lambda, f, c_0) \mapsto (r_i \cdot n_i)_{|\Gamma},
\]

where \((c_i, r_i), \ i = 1, 2\), is the solution of

\[
\mathcal{L}(c_i, r_i) = f, \quad \text{in } \Omega_i \times (0, T),
\]

\[
\mathcal{M}(c_i, r_i) = 0, \quad \text{in } \Omega_i \times (0, T),
\]

\[
c_i = \lambda, \quad \text{on } \gamma \times (0, T),
\]

\[
c_i(\cdot, 0) = c_0, \quad \text{in } \Omega_i.
\]

Different space-time interface problem:

\[
\mathcal{L}_{\gamma}(\lambda, r_\gamma) + S\lambda = \chi + f_\gamma, \quad \text{in } \gamma \times (0, T),
\]

\[
\mathcal{M}_{\gamma}(\lambda, r_\gamma) = 0 \quad \text{in } \gamma \times (0, T),
\]

\[
\lambda(\cdot, 0) = c_{0,\gamma}, \quad \text{in } \gamma.
\]

Two possible preconditionners:

- a Neumann-Neumann preconditionner with weights
Formulation as an interface problem (GTP Schur)

- The same (as with simple DD) Dirichlet-to-Neumann operators, for \( i = 1, 2 \):
  \[
  S_i^{DtN} : (\lambda, f, c_0) \mapsto (r_i \cdot n_i)|_\Gamma,
  \]
  where \((c_i, r_i), \ i = 1, 2\), is the solution of

  \[
  \begin{align*}
  \mathcal{L}(c_i, r_i) &= f, \quad \text{in } \Omega_i \times (0, T), \\
  \mathcal{M}(c_i, r_i) &= 0, \quad \text{in } \Omega_i \times (0, T), \\
  c_i &= \lambda, \quad \text{on } \gamma \times (0, T), \\
  c_i(\cdot, 0) &= c_0, \quad \text{in } \Omega_i.
  \end{align*}
  \]

- Different space-time interface problem:

  \[
  \begin{align*}
  \mathcal{L}_\gamma(\lambda, r_\gamma) + S\lambda &= \chi + f_\gamma, \quad \text{in } \gamma \times (0, T), \\
  \mathcal{M}_\gamma(\lambda, r_\gamma) &= 0 \quad \text{in } \gamma \times (0, T), \\
  \lambda(\cdot, 0) &= c_{0,\gamma}, \quad \text{in } \gamma.
  \end{align*}
  \]

- Two possible preconditioners:
  - a Neumann-Neumann preconditionner with weights
  - a local preconditioner (coming from the observation that the interface problem is dominated by the 2nd order operator)
Transmission conditions for a GTO Schwarz method

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

\[-r_1 \cdot n_1 + \alpha_1 c_{1,\gamma} + \phi_\gamma \partial_t c_{i,\gamma} + \text{div}_\tau r_{\gamma,1} = -r_2 \cdot n_1 + \alpha_1 c_{2,\gamma} + f_\gamma\]
\[r_{\gamma,1} = -D_\gamma \delta \nabla_\tau c_{1,\gamma}\]

\[-r_2 \cdot n_2 + \alpha_2 c_{2,\gamma} + \phi_\gamma \partial_t c_{2,\gamma} + \text{div}_\tau r_{\gamma,2} = -r_1 \cdot n_2 + \alpha_2 c_{1,\gamma} + f_\gamma\]
\[r_{\gamma,2} = -D_\gamma \delta \nabla_\tau c_{2,\gamma}\]
We use Ventcell to Robin operators, for $i = 1, 2$:

$$S_i^{VtR} : (\theta_i, f, c_0, f_{\gamma}, c_{0,\gamma}) \mapsto (-r_i \cdot n_j + \alpha c_i)|\Gamma,$$

where $(c_i, r_i, c_{i,\gamma}, r_{\gamma,i})$, $i = 1, 2$, is the solution of

$$\mathcal{L}(c_i, r_i) = f, \quad \text{in } \Omega_i \times (0, T),$$

$$\mathcal{M}(c_i, r_i) = 0, \quad \text{in } \Omega_i \times (0, T),$$

$$-r_i \cdot n_i + \alpha c_{i,\gamma} + \phi_{\gamma} \partial_t c_{i,\gamma} + \text{div}_\tau r_{\gamma,i} = \theta_i, \quad \text{on } \gamma \times (0, T),$$

$$r_{\gamma,i} + D_{\gamma} \delta \nabla_\tau c_{i,\gamma} = 0, \quad \text{on } \gamma \times (0, T),$$

$$c_i(\cdot, 0) = c_0, \quad \text{in } \Omega_i$$

$$c_{i,\gamma}(\cdot, 0) = c_{0,\gamma}, \quad \text{in } \gamma.$$
Formulation as an interface problem (GTO Schwarz)

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

$$S_i^{VtR} : (\theta_i, f, c_0, f_\gamma, c_{0,\gamma}) \mapsto (-r_i \cdot n_j + \alpha c_i)|_{\Gamma},$$

where $(c_i, r_i, c_{i,\gamma}, r_{\gamma,i})$, $i = 1, 2$, is the solution of

- $\mathcal{L}(c_i, r_i) = f$, in $\Omega_i \times (0, T)$,
- $\mathcal{M}(c_i, r_i) = 0$, in $\Omega_i \times (0, T)$,
- $-r_i \cdot n_i + \alpha c_{i,\gamma} + \phi_\gamma \partial_t c_{i,\gamma} + \text{div}_\tau r_{\gamma,i} = \theta_i$, on $\gamma \times (0, T)$,
- $r_{\gamma,i} + D_\gamma \delta \nabla_\tau c_{i,\gamma} = 0$, on $\gamma \times (0, T)$,
- $c_i(\cdot, 0) = c_0$, in $\Omega_i$
- $c_{i,\gamma}(\cdot, 0) = c_{0,\gamma}$, in $\gamma$.

Space-time interface problem:

$$\theta_1 = S_2^{VtR}(\theta_2, f, c_0, f_\gamma, c_{0,\gamma}) + f_\gamma, \quad \text{on } \gamma \times (0, T),$$
$$\theta_2 = S_1^{VtR}(\theta_1, f, c_0, f_\gamma, c_{0,\gamma}) + f_\gamma, \quad \text{on } \gamma \times (0, T).$$
Numerical results

Geometry and boundary conditions.

- Isotropic coefficients: $D_i = 1$, $i = 1, 2$, and $D_\gamma = 1/\delta = 1000$. 

Numerical results

Geometry and boundary conditions.

- Isotropic coefficients: $D_i = 1$, $i = 1, 2$, and $D_\gamma = 1/\delta = 1000$.
- Zero source terms and initial condition.
- Spatial discretization: uniform rectangular mesh $h = 1/100$ → 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 $c$

$t = \Delta t$

$t = T/4$

$t = T/2$

$t = T$
Snapshots of solution - diffusive flux $r$

$t = \Delta t$

$t = T/4$

$t = T/2$

$t = T$
Convergence - GMRES

- L² concentration errors (c)
- L² flux errors (r)
- L² error versus α

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

- Coupling with advection in the fractures: the GTO Schwarz gives a rather remarkable convergence speed. With an explicit time scheme for advection, using smaller time steps in the fracture avoid imposing a time step in the two subdomains dictated by the CFL number of the equation in the fracture.

- Develop stopping criteria to stop the DD iterations as soon as the discretization error is reached, with a posteriori estimates (with Sarah Ali Hassan (PhD), Martin Vohralík & Michel Kern).