Analysis of numerical methods for coupling transport and geochemistry equations.

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SIAM conference on Computational Geosciences

Leipzig, June 2009

Outline

- Chemistry model
- Transport model and coupled model
- SNIA method
- SIA method
- Global-ODE method
- Global-DSA method
- Global-DAE method
- Numerical results

Joint work with C. de Dieuleveult

Work supported by ANDRA and by GdR MOMAS from PACEN

Chemistry model

Mass action laws (no precipitation)

$$\log x = S \log c + \log K_c$$

$$\log y = A \log c + B \log s + \log K_s$$

- $c \in \mathbb{R}^{N_c}$: aqueous components
- $s \in \mathbb{R}^{N_s}$: sorbed components
- $x \in \mathbb{R}^{N_x}$: secondary aqueous species
- $y \in \mathbb{R}^{N_y}$: secondary sorbed species
- $K_c \in \mathbb{R}^{N_x}$ and $K_s \in \mathbb{R}^{N_y}$: equilibrium constants
- $\overline{S} = \begin{pmatrix} S & 0 \\ A & B \end{pmatrix} \in \mathbb{R}^{N_x+N_y, N_c+N_s}$: stoichiometric coefficients

Chemistry model

Mass conservation

$$
\begin{aligned}
T &= c + S^T x + A^T y \\
W &= s + B^T y
\end{aligned}
$$

- W fixed and given
- T given or coupled with transport model
- aqueous total $C = c + S^T x$
- fixed total $F = A^T y$

Chemistry model

Nonlinear equations

$$\Phi(a) - \begin{pmatrix} T \\ W \end{pmatrix} = 0$$

- $\Phi(a) = \exp(a) + \overline{S}^T exp(K + \overline{S}a)$
- $a = (\log c, \log s)^T$
- $K = (\log K_c, \log K_s)^T$

Jacobian matrix

$$J_c(a) = \operatorname{diag}(\exp(a)) + \overline{S}^T \operatorname{diag}(\exp(K + \overline{S}a))\overline{S}$$

Newton iterative method

Global method with line search or trust region

Chemistry model with precipitation

Mass Conservation $p \in \mathbb{R}^{N_p}$: precipitated species

$$F = A^T y + D^T p$$

Mass action laws

Π : saturation index

$$\Pi = \log K_p + D \log c$$
$$\begin{cases} p_i = 0 & \text{if } \Pi_i < 1 \\ \Pi_i = 1 & \text{otherwise .} \end{cases}$$

Non differentiable equations

Complementarity problem and semi-smooth Newton methods

Coupled transport and chemistry models

Advection-dispersion

$$\mathcal{L}(C) = \nabla.\left(C\vec{V}\right) - \nabla.\left(D\nabla C\right)$$

Transport of each chemical component

Linear transport equations

$$\omega\frac{\partial T_j}{\partial t} + \mathcal{L}(C_j) = 0, \quad j = 1, \dots, N_c$$

Chemistry equations

Precipitation with a fixed number of species

$$\begin{aligned}
& a = (\log c, \log s)^T \\
& C = c + S^T \exp(\log K_c + S \log c) = C(a) \\
& \Phi(a) - \begin{pmatrix} T \\ W \end{pmatrix} = 0
\end{aligned}$$

Discrete coupled model

Method of Lines :

Space discretization with a Finite Volume method

with N_m points.

Discrete transport operator.

Variables T, C, F of order $N_m N_c$ and a of order $N_m(N_c + N_s)$.

SNIA approach

TC formulation with explicit chemistry

$$\begin{cases} \frac{dT}{dt} + (L \otimes I)C = 0, N_m \times N_c \text{ equations} \\ \Phi(a) - \begin{pmatrix} T \\ W \end{pmatrix} = 0, (N_c + N_s + N_p) \times N_m \text{ equations} \\ C - C(a) = 0. \end{cases}$$

explicit Euler scheme

$$\begin{cases} \frac{T^{n+1} - T^n}{\Delta t} + (L \otimes I)C^n = 0, \\ \Phi(a) - \begin{pmatrix} T^{n+1} \\ W \end{pmatrix} = 0, \\ C^{n+1} - C(a) = 0. \end{cases}$$

