Numerical methods for reactive transport

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Outline

- reactive transport model
- some numerical methods
- numerical results in Rennes
- numerical results in Rocquencourt

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

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

Chemistry equations

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

Discrete coupled model

Method of Lines :

Spatial discretization with N_m points.

Discrete transport operator.

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

SNIA approach

TC formulation

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

explicit Euler scheme

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

SIA and Global approaches

TC formulation

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

implicit Euler scheme

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

SIA approach :fixed-point method

SIA-TC

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

SIA-CC

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

Global approach with DSA framework

Direct Substitution Approach

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

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

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

with A_k Jacobian of G

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 $k = 1, ...$until convergence

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

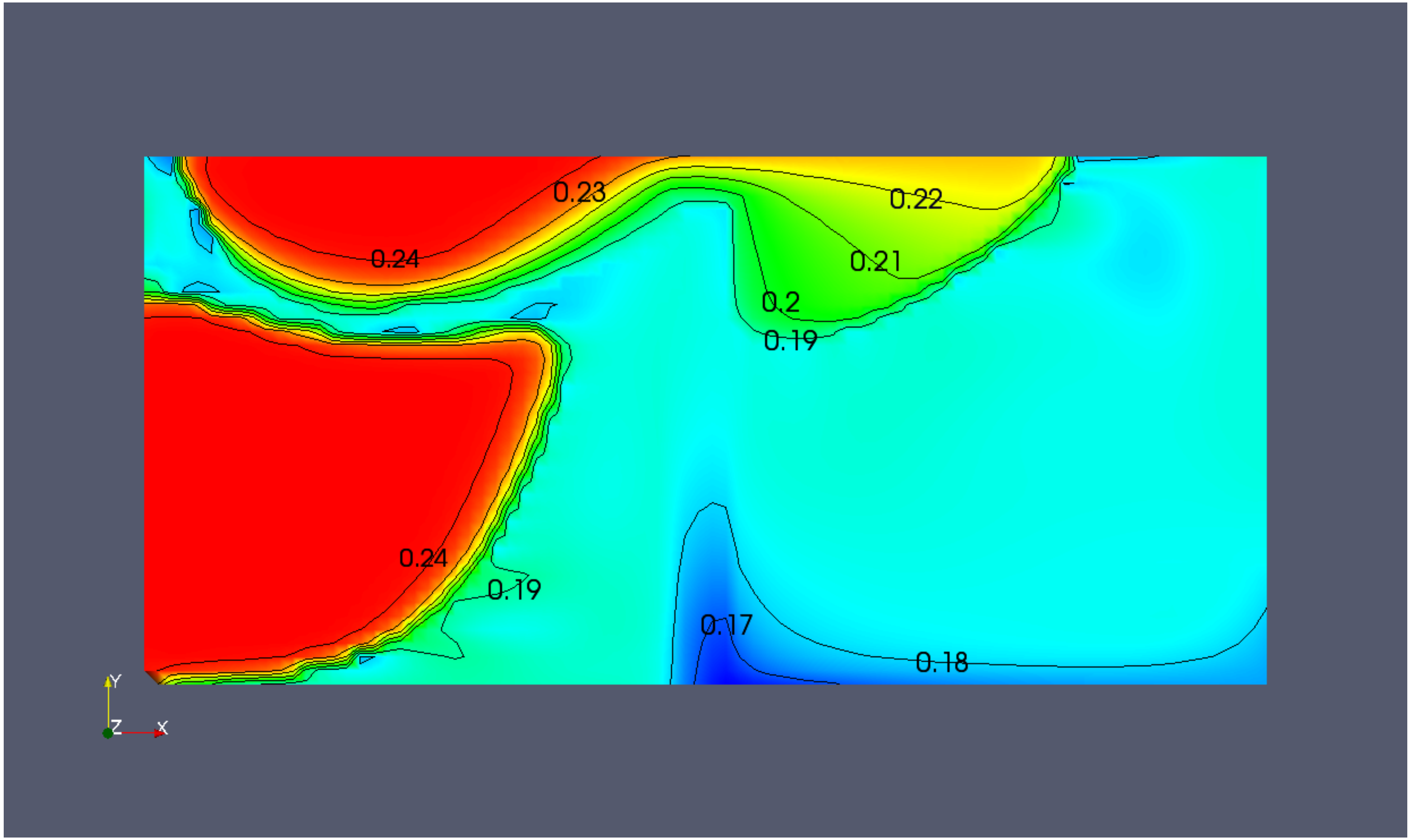
End

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

Global strategy and software in Rennes

- MOL and implicit scheme with DAE formulation
- finite difference first order upwind scheme (MT3D)
- restricted precipitation-dissolution
- 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 : Momas benchmark 2D test case



