Time Space Domain Decomposition Methods for Reactive Transport

Application to CO$_2$ Geological Storage

Florian Haeberlein

Ph. D. Supervisor: Laurence Halpern
Scientific Supervisor: Anthony Michel
Outline

- Context — Problems and Challenges
- Linear Coupled Two Species System
- Nonlinear Coupled Two Species System
- Nonlinear Coupled Multispecies System
- Conclusion and Perspectives
Physical and chemical phenomena:

- $\text{CO}_2$ dissolves partially in water and changes pH
- Acid water attacks rock matrix
- Change in geophysical properties has impact on Darcy flow
Challenges in Reactive Transport Numerical Simulation

Physical challenges:
- Large domains and long simulation times
- Strong heterogeneity in time and space
- Occurring effects on different time scales
- Many chemical species (mobile and fixed)

Numerical challenges:
- Large coupled systems
- Strong nonlinearities
Existing Approaches for Reactive Transport

- **Splitting methods:**
  - Highly developed solvers for subproblems
  - Poor performance for long-term simulations with strong chemistry
    - local time-stepping for pure advective cases

- **Global Implicit Approach:**
  - High-performing approaches for long-term simulation
    - Different formulations
    - local time-stepping not yet developed
Approach in this Work

Reactive Transport Model
- Global implicit approach
- Multispecies reactive transport
- Global-DAE formulation [Amir, Dieuleveult, Erhel, Kern] extended to kinetic reactions and mineral species

Domain Decomposition Approach
- Schwarz Waveform Relaxation (SWR)
- Localising heterogeneity affecting the performance of the non-linear solver
- Individual per subdomain time-stepping
Global Problem in $\Omega \times [0, T]$
Classical Strategy for Time-Dependant Problems

\[ \Omega_1 \times [0, T] \]

\[ \Omega_2 \]

\[ \Delta t \]
SWR
Schwarz Waveform Relaxation
Numerical Discretisation Using DD in the FV Context

- Implicit Euler method in time

- Hybrid Finite Volume scheme in space [Eymard, Gallouët, Herbin]

- Projection algorithm in space and time [Achdou, Japhet, Maday, Nataf], [Gander, Japhet]

- Numerical study of the influence of projections
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■ Context — Problems and Challenges
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The Coupled System

\[
\phi \partial_t u + \text{div}(-a \vec{\nabla} u + \vec{b} u) - k(v - cu) = 0 \quad \text{on } \Omega \times (0, T)
\]
\[
\phi \partial_t v + k(v - cu) = 0 \quad \text{on } \Omega \times (0, T)
\]

\(u\): Mobile species
\(v\): Fixed species

\(\phi\): Porosity
\(a\): Scalar diffusion coefficient
\(\vec{b}\): Darcy field
\(k\): Reaction rate coefficient
\(c\): Equilibrium constant
SWR Algorithm for the Coupled System

\[
\phi \partial_t u_1^{k+1} + \mathcal{L}(u_1^{k+1}) - k(v_1^{k+1} - c u_1^{k+1}) = 0 \quad \text{on } \Omega_1 \times (0, T)
\]
\[
\phi \partial_t v_1^{k+1} + k(v_1^{k+1} - c u_1^{k+1}) = 0 \quad \text{on } \Omega_1 \times (0, T)
\]
\[
(u_1^{k+1}(x, 0), v_1^{k+1}(x, 0)) = (u_0, v_0) \quad \text{on } \Omega_1
\]
B. C.
\[
\mathcal{B}_1 \left( u_1^{k+1}, v_1^{k+1} \right) = \mathcal{B}_1 \left( u_1^k, v_1^k \right) \quad \text{on } \Gamma_1 \times (0, T)
\]

\[
\phi \partial_t u_2^{k+1} + \mathcal{L}(u_2^{k+1}) - k(v_2^{k+1} - c u_2^{k+1}) = 0 \quad \text{on } \Omega_2 \times (0, T)
\]
\[
\phi \partial_t v_2^{k+1} + k(v_2^{k+1} - c u_2^{k+1}) = 0 \quad \text{on } \Omega_2 \times (0, T)
\]
\[
(u_2^{k+1}(x, 0), v_2^{k+1}(x, 0)) = (u_0, v_0) \quad \text{on } \Omega_2
\]
B. C.
\[
\mathcal{B}_2 \left( u_2^{k+1}, v_2^{k+1} \right) = \mathcal{B}_2 \left( u_2^k, v_2^k \right) \quad \text{on } \Gamma_2 \times (0, T)
\]
Evolution from Scalar Equation to Coupled System

