Coupling transport with geochemistry
Applications to CO2 sequestration

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Outline

- Motivations and problem statement
- Formulations and solution methods
    - Coupled problem and coupling algorithms
    - A simplified model, and Jacobian precondtioning
- Examples
    - MoMaS benchmark
    - CO2 test case

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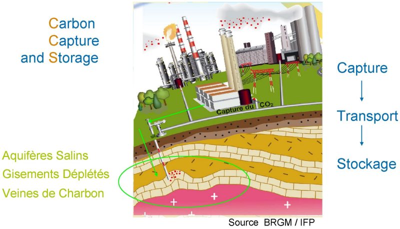
Motivation

Multi-species reactive transport

- Chemistry with equilibrium reactions
- Transport of aqueous species
- Large nonlinear system

Large scale geologic model for CO2 sequestration project (A. Michel, IFP)



Source BRGM / IFP

Numerical issues

- Formulation of coupled problem
- Iterative method: Fixed point vs Newton(–Krylov)
- Preconditioning for Newton–Krylov

Modeling chemical equilibrium systems

$$\sum_{j=1}^{N_s+\bar{N}_S} \nu_{ij} Y_j \leftrightarrows 0, \quad i = 1, \dots, N_r \qquad N_s + \bar{N}_S \text{ species }, N_r \text{ reactions.}$$

Mass action law $\nu \log \begin{pmatrix} c \\ \bar{c} \end{pmatrix} + \log K = 0$

Mass conservation $\nu^T \begin{pmatrix} c \\ \bar{c} \end{pmatrix} = \begin{pmatrix} T \\ W \end{pmatrix}$

System of non-linear equations T known from transport, W imposed

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Role of chemical model

Given totals T (and W, known), split into mobile (C) and immobile ($\bar{C}$) total concentrations

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Chemistry solver

$$\bar{C} = \Psi_C(T, W)$$

Transport with chemical reactions

Mobile species

$$\omega \partial_t c_i + \underbrace{\nabla \cdot (\mathbf{u} c_i - \mathbf{D} \nabla c_i)}_{L(c)} = \sum_{j=1}^{N_R} \nu_{ij} R_j, \quad i = 1, \dots, N_S$$

- c_i: concentration of *i*th species $[\mathrm{mol}/\mathrm{l}]$
- **D** Dispersion – diffusion tensor $[\mathrm{m}^2/\mathrm{s}]$
- R_j reaction term (unknown)
- ω: porosity [–]
- **u** Darcy velocity $[\mathrm{m}/\mathrm{s}]$
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Mass balance for immobile species

$$\rho_s\partial_t \bar{c}_i = \sum_{j=1}^{N_R} \nu_{ij} R_j, \quad i = 1,\dots,\bar{N}_S$$

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Formulations and solution strategies

Eliminate unkown equilibrium reaction rates by introducing mobile and immobile totals.

$$\left.\begin{aligned}\phi\partial_t C + \partial_t \bar{C} + LC &= 0\\ \bar{C} &= \Psi_c(T)\end{aligned}\right., \text{ with } T = C + \bar{C}$$

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Others

- Formulation as DAE (Erhel, de Dieuleveutl, Sabit)
- Elimination technique (Knabner, Kraütle, Hoffmann)
- Nonlinear CG (Bouillard, Herbin, Montarnal)

De Dieuleveult, Erhel, MK (JCP '09)

A global method from the fixed–point formulation

Discrete non-linear system

$$\begin{cases} C^{n+1} = \Psi_T\left(\phi\dfrac{\bar{C}^n - \bar{C}^{n+1}}{\Delta t}, C^n\right) \\ \bar{C}^{n+1} = \Psi_C(C^{n+1} + \bar{C}^{n+1}) \end{cases}$$

uncoupled

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Discrete non-linear system

$$\left\{\begin{aligned} C^{n+1} &= \Psi_T\left(\phi\,\frac{\bar{C}^n - \bar{C}^{n+1}}{\Delta t}, C^n\right) && \text{solve transport} \\ \bar{C}^{n+1} &= \Psi_C(C^{n+1} + \bar{C}^{n+1}) && \text{solve chemistry} \end{aligned}\right. \qquad \text{uncoupled}$$

