# Solving Partial Differential Algebraic Equations and reactive transport models

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co-authors
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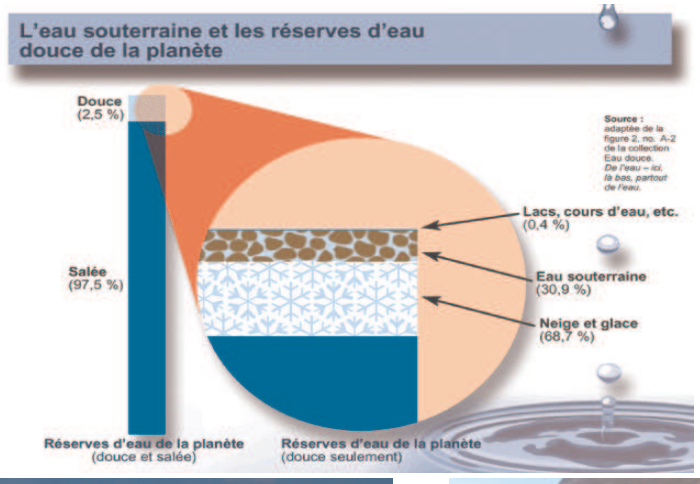
# 1 Introduction

# Water resources




Pictures: Yves Chaux, Rennes, France

Diagram: `http://www.ec.gc.ca/water/f_main.html`

## Reactive transport modeling

- Coupling transport by advection-dispersion with geochemistry
- System of Partial Differential Algebraic equations
- Model with thermodynamic equilibrium
- Method of lines: first discretize in space then in time $\Rightarrow$ DAE system
- Explicit scheme (SNIA): decoupling but stability restrictions
- Implicit scheme (Global): stability but nonlinear coupled system

**Our method: global approach GDAE**

 S. Kräutle, P. Knabner, (2005); A new numerical reduction scheme for fully coupled multicomponent transport-reaction problems in porous media; Water Resources Research, Vol. 41, W09414, 17 pp.

 S. Molins, J. Carrera, C. Ayora, Carlos and M.W. Saaltink, (2004); A formulation for decoupling components in reactive transport problems; Water Resources Research, Vol.40, W10301, 13 pp.

 C. de Dieuleveult, J. Erhel , M. Kern; A global strategy for solving reactive transport equations; Journal of Computational Physics,2009.

# Mass action laws

## Aqueous reactions

$$x_i(c) = K_{ci} \prod_{j=1}^{N_c} c_j^{S_{ij}}, \quad i = 1, \dots N_x \tag{1}$$

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## Precipitation reactions

$$\Pi_i(c) = K_{pi} \prod_{j=1}^{N_c} c_j^{E_{ij}}, \quad i = 1, \dots N_p \tag{3}$$

# Mass conservation laws

## Chemical variables and functions

$$X = \begin{pmatrix} c \\ s \\ p \end{pmatrix}, \quad \Phi(X) = \begin{pmatrix} c + S^T x(c) + A^T y(c,s) + E^T p \\ s + B^T y(c,s) \\ \Pi(c) \end{pmatrix} \tag{4}$$

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## Chemical model

$$\begin{cases} \Phi(X) = \begin{pmatrix} T \\ W \\ 1 \end{pmatrix}, \\ c \geq 0, \\ s \geq 0, \\ p > 0. \end{cases} \tag{5}$$

# Transport model

## Advection-Dispersion operator

$$\mathcal{L}(u) = \nabla \cdot (vu - D\nabla u)$$

$$D = d_m I + \alpha_T \|v\| I + (\alpha_L - \alpha_T) \frac{vv^T}{\|v\|}$$

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## Transport of mobile species

$$C(X) = c + S^T x(c) \tag{6}$$

$$\omega \frac{\partial T_i}{\partial t} + \mathcal{L}(C_i) = Q_i, \quad i = 1, \ldots, N_c \tag{7}$$

with boundary and initial conditions

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## Space discretization

with (for example) a finite difference method

$$T = (T_1, \ldots, T_{N_m}) \tag{8}$$

# Coupling transport with chemistry

## Semi-discrete reactive transport model

$$\begin{cases} \omega \frac{dT_i}{dt} + LC_i(X) = Q_i + G_i, \quad i = 1, \ldots, N_c, \\ \Phi(X_j) - \begin{pmatrix} T_j \\ W_j \\ 1 \end{pmatrix} = 0 \quad j = 1, \ldots, N_m, \\ \text{initial condition for } T, \end{cases} \tag{9}$$

