

Time Space Domain Decomposition Methods for Reactive Transport *Application to CO₂ Geological Storage*

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Outline

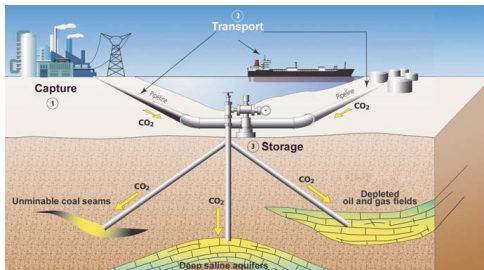


- Context — Problems and Challenges
- Linear Coupled Two Species System
- Nonlinear Coupled Two Species System
- Nonlinear Coupled Multispecies System
- Conclusion and Perspectives

CCS

Carbon Capture and Storage

Technical process:



Physical and chemical phenomena:

- CO₂ 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
 - o local time-stepping for pure advective cases

- Global Implicit Approach:
 - + High-performing approaches for long-term simulation
 - o Different formulations
 - o local time-stepping not yet developed

Approach in this Work



Reactive Transport Model

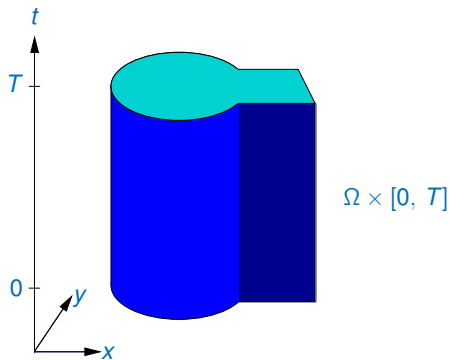
- Global implicit approach
- Multispecies reactive transport
- Global-DAE formulation [Amir, Dieuleveult, Erhel, Kern] extended to kinetic reactions and mineral species

Domain Decomposition Approach

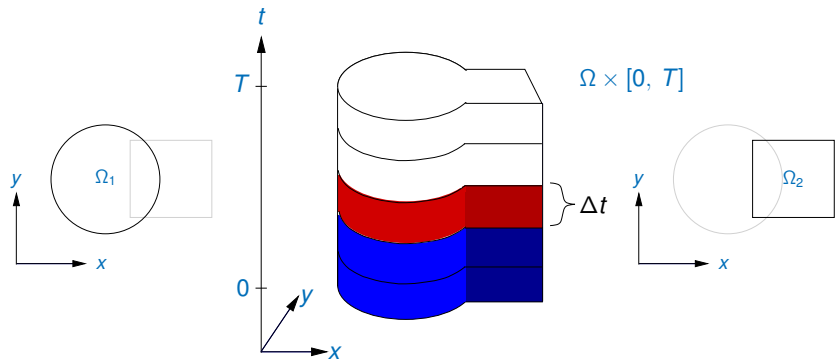
- Schwarz Waveform Relaxation (SWR)
- Localising heterogeneity affecting the performance of the non-linear solver
- Individual per subdomain time-stepping



Global Problem in $\Omega \times [0, T]$

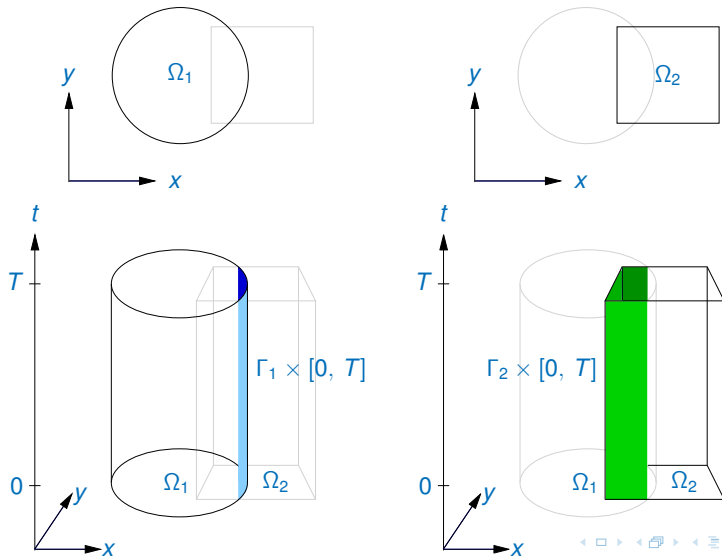


Classical Strategy for Time-Dependant Problems



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

Outline



- Context — Problems and Challenges
- **Linear Coupled Two Species System**
- Nonlinear Coupled Two Species System
- Nonlinear Coupled Multispecies System
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The Coupled System

