SHPCO2

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Reactive transport in porous media: formulations, non-linear solvers and preconditioners

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Institut National de Recherche en Informatique et Automatique

High Performance Computing for CO2 Geological Storage
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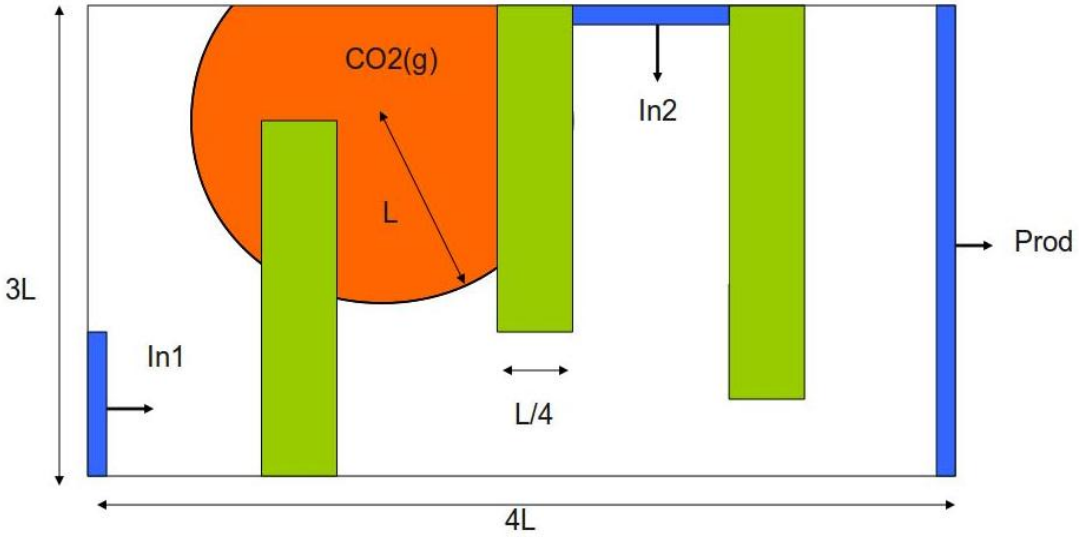
CO_2 sequestration: a synthetic model

Minimal chemical system that still ”looks like” realistic for CO_2 storage



Dissolution of CO_2 in water, dissolution of calcite. Gas assumed immobile (capillary trapping), decouples two phase flow from reactive transport.

Chemical system

- $H_2O \rightleftharpoons H^+ + OH^-$ water dissociation
- $CO_{2\,(g)} \rightleftharpoons CO_{2\,(aq)}$ gas dissolution
- $H_2O + CO_{2\,(aq)} \rightleftharpoons HCO_3^- + H^+$ dissociation of aqueous CO_2
- $CaCO_3 + H^+ \rightleftharpoons Ca_2^+ + HCO_3^-$ Dissolution of calcite

Outline

Chemical phenomena

Different reaction types

According to nature of reaction

Homogeneous	In the same phase (aqueous, gaseous, ...)
Heterogeneous	Involve different phases: gas dissolution, precipitation / dissolution, ...

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Slow reactions	Irreversible, modeled using kinetic law
Fast reactions	Reversible, modeled using equilibrium

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Morel formalism:

$$\begin{array}{c|c} (c,\ \bar{c}) \text{ primary species} & (x,\ \bar{x}) \text{ secondary species} \\ \hline (c, x) \text{ mobile species} & (\bar{c},\ \bar{x}) \text{ fixed species} \end{array}$$

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Reactive transport model

Balance equations

$$
\begin{aligned}
\phi \partial_t c + L c &= S^T R_e^a + A^T R_e^h + H^T R_k(c, x, \bar{c}, \bar{x}) \\
\phi \partial_t x + L x &= - R_e^a + K^T R_k(c, x, \bar{c}, \bar{x}) \\
\phi \partial_t \bar{c} &= B^T R_e^h + P^T R_k(c, x, \bar{c}, \bar{x}) \\
\phi \partial \bar{x} &= - R_e^h + Q^T R_k(c, x, \bar{c}, \bar{x})
\end{aligned}
$$

L advection diffusion operator

$$
L c = \underbrace{-\operatorname{div}(\mathbf{D} \operatorname{grad} c)}_{\text{dispersion}} + \underbrace{\operatorname{div}(\mathbf{u} c)}_{\text{advection}}
$$

$\mathbf{u}$ Darcy velocity (saturated flow model)

Dispersion tensor: $\mathbf{D} = d_e \mathbf{I} + \alpha_T |\mathbf{u}| I + (\alpha_L - \alpha_T) \dfrac{\mathbf{u} \otimes \mathbf{u}}{|\mathbf{u}|}$