SNIA approach

- Chemistry solver as a black box
- decoupled transport and chemistry equations
- No transport equation to solve
- stability condition : small time steps

SIA approach

CC formulation with explicit chemistry

$$\begin{cases} \frac{dC}{dt} + \frac{dF}{dt} + (L \otimes I)C = 0, \\ \Phi(a) - \begin{pmatrix} C + F \\ W \end{pmatrix} = 0, \\ C - C(a) = 0 \text{ or } F - F(a) = 0. \end{cases}$$

implicit Euler scheme

$$\begin{cases} \frac{C^{n+1} - C^n}{\Delta t} + \frac{F^{n+1} - F^n}{\Delta t} + (L \otimes I)C^{n+1} = 0, \\ T^{n+1} = C^{n+1} + F^{n+1}, \\ \Phi(a) - \begin{pmatrix} T^{n+1} \\ W \end{pmatrix} = 0, \\ C^{n+1} - C(a) = 0 \text{ or } F^{n+1} - F(a) = 0. \end{cases}$$

SIA approach

Fixed-Point iterations (block-SOR-Newton)

$$\left\{ \begin{array}{l} \frac{C^{n+1,k+1}-C^n}{\Delta t} + \frac{F^{n+1,k}-F^n}{\Delta t} + (L \otimes I)C^{n+1,k+1} = 0, \\ T^{n+1,k+1} = C^{n+1,k+1} + F^{n+1,k}, \\ \Phi(a) - \begin{pmatrix} T^{n+1,k+1} \\ W \end{pmatrix} = 0, \\ F^{n+1,k+1} - F(a) = 0. \end{array} \right.$$

Another SIA approach

TC formulation and fixed-Point iterations (block-SOR-Newton)

$$\left\{\begin{array}{l} \frac{T^{n+1,k+1}-T^n}{\Delta t} + (L \otimes I) C^{n+1,k} = 0, \\ \\ \Phi(a) - \begin{pmatrix} T^{n+1,k+1} \\ W \end{pmatrix} = 0, \\ C^{n+1,k+1} - C(a) = 0. \end{array}\right.$$

SIA approach

- Chemistry solver as a black box
- decoupled transport and chemistry equations
- No transport equation to solve
- convergence condition : small time steps

comparison of time steps conditions

between SNIA, CC-SIA, TC-SIA ?

Global approach with ODE framework

TC formulation and implicit chemistry

$$\begin{cases} \frac{dT}{dt} + (L \otimes I) C(\Psi(T)) = 0, \\ a = \Psi(T), \\ C - C(a) = 0. \end{cases}$$

implicit Euler scheme

$$\frac{T^{n+1} - T^n}{dt} + (L \otimes I) C(\Psi(T^{n+1})) = 0.$$

Global approach with ODE framework

Newton iterations

$$\begin{cases} T_1 = T^n \\ \text{For } k = 1, \text{...until convergence} \\ a = \Psi(T_k) \\ C_k = C(a) \\ (I + \Delta t J_k)(T_{k+1} - T_k) = T^n - T_k - \Delta t C_k \\ \text{End} \\ T^{n+1} = T_k \end{cases}$$

with J_k Jacobian of $C(\Psi)$

Global approach with ODE framework

- Chemistry solver as a black box
- No stability condition
- Fast convergence
- Chemistry solver at each Newton iteration
- No explicit Jacobian J_k

Global approach with DSA framework

TC formulation with explicit chemistry

$$\left\{\begin{array}{l} \frac{dT}{dt} + (L \otimes I)C = 0, \\ \Phi(a) - \begin{pmatrix} T \\ W \end{pmatrix} = 0, \\ C - C(a) = 0. \end{array}\right.$$

implicit Euler scheme

$$\left\{\begin{array}{l} \frac{T^{n+1} - T^n}{\Delta t} + (L \otimes I)C^{n+1} = 0, \\ \Phi(a) - \begin{pmatrix} T^{n+1} \\ W \end{pmatrix} = 0, \\ C^{n+1} - C(a) = 0. \end{array}\right.$$