Solution by Newton–Krylov method

- Solve the linear system by an iterative method (GMRES)
- Requires only Jacobian matrix by vector products, Jacobian not stored
- Keep transport and chemistry as black–boxes
- Theoretical framework: inexact Newton's method (Eisenstat and Walker)

Hammond, Valocchi, Lichtner (05), L. Amir's thesis, Amir, MK (09)

A simplified model: single species with explicit sorption

c mobile concentration, $\bar{c}$ fixed concentration.

$$\begin{cases} \omega \partial_t c + (1-\omega)\rho_S \partial_t \bar{c} - \nabla.(\mathbf{D}\nabla c - qc) = 0 \\ \bar{c} = \Psi(c) = \dfrac{k_f \sigma c}{k_b + k_f c} \quad \text{(Langmuir isotherm)} \end{cases}$$

Structure similar to multicomponent system

Barrett and Kanbner, Knabner and Van Duijn, Frolkovič, Kačur et al.

3 formulations

$\Psi_C(\mathbf{c}) = (\Psi_C(c_T))_T,\ T \in \mathscr{T}_h$

Coupled system $F_c \begin{pmatrix} \mathbf{c} \\ \bar{\mathbf{c}} \end{pmatrix} := \begin{pmatrix} (\mathbf{M} + \Delta t\, \mathbf{L})\mathbf{c} + \mathbf{M}\bar{\mathbf{c}} - \mathbf{b}^n \\ \bar{\mathbf{c}} - \Psi_C(\mathbf{c}) \end{pmatrix} = 0$

Elimination of $\bar{c}$ $F(\mathbf{c}) := (\mathbf{M} + \Delta t\, \mathbf{L})\mathbf{c} + \mathbf{M}\Psi_C(\mathbf{c}) - \mathbf{b}^n = 0$

Elimination of c $\tilde{F}(\bar{\mathbf{c}}) := \bar{\mathbf{c}} - \Psi_C\left((\mathbf{M} + \Delta t\, \mathbf{L})^{-1}(\mathbf{b}^n - \mathbf{M}\bar{\mathbf{c}})\right) = 0$

Jacobian preconditioning

- Essential for good linear performance
- Difficult for matrix free formulation
- Only block preconditioning, respect structure of coupled system

Algebraic elimination of mobile concentration equivalent to Schur complement of block Gauss–Seidel precond.

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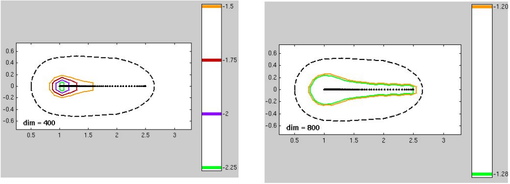
Algebraic elimination of mobile concentration equivalent to Schur complement of block Gauss–Seidel precond.

Can show eigenvalues of preconditioned op. bounded away from 0, independent of *h*, but convergence of GMRES not determined by eigenvalues

Field of values analysis ?



Eingenvalues, field of values and pseudospectrum for GS preconditioning

Preconditioner performance

1D model (Matlab + Sundials), $h = 0.05$, $K_L = 1.$, $\sigma = 1.5$, and $\Delta t = 0.0135$.

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	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
None	3	104	3	167	3	267	3	453

Mesh dependance : constant forcing term

NI: # nonlinear iters, NLI: total # linear iters.

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Elimination	3	41	3	41	3	41	3	40

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BGS	8	23	7	24	7	22	8	25
Elimination	5	15	5	15	5	15	5	15

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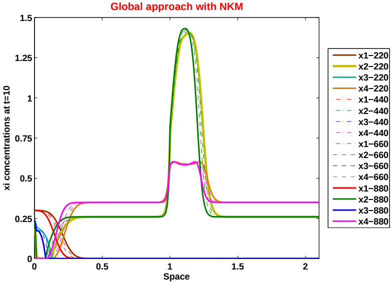
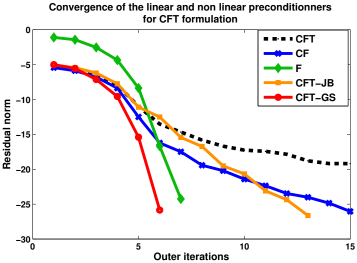
The 1D MoMaS benchmark

- 4 aqueous, 1 sorbed primary, 5 aqueous, 2 sorbed secondary species.
- Huge variation in equilibrium constants, large stoichiometric coeffs.
- Long simulation time (not this talk !)



