Coupled formulations and coupling algorithms for reactive transport in porous media

Michel Kern
with L. Amir, B. Gueslin, A. Taakili

INRIA Rocquencourt

DyCap Workshop
Microbiology and Reactive Transport in the Capilary Fringe

Heidelberg, October 7-8, 2010

1. Motivations

2. Basic models and methods
   - Flow model
   - Transport model
   - Chemistry

3. Formulations and solution methods

4. Examples
   - Ion exchange
   - CO2 example

5. Conclusions

Outline

1 Motivations

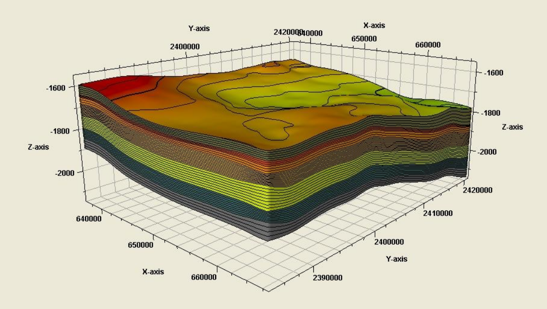
2 Basic models and methods
- Flow model
- Transport model
- Chemistry

3 Formulations and solution methods

4 Examples
- Ion exchange
- CO2 example

5 Conclusions

CO_2 sequestration



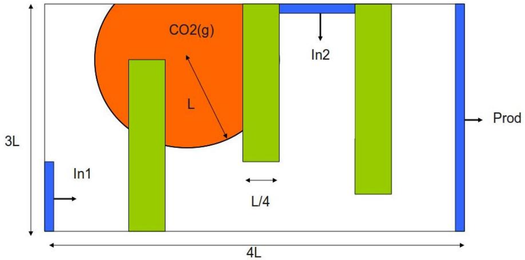
Geological model, BRGM (21 million grid points)

- Long term capture of CO_2 in saline aquifer
- Simulation to understand CO_2 migration through salt
- Coupling of liquid and gas phase, reactive transport

SHPCO2 project (funded by ANR) High Performance Simulation of CO_2 sequestration

CO_2 sequestration : a synthetic model

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



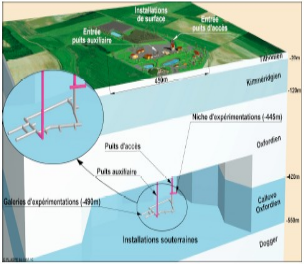
Dissolution of CO_2 in water, dissolution of calcite. Gas assumed immobile (capillary trapping), decouples two phase flow from reactive transport.

Chemical system

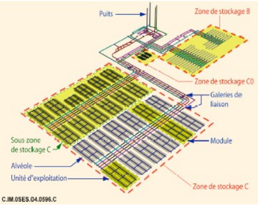
- $H_2O \rightleftharpoons H^+ + OH^-$ Water dissociation
- $CO_{2\,(g)} \rightleftharpoons CO_{2\,(aq)}$ Gas dissolution
- $H_2O + CO_{2\,(aq)} \rightleftharpoons HCO_3^- + H^+$ Dissociation of aqueous CO_2
- $CaCO_3 + H^+ \rightleftharpoons Ca_2^+ + HCO_3^-$ Dissolution of calcite

Nuclear waste storage

- Assess safety of deep geological nuclear waste storage (clay layer)
- Long term simulation of radionuclide transport (one million years)
- Wide variation of scales : from package (meter) to regional (kilometers)
- Geochemistry : large number of species
- Strong government regulation



ANDRA



Present choice in France : a sedimentary geological formation (in the Meuse region)

Research in mathematical and numerical modeling is conducted in the CNRS MOMAS group (Director A. Ern).

Outline

1. Motivations

2. Basic models and methods
   - Flow model
   - Transport model
   - Chemistry

3. Formulations and solution methods

4. Examples
   - Ion exchange
   - CO2 example

5. Conclusions

Flow model

Flow equations : Darcy's law

$$q = -K\nabla h$$
$$\nabla \cdot q = 0$$

- h piezometric head
- q Darcy velocity

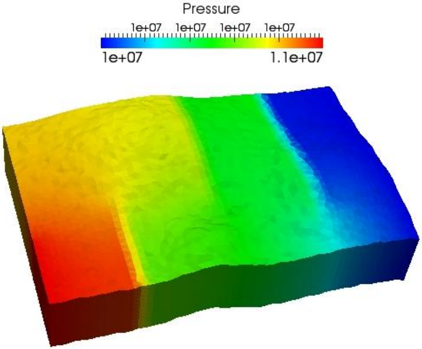
- K permeability tensor (heterogeneous, anisotropic)