Scalar equation:

\[ \phi \frac{\partial}{\partial t} u + \text{div}(-a \vec{\nabla} u + \vec{b} u) - cu = 0 \quad \text{on } \Omega \times (0, T) \]


Coupled system:

\[ \phi \frac{\partial}{\partial t} u + \text{div}(-a \vec{\nabla} u + \vec{b} u) - k(v - cu) = 0 \quad \text{on } \Omega \times (0, T) \]
\[ \phi \frac{\partial}{\partial t} v + k(v - cu) = 0 \quad \text{on } \Omega \times (0, T) \]
Well-posedness of the SWR Algorithm

- Well-posedness (energy estimates, Galerkin method)
  - Global problem
  - Sub-Problems using Robin/Ventcel conditions
  - SWR algorithm with different transmission conditions \( L \geq 0 \)

**Theorem**

Let \( p > 0 \) be given and \( L > 0 \). If \((u_0, v_0) \in H^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)\) and \( g_{b_i}^0 \in H^{\frac{1}{4}}(0, T; L^2(\Gamma_i)) \cap L^2(0, T; H^{\frac{1}{2}}(\Gamma_i)), i = 1, 2, \) are given, then the SWR algorithm with the transmission operators defined by

\[
B_1(u, v) = \frac{\partial u}{\partial n_1} - \frac{b_x - p}{2a} u, \quad B_2(u, v) = \frac{\partial u}{\partial n_2} + \frac{b_x + p}{2a} u,
\]

defines a unique sequence of iterates \(((u_1^k, v_1^k), (u_2^k, v_2^k))\) such that

\[
u_i^k \in L^2(0, T; H^2(\Omega_i)) \cap H^1(0, T; L^2(\Omega_i)), \quad v_i^k \in H^1(0, T; L^2(\Omega_i)), \quad i \in \{1, 2\}.
\]
Convergence of the SWR Algorithm

- Convergence and convergence factor of the SWR algorithm with different transmission conditions with/without overlap (energy estimates, Fourier transform)

Theorem

Let $L > 0$ and suppose that the advection speed $b$ is such that $b_x \neq 0$. Let $p > 0$. Then the sequence $((u^k_1, v^k_1), (u^k_2, v^k_2))$ defined by the SWR algorithm with Robin transmission operators converges to $((u, v)|_{\Omega_1}, (u, v)|_{\Omega_2})$, in $\prod_{i=1}^{2} (L^2(0, T; L^2(\Omega_i))) \times L^2(0, T; L^2(\Omega_i)))$ for $k \to \infty$. 
Convergence of the SWR Algorithm

![Graph showing convergence of the SWR Algorithm with different boundary conditions: Dirichlet overlap dx, Optimised Robin no overlap, Optimised Robin overlap dx, Optimised Ventcel no overlap, and Optimised Ventcel overlap dx. The graph plots interface error against iteration number, with error decreasing significantly with each iteration.]
Optimised Transmission Conditions

- Numerical optimisation of parameters: Comparison between scalar adv.-diff. equation and coupled system
  - Parameters of scalar advection-diffusion equation applicable even for strong chemistry (Ventcel 1D; Robin and Ventcel in 2D, 3D)
  - Significant differences for Robin in 1D

![Graph showing error after 10 iterations and optimised parameters for adv−diff−reaction and adv−diff]
Analytical Formula for Optimised Parameter in 1D

- Analytical solution for Robin without overlap in 1D following [Bennequin, Gander, Halpern 2009]

\[ p^* = \sqrt{2\Re \left( \sqrt{b_X^2 + 4ad(\tau_m)} \right) \Re \left( \sqrt{b_X^2 + 4ad(\tau_M)} \right)}, \quad d(\tau) = \phi i\tau - \frac{k^2 c}{\phi i\tau + k} + kc \]
Application of 1D Parameter in 2D/3D cases

