Numerical Methods for the reactive transport : Global DAE approach

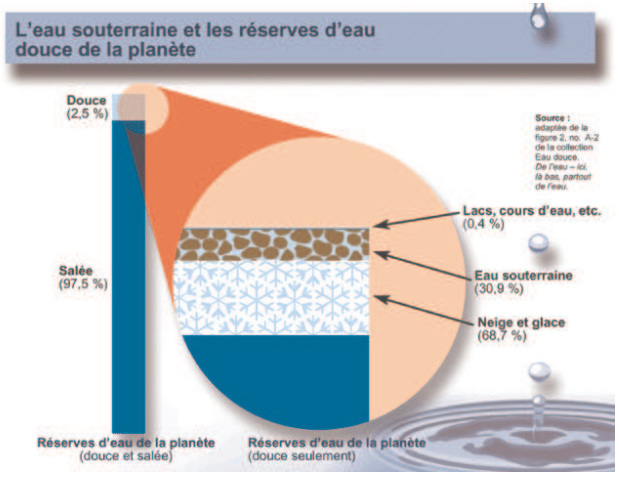
Souhila Sabit
SAGE-INRIA, RENNES

co-authors

Jocelyne Erhel (IRISA, Rennes, France)
Édouard Canot (IRISA, Rennes, France)

Sophia Antipolis, July 2012

1 Introduction


L'eau souterraine et les réserves d'eau douce de la planète
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)

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 method of lines, corresponding to the discretization in space only, leads to a differential algebraic system (DAE).
- Use a solver appropriate to solve this differential algebraic system (DAE).
- Use a solver based on an implicit method, in order and variable step, which requires at each time step, the iterative solution of large nonlinear system based on the Jacobian matrix
- Use Newton method to solve the nonlinear chimical systems.

our method **Global approach DAE**

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

Chemical model (1)

- **Chemical reactions :**

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

Chemical model (1)

- **Chemical reactions :**

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

- **Chemical equilibrium:**

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

Chemical model (1)

- **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 model (2)

Chemical system

$$\begin{pmatrix} \mathbf{T}_a(x,t) - \mathcal{C}_a(\mathbf{lc}_a(x,t)) - \mathcal{F}_a(\mathbf{lc}_a(x,t), \mathbf{lc}_s(x,t), \mathbf{c}_\pi(x,t)) \\ \mathbf{T}_s(x,t) - \mathcal{F}_s(\mathbf{lc}_a(x,t), \mathbf{lc}_s(x,t)) \\ \mathcal{E}_\pi(\mathbf{lc}_a(x,t)) \end{pmatrix} = \mathbf{0} \quad (3)$$

Transport model (1)

The transport of these elements may be related to two phenomena, **advection** and **dispersion**.

- **Advection :**

$$-\nabla.(c\mathbf{q}) = \mathcal{L}_{adv}(c) \tag{4}$$

- **Dispersion :**

$$\nabla.(\mathbf{D}\nabla c) = \mathcal{L}_{disp}(c) \tag{5}$$

- **Transport equation :**

$$\varepsilon \frac{\partial c}{\partial t} = \mathcal{L}_{adv}(c) + \mathcal{L}_{disp}(c) = \mathcal{L}(c) \tag{6}$$

Coupling between chemistry and transport

- From the equations defined above, we obtain the following system:

$$\begin{cases} \varepsilon \frac{\partial \mathbf{T}_a}{\partial t} & = & \mathcal{L}(\mathbf{C}_a) - \mathbf{f}, \\ \Phi(\mathbf{T}_a, \mathbf{y}) & = & \mathbf{0} \\ \mathbf{C}_a - \mathcal{C}_a(\mathbf{y}) & = & \mathbf{0} \\ + \text{ boundary conditions} \\ + \text{initial conditions} \end{cases} \tag{7}$$

Where :

- The vector $\mathbf{y} = \begin{pmatrix} \mathbf{lc}_a \\ \mathbf{lc}_s \\ \mathbf{c}_\pi \end{pmatrix}$ corresponds to the unknown chemical system.
- Φ is the function describing the chemical phenomena defined in the system (3).

The global approach DAE

- We will write the **coupled** model as a **differential-algebraic** system and solve it by an appropriate solver after space discretization.