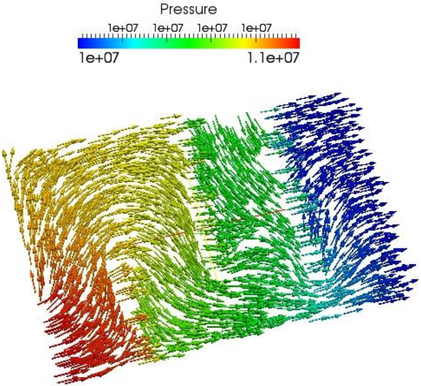
Mixed finite elements

- Approximate both head and velocity
- Continuous flux across element faces

- Locally mass conservative
- Allows full diffusion tensor

Pressure and velocity for CO2 example (A. Fumagalli, M. Franco)





Transport model

Convection–diffusion equation

$$\phi \frac{\partial c}{\partial t} - \underset{\text{dispersion}}{\mathrm{div}(\mathbf{D}\,\mathrm{grad}\, c)} + \underset{\text{advection}}{\mathrm{div}(\mathbf{u} c)} + \phi \lambda c = f$$

- c : concentration $[\mathrm{mol}/\mathrm{l}]$
- ϕ : porosity [–]
- λ radioactive decay $[\mathrm{s}^{-1}]$
- $\mathbf{u}$ Darcy velocity $[\mathrm{m}/\mathrm{s}]$

Dispersion tensor

$$\mathbf{D} = d_e \mathbf{I} + |\mathbf{u}|[\alpha_l \mathbf{E}(\mathbf{u}) + \alpha_t (I - \mathbf{E}(\mathbf{u}))], \quad E_{ij}(\mathbf{u}) = \frac{u_i u_j}{|\mathbf{u}|}$$

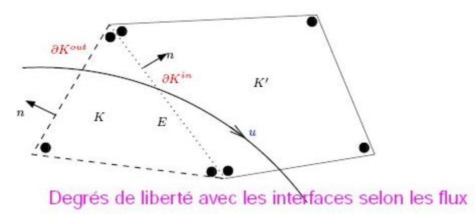
α_l, α_t dispersivity coeff. $[\mathrm{m}]$, d_e molecular diffusion $[\mathrm{m}/\mathrm{s}^2]$

Solution by operator splitting

Advection step

Explicit, finite volumes / discontinuous Galerkine

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



Degrés de liberté avec les interfaces selon les flux

Dispersion step

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

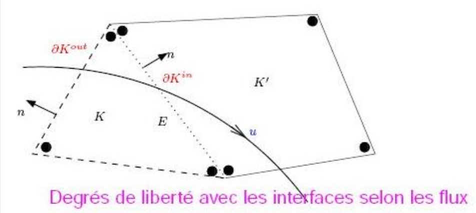
See Ackerer et al., Putti et al., Arbogast et al., ...

Solution by operator splitting

Advection step

Explicit, finite volumes / discontinuous Galerkine

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



Degrés de liberté avec les interfaces selon les flux

Dispersion step

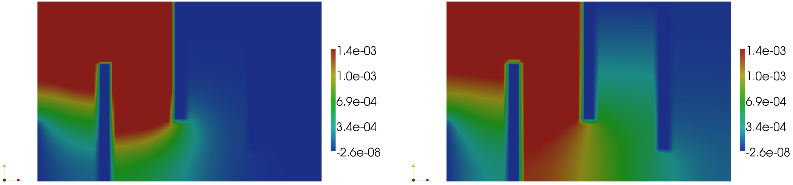
Like flow equation (time dependent) : mixed finite elements (implicit)

See Ackerer et al., Putti et al., Arbogast et al., ...

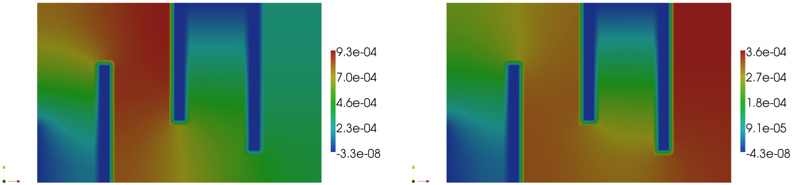
Condense transport solver, one time step

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

Transport for synthetic CO_2 example



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



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

Classification of chemical reactions

According to nature of reaction

Homogeneous	In the same phase (aqueous, gaseous, ...) Examples : Acid base, oxydo–reduction
Heterogeneous	Involve different phases Examples : Sorption, precipitation – dissolution, ...