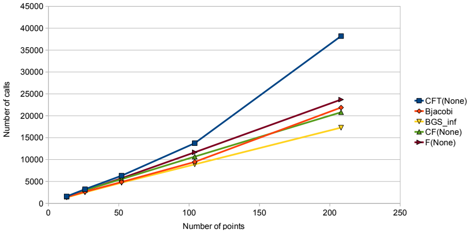
Components concentrations $t = 10$



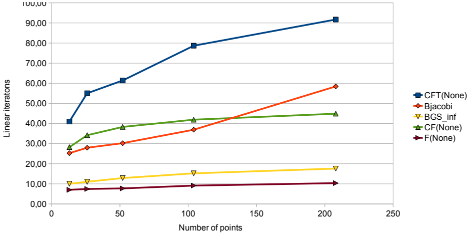
Performance of Newton-Krylov for different preconditioner

MoMaS benchmark: performance of different formulations

Number of calls to nonlinear function



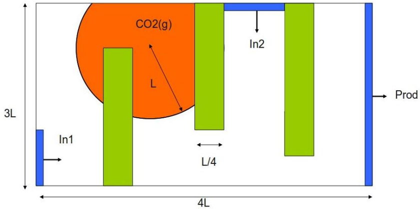
Number of linear iterations



- Basic method (CFT) not *h* independant, other methods OK
- Elimination method has least number of linear iterations, but not least number of *F* calls (why ?)
- Block Gauss-Seidel most efficient as preconditioners

CO$_2$ sequestration: a synthetic model

Minimal chemical system that still "looks" realistic for CO$_2$ storage



Dissolution of CO$_2$ in water, dissolution of calcite. Gas assumed immobile (capillary trapping), decouples flow from reactive transport.

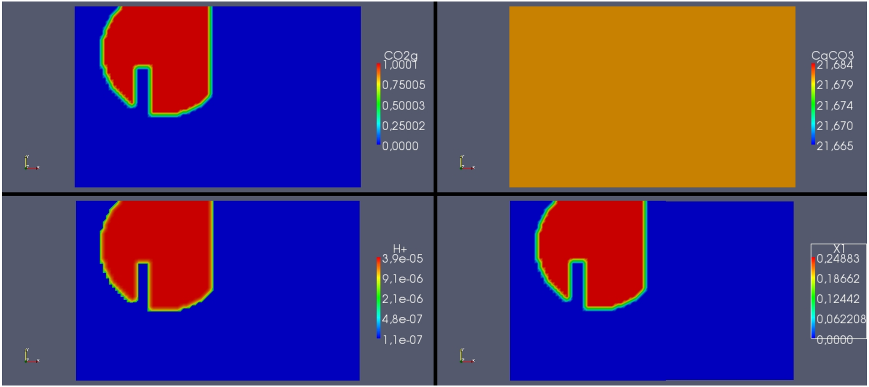
Chemical system

- $H_2O \rightleftharpoons H^+ + OH^-$ water dissociation
- $H_2O + CO_{2\,(aq)} \rightleftharpoons HCO_3^- + H^+$ dissociation of aqueous CO$_2$
- $CO_{2\,(g)} \rightleftharpoons CO_{2\,(aq)}$ gas dissolution
- $CaCO_3 + H^+ \rightleftharpoons Ca_2^+ + HCO_3^-$ Dissolution of calcite

Simulation code LifeV (EPFL, MOX, INRIA), nonlinear solver Kinsol (LLNL).