Flow and transport solution

Flow computation: mixed finite elements

- Approximate both head and velocity
- Continuous flux across element faces
- Locally mass conservative
- Allows full diffusion tensor

Transport simulation by operator splitting

Advection step Explicit, finite volumes / discontinuous Galerkine

- Locally mass conservative
- Allows unstructured meshes
- CFL condition: use sub–time–steps

Dispersion step Like flow equation (time dependent): mixed finite elements (implicit)

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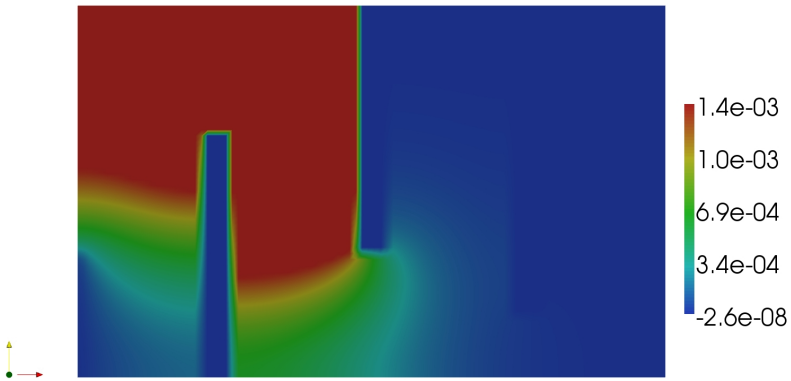
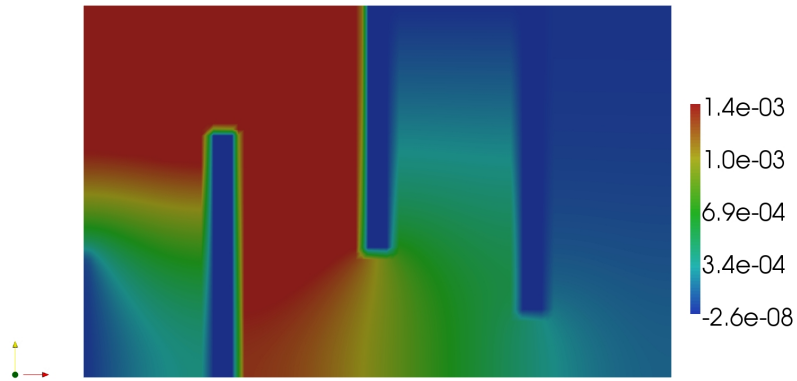
Condense transport solver, one time step

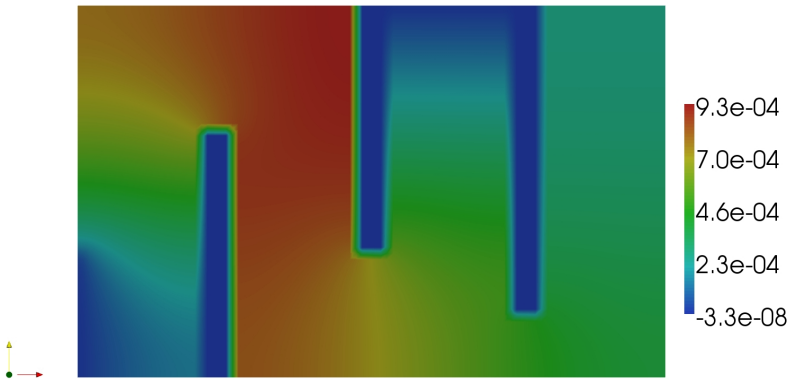
$$C^{n+1} = \Psi_T(f^n, C^n)$$

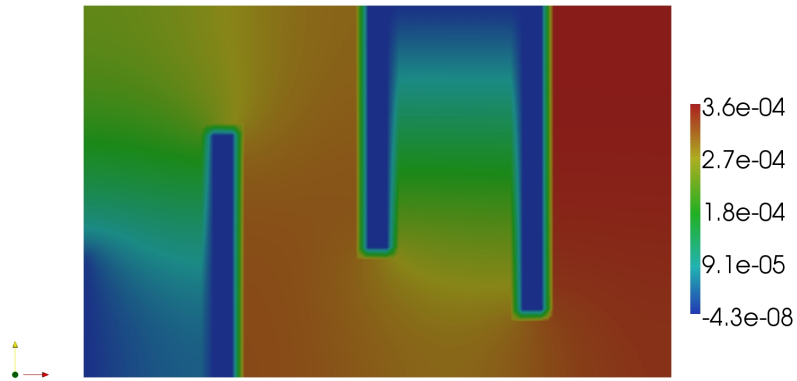
Transport for synthetic CO_2 example (M. Franco)





Left $T = 1$ day, right $T = 6$ days





Left $T = 12$ day, right $T = 37$ days

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Numerical solution of chemical equilibrium

