

Krylov methods applied to reactive transport models

Jocelyne Erhel

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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

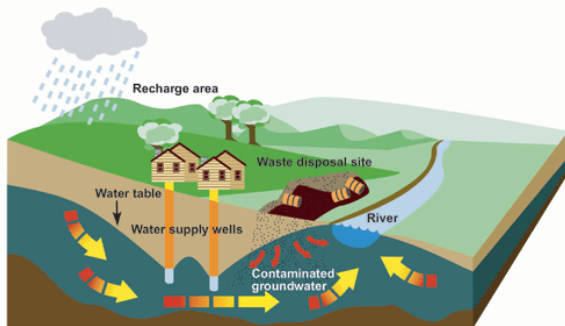
1 Reactive transport model

- 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

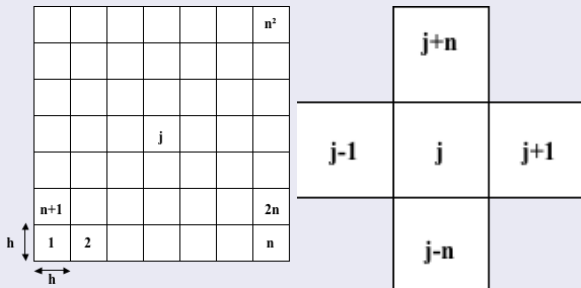
- Thermodynamical equilibrium
- Aqueous, fixed and mineral reactions
- N_c mobile primary species and N_s fixed primary species
- Secondary species function of primary species
- Minerals at saturation

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

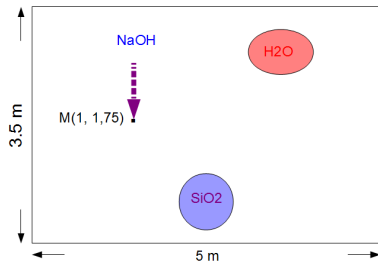
$$\begin{cases} J_F(c, s) = J_g(c, s) + \Delta t \begin{pmatrix} J_f(c) & 0 \\ 0 & 0 \end{pmatrix}, \\ J_g(c, s) = \mathbf{diag}(J_{\bar{g}}(c_j, s_j)), \\ J_f = (L \otimes I_{N_m}) \mathbf{diag}(dC_j(c)/dc_j) \end{cases}$$

Preconditioning M

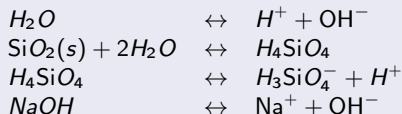
$$M = J_g(c, s)$$

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



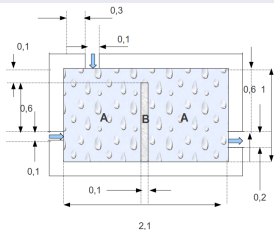
Computations done using GRT3D (Inria and ANDRA software)



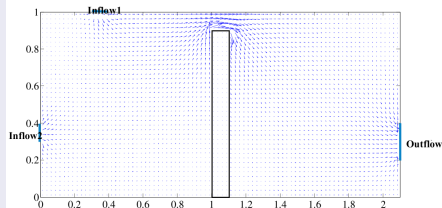
J. Erhel, S. Sabit and C. de Dieuleveult, Solving Partial Differential Algebraic Equations and Reactive Transport Models , Computational Science, Engineering and Technology Series, 2013

Numerical experiment: MoMaS 2D easy test case

Flow conditions

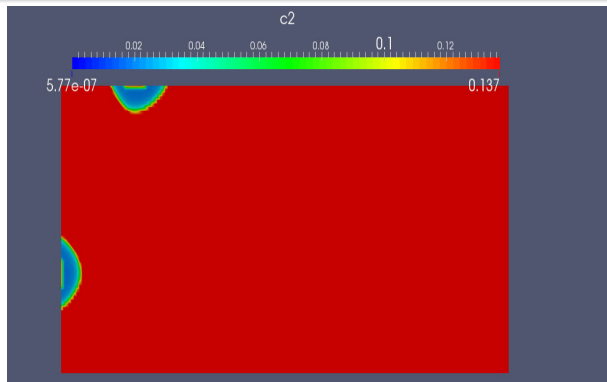


Velocity



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 80×168 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/>