Coupling flow, transport and geochemistry

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team SAGE

Workshop on model order reduction,

coupled problems and optimization

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Outline

- Transport of contaminant in groundwater flow :
  coupling transport and chemistry
- Saltwater intrustion :
  coupling salt transport and density-driven flow

Reactive transport coupled models

Joint work with M. Kern, INRIA-Rocquencourt

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
- $\overline{S} \in \mathbb{R}^{N_x+N_y, N_c+N_s} = \begin{pmatrix} S & 0 \\ A & B \end{pmatrix}$: stoechiometric coefficients

Chemistry model

Mass conservation

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

- W fixed and given
- T given or coupled with transport model

For W and T given, nonlinear equations solved by Newton

Chemistry model with precipitation

Mass Conservation

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

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

Mass action laws

Π : saturation index

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

Coupled transport and chemistry models

Convection-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 (no precipitation)

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

Sequential Iterative method

Implicit Euler scheme - Formulation TCF

$$\begin{aligned}
&C^{n+1} + F^{n+1} + \Delta t \mathcal{L}(C^{n+1}) - T^n = 0,\\
&T^{n+1} = C^{n+1} + F^{n+1},\\
&C^{n+1} = c + S^T x,\\
&F^{n+1} = A^T y,\\
&W = s + B^T y
\end{aligned}$$

SOR-Newton iterations

$$\begin{cases}
C^{n+1,k+1} + F^{n+1,k} + \Delta t \mathcal{L}(C^{n+1,k+1}) - T^n = 0\\
T^{n+1,k+1} = C^{n+1,k+1} + F^{n+1,k}\\
c + S^T x + A^T y = T^{n+1,k+1}\\
s + B^T y = W\\
F^{n+1,k+1} = A^T y
\end{cases}$$

Sequential Iterative method

- Decoupled transport and chemistry solvers
- Precipitation easy to include
- Nonlinear transport and nonlinear chemistry at each iteration
- slow convergence

Global method

System of ODE with one unknown T

$$\frac{dT}{dt} + \mathcal{L}(C) = 0,$$
$$T - (c + S^T x) - A^T y = 0,$$
$$W - (s + B^T y) = 0,$$
$$C = c + S^T x$$

- ODE solver
- nonlinear chemistry at each function evaluation
- Jacobian computed by finite differences
- Precipitation can be included

Global method

System of DAE with unknowns X=(C,F,c,s)

$$\frac{dC}{dt} + \frac{dF}{dt} + \mathcal{L}(C) = 0,$$

$$F - A^T y = 0,$$
$$C + F - (c + S^T x) - A^T y = 0,$$
$$W - (s + B^T y) = 0$$

Implicit scheme and Newton method

$$\begin{pmatrix} M dX/dt + \Phi(X) = 0, \\ M X^{n+1} + \Delta t \Phi(X^{n+1}) = M X^n \end{pmatrix}$$

Global method

- DAE solver
- Linearised transport and linearised chemistry at each Newton iteration
- fast convergence
- Coupled large sparse linear system
- Precipitation not yet included