System of non-linear equations

Mass action law

$$\log x = S \log c + \log K,$$
$$\log \bar{x} = A \log c + B \log \bar{c} + \log \bar{K}.$$

Mass conservation

$$c + S^T x + A^T \bar{x} = T, \quad T \text{ known from transport}$$
$$\bar{c} + B^T \bar{x} = W, \quad W \text{ imposed}$$

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Role of chemical model

Given totals T (and W, known), split into

Mobile $C = c + S^T x$,

Fixed $F = A^T \bar{x}$.

total concentrations

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T known from transport

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Chemistry solver

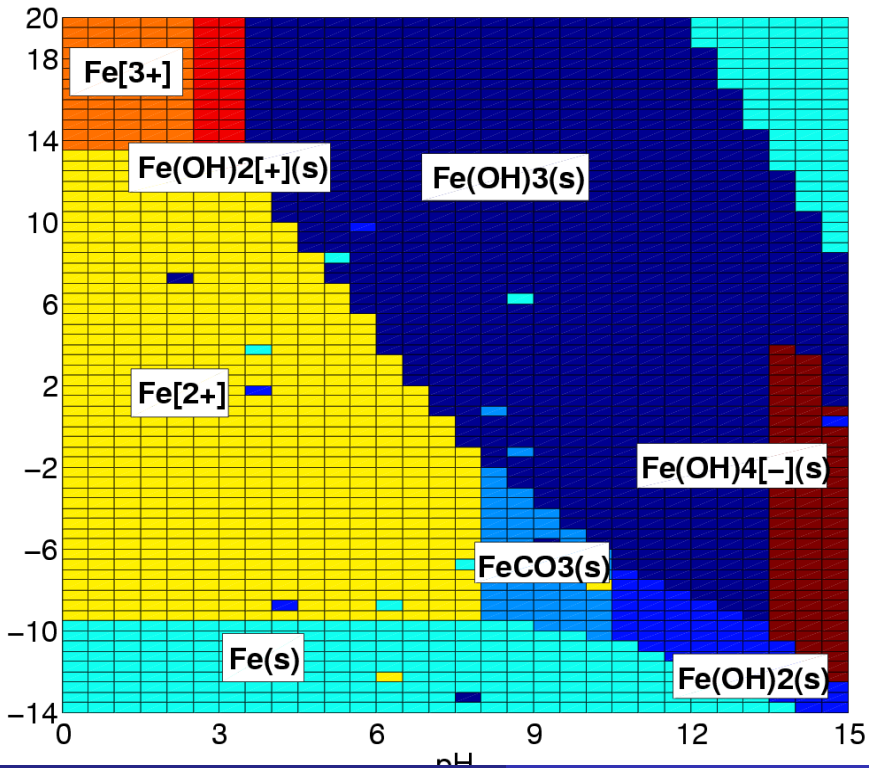
$$H \begin{pmatrix} \log c \\ \log \bar{c} \end{pmatrix} = \begin{pmatrix} T \\ W \end{pmatrix}$$

$$F = \Psi_C(T, W)$$

Handling minerals

- Reactions with threshold, which species appear unknown a priori.
- Standard procedure: combinatorial search, sequence of standard problems
- Reformulate as complementarity problem
- Interior point algorithm (Saaf et al. ('96), J.-Ch. Gilbert, I. Ben Gharbia)
- Also semi–smooth Newton (Kräutle)

pH-pE diagram for iron



Coupled formulation

Elimination of equilibrium rates

$$\begin{aligned} \phi \partial_t C + \quad \phi \partial_t F + \quad LC &= \quad S_T R_k(T, W) \\ \phi \partial_t W \qquad\qquad\quad &= \quad S_W R_k(T, W) \end{aligned}$$

$+$ local chemical equilibrium.

Special case: no kinetic reactions

$$\phi \frac{\partial T^{ic}}{\partial t} + L(C^{ic}) = 0, \quad ic = 1, \ldots, N_c$$

$$T^{ic}_{ix} = C^{ic}_{ix} + F^{ic}_{ix} \qquad ic = 1, .., N_c \text{ and } ix = 1, .., N_x$$

$$F_{ix} = \Psi(T_{ix}) \qquad ix = 1, \ldots, N_x.$$

Solution strategies

Fixed point (aka OS) Yeh–Tripathi, Carrayrou et al., Carrera et al.

- + easy to program, code reuse
- − not robust, small time steps

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DAE formulation Erhel and de Dieuleveult

- + use quality DAE software, accurate
- − expensive

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Elimination technique Knabner et al.