Evolution of concentrations

Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 0$

Evolution of concentrations

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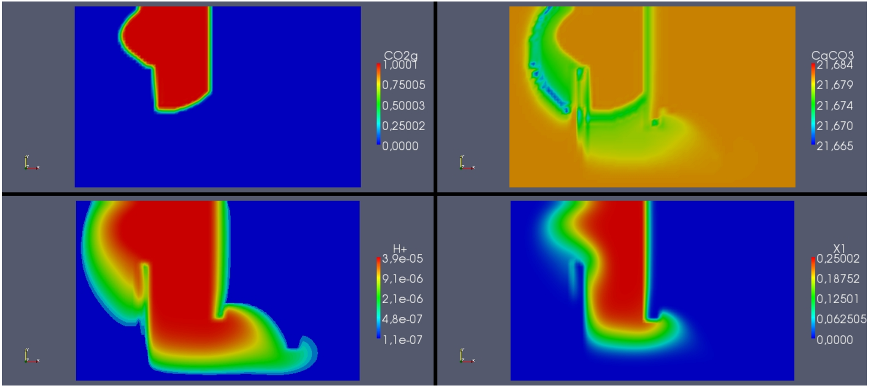
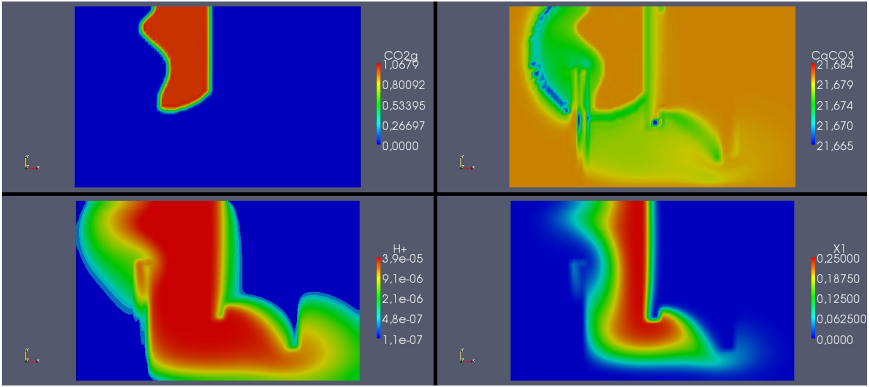


$t =$ 400 years

Evolution of concentrations

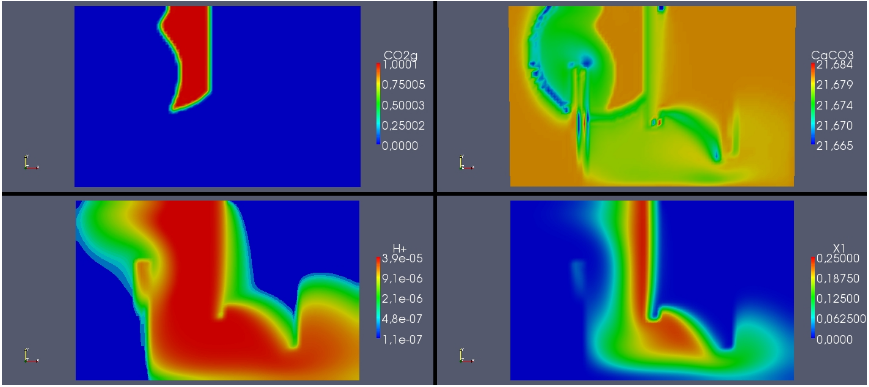
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t =$ 100 years, simulate 10 000 years.



$t =$ 800 years

Evolution of concentrations

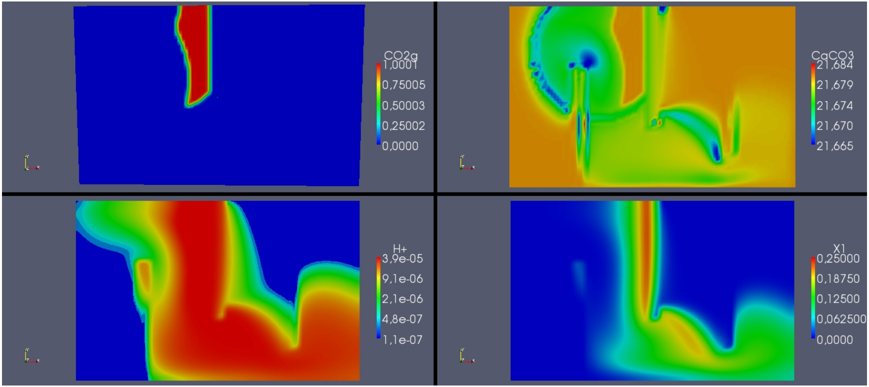
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 1200$ years