- Localised strategy in 2D/3D for advection-dominant cases:
  \[ \rho = \text{const} \implies \rho(x) \text{ on } \Gamma \]
  1D optimisation or Taylor approximation on every face

![Graph showing interface error over iterations for constant and local parameters](image-url)
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The Nonlinear Coupled System

\[\phi \partial_t u + \text{div}(\vec{a} \vec{\nabla} u + \vec{b} u) - R(u, v) = 0 \quad \text{on } \Omega \times (0, T)\]

\[\phi \partial_t v + R(u, v) = 0 \quad \text{on } \Omega \times (0, T)\]

\[R : \mathbb{R}^2 \rightarrow \mathbb{R} \text{ nonlinear function}\]
Optimised Transmission Conditions

- Robin transmission condition
  - Realisation as in the linear cases
  - Accordance of optimised parameter with linear case

BET Isotherm

\[ R(u, v) = \exp(10(2v - 3u)) - 1 \]
Mixing Newton and SWR

1. Classical approach:
   - Fixpoint \((\text{SWR ( NLPb)})\)
   - Nonlinear subproblems at every iteration

2. Nested Iteration Approach (NIA):
   - Newton-Krylov \((\text{SWR ( NLPb)})\)
   - Linearised problems for Jacobian evaluation
   - Nonlinear problems for residual evaluation

3. Common Iteration Approach (CIA):
   - Krylov-SWR \((\text{Newton ( NLPb)})\)
   - Linearised problems for Jacobian evaluation
   - Linearised problems for residual evaluation

[Haeberlein, Halpern, Michel, DD20, 2011, submitted]
Mixing Newton and SWR

Numerical Results

+ Easy to add to standard approach
+ Accelerating properties
Mixing Newton and SWR Numerical Results

- Easy to add to standard approach
- Accelerating properties
Mixing Newton and SWR Numerical Results

+ Easy to add to standard approach
+ Accelerating properties

![Graph showing numerical results](graph.png)

Number of grid cells per dimension, \( N_x = N_y \)

- Classical Approach: \( O(N^{1/2.75}) \)
- Nested Iteration Approach: \( O(N^{1/7}) \)
- Common Iteration Approach: \( O(N^{1/7}) \)
Mixing Newton and SWR

Numerical Results

+ Easy to add to standard approach
+ Accelerating properties

<table>
<thead>
<tr>
<th>Number of matrix inversions</th>
<th>Stopping criterion</th>
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<tr>
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<td>$10^0$</td>
</tr>
<tr>
<td>500</td>
<td>$10^{-5}$</td>
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<td>$10^{-10}$</td>
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<td>1500</td>
<td>$10^{-15}$</td>
</tr>
<tr>
<td>2000</td>
<td>$10^{-20}$</td>
</tr>
</tbody>
</table>

Classical Approach
Nested Iteration Approach
Common Iteration Approach
Mixing Newton and SWR

Numerical Results

+ Easy to add to standard approach
+ Accelerating properties

- Needs adaptive strategy for linear solver to be performant
- Overhead cost for coarse discretisation $\Rightarrow$ No acceleration
- Storage cost for CIA
- Dependence of the performance on the character of the test case
Performance Results for Nonlinear Two Species System

- Advection-dominant cases
- Time-space localisation of chemical disequilibria
- Overlap
- Taylor approximation for Robin condition
- Initial state as guess for SWR

$\Rightarrow \approx 3$ SWR iterations.

- Isolation of disequilibria in separate subdomain $m(\Omega_R) \leq 0.3 \cdot m(\Omega)$
- Different time steps in subdomains $3\Delta t_R \leq \Delta t_{NR}$

$\Rightarrow \approx 20\%$ gain in CPU time.
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The Treated Problem
Phases and Species

mobile phase

fixed phases

sorbed phase

mineral phases

$c_1$

$x_1$

$c_2$

$x_2$

$s_1$

$s_2$

$y_1$

$q_1$

$q_2$

$z_1$
Equilibrium reactions are represented by a Morel tableau:

<table>
<thead>
<tr>
<th></th>
<th>$c$</th>
<th>$s$</th>
<th>$q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c$</td>
<td>$ld$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$s$</td>
<td></td>
<td>$ld$</td>
<td></td>
</tr>
<tr>
<td>$q$</td>
<td></td>
<td></td>
<td>$ld$</td>
</tr>
<tr>
<td>$x$</td>
<td>$S_c^x$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$y$</td>
<td>$S_c^y$</td>
<td>$S_s^y$</td>
<td></td>
</tr>
<tr>
<td>$z$</td>
<td>$S_c^z$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Ideal activity model: $a_i = c_i$. 
The Treated Problem

The Chemical Flash

\[ \theta_w c + \theta_w (S_c^x)^t x + \theta_s (S_c^y)^t y + (S_c^z)^t (\theta_z \cdot z) = T, \]
\[ \theta_s s + \theta_s (S_s^y)^t y = W, \]
\[ \theta_q \cdot q = Q, \]
\[ \ln(a_x) - (S_c^x) \ln(a_c) = \ln K_x, \]
\[ \ln(a_y) - (S_c^y) \ln(a_c) - (S_s^y) \ln(a_s) = \ln K_y, \]
\[ \ln(a_z) - (S_c^z) \ln(a_c) = \ln K_z, \]
\[ \sum_{i=1}^{N_c} c_i + \sum_{i=1}^{N_x} x_i = 1, \quad \text{(mobile phase)}, \]
\[ \sum_{i=1}^{N_s} s_i + \sum_{i=1}^{N_y} y_i = 1, \quad \text{(sorbed phase, if present)}, \]
\[ q_i = 1, \quad i = 1, \ldots, N_q, \]
\[ z_i = 1, \quad i = 1, \ldots, N_z. \]
The Treated Problem
Total Component RT Problem

\[ \partial_t (\phi C) + \partial_t (\phi F) + \mathcal{L}(C) + R_{T,\text{kin}} = 0 \] (#C),

\[ \partial_t W + R_{W,\text{kin}} = 0 \] (#W),

\[ \partial_t Q + R_{Q,\text{kin}} = 0 \] (#Q),

\[ T - \phi C - \phi F = 0 \] (#T),

\[ \phi F - \Psi(T, W, Q) = 0 \] (#F),

\[ R_{T,\text{kin}} - \Theta(T, W, Q) = 0 \] (#R_{T,\text{kin}}),

\[ R_{W,\text{kin}} - \Upsilon(T, W, Q) = 0 \] (#R_{W,\text{kin}}),

\[ R_{Q,\text{kin}} - \Xi(T, W, Q) = 0 \] (#R_{Q,\text{kin}}).
Numerical Approach for Reactive Transport Problem

- Adaptive time stepping strategy
- Hybrid finite volume scheme in space and implicit Euler in time discretisation
- Global Implicit Approach
- Solve complementary condition in algebraic equivalent version by semi-smooth Newton method [Hoffmann, Knabner, Kräutle]
  - prevent from negative concentrations for mineral species in global problem
  - manage disappearing mineral phases in local problem
Numerical Results
Cement Attack by CO$_2$

image source: Princeton University

image sources: Thesis Th. Millan,
IFP EN - Ecole des Mines de St Etienne
Numerical Results
Cement Attack by CO$_2$

image sources: Thesis Th. Millan, IFP EN - Ecole des Mines de St Etienne
Numerical Results
Cement Attack by CO$_2$

Mobile species: H$_2$O, tracer, CO$_2$(aq), CaO(aq), SiO$_2$(aq)
Mineral species: Calcite, Wollastonite, Portlandite, Silica

Kinetic reactions:
- Portlandite Dissolution: Portlandite + CO$_2$(aq) $\rightarrow$ Calcite
- Wollastonite Dissolution: Wollastonite + CO$_2$(aq) $\rightarrow$ CaO(aq) + Silica
- Calcite Precipitation: CaO(aq) + CO$_2$(aq) $\rightarrow$ Calcite
- Silica Dissolution: Silica + CaO(aq) $\rightarrow$ SiO$_2$(aq)
Numerical Results
Cement Attack by CO$_2$
Numerical Results
Cement Attack by CO$_2$
Numerical Results
Cement Attack by CO$_2$
Numerical Results
SHPCO2 Test Case

Injector 1
Productor
Injector 2
Numerical Results
SHPCO2 Test Case

Water
Salt
Carbonates
Silicates

H₂O
H⁺ OH⁻
Na⁺
Cl⁻ HCO₃⁻
Ca²⁺

CO₂(g)