$$\begin{aligned} \phi \partial_t u + \operatorname{div}(-a \vec{\nabla} u + \vec{b} u) - k(v - cu) &= 0 & \text{on } \Omega \times (0, T) \\ \phi \partial_t v &+ k(v - cu) = 0 & \text{on } \Omega \times (0, T) \end{aligned}$$

u : Mobile species

v : Fixed species

ϕ : Porosity

a : Scalar diffusion coefficient

\vec{b} : Darcy field

k : Reaction rate coefficient

c : Equilibrium constant

SWR Algorithm for the Coupled System



$$\begin{aligned} \phi \partial_t u_1^{k+1} + \mathcal{L}(u_1^{k+1}) - k(v_1^{k+1} - cu_1^{k+1}) &= 0 && \text{on } \Omega_1 \times (0, T) \\ \phi \partial_t v_1^{k+1} + k(v_1^{k+1} - cu_1^{k+1}) &= 0 && \text{on } \Omega_1 \times (0, T) \\ (u_1^{k+1}(x, 0), v_1^{k+1}(x, 0)) &= (u_0, v_0) && \text{on } \Omega_1 \\ \text{B. C.} &&& \text{on } \partial\Omega \cap \partial\Omega_1 \times (0, T) \\ \mathcal{B}_1(u_1^{k+1}, v_1^{k+1}) &= \mathcal{B}_1(u_2^k, v_2^k) && \text{on } \Gamma_1 \times (0, T) \end{aligned}$$

$$\begin{aligned} \phi \partial_t u_2^{k+1} + \mathcal{L}(u_2^{k+1}) - k(v_2^{k+1} - cu_2^{k+1}) &= 0 && \text{on } \Omega_2 \times (0, T) \\ \phi \partial_t v_2^{k+1} + k(v_2^{k+1} - cu_2^{k+1}) &= 0 && \text{on } \Omega_2 \times (0, T) \\ \text{B. C.} &&& \text{on } \partial\Omega \cap \partial\Omega_2 \times (0, T) \\ (u_2^{k+1}(x, 0), v_2^{k+1}(x, 0)) &= (u_0, v_0) && \text{on } \Omega_2 \\ \mathcal{B}_2(u_2^{k+1}, v_2^{k+1}) &= \mathcal{B}_2(u_1^k, v_1^k) && \text{on } \Gamma_2 \times (0, T) \end{aligned}$$



Evolution from Scalar Equation to Coupled System

Scalar equation:

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

Gander, Halpern, Kern: *A SWR Method for Advection-Diffusion-Reaction Problems with Discontinuous Coefficients and non-Matching Grids*. DD16, Springer, 2007.

Bennequin, Gander, Halpern: *A Homographic Best Approximation Problem with Application to Optimized SWR*. Math. Comp. 78, no. 265, pp 185—223, 2009.

Coupled system:

$$\begin{aligned} \phi \partial_t u + \operatorname{div}(-a \vec{\nabla} u + \vec{b} u) - k(v - cu) &= 0 & \text{on } \Omega \times (0, T) \\ \phi \partial_t v + k(v - cu) &= 0 & \text{on } \Omega \times (0, T) \end{aligned}$$

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

$$\mathcal{B}_1(u, v) = \frac{\partial u}{\partial n_1} - \frac{b_x - p}{2a} u, \quad \mathcal{B}_2(u, v) = \frac{\partial u}{\partial n_2} + \frac{b_x + p}{2a} u,$$

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

$$u_i^k \in L^2(0, T; H^2(\Omega_i)) \cap H^1(0, T; L^2(\Omega_i)), \quad v_i^k \in H^1(0, T; L^2(\Omega_i)),$$

for $i \in \{1, 2\}$.