- + Efficient, accurate,
- − difficult to code

A global method based on DAE formulation

CC formulation, explicit chemistry

$$\begin{cases} \phi \dfrac{dC}{dt} + \dfrac{dF}{dt} + LC = 0 \\ H(z) - \begin{pmatrix} C+F \\ W \end{pmatrix} = 0 \\ F - F(z) = 0. \end{cases}$$

- $+$ Explicit Jacobian
- $+$ Chemistry function, no chemical solve
- $-$ Intrusive approach (chemistry not a black box)
- $-$ Precipitation not easy to include

Coupled system is index 1 DAE

$$K\frac{dy}{dt} + f(y) = 0$$

Use standard DAE software

C. de Dieuleveult (Andra thesis), J. Erhel, MK (JCP '09)

A global method from the fixed–point formulation (1)

Discrete non-linear system

$$
\begin{aligned}
C^{n+1} &= \Psi_T \left(S_T R_k(T^{n+1}, W^{n+1}) - \phi \frac{F^{n+1} - F^n}{\Delta t}, C^n \right) \\
F^{n+1} &= \Psi_C(T^{n+1}, W^{n+1}) \\
W^{n+1} &= W^n + \frac{\Delta t}{\phi} S_W R_k(T^{n+1}, W^{n+1}) \\
T^{n+1} &= C^{n+1} + F^{n+1}
\end{aligned}
$$

Formulation without kinetic reactions

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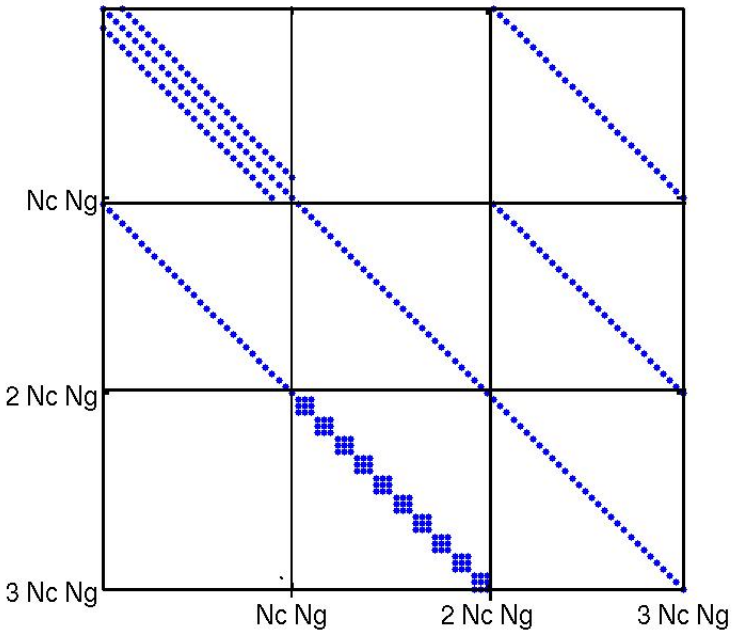
$$

Can be solved by block Gauss Seidel or by Newton's method

A global method from the fixed–point formulation (2)

- + Non-intrusive approach
- + Precipitation can be included
- − One chemical equilibrium solve for each function evaluation

Solution by Newton–Krylov : keep transport and chemistry as black–boxes (up to Jacobian computation)



Jacobian structure

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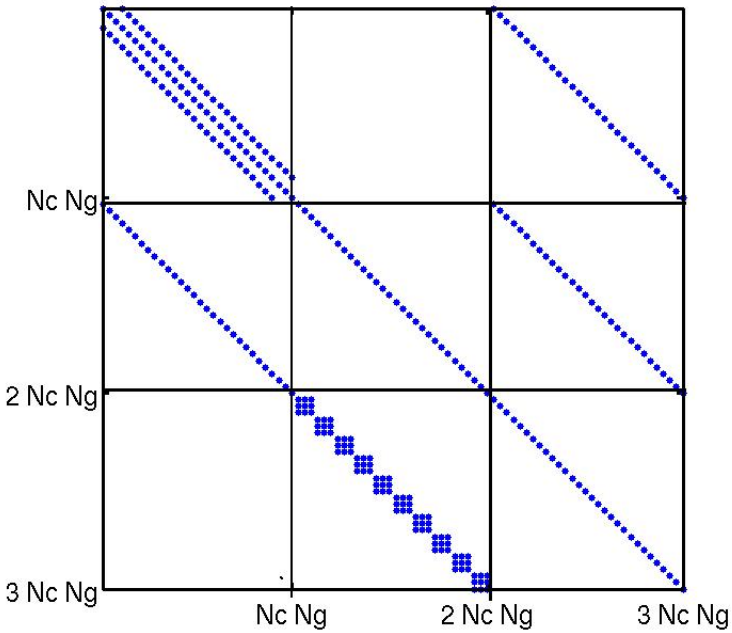

Jacobian structure

Residual computation:

1. Apply Ψ_T : solve transport for each species,
2. Apply Ψ_C: solve chemistry for each grid cell.

Solution by Newton–Krylov

- Solve the linear system by an iterative method (GMRES)
- Requires only jacobian matrix by vector products.