Classification of chemical reactions

According to nature of reaction

Homogeneous In the same phase (aqueous, gaseous, ...)
Examples : Acid base, oxydo–reduction

Heterogeneous Involve different phases
Examples : Sorption, precipitation – dissolution, ...

According to speed of reaction

Fast reactions Reversible, modeled using equilibrium
Examples : Aqueous reactions, sorption, precipitation – dissolution

Slow reactions Irreversible, modeled using kinetic law
Examples : Precipitation – dissolution

Depends on relative speed of reactions and transport.

Chemical equilibrium

c_j aqueous (mobile) species, $\bar{c}_j$ fixed (immobile) species,

Chemical reactions

$$S_{mm} c \Leftrightarrow 0$$

$$S_{mf} c + S_{ff} \bar{c} \Leftrightarrow 0$$

Chemical equilibrium

c_j aqueous (mobile) species, $\bar{c}_j$ fixed (immobile) species,

Chemical reactions

$$S_{mm} c \Leftrightarrow 0$$

$$S_{mf} c + S_{ff} \bar{c} \Leftrightarrow 0$$

Let

$$\begin{pmatrix} P_{mm} & P_{mf} \\ 0 & P_{ff} \end{pmatrix} \begin{pmatrix} S_{mm}^T & S_{mf}^T \\ 0 & S_{ff}^T \end{pmatrix} = 0$$

Chemical equilibrium

c_j aqueous (mobile) species, $\bar{c}_j$ fixed (immobile) species,

Chemical reactions

$$S_{mm} c \Leftrightarrow 0$$

$$S_{mf} c + S_{ff} \bar{c} \Leftrightarrow 0$$

Let

$$\begin{pmatrix} P_{mm} & P_{mf} \\ 0 & P_{ff} \end{pmatrix} \begin{pmatrix} S_{mm}^T & S_{mf}^T \\ 0 & S_{ff}^T \end{pmatrix} = 0$$

System of non-linear equations

Mass action law

$$S_{mm} \log c = \log K,$$

$$S_{mf} \log c + S_{ff} \log \bar{c} = \log \bar{K}.$$

Mass conservation

$$P_{mm} c + P_{mf} \bar{c} = T$$

$$P_{ff} \bar{c} = W,$$

T, W known from transport

Numerical solution of nonlinear problem

Take concentration logarithms as main unknowns
Use globalized Newton's method (line search, trust region).

Mineral reactions

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

Numerical solution of nonlinear problem

Take concentration logarithms as main unknowns

Use globalized Newton's method (line search, trust region).

Mineral reactions

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

Role of chemical model

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

$C = P_{mm}c$, $F = P_{mf}\bar{c}$, $G = P_{ff}\bar{c}$.

Result of chemical problem

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

Outline

1 Motivations

2 Basic models and methods
- Flow model
- Transport model
- Chemistry

3 Formulations and solution methods

4 Examples
- Ion exchange
- CO2 example

5 Conclusions

Reactive transport model

Balance equations

$$
\begin{aligned}
\phi \partial_t c + L c &= S_{mm}^T R_e^a + S_{mf}^T R_e^h + P^T R_k(c, \bar{c}) \\
\phi \partial_t \bar{c} &= \phantom{S_{mm}^T R_e^a +{}} S_{ff}^T R_e^h + Q^T R_k(c, \bar{c})
\end{aligned}
$$

R_e equilibrium rates unknown, R_k kinetic rates, known expression

Reactive transport model

Balance equations

$$\begin{aligned}
\phi \partial_t c + Lc &= S_{mm}^T R_e^a + S_{mf}^T R_e^h + P^T R_k(c, \bar{c}) \\
\phi \partial_t \bar{c} &= S_{ff}^T R_e^h + Q^T R_k(c, \bar{c})
\end{aligned}$$

R_e equilibrium rates unknown, R_k kinetic rates, known expression

Example

$$R_k = \begin{cases} k_d(T)\, Sr_M\, (1 - Q/K) & \text{for dissolution} \\ k_p(T)\, Sr_M\, (Q/K - 1) & \text{for precipitation} \end{cases}$$

Q is solubility product, S_r reactive surface, k speed per unit surface.

Non Lipschitz

Coupled formulation

Elimination of equilibrium rates

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

Coupled formulation

Elimination of equilibrium rates

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

Special case : no kinetic reactions

$$\begin{aligned}
&\phi\frac{\partial T^{ic}}{\partial t} + L(C^{ic}) = 0, && ic = 1, \ldots, N_c \\
&T^{ic}_{ix} = C^{ic}_{ix} + F^{ic}_{ix} && ic = 1, .., N_c \text{ and } ix = 1, .., N_x \\
&F_{ix} = \Psi_C(T_{ix}) && ix = 1, \ldots, N_x.
\end{aligned}$$

Solution strategies

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

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

Solution strategies

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

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

Direct substitution Lichtner et al., Saaltink et al.