Numerical experiment : Alliances 2D test case

Alcaline water and quartz

- three aqueous components, two secondary aqueous components
- one precipitated species (quartz)
- initial injection of NaOH in quartz
- advection and hydrodynamic dispersion
- concentration of sodium at t=30 days

Numerical experiment : Alliances 2D test case

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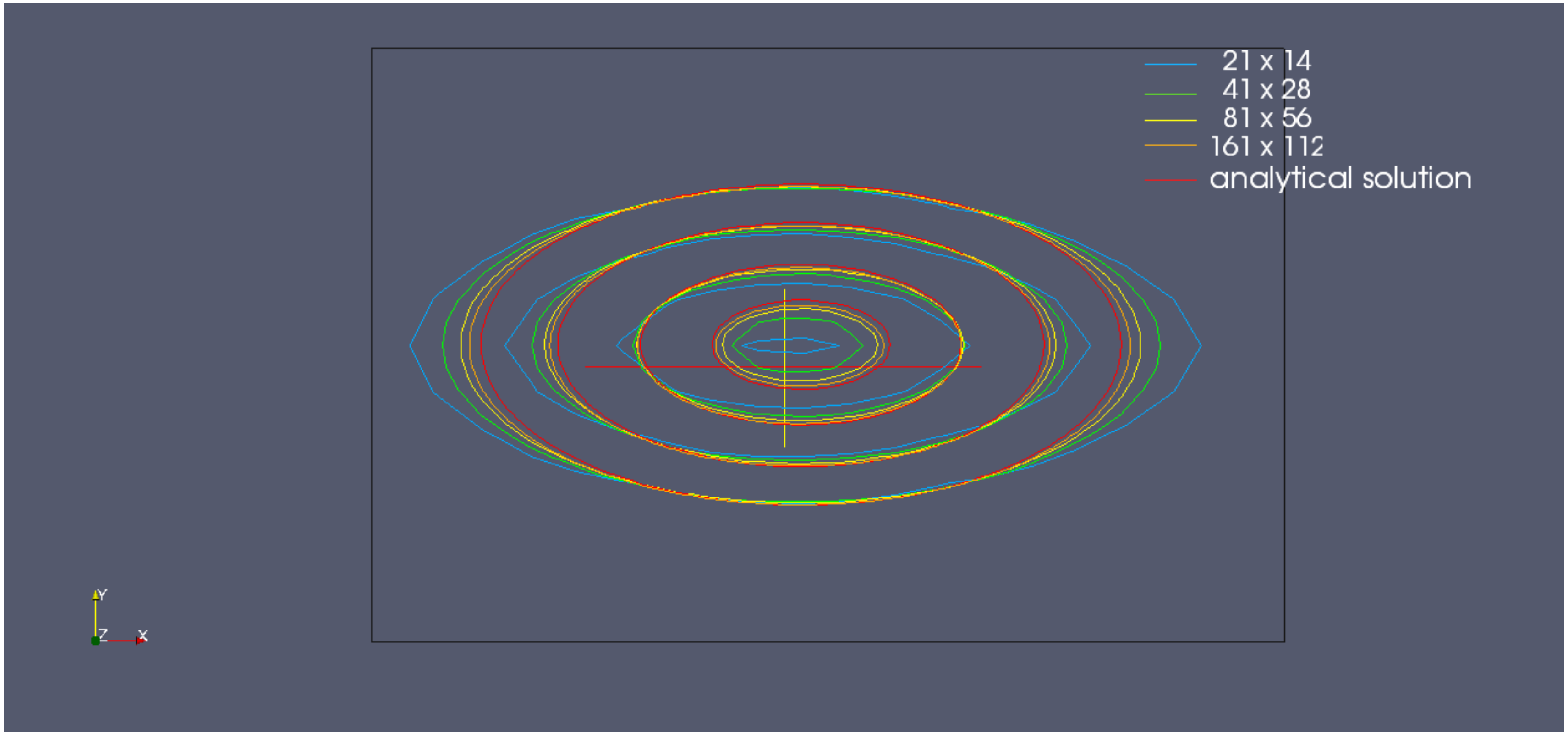