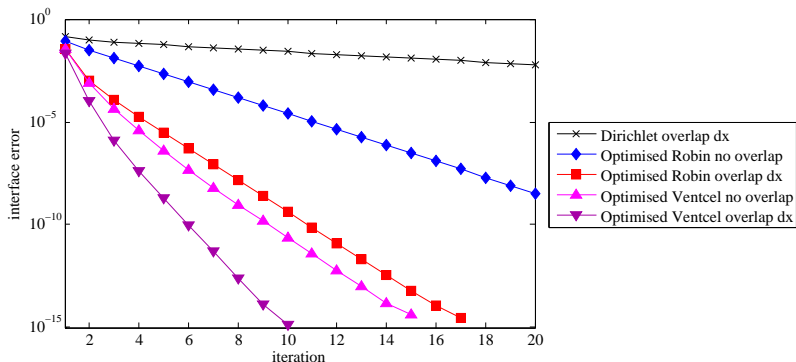
Convergence of the SWR Algorithm

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

Theorem

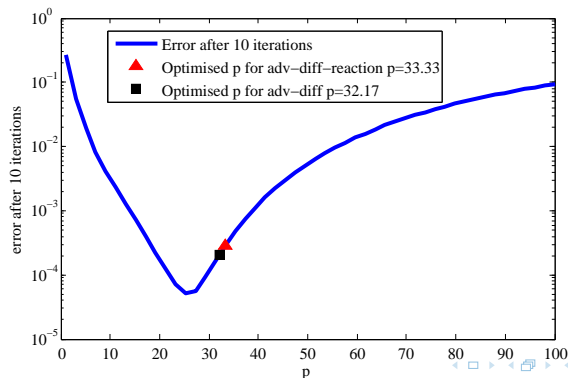
Let $L > 0$ and suppose that the advection speed b is such that $b_x \neq 0$. Let $p > 0$. Then the sequence $((u_1^k, v_1^k), (u_2^k, v_2^k))$ defined by the SWR algorithm with Robin transmission operators converges to $((u, v)|_{\Omega_1}, (u, v)|_{\Omega_2})$, in $\prod_{i=1}^2 (L^2(0, T; L^2(\Omega_i))) \times L^2(0, T; L^2(\Omega_i))$ for $k \rightarrow \infty$.

Convergence of the SWR Algorithm



Optimised Transmission Conditions

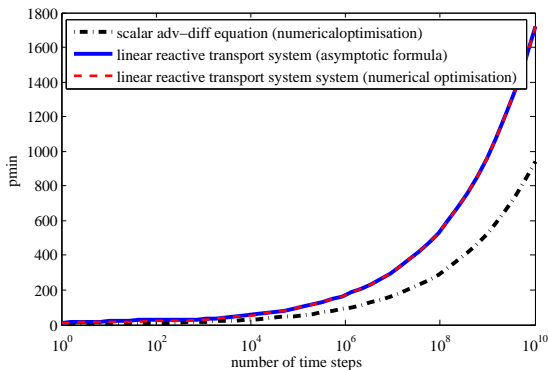
- Numerical optimisation of parameters: Comparison between scalar adv.-diff. equation and coupled system
 - Parameters of scalar advection-diffusion equation applicable even for strong chemistry (Ventcel 1D; Robin and Ventcel in 2D, 3D)
 - Significant differences for Robin in 1D



Analytical Formula for Optimised Parameter in 1D

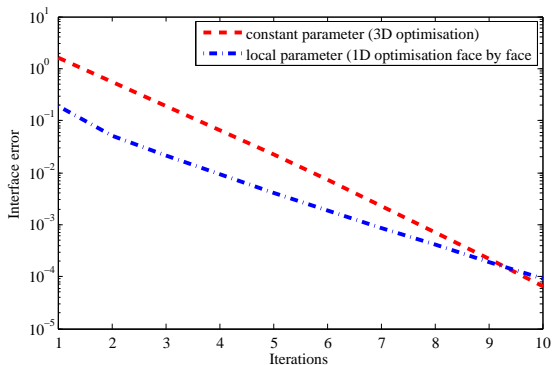
- Analytical solution for Robin without overlap in 1D following [Bennequin, Gander, Halpern 2009]

$$p^* = \sqrt{2\Re\epsilon \left(\sqrt{b_x^2 + 4ad(\tau_m)} \right) \Re\epsilon \left(\sqrt{b_x^2 + 4ad(\tau_M)} \right)}, \quad d(\tau) = \phi i\tau - \frac{k^2 c}{\phi i\tau + k} + kc$$



