Radioactive waste management application

Technical meeting at ANDRA

Numerical models of reactive transport in porous media

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Funded by ANDRA


L'eau potable en Bretagne:
➔ 70% eaux de surface
➔ Quelques captages profonds
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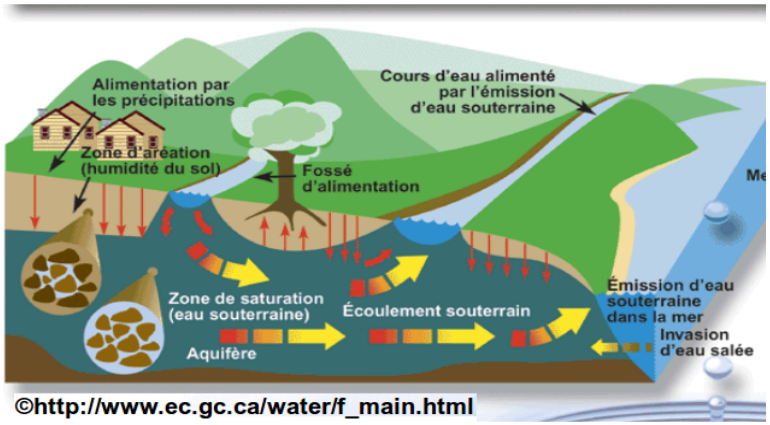
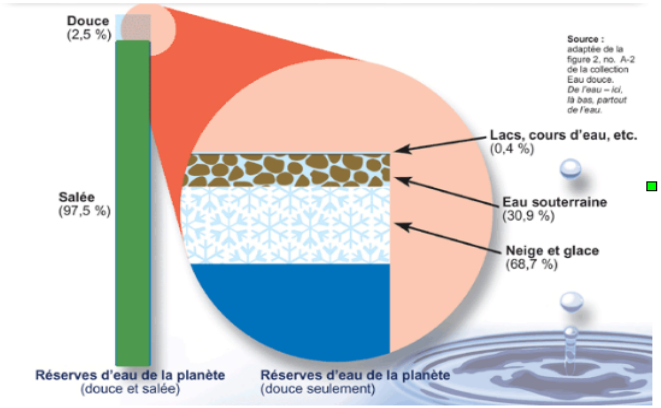

Alimentation par les précipitations
Cours d'eau alimenté par l'émission d'eau souterraine
Zone d'aération (humidité du sol)
Fossé d'alimentation
Zone de saturation (eau souterraine)
Écoulement souterrain
Émission d'eau souterraine dans la mer
Invasion d'eau salée
Aquifère
©http://www.ec.gc.ca/water/f_main.html


Douce (2,5 %)
Salée (97,5 %)
Lacs, cours d'eau, etc. (0,4 %)
Eau souterraine (30,9 %)
Neige et glace (68,7 %)
Réserves d'eau de la planète (douce et salée)
Réserves d'eau de la planète (douce seulement)
©http://www.ec.gc.ca/water/f_main.html

Introduction (1)

- **Modeling** reactive **transport** of contaminants in porous media is a complex problem combining the difficulties of **transport** modeling with those of modeling the **chemistry** and especially the **coupling** between the two.

- This modeling leads to a system of **partial differential equations and algebraic equations** whose unknowns are the quantities of chemical species.


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.

Introduction (2)

- Use a numerical method of lines, which leads to a semi-discrete differential-algebraic equations, after discretization in space.
  - The sequential non-iterative approach (SNIA) uses explicit Euler scheme.
  - The global approach of direct substitution (DSA) uses an implicit Euler scheme and a Newton method.
  - The global approach (GDAE) generalizes (DSA) by using an implicit scheme BDF in order and variable step.


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


C. de Dieuleveult and J. Erhel. A global approach to reactive transport : application to the momas benchmark. Computational Geosciences, 14(3) :451-464, 2010.


J. Erhel, S. Sabit, and C. de Dieuleveult. Computational Technology Reviews, chapter Solving Partial Differential Algebraic Equations and Reactive Transport Models. Saxe-Coburg Publications, 2013.

