Krylov methods applied to reactive transport models

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1. Reactive transport model

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2. Numerical schemes

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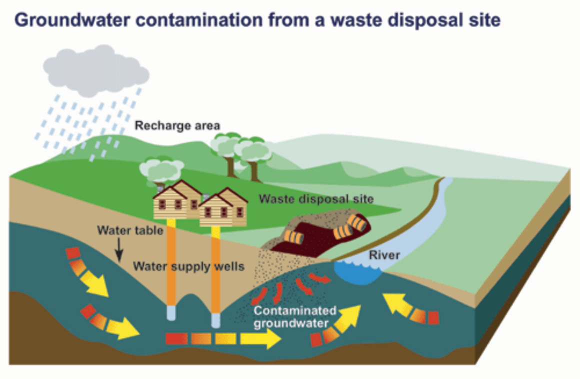
2. Numerical schemes
3. Numerical experiments

Groundwater contamination



- 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

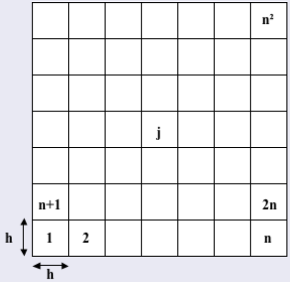
- Thermodynamical equilibrium
- Aqueous, fixed and mineral reactions
- N_c mobile primary species and N_s fixed primary species
- Secondary species function of primary species
- Minerals at saturation

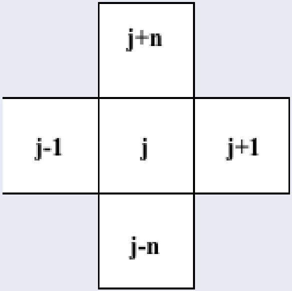
Space discretization

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, $1 \le j \le N_m$

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

Jacobian matrix

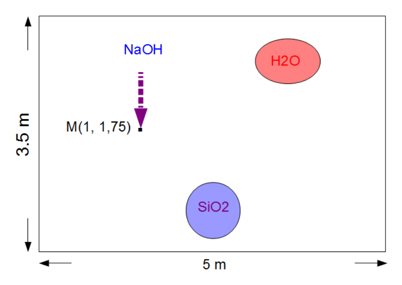
$$\left\{\begin{array}{l} J_F(c,s) = J_g(c,s) + \Delta t \begin{pmatrix} J_f(c) & 0 \\ 0 & 0 \end{pmatrix}, \\ J_g(c,s) = \mathbf{diag}(J_{\overline{g}}(c_j, s_j)), \\ J_f = (L \otimes I_{N_m}) \mathbf{diag}(dC_j(c)/dc_j) \end{array}\right.$$

Preconditioning M

$M = J_g(c,s)$

Numerical example: Andra qualification test

Injection of alcaline water

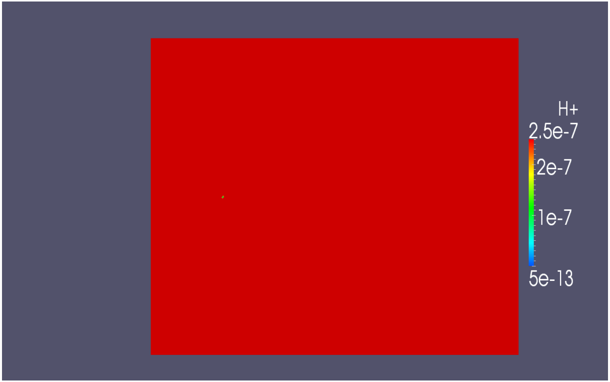


Chemistry

$$
\begin{array}{lcl}
H_2O & \leftrightarrow & H^+ + \mathrm{OH}^- \\
\mathrm{Si}O_2(s) + 2H_2O & \leftrightarrow & H_4\mathrm{Si}O_4 \\
H_4\mathrm{Si}O_4 & \leftrightarrow & H_3\mathrm{Si}O_4^- + H^+ \\
NaOH & \leftrightarrow & \mathrm{Na}^+ + \mathrm{OH}^-
\end{array}
$$

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

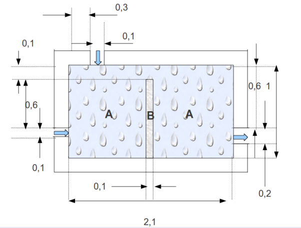


Computations done using GRT3D (Inria and ANDRA software)

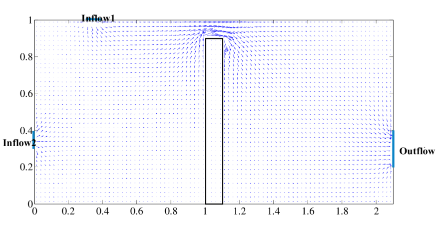
J. Erhel, S. Sabit and C. de Dieuleveult, Solving Partial Differential Algebraic Equations and Reactive Transport Models , Computational Science, Engineering and Technology Series, 2013

Numerical experiment: MoMaS 2D easy test case

Flow conditions

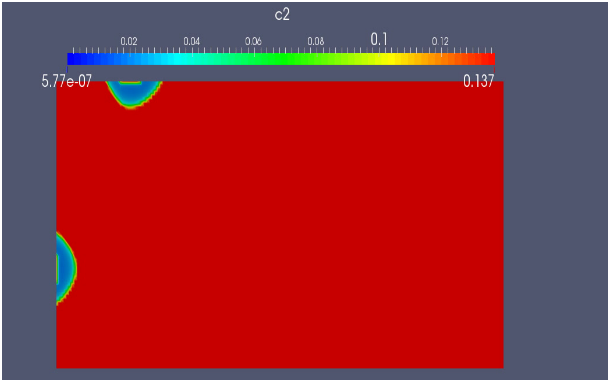


Velocity



J. Carrayrou, 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 GMRES	94 8
MOMAS	40×84	LU GMRES	189 52
MOMAS	80×168	LU GMRES	3012 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/