Application of 1D Parameter in 2D/3D cases

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



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The Nonlinear Coupled System

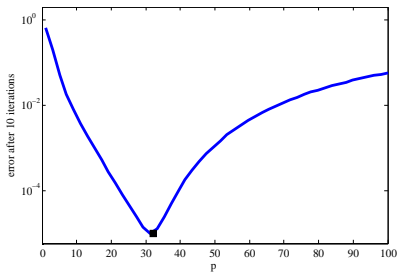
$$\begin{aligned} \phi \partial_t u + \operatorname{div}(-a \vec{\nabla} u + \vec{b} u) - R(u, v) &= 0 & \text{on } \Omega \times (0, T) \\ \phi \partial_t v + R(u, v) &= 0 & \text{on } \Omega \times (0, T) \end{aligned}$$

$R : \mathbb{R}^2 \rightarrow \mathbb{R}$ nonlinear function

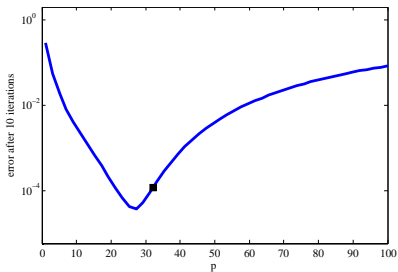
Optimised Transmission Conditions

■ 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 (SWR (NLPb))
- Nonlinear subproblems at every iteration

2. Nested Iteration Approach (NIA):

- Newton-Krylov (SWR (NLPb))
- Linearised problems for Jacobian evaluation
- Nonlinear problems for residual evaluation

3. Common Iteration Approach (CIA):

- Krylov-SWR (Newton (NLPb))
- Linearised problems for Jacobian evaluation
- Linearised problems for residual evaluation

[Haeberlein, Halpern, Michel, DD20, 2011, submitted]



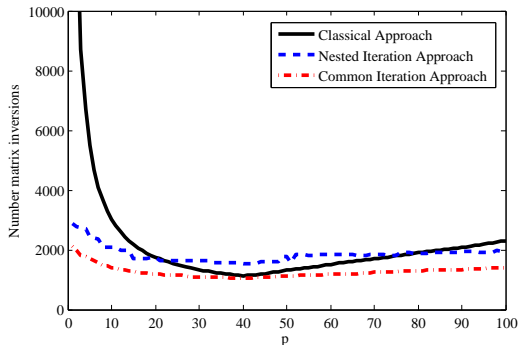
Mixing Newton and SWR Numerical Results

- + Easy to add to standard approach
- + Accelerating properties

Mixing Newton and SWR

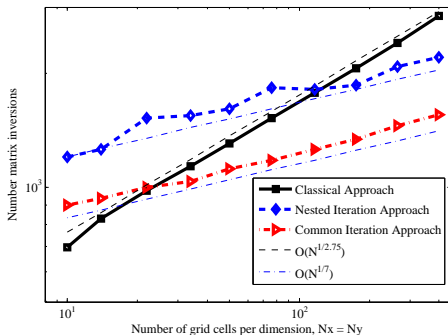
Numerical Results

- + Easy to add to standard approach
- + Accelerating properties



Mixing Newton and SWR Numerical Results

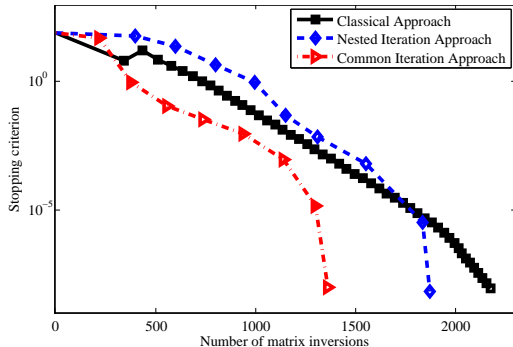
- + Easy to add to standard approach
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Mixing Newton and SWR

Numerical Results

- + Easy to add to standard approach
- + Accelerating properties



Mixing Newton and SWR Numerical Results

- + Easy to add to standard approach
- + Accelerating properties
- o Needs adaptive strategy for linear solver to be performant
 - Overhead cost for coarse discretisation \implies 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

⇒ ≈ 3 SWR iterations.