Evolution of concentrations

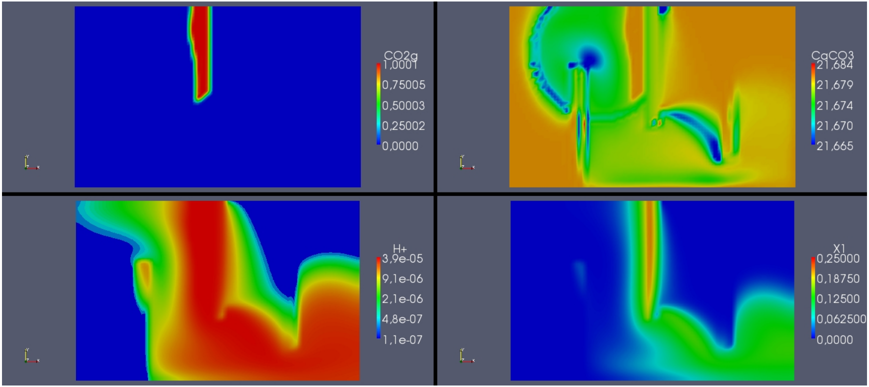
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t =$ 100 years, simulate 10 000 years.



$t =$ 1600 years

Evolution of concentrations

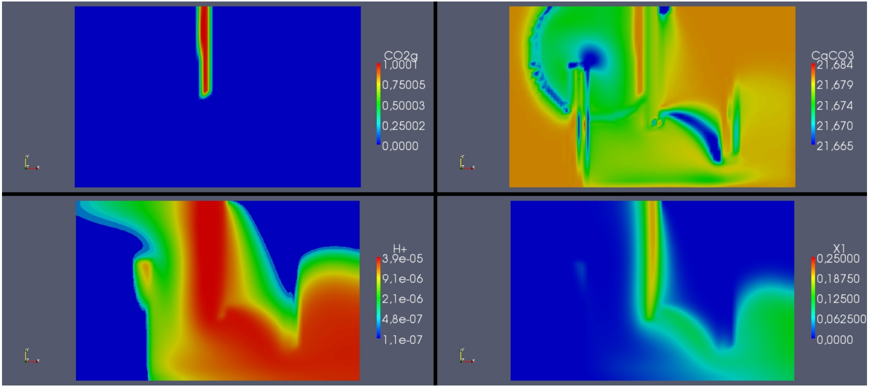
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 2000$ years

Evolution of concentrations

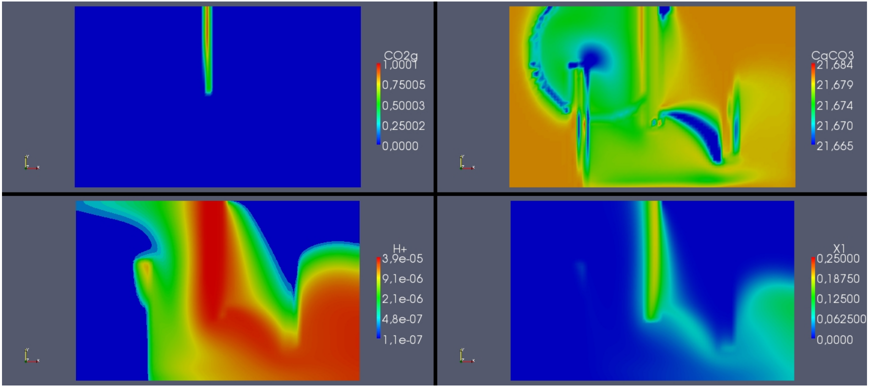
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 2400$ years

Evolution of concentrations

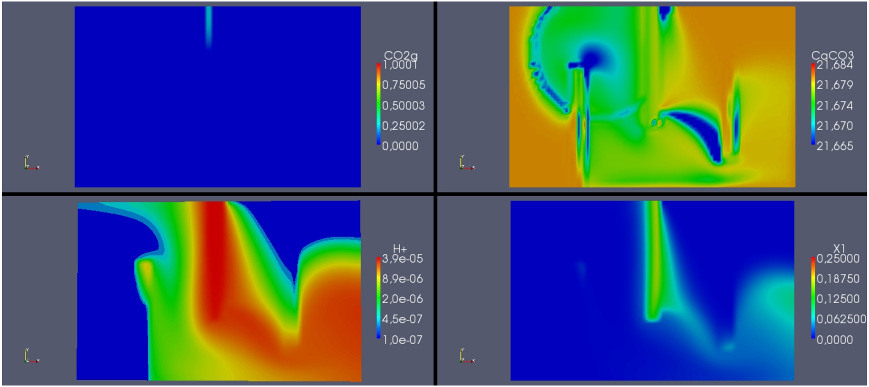
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 2800$ years