- The system (7) is written as:

$$\begin{cases} F(t, \mathbf{Y}, \frac{d\mathbf{Y}}{dt}) = \mathbf{0} \\ + \text{ initials conditions at t=0} \end{cases} \tag{8}$$

- with

$$\mathbf{Y} = \begin{pmatrix} \mathbf{T}_a \\ \mathbf{y} \\ \mathbf{C}_a \end{pmatrix} \text{ and } F\left(t, \mathbf{Y}, \frac{d\mathbf{Y}}{dt}\right) = \begin{pmatrix} \varepsilon \frac{d\mathbf{T}_a}{dt} - L(\mathbf{C}_a) + \mathbf{f} \\ \Phi(\mathbf{T}_a, \mathbf{y}) \\ \mathbf{C}_a - \mathcal{C}_a(\mathbf{y}) \end{pmatrix} \tag{9}$$

- Where $\mathbf{T}_a, \mathbf{y}$ and $\mathbf{C}_a$ are the variables discretized in space of size $N_a \times N_m$, $(N_a + N_s + N_\pi) \times N_m$ and $N_a \times N_m$ respectively.

GRT3D

- We solve the system with the **IDA** solver (**IDA** is a package that solves the Sundials algebraic differential equation (**DAE**) written as **F (t, y, y')= 0**).
- To solve the **chemical system** at the **initial** time **t=0**, we used **Kinsol** (**Kinsol** is a **nonlinear** solver for systems of algebraic equations based on **Newton's** algorithm).
- We provide two calculated functions to the solver, the value of **F** and its the **generalized Jacobian matrix** $J = \frac{\partial F}{\partial \mathbf{Y}} + \alpha \frac{\partial F}{\partial \mathbf{Y}'}$.
- This matrix is written as:

$$J = \begin{pmatrix} \alpha \mathbf{M} & \mathbf{0} & -\mathbf{L} \\ \frac{\partial \Phi}{\partial \mathbf{T}_a} & \frac{\partial \Phi}{\partial \mathbf{y}} & \mathbf{0} \\ \mathbf{0} & \frac{\partial \mathcal{C}_a}{\partial \mathbf{y}} & \mathbf{I}_{N_m N_a} \end{pmatrix} \tag{10}$$

- **M** contains the discretized values of porosity
- α is a term from the time discretization
- **L** is the matrix of spatial discretization of the transport operator.
- The second block of rows contains the chemistry equations
- the third block of rows contains additional chemical equations.

https://computation.llnl.gov/casc/sundials/

GRT3D (2)