1 Geochemical model

Geochemical model

- **Chemical reactions :**

$$\sum_{i=1}^{N_E} \nu_{r,i} E_i \rightleftarrows 0, \ r = 1, N_r \tag{1}$$

- **Chemical equilibrium :**

$$\prod_{i=1}^{N_E} a_i^{\nu_{r,i}} = K_r, \ r = 1, N_r \tag{2}$$

- We assume that the system responses are independent so it is possible to reduce the system. We can express some unknown species which are called secondary, depending on other unknowns known as components .
- $E_\alpha \rightleftarrows \sum_a \nu_{\alpha,a} E_a$
- $E_\sigma \rightleftarrows \sum_a \nu_{\sigma,a} E_a + \sum_s \nu_{\sigma,s} E_s$
- $E_\pi \rightleftarrows \sum_a \nu_{\pi,a} E_a$

Chemical system

- The laws of conservation of mass and the saturation thresholds of minerals are translated into the following system :

$$\Phi(X) = \begin{pmatrix} C_a(\mathbf{c}(x,t)) + F_a(\mathbf{c}(x,t), \mathbf{s}(x,t), \mathbf{p}(x,t)) \\ F_s(\mathbf{c}(x,t), \mathbf{s}(x,t)) \\ \mathcal{E}_\pi(\mathbf{c}(x,t)) \end{pmatrix} \quad (3)$$

With $X = (\mathbf{c}, \mathbf{s}, \mathbf{p})$

- The geochemical model can be written by $\Phi(X) = (T, W, 1)$ with constraints $\mathbf{c} \geq 0, \mathbf{s} \geq 0, \mathbf{p} > 0$,

2
Transport model

Transport model

- The advection and dispersion governing the transport of solutes.
- Under standard assumptions, the transport operator is written as :

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

- The dispersion tensor is defined by $D = d_m I + \alpha_T \|v\| I + (\alpha_L - \alpha_T)\frac{vv^T}{\|v\|}$
- $C(X)$ are the only mobile species
- The transport is modeled by :

$$\omega \frac{\partial T_i}{\partial t} + \mathcal{L}(C_i(X)) = Q_i, \quad i = 1, \ldots, N_c, \tag{4}$$

Spatial discretization

The semi-discrete transport is written as :

$$\begin{cases} \omega \frac{dT_i}{dt} + LC_i(X) = Q_i + G_i, \quad i = 1, \ldots, N_c, \\ \Phi(X_j) = (T_j, W_j, 1), \quad j = 1, \ldots, N_m, \\ \text{initial condition for } T. \end{cases} \tag{5}$$

3
Numerical Methods

Sequential non-iterative approach (SNIA)

- Method based on the explicit Euler scheme.
- With a time step Δt :

$$\begin{cases} \omega T_i^{n+1} + \Delta t L C_i(X^n) = \omega T_i^n + \Delta t (Q_i^n + G_i^n), & i = 1, \ldots, N_c, \\ \Phi(X_j^{n+1}) = (T_j^{n+1}, W_j^{n+1}, 1), & j = 1, \ldots, N_m. \end{cases}$$

- At each time step, we compute explicitly and independently T_i
- In each cell, we solve independently the chemical system.
- We calculate C_i.
- In our software SNIA, we use Kinsol(Sundials) to solve the chemical system.

Global Approach (GDAE)

- The semi-discrete system (5) is a differential-algebraic system index 1.
- We calculate the Jacobian matrix.
- Global approaches DSA are based on implicit time scheme.
- A non-linear system is coupled with each time step.
- Solved globally by a Newton method.


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


J. Erhel, S. Sabit, and C. de Dieuleveult. Computational Technology Reviews, chapter Solving Partial Differential Algebraic Equations and Reactive Transport Models. Saxe-Coburg Publications, 2013.

Global Approach (GDAE)

- The GDAE method uses a scheme BDF.
- The derivatives are approximated by :

$$\frac{dT_i}{dt} \simeq \frac{a}{\Delta t} T_i + \frac{1}{\Delta t} Z_i$$

- Our nonlinear system is written as :

$$\begin{cases} \frac{a\omega}{\Delta t} T_i + LC_i(X) + \ldots = 0 \\ \Phi(X_j) - (T_j, W_j, 1) + \ldots = 0 \end{cases}$$


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


J. Erhel, S. Sabit, and C. de Dieuleveult. Computational Technology Reviews, chapter Solving Partial Differential Algebraic Equations and Reactive Transport Models. Saxe-Coburg Publications, 2013.