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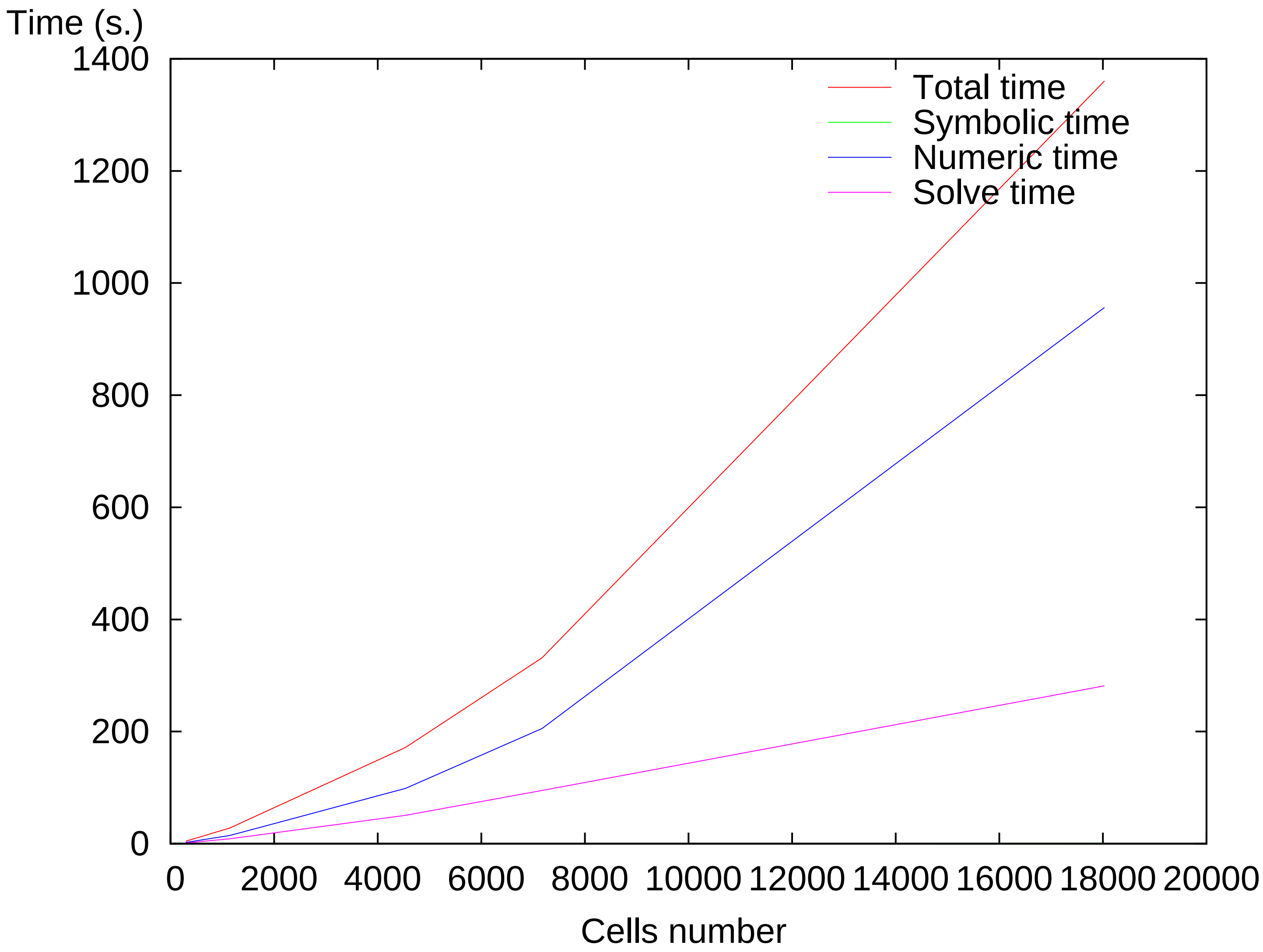

Analysis of 2D results

- good accuracy but not enough points near the front
- some numerical diffusion in the transport engine
- efficient control of time step
- efficient modified Newton : 1 update of J for 11 solvings
- most of the time spent in linear solving
- power law for numerical factorization

Current and future work

Chemistry and transport operators

- reduction of numerical diffusion
- mesh adaptation based on error estimation
- precipitation and dissolution with a variable number of species
- kinetic reactions
- variable diffusion coefficient

DAE solver

- convergence and stability analysis of SIA and SNIA methods
- substitution approach for the linearized equations
- Newton-Krylov method with preconditioner