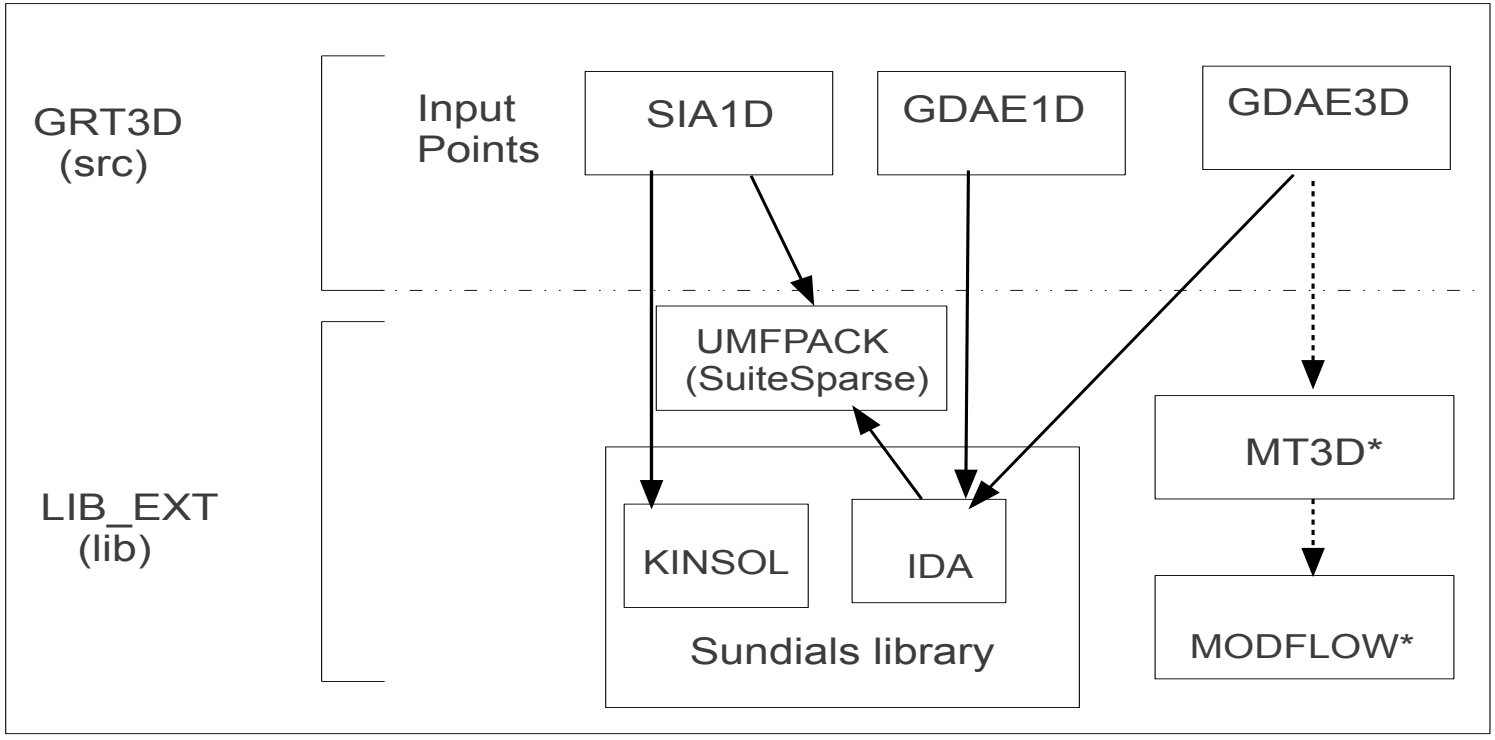


Figure: Description of GRT3D softwar

GRT3DR

- The Jacobian matrix (10) has a particular structure with identity blocks and zero blocks. We then reduce the size of the linear system at each Newton iteration.
- The system

$$J\mathbf{x} = \mathbf{g}$$

is equivalent to:

- $$\begin{cases} (\frac{\partial \Phi}{\partial \mathbf{y}} - \frac{\partial \Phi}{\partial \mathbf{T}_a}\frac{\mathbf{M}^{-1}}{\alpha}\mathbf{L}\frac{\partial \mathcal{C}_a}{\partial \mathbf{y}})\mathbf{x}_2 = \mathbf{g}_2 - \frac{\partial \Phi}{\partial \mathbf{T}_a}\frac{\mathbf{M}^{-1}}{\alpha}(\mathbf{g}_1 + \mathbf{L}\mathbf{g}_3), \\ \mathbf{x}_3 = \mathbf{g}_3 - \frac{\partial \mathcal{C}_a}{\partial \mathbf{y}}\mathbf{x}_2, \\ \mathbf{x}_1 = \frac{\mathbf{M}^{-1}}{\alpha}(\mathbf{g}_1 + \mathbf{L}\mathbf{x}_3), \end{cases} \quad (11)$$