Global approach with DSA framework

Direct Substitution Approach

$$\begin{cases} \frac{C(a^{n+1})+F(a^{n+1})-T^n}{\Delta t} + (L \otimes I)C(a^{n+1}) = 0, \\ W(a^{n+1}) - W = 0, \\ T^{n+1} = C(a^{n+1}) + F(a^{n+1}). \end{cases}$$

nonlinear equations $G(a^{n+1}) = 0$

Newton iterations $J_k(a_{k+1} - a_k) = -G(a_k)$

with J_k Jacobian of G

DSA framework

- no stability condition
- fast convergence
- no chemistry solving
- Explicit Jacobian function
- chemistry functions required
- highly coupled equations
- adaptive time step difficult to implement

Global approach with DAE framework

DAE framework with TC formulation

$$M \frac{dy}{dt} + f(y) = 0.$$

$$y = \begin{pmatrix} T \\ a \\ C \end{pmatrix}, M = \begin{pmatrix} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, f(y) = \begin{pmatrix} (L \otimes I)C \\ \Phi(a) - \begin{pmatrix} T \\ W \end{pmatrix} \\ C - C(a) \end{pmatrix}$$

DAE of index 1

implicit scheme (for example, Euler)

$My^{n+1} + \Delta t f(y^{n+1}) = My^n$

Nonlinear equations at each time step

Global approach and DAE framework

Newton-type method

$y_1 = y^n$

For $k = 1, \ldots$ until convergence

$(M + \Delta t J_k)(y_{k+1} - y_k) = -(M(y_k - y^n) + \Delta t f(y_k))$

End

$$J_k = \begin{pmatrix} 0 & 0 & L \otimes I \\ -\begin{pmatrix} I \\ 0 \end{pmatrix} & \mathrm{diag}(J_c(a_k)) & 0 \\ 0 & -\frac{dC}{da}(a_k) & I \end{pmatrix}$$

Global approach and DAE framework

- no stability condition
- fast convergence
- no chemistry solving
- Explicit Jacobian function
- variable order and adaptive time step
- controlled update of Jacobian
- clear distinction between chemistry and transport functions
- chemistry functions required
- large sparse linear system
- high CPU time

Our global strategy

Transport discrete operator

- MT3D transport engine
- finite difference first order upwind scheme

  other schemes could be used, if they follow the MOL

Chemistry equations

- currently, precipitation-dissolution

  with a given number of precipitated species

DAE framework

- TC formulation with unknowns (T, C, a)

  CC formulation could be used : comparison ?