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

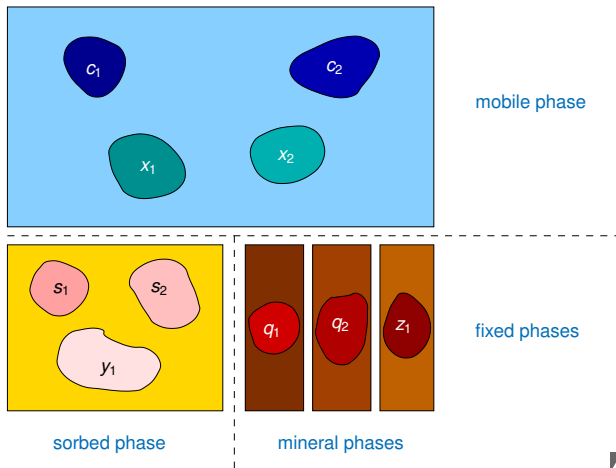
⇒ $\approx 20\%$ gain in CPU time.

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The Treated Problem Phases and Species



The Treated Problem

Components Representation

Equilibrium reactions are represented by a Morel tableau:

	c	s	q
c	Id		
s		Id	
q			Id

x	S_C^x		
y	S_C^y	S_S^y	
z	S_C^z		

Ideal activity model: $a_i = c_i$.

The Treated Problem

The Chemical Flash



$$\begin{aligned}\theta_w c + \theta_w (S_c^x)^t x + \theta_s (S_c^y)^t y + (S_c^z)^t (\theta_z \cdot z) &= T, \\ \theta_s s + \theta_s (S_s^y)^t y &= W, \\ \theta_q \cdot q &= Q,\end{aligned}$$

$$\ln(a_x) - (S_c^x) \ln(a_c) = \ln K_x,$$

$$\ln(a_y) - (S_c^y) \ln(a_c) - (S_s^y) \ln(a_s) = \ln K_y,$$

$$\ln(a_z) - (S_c^z) \ln(a_c) = \ln K_z,$$

$$\sum_{i=1}^{N_c} c_i + \sum_{i=1}^{N_x} x_i = 1, \quad (\text{mobile phase}),$$

$$\sum_{i=1}^{N_s} s_i + \sum_{i=1}^{N_y} y_i = 1, \quad (\text{sorbed phase, if present}),$$