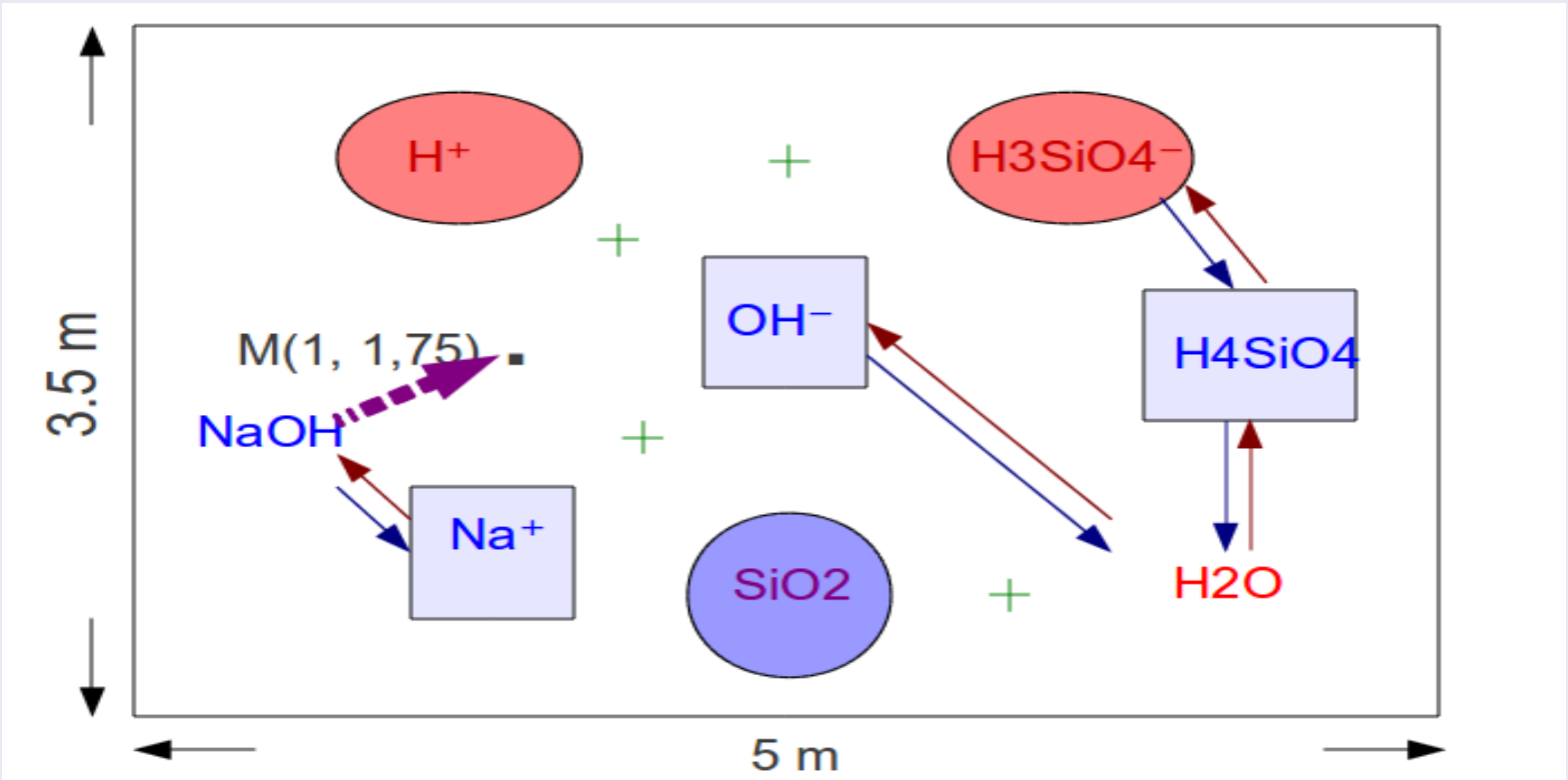
- When $\mathbf{x} = (\mathbf{x}_1^T, \mathbf{x}_2^T, \mathbf{x}_3^T)^T$ and $\mathbf{g} = (\mathbf{g}_1^T, \mathbf{g}_2^T, \mathbf{g}_3^T)^T$. Thus solving the linear system is reduced to $(N_a + N_s + N_\pi) \times N_m$ instead of $(3N_a + N_s + N_\pi) \times N_m$.
  This method is implemented in **GRT3DR software.**

GRT3DR_SL

The use of the logarithm of the concentrations:

- We have the product of concentrations with constant exponent (2).
- We linearize all the equations
- The computation of Jacobian matrix is very easy.
- All the concentrations are possitive (exponential).
- When concentrations are very small, the Jacobian matrix is ill conditioned.
- We have zero initial concentrations,, we approach the value by 10^{-10}
- We can also remove the spectator ion of the Chemical system.
- We use concentrations without logarithm, (Sans Log) then, we have the software GRT3DR-SL ,

test case Andra 2D (1)



- $\varepsilon = 1$ and $T_{final} = 1000$ 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.

test case Andra 2D (2)