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## DAE formulation

$$\begin{cases} \omega \frac{d\mathbf{vec}\, T}{dt} + (L \otimes I)\mathbf{vec}\, C(X) - \mathbf{vec}\, Q - \mathbf{vec}\, G = 0, \quad i = 1, \ldots, N_c, \\ \mathbf{vec}\, \Phi(X) - (I \otimes N)\mathbf{vec}\, T - \mathbf{vec}\, F = 0 \end{cases} \tag{10}$$

# DAE Global approach with substitution

## Time discretization: BDF scheme

$$\frac{d\mathbf{vec}\, T}{dt} \simeq \frac{a}{\Delta t}\mathbf{vec}\, T + \frac{1}{\Delta t}\mathbf{vec}\, Z,$$

$$\begin{cases} \frac{a\omega}{\Delta t}\mathbf{vec}\, T + (L \otimes I)\mathbf{vec}\, C(X) - \ldots = 0, \\ -(I \otimes N)\mathbf{vec}\, T + \mathbf{vec}\, \Phi(X) - \ldots = 0, \end{cases}$$

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## Substitution

$$R(X) = \frac{\Delta t}{a\omega}(L \otimes N)\,\mathbf{vec}\, C(X) + \mathbf{vec}\, \Phi(X) - \ldots$$

The Jacobian of $R$ is

$$J_R(X) = \frac{\Delta t}{a\omega}(L \otimes N)\,\mathbf{diag}\,(\frac{dC}{dX}(X_j)) + \mathbf{diag}(J_\Phi(X_j)).$$

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## Nonlinear system

$$R(X) = 0$$

solved with Newton method

# GRT3D software

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## Coupling modules

- The function $R(X)$
- The derivative $J_R(X)$
- The DAE solver IDA in SUNDIALS using Newton-LU method
- The sparse linear solver UMFPACK

# Versions of GRT3D

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No elimination of $T$ and $C$

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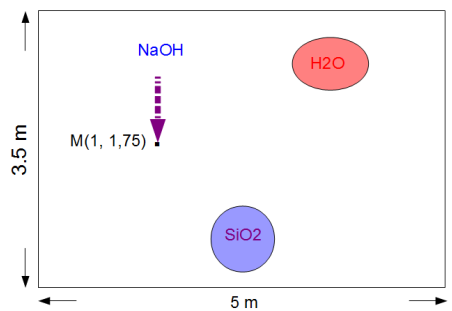
**Optimized version without logarithms**

Elimination of $T$ and $C$ in the linearized equations

# Numerical experiment

## Andra qualification test

Injection of alcaline water $NaOH$ in a porous medium with quartz $SiO_2$




$$\begin{cases} \epsilon = 1. \\ v = \begin{pmatrix} 5.7\,10^{-7} \\ 0. \end{pmatrix} \text{m.s}^{-1} \\ d_m = 0 \\ \alpha_L = 0.2\,\text{m} \\ \alpha_T = 0.05\,\text{m} \\ T = 30\,\text{days} \\ \text{no flux boundary conditions} \end{cases}$$

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.

# Chemistry conditions

## Chemistry equations

$$\begin{array}{lcll} H_2O & \leftrightarrow & H^+ + \mathrm{OH}^- & K_1 = 10^{-14} \\ H_4SiO_4 & \leftrightarrow & H_3SiO_4^- + H^+ & K_2 = 10^{-9.8} \\ H_4SiO_4 & \leftrightarrow & SiO_2(s) + 2H_2O & K_3 = 10^{3.6} \end{array} \tag{11}$$

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## Stoichiometric coefficients

| | $Na^+$ | $OH^-$ | $H4SiO4$ |
|---|---|---|---|
| $H^+$ | 0 | -1 | 0 |
| $H3SiO4^-$ | 0 | 1 | 1 |
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## Initial values

| | $Na^+$ | $OH^-$ | $SiO2$ |
|---|---|---|---|
| Outside $M$ | 0 | 0 | 10. |
| At $M$ | $10^{-2}$ | $10^{-2}$ | 10. |