Software GRT3D

- MT3D software to discretize the transport.
- Sundials (IDA) to integrate the differential-algebraic system.
- UMFPACK to solve the linearized systems.
- GRT3DR : we reduce the size of system because our Jacobian matrix contains null block and identity.
- GRT3DRSL : we use the concentration without logarithm.


C. Zheng and G. D. Bennett. Applied Contaminant Transport Modeling, second edition. John Wiley and Sons, New-York, 2002.

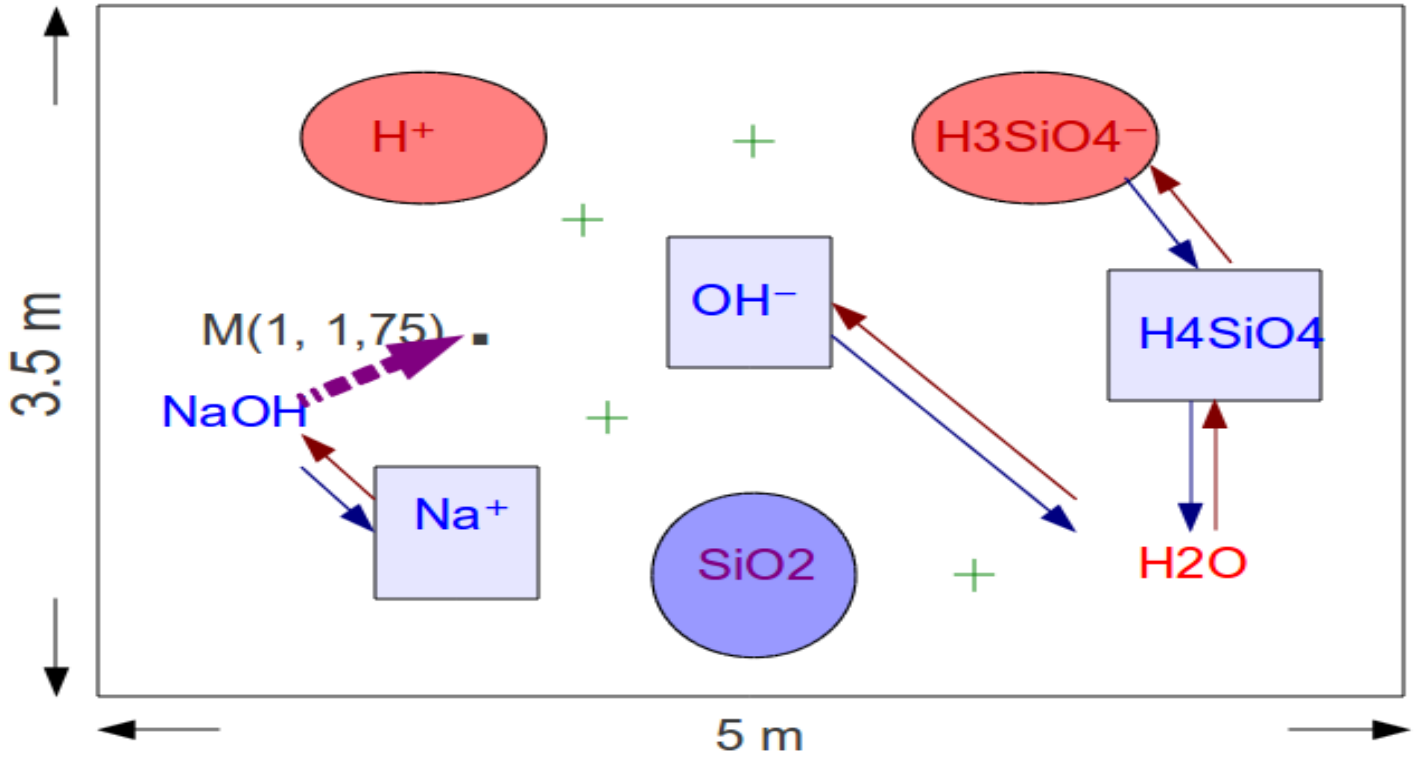

S. Sabit and N. Soualem. Suite logicielle grt3d (global reactive transport 3d). Rapport de contrat andra, INRIA, 2011.


A. C. Hindmarsh, P. N. Brown, K. E. Grant, S. L. Lee, R. Serban, D. E. Shumaker,and C. S. Woodward. SUNDIALS : Suite of nonlinear and differential/algebraic equation solvers. ACM Transactions on Mathematical Software, 31 :363–396, 2005. Also available as LLNL technical report UCRL-JP-200037.


T. Davis.Algorithm 832 : Umfpack, an unsymmetric-pattern multifrontal method. ACM Transactions on Mathematical Software, 30 :196–199, 2004.

4
Numerical results
ANDRA test 2D

Numerical results ANDRA test 2D



- $\omega = 1$, $v = (5.7 \times 10^{-7}, 0)^T$ m.s^{-1}, $d_m = 0$, $\alpha_L = 0.2$ m, $\alpha_T = 0.05$ m.
- A zero flux is imposed at the boundary of the domain and the simulation takes 30 days.

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.

ANDRA test 2D

- Initial values of T and the constant reaction

	Na^+	OH^-	$H4SiO4$
Initial values of T	0	0	10
K	10^{-14}	$10^{+4.2}$	$10^{+3.6}$

- The stoichiometric coefficient matrices

	Na^+	OH^-	$H4SiO4$	quartz
H^+	0	-1	0	0
$H3SiO4^-$	0	1	1	0
quartz	0	0	0	1

