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# Krylov methods applied to reactive transport models

**Jocelyne Erhel**

Inria/IRMAR, RENNES

Joint work with C. de Dieuleveult, S. Sabit and Y. Crenner (Inria)  
F. Pacull, P.-M. Gibert and D. Tromeur-Dervout (university of Lyon)

**SIAM conference on Geosciences**

**Erlangen, September 2017**

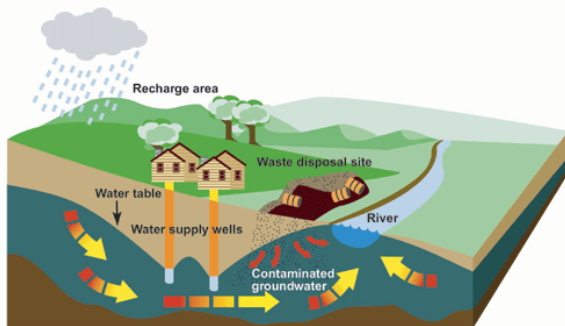
## 1 Reactive transport model

- 1 Reactive transport model
- 2 Numerical schemes

- 1 Reactive transport model
- 2 Numerical schemes
- 3 Numerical experiments

## Groundwater contamination

Groundwater contamination from a waste disposal site



- Manage groundwater resources
- Prevent pollution
- Store waste, store energy, capture  $CO_2$
- Use geothermal energy
- ...

## Reactive transport model

### Transport: Partial Differential Equations

- Single aqueous phase in porous medium
- Advection and dispersion
- Linear transport operator

### Chemistry: Algebraic Equations

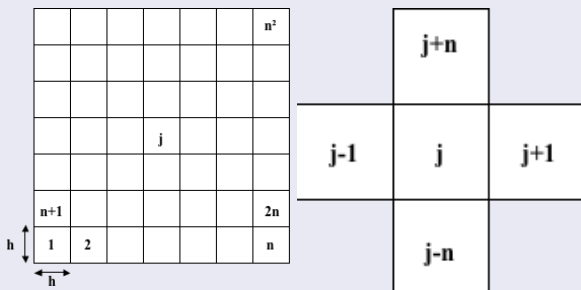
- Thermodynamical equilibrium
- Aqueous, fixed and mineral reactions
- $N_c$  mobile primary species and  $N_s$  fixed primary species
- Secondary species function of primary species
- Minerals at saturation

## Space discretization

### Discretization schemes

- Mesh of computational domain with  $N_m$  points (cells, nodes, ...)
- Eulerian discretization (Mixed Finite Element, Finite Volume, ...)
- Algebraic chemistry at each point

### 2D regular mesh





## Semi-discrete reactive transport model

## Mass conservation equations

$$\begin{cases} dy/dt + f(c) = q, \\ -y + g_c(c, s) = 0, \\ g_s(c, s) = 0, \\ y(t = 0) = y_0. \end{cases}$$

- $y$ : total analytical concentrations  $y \in R^{N_c \times N_m}$
- $c$ : mobile species  $c \in R^{N_c \times N_m}$  (ions, etc)
- $s$ : fixed species  $s \in R^{N_s \times N_m}$  (sorbed species, minerals, etc)
- $f(c)$ : discrete transport applied to mobile species
- $q$ : boundary conditions
- $y_0$ : initial conditions
- $g_c(c, s)$ : total mass of mobile species (involving secondary species)
- $g_s(c, s)$ : total mass of fixed species (involving secondary species) and saturation thresholds of minerals

## Time discretization and nonlinear solver

### Implicit Euler

$$\begin{cases} y + \Delta t f(c) - y^n = \Delta t q, \\ -y + g_c(c, s) = 0, \\ g_s(c, s) = 0. \end{cases}$$

### Nonlinear equations at each time step

$$\begin{cases} g_c(c, s) + \Delta t f(c) - y^n - \Delta t q = 0, \\ g_s(c, s) = 0. \end{cases}$$

### Nonlinear solver: Newton's method

- linearization of equations
- Newton-LU: direct linear solver (LU)
- Newton-GMRES: iterative Krylov solver (GMRES)

## Newton's method

Function  $F(c, s)$  at each point  $j$ ,  $1 \leq j \leq N_m$

$$\begin{cases} F_j(c, s) = \begin{pmatrix} g_{c,j}(c, s) + \Delta t f_j(c) - y_j^n - \Delta t q_j \\ g_{s,j}(c, s) \end{pmatrix}, \\ g_{c,j}(c, s) = \bar{g}_c(c_j, s_j), \\ g_{s,j}(c, s) = \bar{g}_s(c_j, s_j), \\ f(c) = (L \otimes I_{N_m}) \text{vec}(C(c)) \end{cases}$$