$$q_i = 1, \quad i = 1, \dots, N_q,$$

$$z_i = 1, \quad i = 1, \dots, N_z.$$

The Treated Problem

Total Component RT Problem

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

$$\partial_t W + R_{W,\text{kin}} = 0 \quad (\#W),$$

$$\partial_t Q + R_{Q,\text{kin}} = 0 \quad (\#Q),$$

$$T - \phi C - \phi F = 0 \quad (\#T),$$

$$\phi F - \Psi(T, W, Q) = 0 \quad (\#F),$$

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

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

$$R_{Q,\text{kin}} - \Xi(T, W, Q) = 0 \quad (\#R_{Q,\text{kin}}).$$

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 CO₂

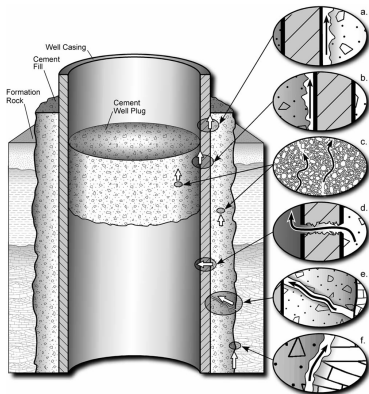


image source: Princeton University

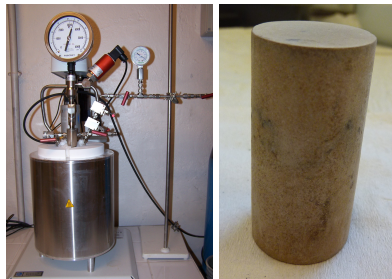


image sources: Thesis Th. Millan,
IFP EN - Ecole des Mines de St Etienne



Numerical Results

Cement Attack by CO₂

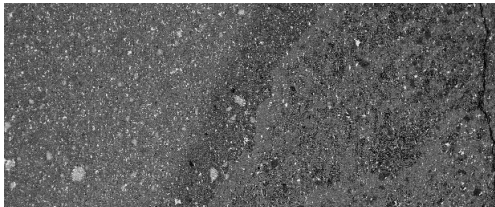


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Numerical Results

Cement Attack by CO₂

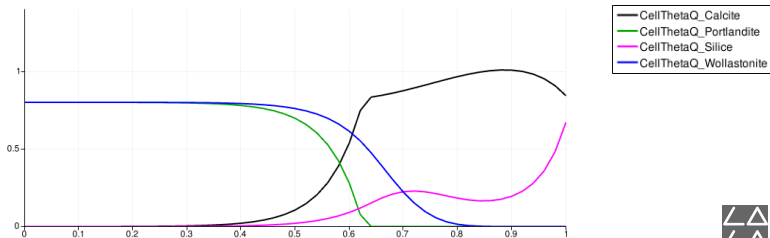
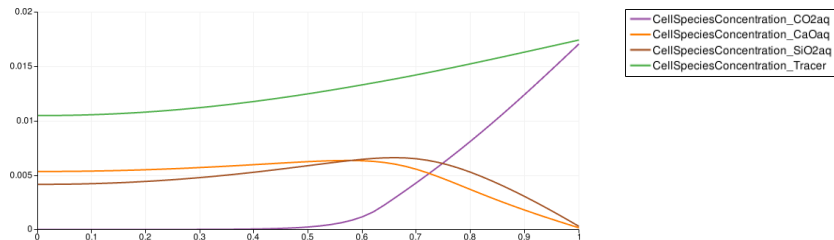
Mobile species: H₂O, tracer, CO₂(aq), CaO(aq), SiO₂(aq)
Mineral species: Calcite, Wollastonite, Portlandite, Silica

Kinetic reactions:

- Portlandite Dissolution: Portlandite + CO₂(aq) → Calcite
- Wollastonite Dissolution: Wollastonite $\xrightarrow{\text{CO}_2(\text{aq})}$ CaO(aq) + Silica
- Calcite Precipitation: CaO(aq) + CO₂(aq) → Calcite
- Silica Dissolution: Silica $\xrightarrow{\text{CaO}(\text{aq})}$ SiO₂(aq)

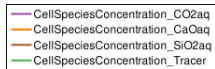
Numerical Results

Cement Attack by CO_2

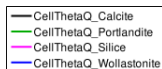


Numerical Results

Cement Attack by CO₂

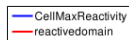


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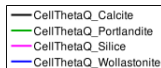