- + accurate, robust,
- − difficult to code, large non-linear system

Solution strategies

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

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

Direct substitution Lichtner et al., Saaltink et al.

- + accurate, robust,
- − difficult to code, large non-linear system

DAE formulation Erhel and de Dieuleveult

- + use quality DAE software, accurate
- − expensive

Solution strategies

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

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

Direct substitution Lichtner et al., Saaltink et al.

- + accurate, robust,
- – difficult to code, large non-linear system

DAE formulation Erhel and de Dieuleveult

- + use quality DAE software, accurate
- – expensive

Elimination technique Knabner et al.

- + Efficient, accurate,
- – difficult to code

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

Discrete non-linear system

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

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

Discrete non-linear system

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

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

Discrete non-linear system

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

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

Discrete non-linear system

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

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

Discrete non-linear system

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

Formulation without kinetic reactions

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

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

Discrete non-linear system

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

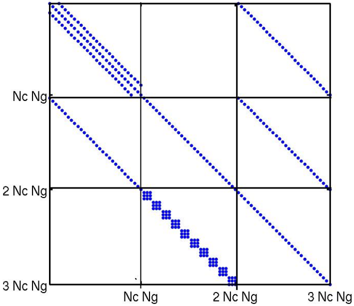
Formulation without kinetic reactions

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

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)

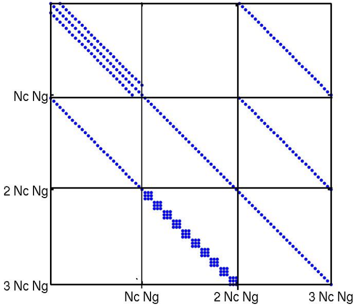


Jacobian structure

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

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)

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)

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)

Outline

1. Motivations

2. Basic models and methods
   - Flow model
   - Transport model
   - Chemistry

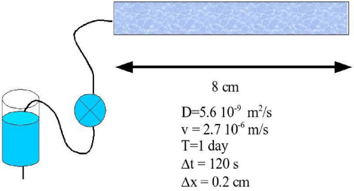
3. Formulations and solution methods

4. Examples
   - Ion exchange
   - CO2 example

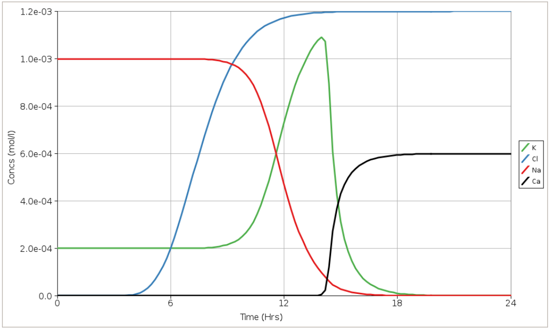
5. Conclusions

Example : ion exchange

Column experiment (Phreeqc ex. 11)

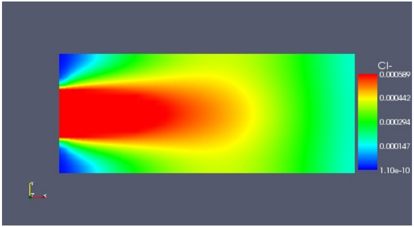


Column contains a solution with $1\mathrm{mmol}$ Na, $0.2\mathrm{mmol}$ K and $1.2\mathrm{mmol}$ NO_3. Inject solution with $1.2\mathrm{mmol}CaCl_2$. $CEC = 1.1\,10^{-3}$.

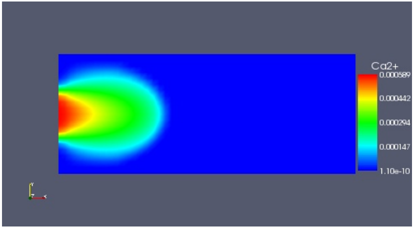


Ion exchange example (ctd)