Our implementation

DAE solver

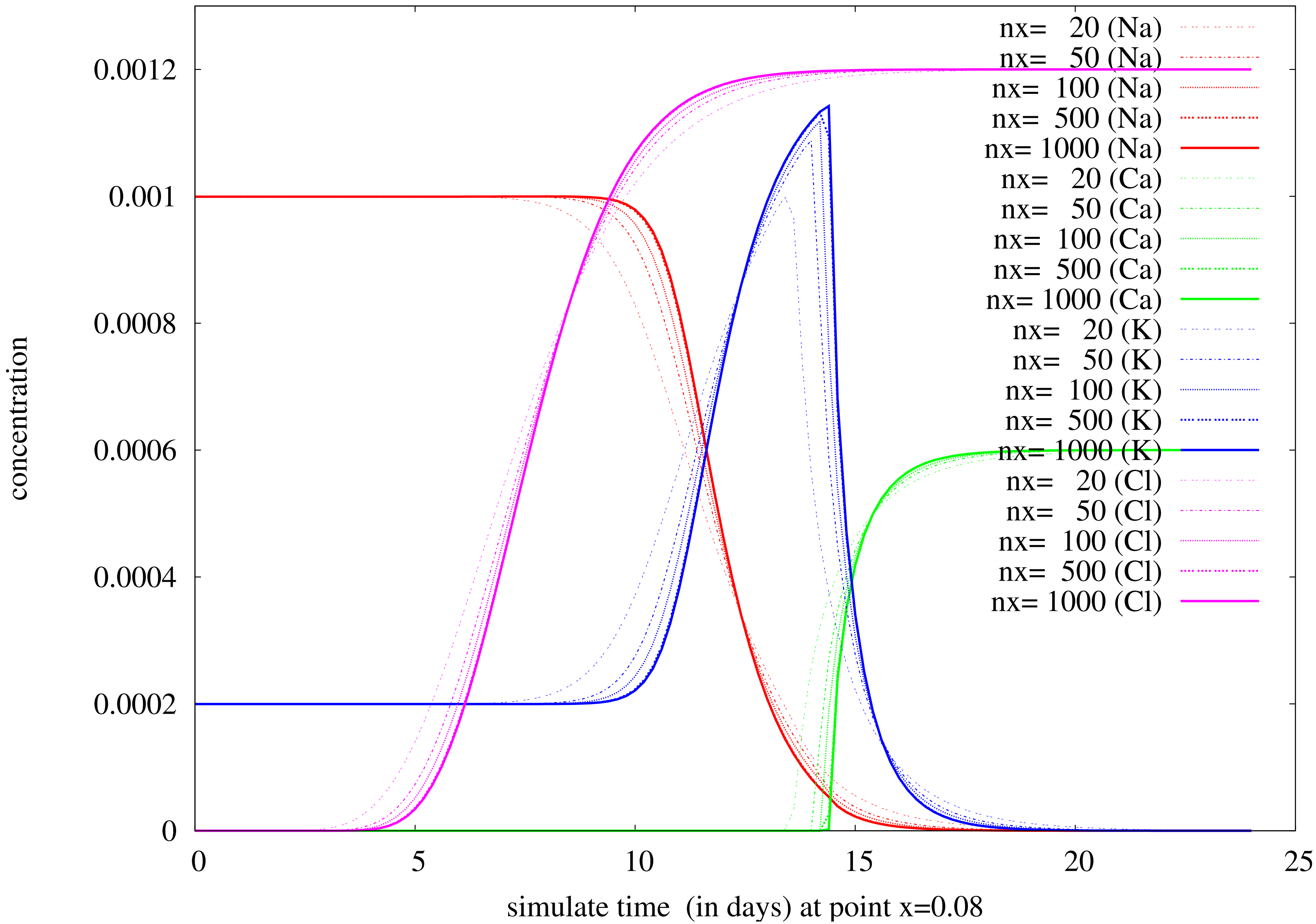
- variable order and adaptive time step (BDF method)
- modified Newton method with adaptive update of Jacobian
- control of convergence with adaptive time step
- Newton-LU solver with direct multifrontal sparse linear solver
- libraries SUNDIALS and UMFPACK

Numerical experiment : Ex11

Ex11 : example 11 from PhreeqC package

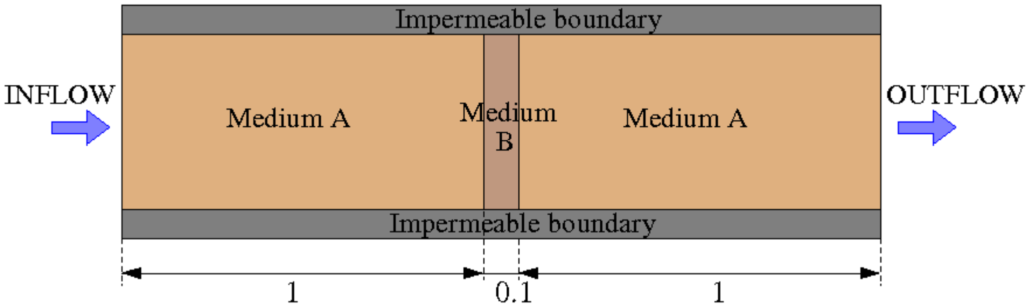
- column with potassium, sodium and nitrate in equilibrium with a cation exchanger
- injection of a calcium chloride solution
- transport by advection and diffusion