SiO₂(aq)

CO₂(aq)

Calcite

Quartz

Tracer

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Numerical Results
SHPCO2 Test Case

Primary species:
\[
c = \begin{pmatrix}
c_1 \\
c_2 \\
c_3 \\
c_4 \\
c_5 \\
c_6 \\
c_7 \\
c_8 \\
\end{pmatrix} = \begin{pmatrix}
\text{H}_2\text{O} \\
\text{Tracer} \\
\text{CO}_2(\text{aq}) \\
\text{Cl}^- \\
\text{H}^+ \\
\text{Na}^+ \\
\text{Ca}^{++} \\
\text{SiO}_2(\text{aq}) \\
\end{pmatrix}
\]

Secondary species:
\[
x = \begin{pmatrix}
x_1 \\
x_2 \\
\end{pmatrix} = \begin{pmatrix}
\text{HCO}_3^- \\
\text{OH}^- \\
\end{pmatrix}
\]

\[
q = \begin{pmatrix}
q_1 \\
q_2 \\
\end{pmatrix} = \begin{pmatrix}
\text{Calcite} \\
\text{Quartz} \\
\end{pmatrix}
\]

\[
z = \begin{pmatrix}
z_1 \\
\end{pmatrix} = \begin{pmatrix}
\text{CO}_2(\text{solid}) \\
\end{pmatrix}
\]
Numerical Results
SHPCO2 Test Case

Equilibrium reactions:

- $\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$
- $\text{CO}_2(\text{g}) \rightleftharpoons \text{CO}_2(\text{aq})$
- $\text{H}_2\text{O} + \text{CO}_2(\text{aq}) \rightleftharpoons \text{HCO}_3^- + \text{H}^+$

Kinetic reactions:

- Calcite + $\text{H}^+$ $\rightleftharpoons$ Ca$^{++}$ + HCO$_3^-$
- Quartz $\rightleftharpoons$ SiO$_2$(aq)
Numerical Results
SHPCO2 Test Case
Numerical Results
SHPCO2 Test Case
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Conclusion:

- Application of previously developed theory and techniques to a coupled system
- Confirmation of results similar to scalar equations
  - Only optimised parameters offer fast convergence
  - Good accordance between theory and numerics

Perspectives:

- Optimised transmission conditions
  - for unknown temporal discretisation and
  - in the nonlinear case
- Comparative numerical tests for different proposed Ventcel conditions in the nonlinear case
Conclusion:
- Two new numerical approaches developed
- Tested with success on nonlinear coupled system
  - Accelerating properties
  - Less sensibility to transmission condition parameter
  - Better asymptotic behaviour

Perspectives:
- More tests on other types of equations and other test cases
- Investigation for eliminating overhead cost
Multispecies RT Formulation and DD Approach

Conclusion:
- Extension of existing formulation to kinetic reactions and minerals
- First approach of domain decomposition on nonlinear coupled multispecies reactive transport systems

Perspectives:
- Study of numerical formulation (stability, conditioning,...)
- Study of well-posedness of multispecies reactive transport formulation with given boundary data by domain decomposition algorithm
Limiting of Kinetic Reaction Rates

\[ M \rightarrow A + B, \text{ reaction rate } k > 0 \]

\[
\frac{M^{n+1} - M^n}{\Delta t} + k = 0 \quad \text{if } M^{n+1} \geq 0
\]

\[ M^{n+1} = 0 \quad \text{else} \]

\[
\frac{M^{n+1} - M^n}{\Delta t} + \min \left\{ k, \frac{M^n}{\Delta t} \right\} = 0.
\]
Mineral Equilibrium Limiting

\[
\ln(a_z) - (S^z_c) \ln(a_c) - \ln K_z \bigg|_i = 0 \quad \text{if mineral phase } i \text{ is present}
\]

\[
\theta_{z_i} = 0 \quad \text{if mineral phase } i \text{ is not present}
\]

\[
f := \ln(a_z) - (S^z_c) \ln(a_c) - \ln K_z
\]

\[
\varphi(f, \theta_{z_i}) = f + \theta_{z_i} - \sqrt{f^2 + (\theta_{z_i})^2} = 0
\]