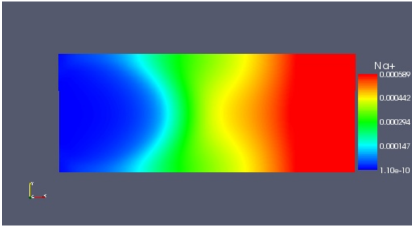
Snapshots at $t = 35$



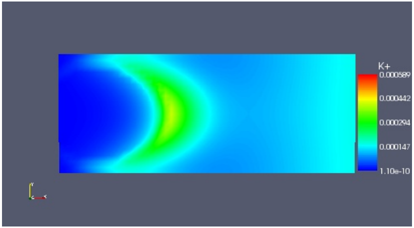
Cl



Ca



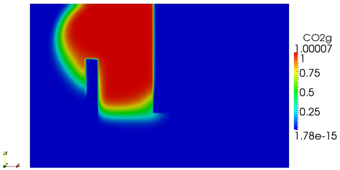
Na



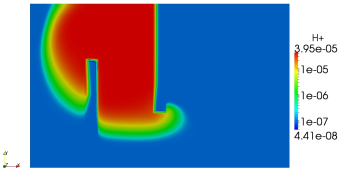
K

Application to CO2 model (LifeV, Kinsol)

Gas concentration

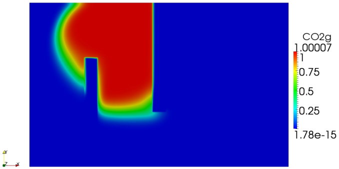


pH

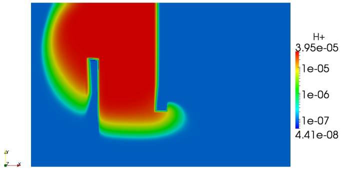


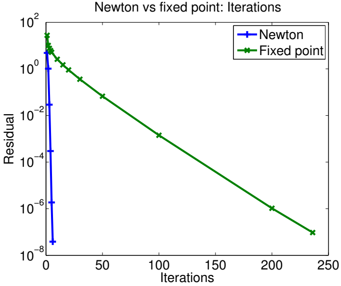
Application to CO2 model (LifeV, Kinsol)