Results for Ex11



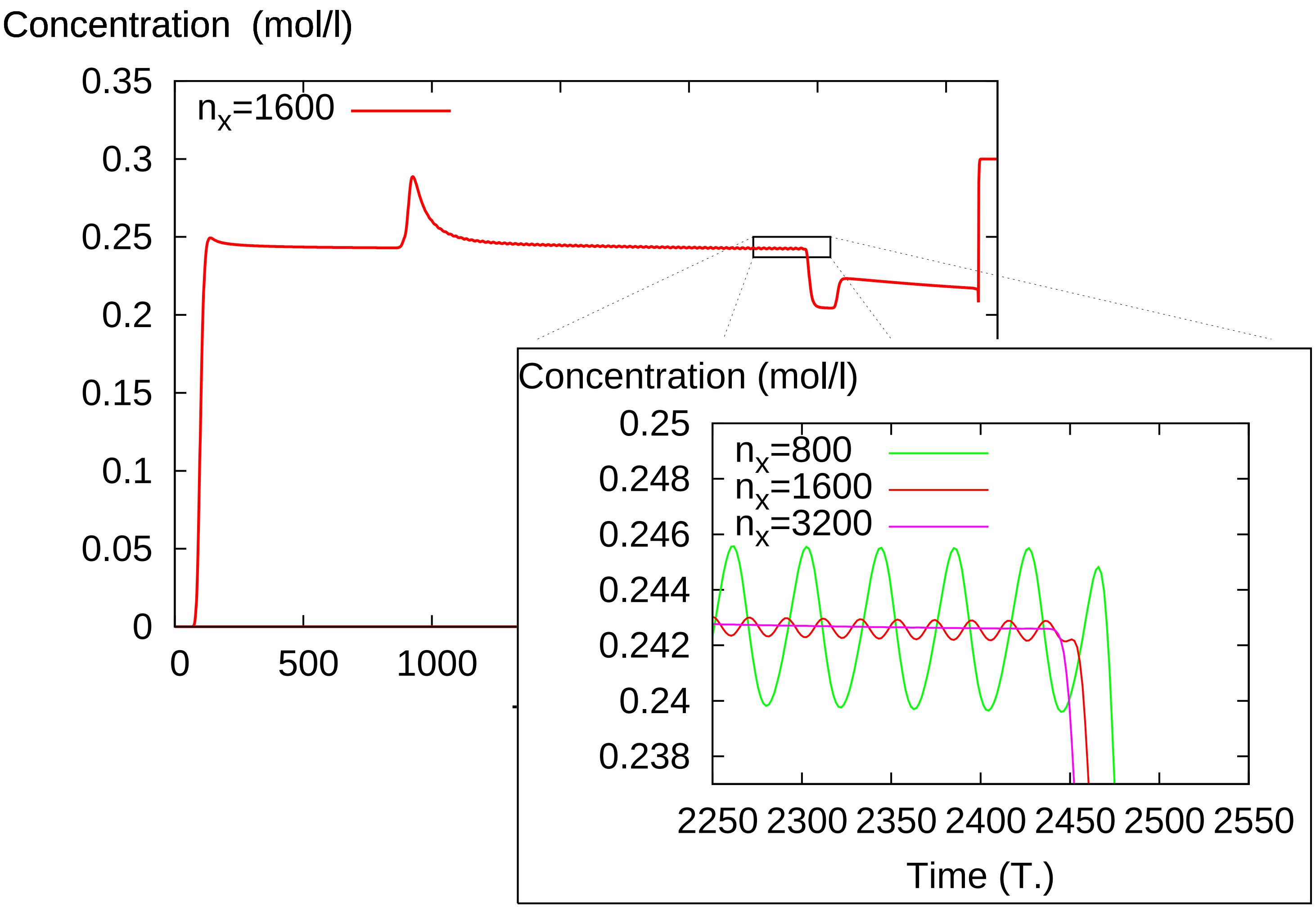
Numerical experiment : Momas benchmark

easy 1D test case



- four aqueous components, one sorbed component
- five aqueous secondary species, two sorbed secondary species
- different porosity and dispersion in medium A and medium B

Results for Momas benchmark



Future work

Chemistry and transport operators

- reduction of numerical diffusion in the transport engine
- precipitation and dissolution with a variable number of species

DAE solver

- complexity analysis and reduction of computational costs
- convergence and stability analysis of SIA and SNIA methods
- Newton-Krylov method with preconditioner