

A Newton-Krylov method for coupling transport with chemistry in porous media

Laila Amir^{1,2} Michel Kern²

¹ITASCA Consultants

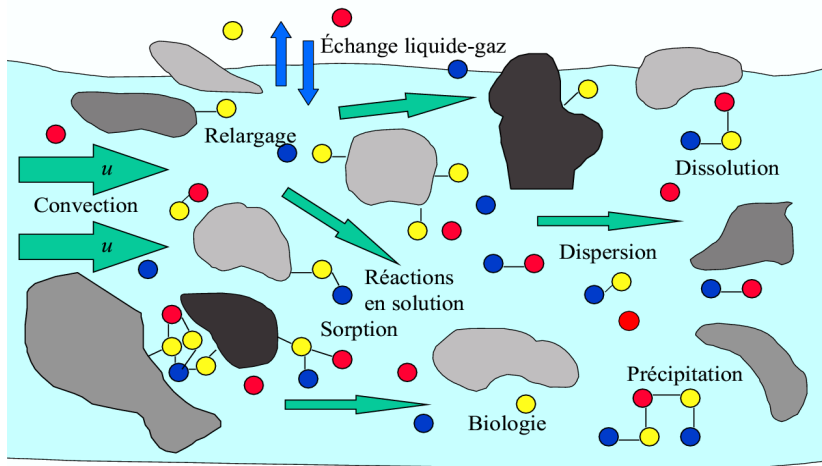
²INRIA Rocquencourt

Colloque GDR MoMaS

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- 1 Solving chemical equilibrium problems
- 2 Transport in a heterogeneous medium
- 3 Coupled models
- 4 Résultats numériques

Chemical and hydrogeological phenomena



Chemical reactions :

$$x_i \rightleftharpoons \sum_{j=1}^{N_c} S_{ij} c_j, \quad i = 1, \dots, N_x$$

$$y_i \rightleftharpoons \sum_{j=1}^{N_c} A_{ij} c_j + \sum_{j=1}^{N_s} B_{ij} s_j, \quad i = 1, \dots, N_y,$$

c_j aqueous (mobile) components, s_j sorbed (immobile) components,
 x_i aqueous secondary species, y_i fixed secondary species.

System of non-linear equations

Mass action law

$$\log x = S \log c + \log K_x,$$

$$\log y = A \log c + B \log s + \log K_y.$$

Mass conservation

$$c + S^t x + A^T y = T, \quad T \text{ known from transport}$$

$$s + B^T y = W, \quad W \text{ imposed}$$

Dissolved total : $C = c + S^T x$, Fixed total : $F = A^T y$.

$$C = \Phi(T), \quad F = \Psi(T)$$

Role of chemical model

Given totals T (and W , known), split into mobile and immobile total concentrations

$$C = \Phi(T), \quad F = \Psi(T)$$

Take concentration **logarithms** as main unknowns

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

Diffusion–convection equation

$$\omega \frac{\partial c}{\partial t} + \underbrace{\frac{\partial}{\partial x} \left(\mathbf{u}c - \mathbf{D} \frac{\partial c}{\partial x} \right)}_{L(c)} = f \quad \text{for } 0 < x < L \quad + \text{IC}$$

$$c = c_d \text{ at } x = 0 \quad - \mathbf{D} \frac{\partial c}{\partial x} = 0 \text{ at } x = L.$$

Desirable properties

- **monotonicity** of the scheme
- Control of **numerical diffusion**
- **Implicit** treatment of diffusion
- Handling of **heterogeneities**

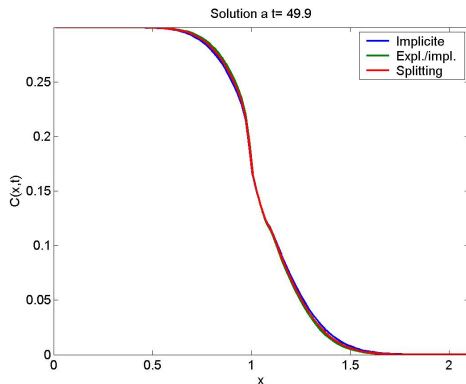
Numerical schemes for transport

3 schemes

Fully implicit

Implicit diffusion, explicit convection

Operator splitting



1D medium with 3 layers,
like TR benchmark

The coupled formulation

Transport for each species and component

$$\begin{aligned}\frac{\partial \mathbf{x}_i}{\partial t} + L(\mathbf{x}_i) &= r_i^{\mathbf{x}}, & \frac{\partial \mathbf{c}_j}{\partial t} + L(\mathbf{c}_j) &= r_j^{\mathbf{c}}, \\ \frac{\partial \mathbf{y}_i}{\partial t} &= r_i^{\mathbf{y}}, & \frac{\partial \mathbf{s}_j}{\partial t} &= r_j^{\mathbf{s}},\end{aligned}$$