CPU time for the test Andra 2D (1)

- CPU time for the test Andra 2D with GRT3D

Mesh	GRT3D with spectator ion		GRT3D without spectator ion	
	size	CPU	size	CPU
21x14	2940	1 min 50 s	2058	18 s
48x28	13440	8 min	9408	1 min 36 s
81x56	45360	56 min	31752	6 min 33 s
71x101	71710	1h 20 min	50197	11 min 55 s
161x112	180320	3h	126224	32 min 43 s
322x224	721280	(1)	504896	(1)

(1) : initial chemical balance not found

CPU time for the test Andra 2D (2)

- CPU time for the test Andra 2D without spectator ion for GRT3DR and GRT3DR-SL

Mesh	GRT3DR	GRT3DR-SL	Gain/GRT3D		size
21x14	4 s	2 s	0.5	0.11	882
48x28	21 s	8s	0.22	0.084	4032
81x56	1 min 53 s	50 s	0.29	0.13	13608
71x101	3 min 28 s	1 min 21 s	0.29	0.11	21513
161x112	16 min 30 s	4 min 32 s	0.5	0.14	54096
322x224	1 h 52 min	37 min 38 s			216384

ANDRA test 2D

- the component Na^+ satisfies a transport equation whose analytical solution is :

$$x_{Na^+} = \frac{0.01\delta_M}{4\upsilon\pi\sqrt{\alpha_L\alpha_T}t}\exp\left(-\frac{(x-x_M-\upsilon t)^2}{4\upsilon\alpha_L t} - \frac{(y-y_M)^2}{4\upsilon\alpha_T t}\right) \quad (6)$$

  with $(x_M, y_M) = (1, 1.75)$
- The domain is meshed with regular cells $N_m = n_1 \times n_2$.
- With SNIA, the time step $\triangle t_e$ is chosen to ensure numerical stability, while it is dynamically adapted with GDAE.

ANDRA test 2D

- From equation (6), we can compute the analytical solution $x_{Na^+}(m_j, t_n)$ at each point $m_j, j = 1....N_m$ and at each instant $t_n, n = 1...N_t$.
- The error E_{Na^+} is defined by :

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

with $\tilde{x}_{Na^+}(m_j, t_n)$ is the solution calculated by GRT3DRSL or SNIA.