Numerical Results

Cement Attack by CO₂

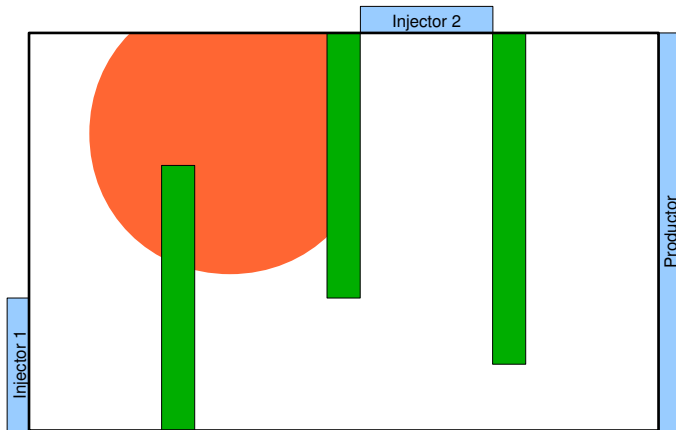


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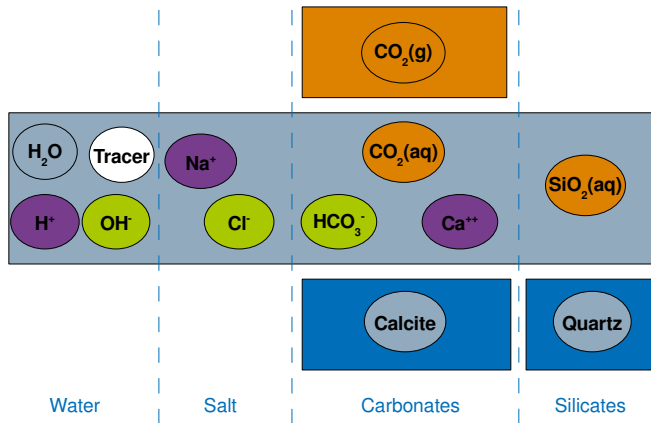
Numerical Results

SHPCO₂ Test Case



Numerical Results

SHPCO₂ Test Case



Numerical Results

SHPCO2 Test Case



Primary species:

$$c = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ c_7 \\ c_8 \end{pmatrix} = \begin{pmatrix} \text{H}_2\text{O} \\ \text{Tracer} \\ \text{CO}_2(\text{aq}) \\ \text{Cl}^- \\ \text{H}^+ \\ \text{Na}^+ \\ \text{Ca}^{++} \\ \text{SiO}_2(\text{aq}) \end{pmatrix}, \quad q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} \text{Calcite} \\ \text{Quartz} \end{pmatrix}$$

Secondary species:

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \text{HCO}_3^- \\ \text{OH}^- \end{pmatrix}, \quad z = (z_1) = (\text{CO}_2(\text{solid}))$$

Numerical Results

SHPCO₂ Test Case



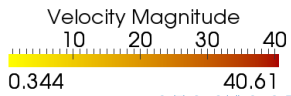
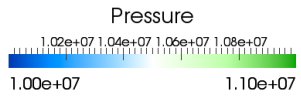
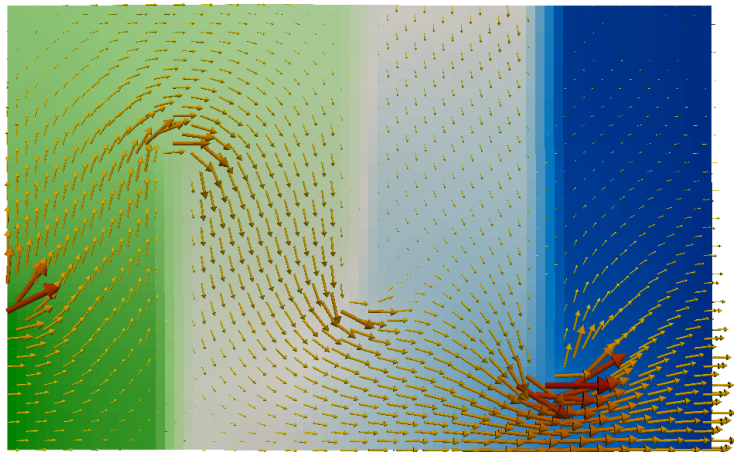
Equilibrium reactions:

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

Kinetic reactions:

- $\text{Calcite} + \text{H}^+ \longleftrightarrow \text{Ca}^{++} + \text{HCO}_3^-$
- $\text{Quartz} \longleftrightarrow \text{SiO}_2(\text{aq})$

Numerical Results SHPCO2 Test Case



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Numerical Results

SHPCO2 Test Case



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SWR Domain Decomposition for Coupled Systems

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

SWR and Krylov Accelerators 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

$M \rightarrow A + B$, 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

$$\begin{aligned} [\ln(a_z) - (S_C^Z) \ln(a_c) - \ln K_Z]_i &= 0 && \text{if mineral phase } i \text{ is present} \\ \theta_{z_i} &= 0 && \text{if mineral phase } i \text{ is not present} \end{aligned}$$



$$f := [\ln(a_z) - (S_C^Z) \ln(a_c) - \ln K_Z]_i$$

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