Jacobian matrix

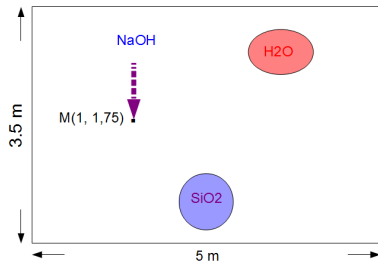
$$\begin{cases} J_F(c, s) = J_g(c, s) + \Delta t \begin{pmatrix} J_f(c) & 0 \\ 0 & 0 \end{pmatrix}, \\ J_g(c, s) = \mathbf{diag}(J_{\bar{g}}(c_j, s_j)), \\ J_f = (L \otimes I_{N_m}) \mathbf{diag}(dC_j(c)/dc_j) \end{cases}$$

Preconditioning  $M$

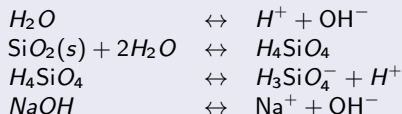
$$M = J_g(c, s)$$

## Numerical example: Andra qualification test

### Injection of alkaline water



### Chemistry



Mugler, G. and Bernard-Michel, G. and Faucher, G. and Miguez, R. and Gaombalet, J. and Loth, L. and Chavant, C., Projet ALLIANCES: plan de qualification, CEA, ANDRA, EDF

## Results of simulations: Andra test case



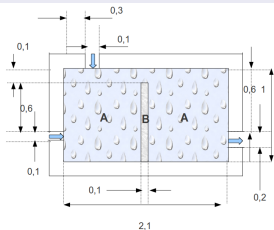
Computations done using GRT3D (Inria and ANDRA software)



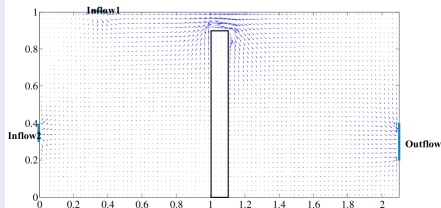
J. Erhel, S. Sabit and C. de Dieuleveult, Solving Partial Differential Algebraic Equations and Reactive Transport Models , Computational Science, Engineering and Technology Series, 2013

## Numerical experiment: MoMaS 2D easy test case

### Flow conditions

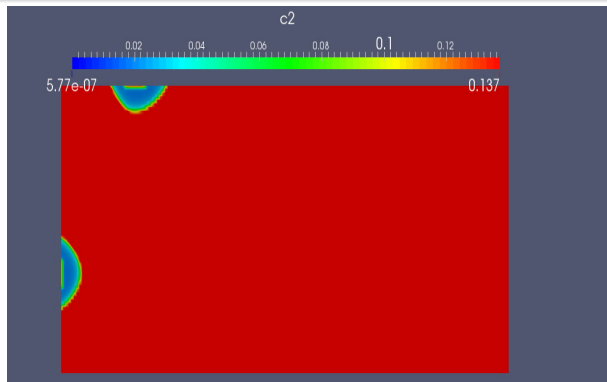


### Velocity



J. Carayrou, M. Kern and P. Knabner, Reactive transport benchmark of MoMaS, Computational Geosciences, 2010

## Results of simulations: MoMaS 2D easy test case



Computations done using GRT3D (Inria and ANDRA software) with a mesh of  $80 \times 168$  cells



J. Erhel and S. Sabit, Analysis of a global reactive transport model and results for the MoMaS benchmark, Mathematics and Computers in Simulation, 2017

## Comparison of Newton-LU and Newton-GMRES

## Newton-LU with UMFPACK and Newton-GMRES with PETSC

Test case	Mesh	Solver	CPU Time (minutes)
ANDRA	322 × 224	LU	94
		GMRES	8
MOMAS	40 × 84	LU	189
		GMRES	52
MOMAS	80 × 168	LU	3012
		GMRES	621



F. Pacull, P.-M. Gibert, S. Sabit, J. Erhel and D. Tromeur-Dervout, Parallel Preconditioners for 3D Global Reactive Transport, Parallel CFD, Norway, 2014



## Concluding remarks

### Efficiency of the software GRT3D

- global approach (implicit scheme and Newton's method)
- adaptive time step and modified Newton iterations (convergence monitoring)
- Newton-GMRES using the specific structure

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### Future work

- Adaptive mesh refinement
- Kinetic reactions

## Announcement



Computational Methods for Water Resources  
Saint-Malo, France, June 3-7, 2018  
Website: <http://cmwrconference.org/>