Used for CFD, shallow water, radiative transfer(Keyes, Knoll, JCP 04), and for reactive transport (Hammond, Valocchi, Lichtner, Adv. Wat. Res. 05)

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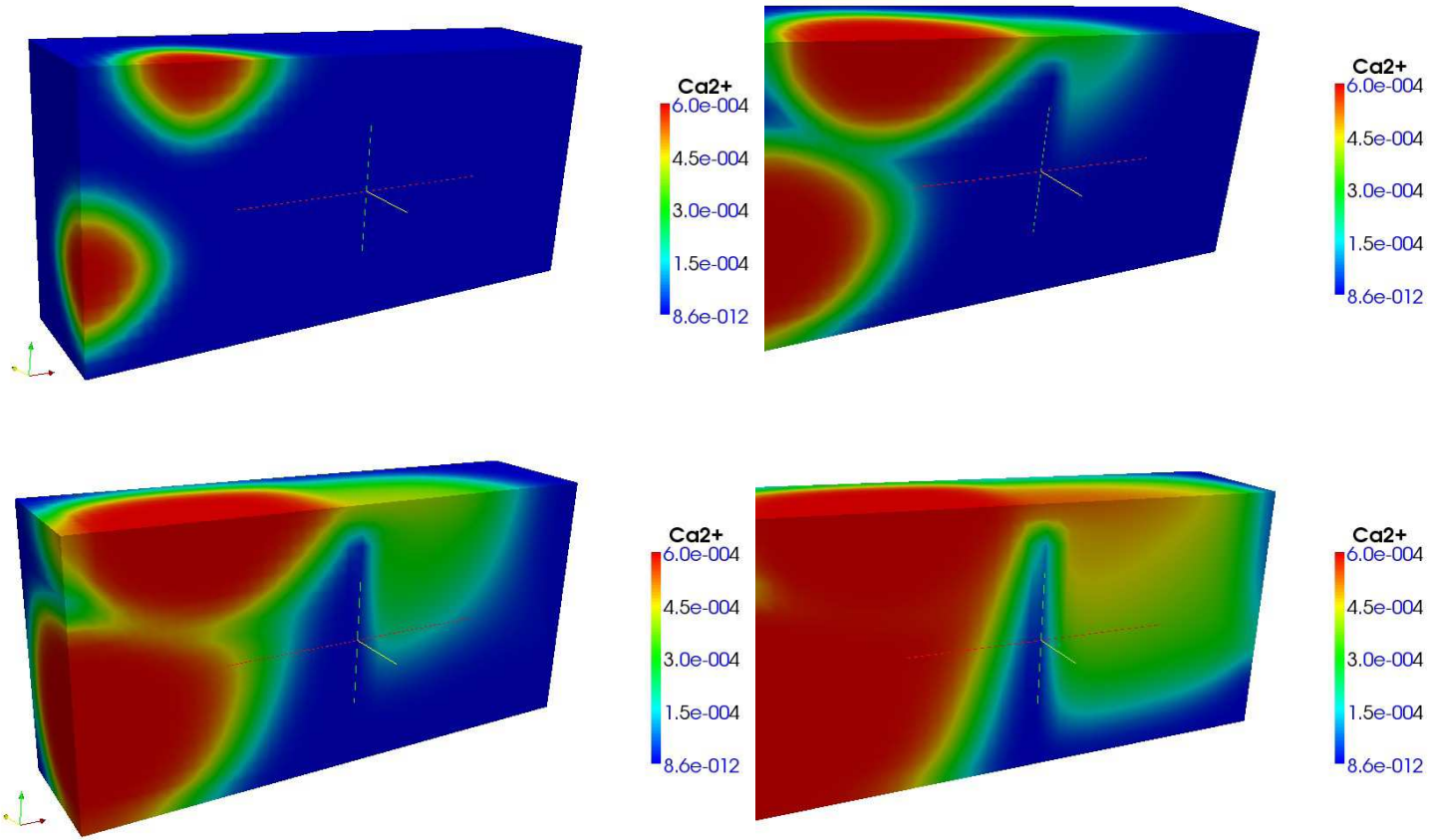
Inexact Newton

- Approximation of the Newton's direction $\|f'(x_k)d + f(x_k)\| \leq \eta \|f(x_k)\|$
- Choice of the forcing term η?
  - Keep quadratic convergence (locally)
  - Avoid oversolving the linear system
- $\eta = \gamma \|f(x_k)\|^2 / \|f(x_{k-1})\|^2$ (Kelley, Eisenstat and Walker)

L. Amir's thesis, Amir, MK (Comp. Geosci. 09)

3D ion exchange example (O. Saouli)