Evolution of concentrations

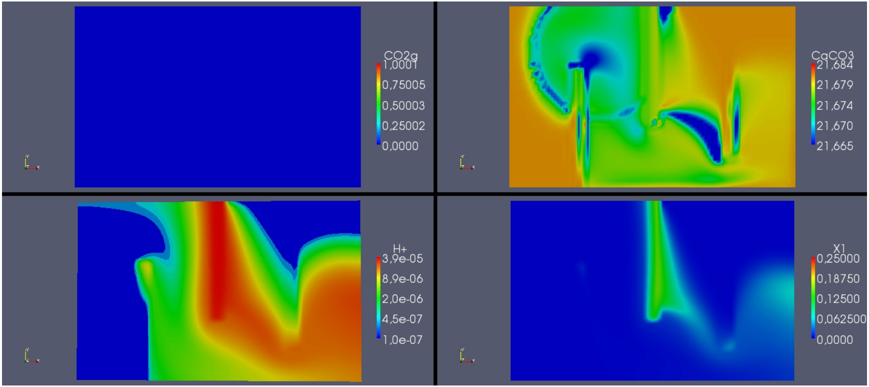
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 3200$ years

Evolution of concentrations

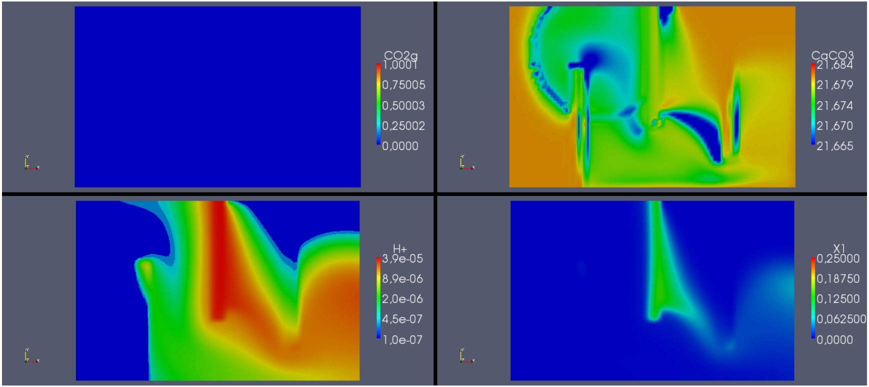
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t =$ 100 years, simulate 10 000 years.



$t =$ 3600 years

Evolution of concentrations

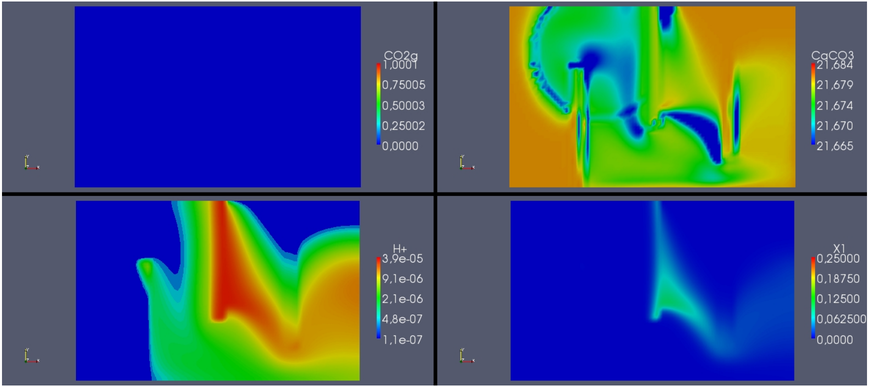
Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 4000$ years

Evolution of concentrations

Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.