The coupled formulation

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Eliminate the terms of reactions r_i and r_j (unknowns)
by using conservation laws, discretize in time

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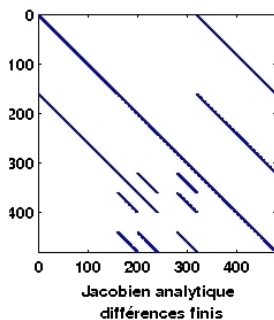
$$\begin{cases} \frac{C^{n+1} - C^n}{\Delta t} + \frac{F^{n+1} - F^n}{\Delta t} + L(C^{n+1}) = 0 \\ T^{n+1} = C^{n+1} + F^{n+1} \\ F^{n+1} = \Psi(T^{n+1}) \end{cases}$$

Non-linear system, resolution by Newton's method?
Exact or inexact Newton method?

Structure of Jacobian matrix

$$\text{Jacobian : } f'(C, T, F) = \begin{pmatrix} (I + \Delta t L) & 0 & I \\ -I & I & -I \\ 0 & -\Psi'(T) & I \end{pmatrix}$$

$\Psi'(T)$ jacobian of chemistry



Storage of jacobian matrix is expensive,
size of matrix is $3N_x N_c \times 3N_x N_c$

Newton Krylov method

- Solve the linear system by an **iterative** method
- GMRES, TFQMR and BiCGStab require only jacobian matrix by vector products.
Can be approximated by finite differences or computed analytically.

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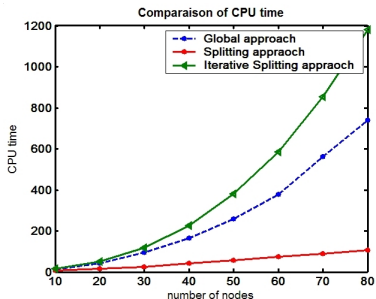
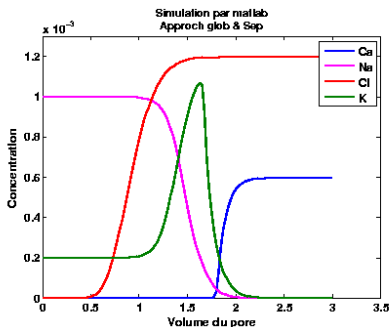
Inexact Newton

- **Approximation** of the Newton's direction :

$$\|f'(x_k)d + f(x_k)\| \leq \eta \|f(x_k)\| \quad (0 < \eta < 1)$$

- 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)

Validation of coupled code



Results from PhreeqC ion exchange example

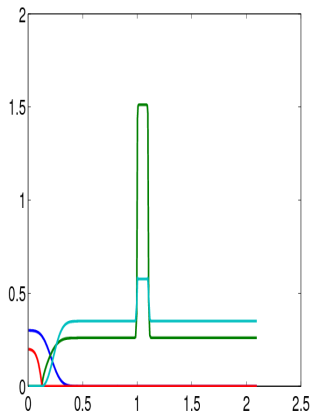
CPU time vs number of function evaluations for 3 methods

MoMaS benchmark : a first attempt

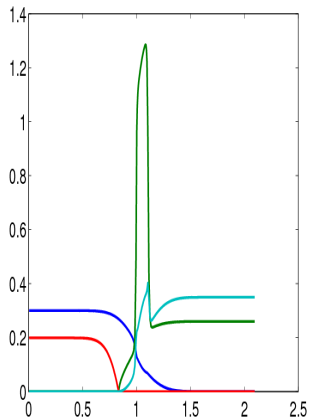
Concentration of components in the column

X1, X2, X3, X4.

t=10.00



t=50.00



Problem with the chemistry solver ?

Easy benchmark : validated initial and boundary conditions

3.0000000e-01	3.0000000e-01	9.3576230e-20	7.6812047e-21
8.0993946e-03	2.4161985e-01	2.5971841e-01	1.5115502e+00
2.0161118e-01	2.4161985e-01	5.0762747e-18	2.0767417e-17
1.0526649e-34	1.4448106e-41	3.4953787e-01	5.7561100e-01
9.0324411e-01	1.1642278e-13	3.9074372e-01	7.9128388e+00
cL1	cL0	clnitA	clnitB

Computation with Maple : symbolic methods for polynomial systems
Compute (lexicographic) Gröbner basis, solve polynomial in one variable (high degree), then back substitute. **FGb/RS** software by Faugère and Rouiller
Doesn't yet work for full system (no lex basis)

- Fix chemistry solver
- Solve 1D easy benchmark
- Extend to 2D geometry
- Include minerals, kinetic reactions
- Find **good** preconditionner (operator split, block factorization)