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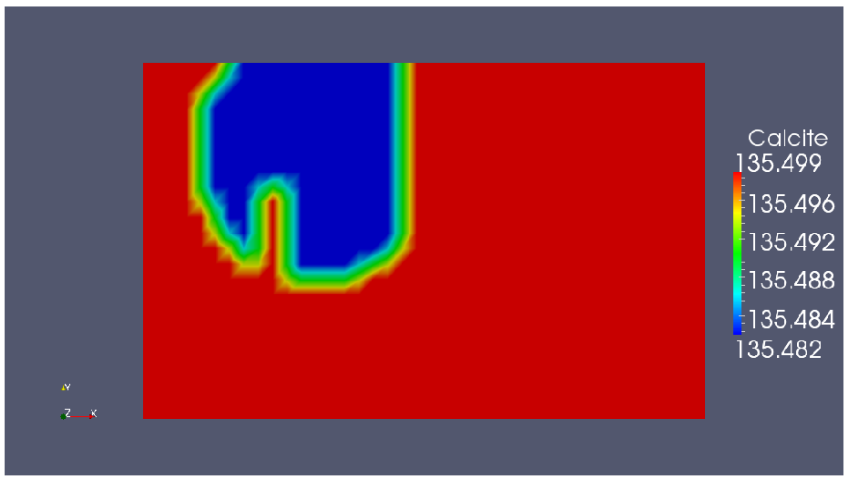
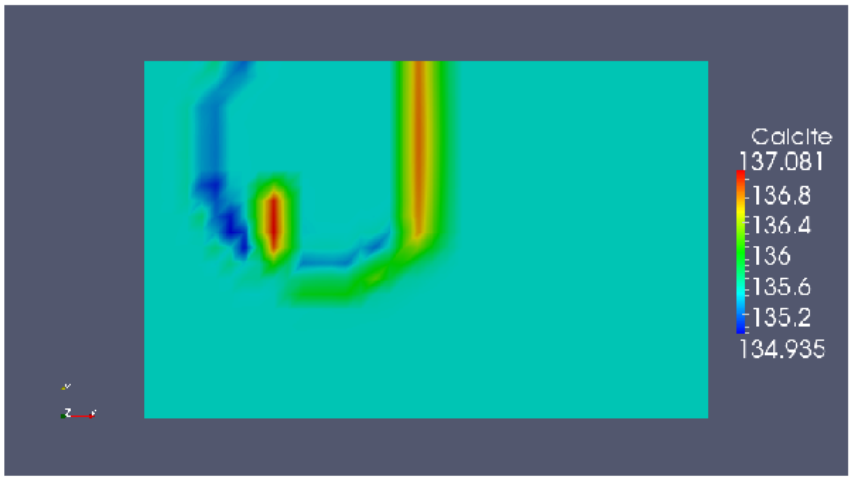
Application to SHPCO2 model

Aqueous species, gas (Henry's law), equilibrium mineals

Calcite concentration: left $t = 0$, right $t = 115$ days





Computations by B. Gueslin.
LifeV library (EPFL, Milano, INRIA), Kinsol (LLNL)

A simplified one species model, with sorption

Coupled model

$$\phi \frac{\partial C}{\partial t} + \phi \frac{\partial F}{\partial t} + LC = 0,$$

$$F = \Psi(C) = \frac{k_f \sigma_0 C}{k_f C + k_b}.$$

Mathematical, numerical analysis: van Duijn, Knabner, Frolkovic

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Coupled problem

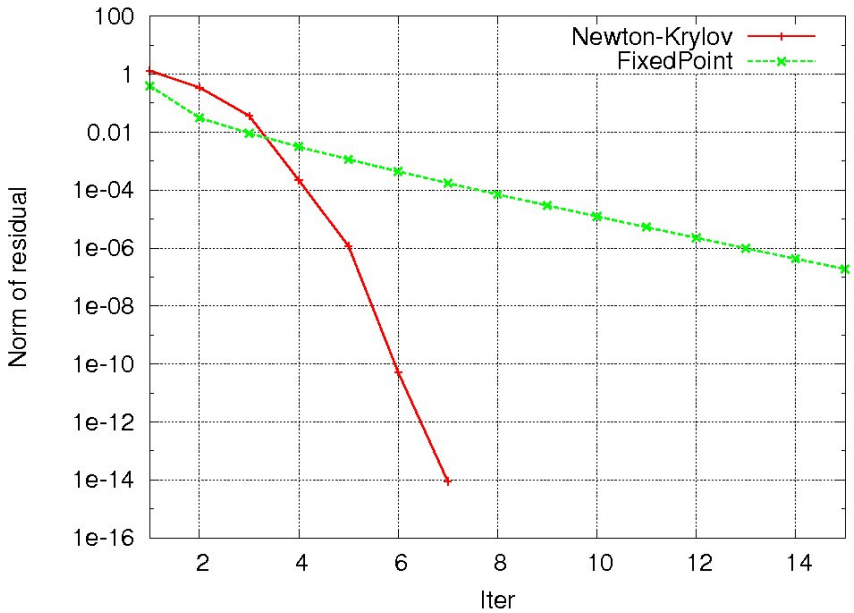
Coupled formulation

$$F\begin{pmatrix} C \\ F \end{pmatrix} = \begin{pmatrix} (\mathbf{M} + \Delta t \mathbf{L})C + \mathbf{M}F + b \\ F - \Psi(C) \end{pmatrix} = 0$$