$t = 5000$ years

Evolution of concentrations

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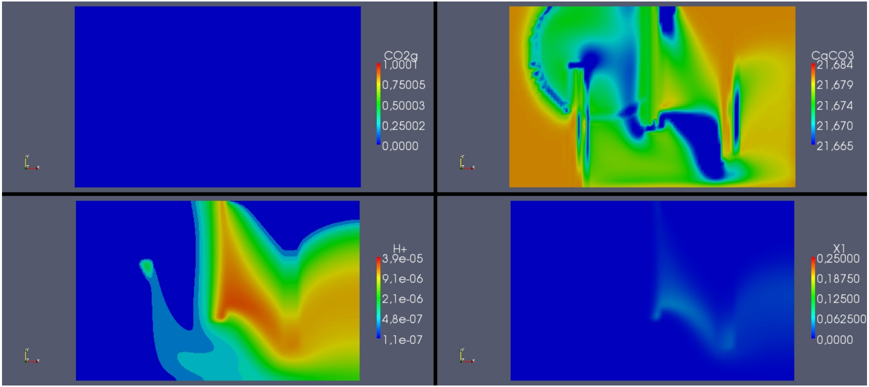
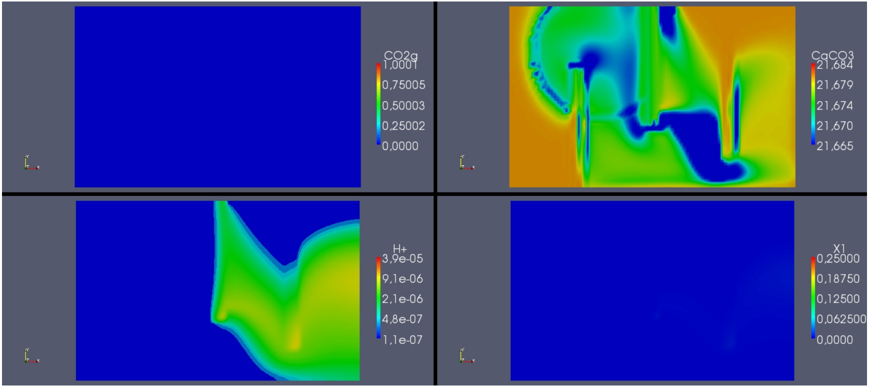


$t = 7000$ years

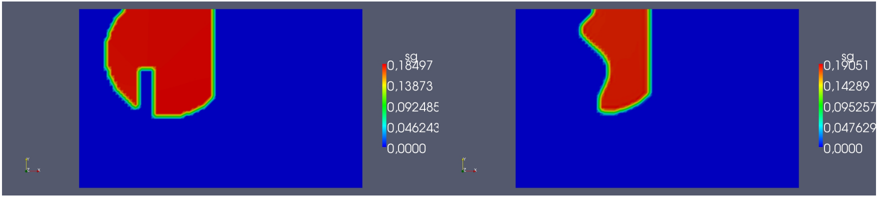
Evolution of concentrations

Grid with 5700 cells, $\Delta x = 50\mathrm{m}$, $\Delta t = 100$ years, simulate 10 000 years.

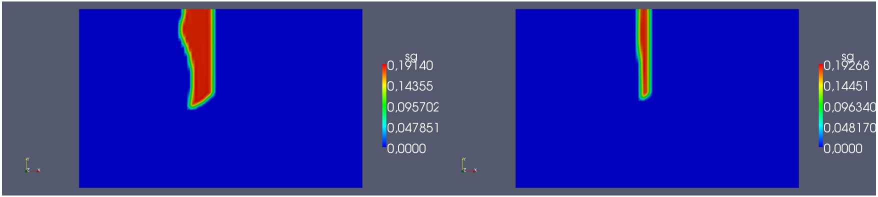


$t = 10000$ years

Evolution of gas saturation



$t = 0$ $t = 800$ years



$t = 1600$ $t = 2400$ years

Conclusions

- Formulation for coupled problem, separate transport and chemistry
- Newton–Krylov method can be applied on “fixed–point” formulation
- Connection between block–preconditioning and elimination at non-linear level
- Inverting transport gives mesh independent convergence for both linear (LI) and nonlinear (NI) iterations.
- In practice: approximate inverse should give spectral equivalence
- Future work: Prove FOV results, more tests on mulitcomponent chemistry, extension to two-phase flow

Università degli Studi di Padova

Dipartimento di Matematica

2013 SIAM Conference on Mathematical and Computational Issues in the Geosciences

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SUBMISSION DEADLINES

November 19, 2012	Minisymposium proposals
December 20, 2012	Abstracts for contributed and minisymposium speakers

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