# Accuracy results

## Accuracy of computed pH

$$E_{H^+} = \|\tilde{x}_{H^+} - x_{H^+}\|$$

| Mesh | first GRT3D | reduced GRT3D | optimized GRT3D |
|---|---|---|---|
| 21x14 | 1.333005E-11 | 1.591450E-11 | 8.040057E-11 |
| 41x28 | 2.489791E-09 | 2.489787E-09 | 8.113751E-11 |
| 81x56 | 7.640456E-09 | 7.640825E-09 | 3.055914E-10 |
| 71x101 | 7.747011E-09 | 7.746415E-09 | 4.161827E-10 |
| 161x112 | 7.9736E-09 | 7.9738E-09 | 2.6672E-10 |
| 322x224 | - | 3.0871E-09 | 4.3067E-10 |

# Performance results

## CPU time of GRT3D

Computations done on two six-core Intel Xeon processors X5690, with a frequence of 3.46 GHz and 4GB of RAM per core.

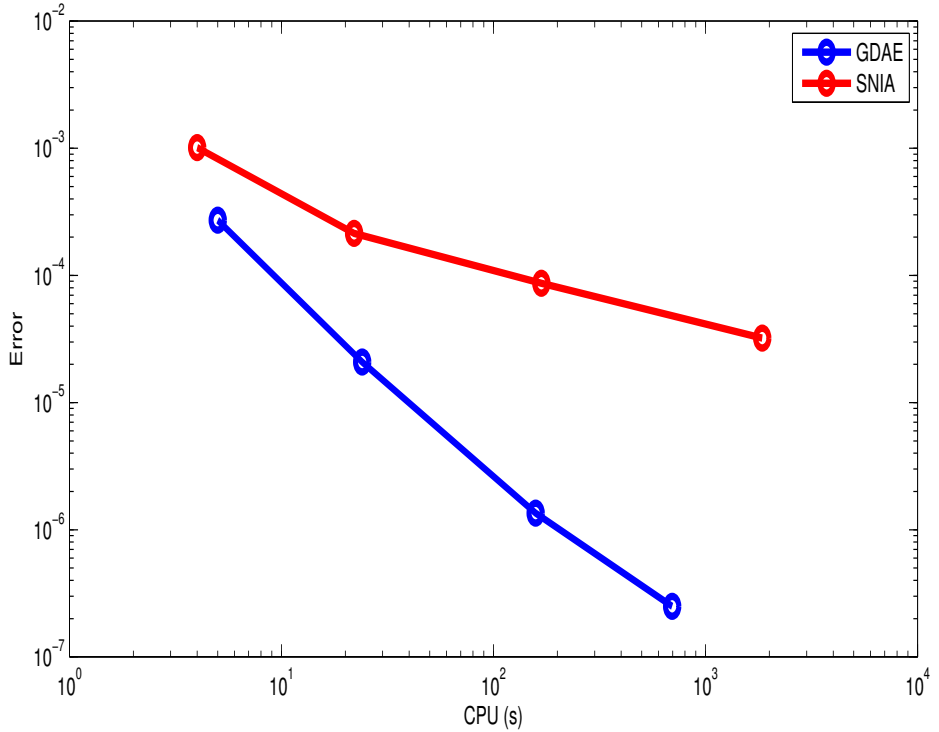
| Mesh | first GRT3D | reduced GRT3D | optimized GRT3D |
|---|---|---|---|
| 21x14 | 18 s | 4 s | 2 s |
| 48x28 | 1 min 36 s | 21 s | 8s |
| 81x56 | 6 min 33 s | 1 min 53 s | 50 s |
| 71x101 | 11 min 55 s | 3 min 28 s | 1 min 21 s |
| 161x112 | 32 min 43 s | 16 min 30 s | 4 min 32 s |
| 322x224 | - | 1 h 52 min | 37 min 38 s |

# Comparison results

## Performance/Accuracy results

Comparison with an analytical solution

$$E_{Na^+} = [\frac{1}{N_m N_t} \sum_{n,j} (\tilde{x}_{Na^+}(m_j, t_n) - x_{Na^+}(m_j, t_n))]^{1/2}$$



# Conclusion

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- The DAE global approach (implicit scheme and Newton method) is very efficient
- Substitution is very efficient
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## Future work

- Precipitation-dissolution with vanishing $p$
- Parallel computations