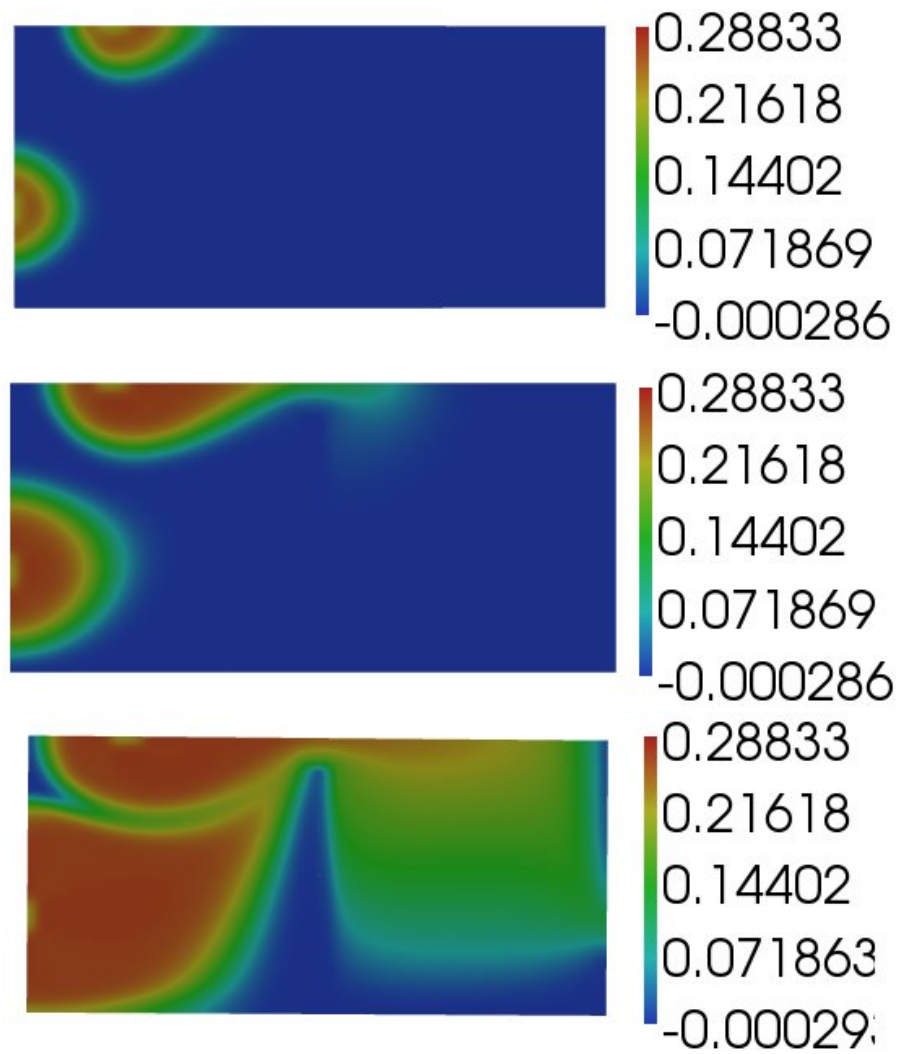
Eliminate F $F_1(C) = (\mathbf{M} + \Delta t \mathbf{L})C + \mathbf{M}\Psi(C) - b^n$

Eliminate C $F_2(F) = F - \Psi\left((\mathbf{M} + \Delta t \mathbf{L})^{-1}(b - \mathbf{M}F)\right)$

Performance of Newton's method



Convergence of Newton and fixed point



Jacobian preconditioning

Jacobian for coupled formulation,with $D = \mathrm{diag}(\Psi'(C_1), \ldots, \Psi'(C_N))$

$$J = \begin{pmatrix} \mathbf{M} + \Delta t \mathbf{L} & \mathbf{M} \\ -\mathbf{D} & I \end{pmatrix}$$

$J_2 = I + \mathbf{D}(\mathbf{M} + \Delta t \mathbf{L})^{-1}\mathbf{M}$ is Schur complement of J

Block preconditioning

Jacobi Solve transport at each step

$$\mathbf{P} = \begin{pmatrix} \mathbf{M} + \Delta t \mathbf{L} & 0 \\ 0 & \mathbf{I} \end{pmatrix}$$

Gauss–Seidel Solve transport at each step, some coupling

$$\mathbf{P} = \begin{pmatrix} \mathbf{M} + \Delta t \mathbf{L} & 0 \\ -\mathbf{D} & \mathbf{I} \end{pmatrix}$$

Elimination of C is equivalent to Schur complement of Gauss–Seidel.