- Initial values of T and logarithm

	Na^+	OH^-	$H4SiO4$
Initial values of T	0	0	10
log K	-32.2362	9.67086	8.28931

- 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

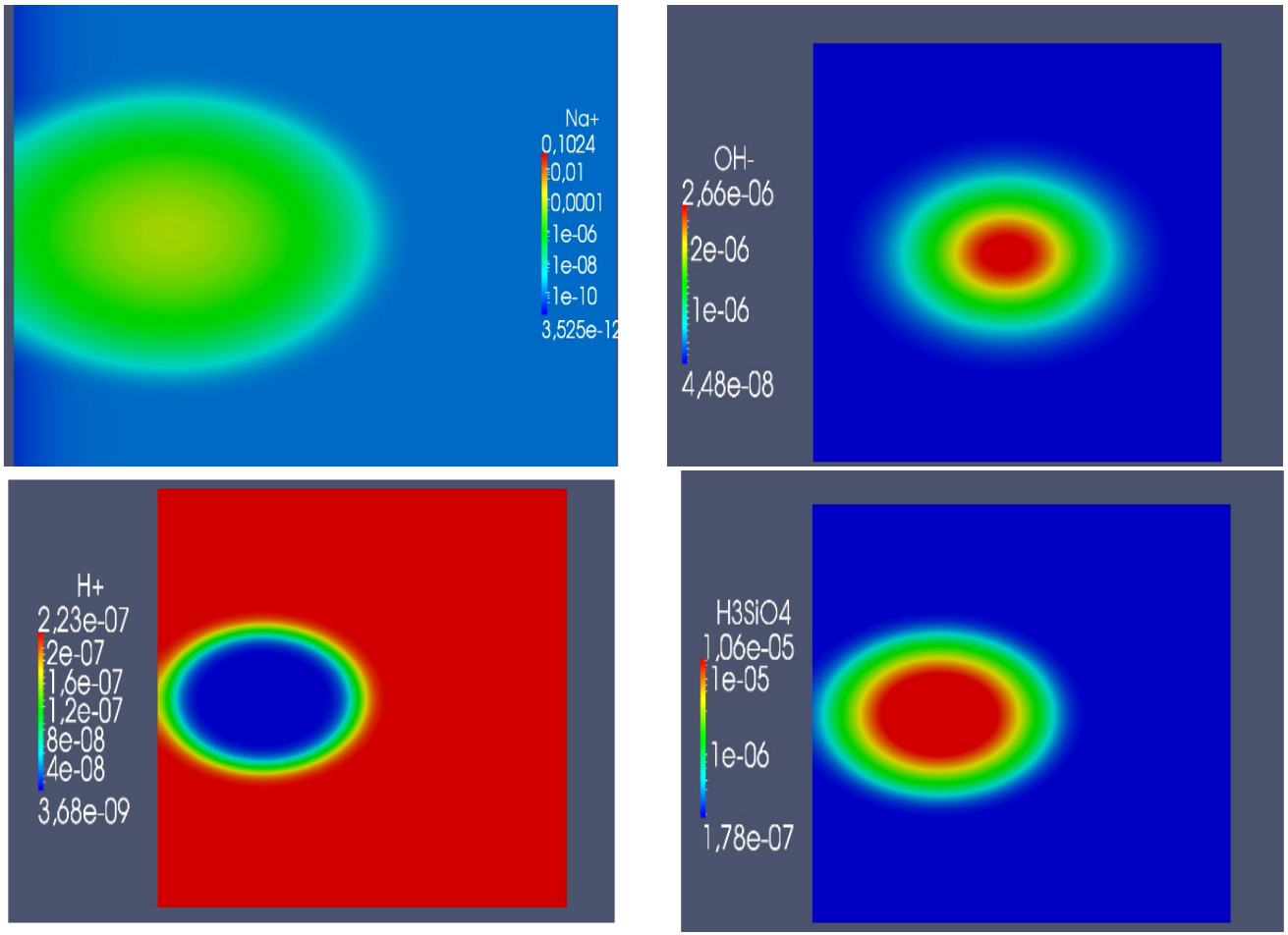
Mesh	GRT3D with spectator ion		GRT3D without spectator ion	
	size	CPU	size	CPU
21x14	2940	1 min 50 s	2058	18 s
48x28	13440	8 min	9408	1 min 36 s
81x56	45360	56 min	31752	6 min 33 s
71x101	71710	1h 20 min	50197	11 min 55 s
161x112	180320	3h	126224	32 min 43 s
322x224	721280	(1)	504896	(1)

- 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

(1): initial chemical balance not found

CPU time for the test Andra 2D (2)



Conclusion & perspectives

ⓐ 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.

ⓑ Perspectives

- apply the SNIA method (Non-iterative sequential methods) and compare the CPU time.
- study the nonlinear complementarity problem.
- use semi-smooth Newton method.
- Parallelism through the components or the mesh.

Thank

Thank you for your attention