ANDRA test 2D

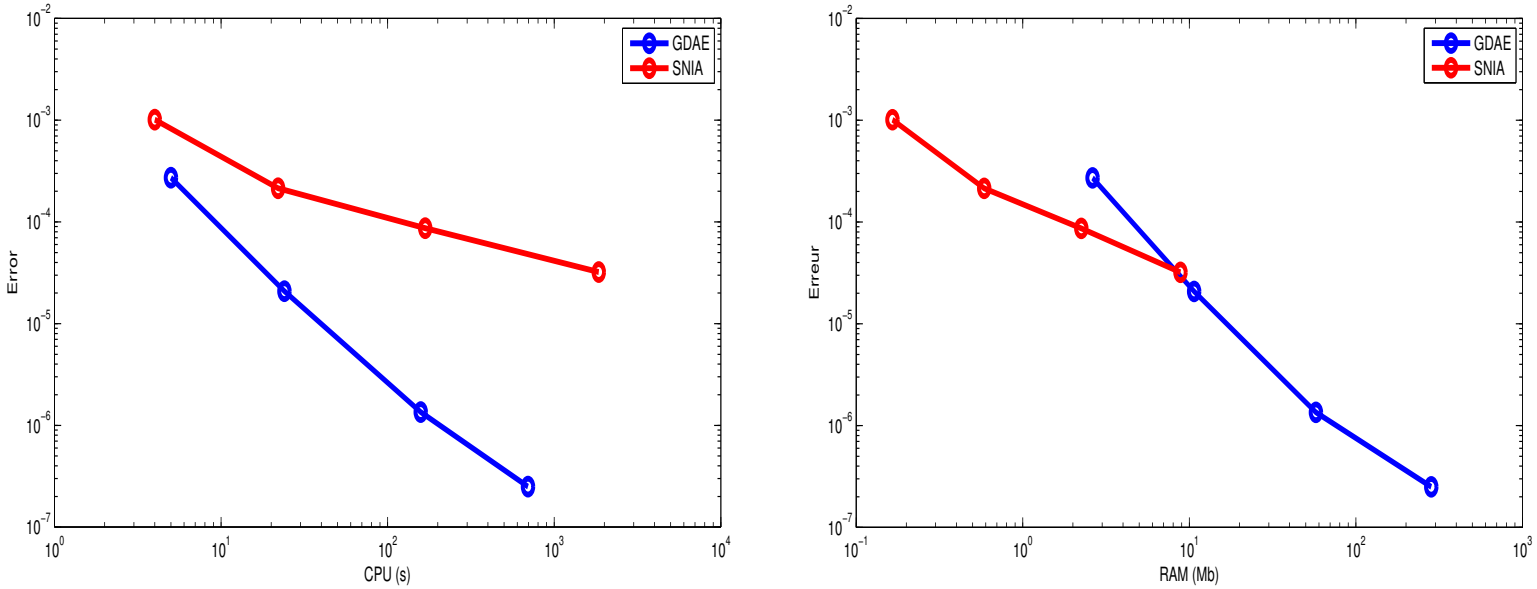


FIGURE: Error E_{Na^+} for GDAE (blue) and SNIA (in red) for 4 meshes :
$N_m = 21 \times 14$, $\triangle t_e = 3600$; $N_m = 41 \times 28$, $\triangle t_e = 1296$;
$N_m = 81 \times 56, \triangle t_e = 432$; $N_m = 161 \times 112, \triangle t_e = 120$;
Left : CPU times (s) ;
Right : ram memory (MB).

ANDRA test 2D

5
Conclusion

Conclusion

- removing the spectator ion $\Rightarrow$ reduce the CPU time by a factor of six
- GRT3DR $\Rightarrow$ gain a factor two CPU time with respect to the CPU time of GRT3D
- GRT3DR-SL $\Rightarrow$ reduce the CPU time by a factor between two and four compared to the CPU time of GRT3DR.
- The global method GDAE is much more accurate and faster than the explicit method SNIA.
- The global method GDAE uses more memory than the explicit method SNIA, but still less than 1 GB for the finer mesh.

Perspectives

- study the nonlinear complementarity problem.
- use semi-smooth Newton method.
- Parallelism through the components or the mesh.

Thank you

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