Gas concentration

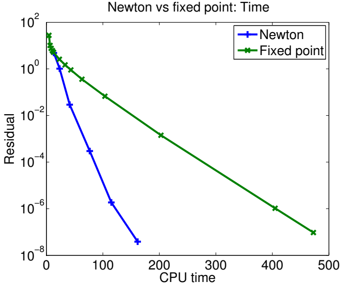


pH



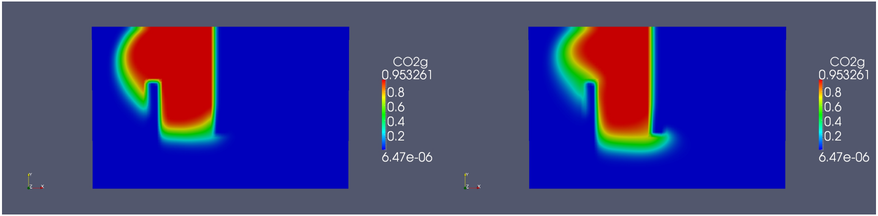


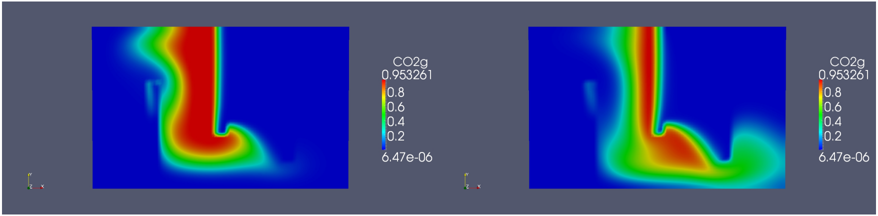
Iterations



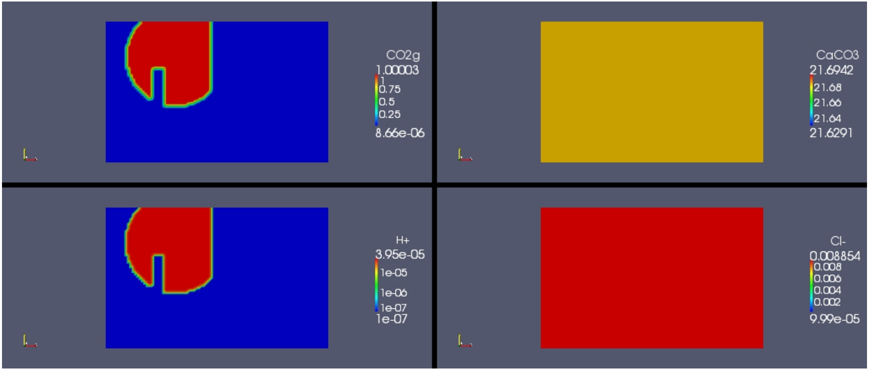
time

Evolution of CO2 concentration

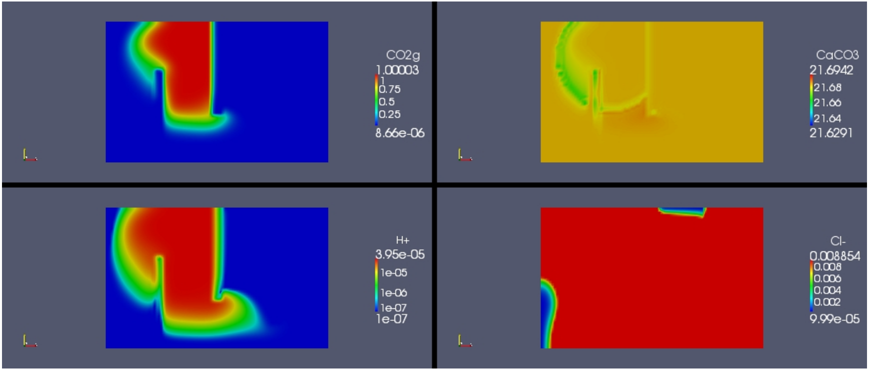




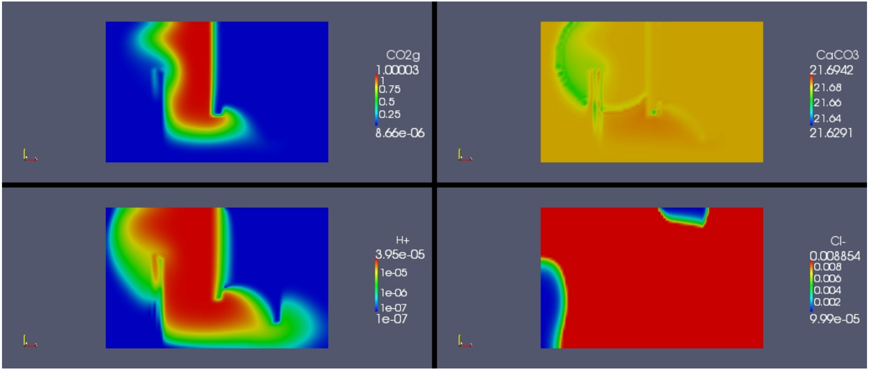
Evolution of concentrations



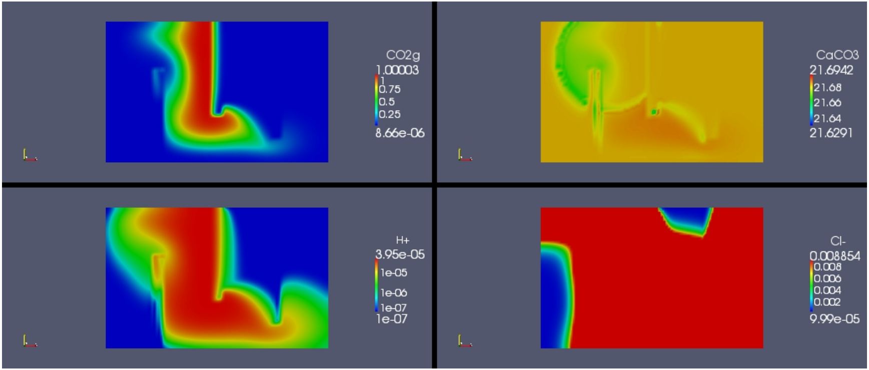
Evolution of concentrations



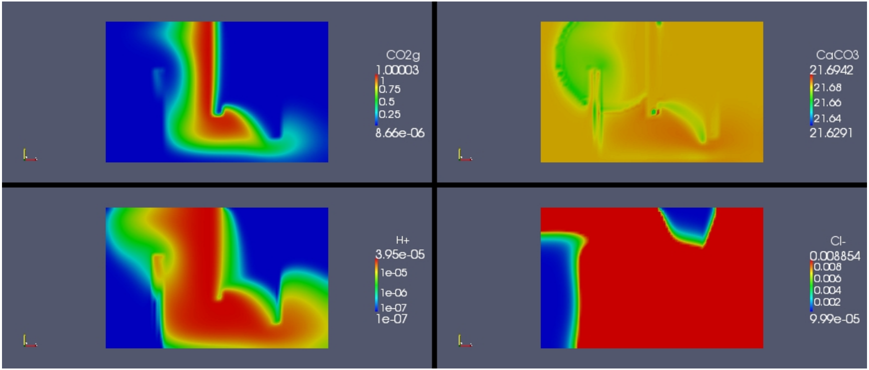
Evolution of concentrations



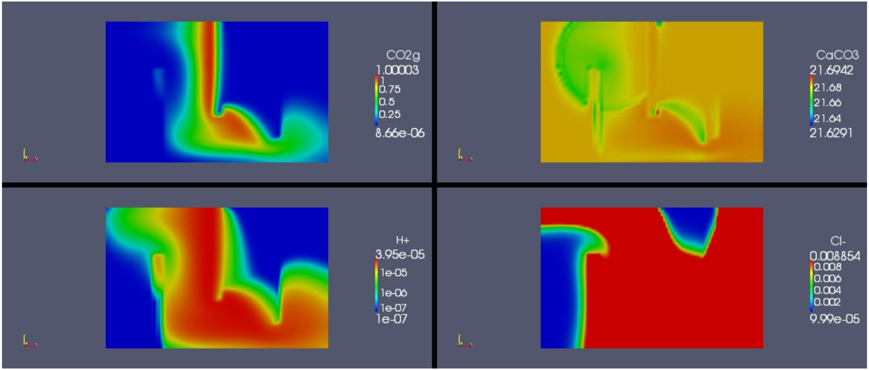
Evolution of concentrations



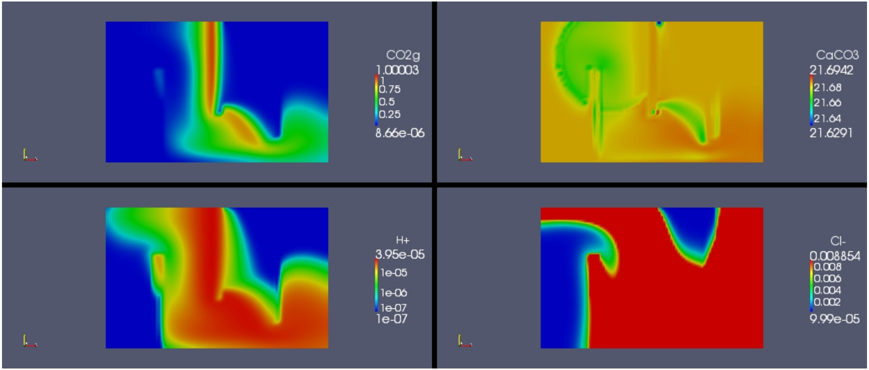
Evolution of concentrations



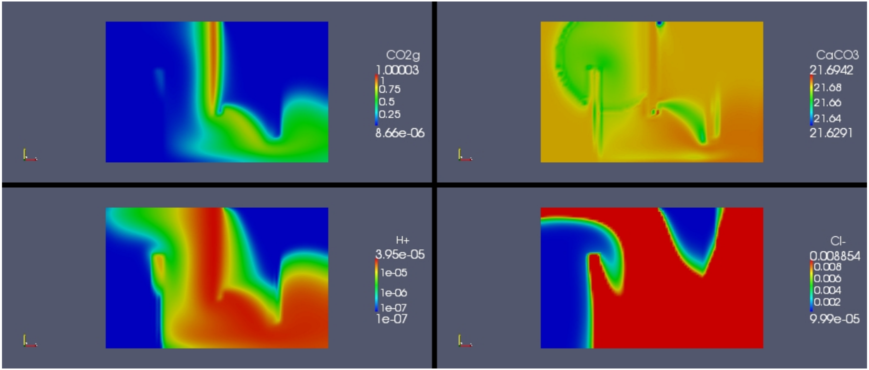
Evolution of concentrations



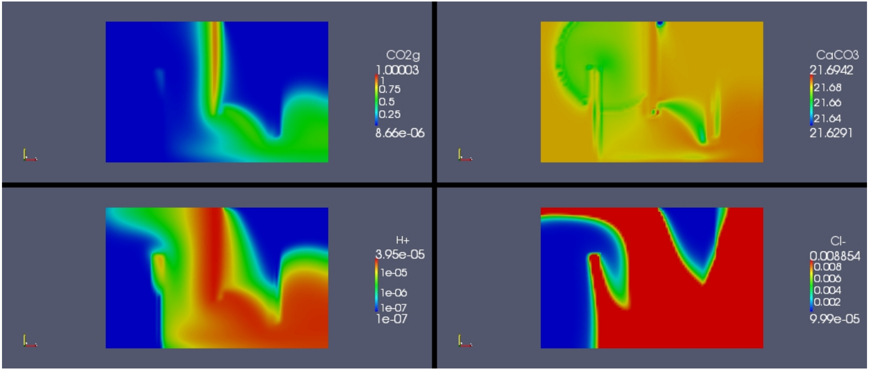
Evolution of concentrations



Evolution of concentrations

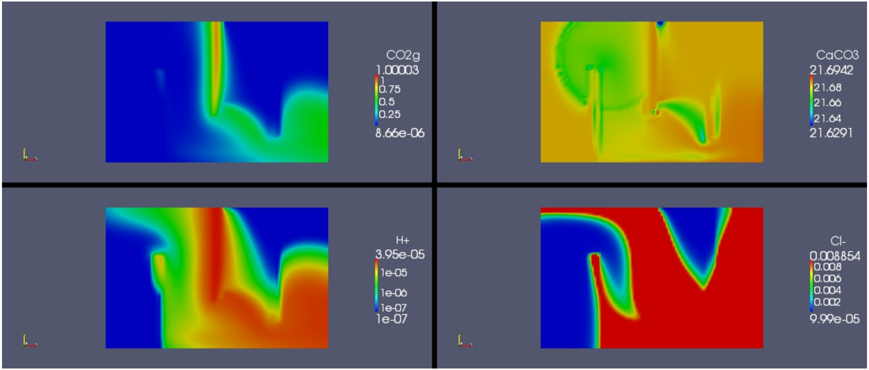


Evolution of concentrations

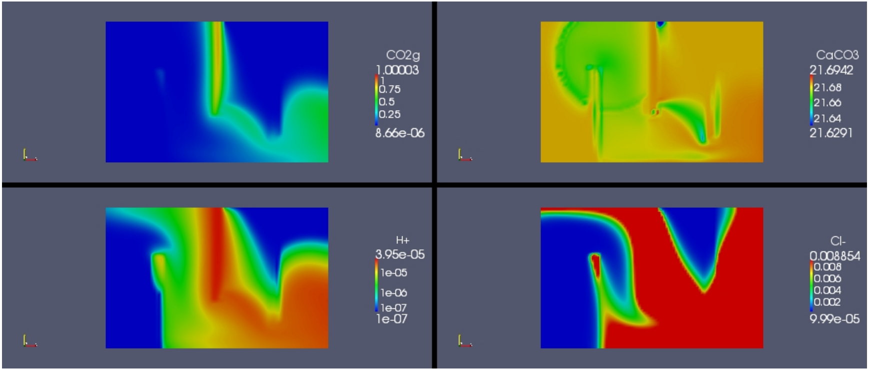


INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE INRIA centre de recherche PARIS - ROCQUENCOURT

Evolution of concentrations



Evolution of concentrations



Outline

1. Motivations
2. Basic models and methods
   - Flow model
   - Transport model