Gmres convergence: field of values analysis

Convergence of GMRES not determined by eigenvalues (Greenbaum, Strakos).

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Nevertheless ...

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Eigenvalues of preconditioned operators

Assume spectrum$(\mathbf{M} + \delta t \mathbf{L}) \approx O(1/h^2)$.

Jacobi $\Lambda(P^{-1}J) \subset [1 - iCh, 1 + iCh]$

Gauss-Seidel $\Lambda(P^{-1}J) \subset [1, 1 + Ch^2]$, 1 is multiple ev

Schur $\Lambda(J_2) \subset [1, 1 + Ch^2]$

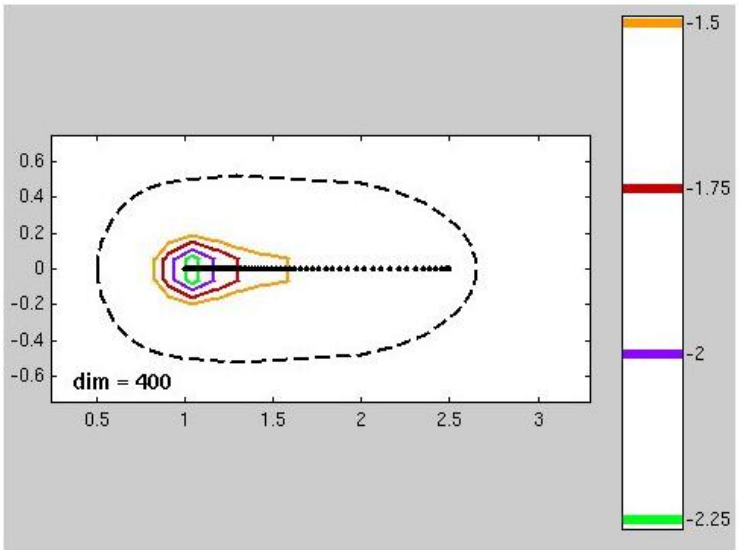
Bounded independent of h.

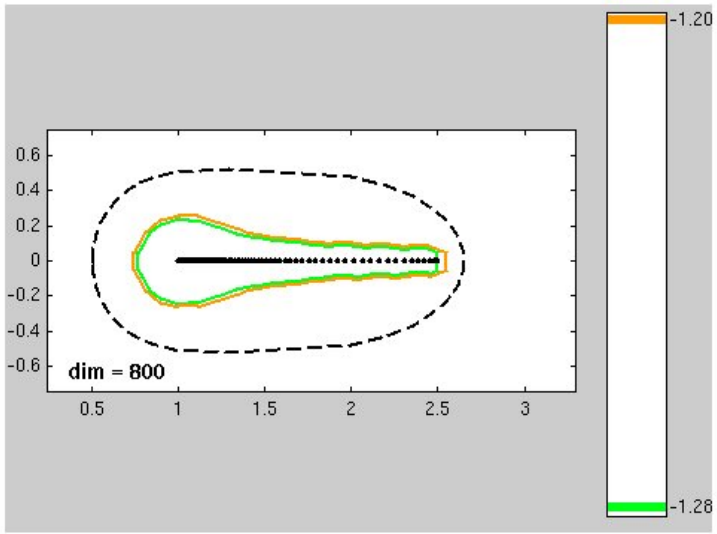
Field of value analysis

GMRES convergence

$$W(A) \equiv \left\{ \frac{x^* A x}{x^* x} | x \in \mathbb{C}^n, x \neq 0 \right\}, \text{ convex set, contains eigenvalues of } A$$

$$\frac{\|r_k\|_2}{\|r_0\|_2} \leq 2 \min_{p \in \mathcal{P}_k^*} \max_{z \in W(A)} \|p(z)\|_2.$$





Eingenvalues, field of values and pseudospectrum for GS preconditioning

Preconditioner performance

	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
None	8	54	10	100	17	238	33	658

Preconditioner performance

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	Nl	Ll	Nl	Ll	Nl	Ll	Nl	Ll
None	8	54	10	100	17	238	33	658
BGS	8	11	10	15	14	22	21	36

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None	8	54	10	100	17	238	33	658
BGS	8	11	10	15	14	22	21	36
Elimination	6	25	6	25	6	25	6	25

Inverting transport gives mesh independent convergence for both linear (LI) and nonlinear (NI) iterations.

In practice: approximate inverse should give spectral equivalence