   - Chemistry
3. Formulations and solution methods
4. Examples
   - Ion exchange
   - CO2 example
5. Conclusions

Conclusions – perspectives

- Robust methods for flow and transport
- Newton–Krylov as a framework for code coupling
- Extension of chemical solver to handle minerals and gas
- Preconditioner for simplified system, mesh independent convergence

Conclusions – perspectives

- Robust methods for flow and transport
- Newton–Krylov as a framework for code coupling
- Extension of chemical solver to handle minerals and gas
- Preconditioner for simplified system, mesh independent convergence

- Implement analytical Jacoban – vector product
- Implement kinetic reactions
- Parallel computing (w. MOX, Milano)
- Extension to multiphase (compositional) flow

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

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

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

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

Jacobian preconditioning

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

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

Block preconditioning

Jacobi $\mathbf{P_J} = \begin{pmatrix} \mathbf{M} + \Delta t \, \mathbf{L} & 0 \\ 0 & \mathbf{I} \end{pmatrix}$, $\Lambda(P_J^{-1} J) \subset [1 - iCh, 1 + iCh]$

Gauss–Seidel $\mathbf{P_{GS}} = \begin{pmatrix} \mathbf{M} + \Delta t \, \mathbf{L} & 0 \\ -\mathbf{D} & \mathbf{I} \end{pmatrix}$, $\Lambda(P_{GS}^{-1} J) \subset [1, 1 + Ch^2]$

Schur $J_2 = I + \mathbf{D}(\mathbf{M} + \Delta t \mathbf{L})^{-1} \mathbf{M}$, $\Lambda(J_2) \subset [1, 1 + Ch^2]$

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

Preconditioner performance

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

Preconditioner performance

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

Nevertheless ...

Preconditioner performance

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

Nevertheless ...

	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

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

Nevertheless ...

	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
None	8	54	10	100	17	238	33	658
BGS	8	11	10	15	14	22	21	36

Preconditioner performance

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

	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
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