Preliminary results

Pyrite test case

4 components, 39 aqueous species and 13 fixed species

Somehow artificial with no precipitation

Comparison between Sequential Iterative and Global DAE methods

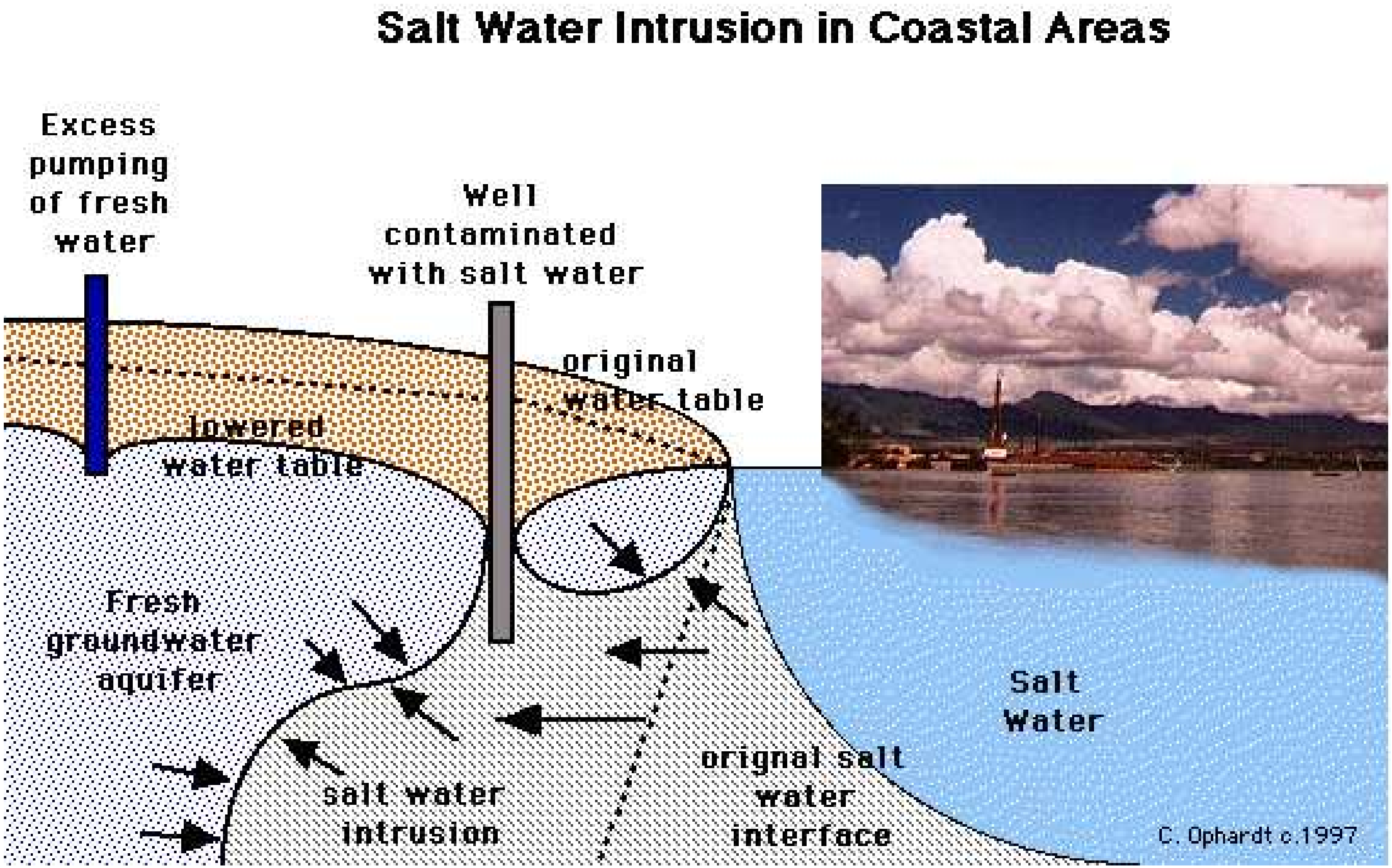
CPU times on a PC using Matlab

- SI, timestep $5.5 10^{-4}$: 4212 CPU seconds
- SI, timestep 10^{-3} : 2465 CPU seconds
- DAE, timestep $5.5 10^{-4}$: 409 CPU seconds

Reactive transport - open questions

- DAE system with precipitation-dissolution ?
- Large 2D and 3D problems ?
- Reduced Coupled Model ?

Saltwater intrusion



Density-driven flow

Joint work with E. Canot, C. de Dieuleveult, INRIA-Rennes

Based on work and software developed at IMFS-Strasbourg

Ph. Ackerer, A. Younes, and R. Mosé
Modeling variable density flow and solute transport in porous medium : 1. numerical model and verification,
Transport in Porous Media, 35 :345–373, 1999.

Density-driven flow

Mass conservation

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla.\left(\varepsilon\rho\vec{V}\right) = \rho Q_S$$

Generalized Darcy law

$$\varepsilon\vec{V} = -\frac{1}{\mu}\mathbb{k}(\nabla P + \rho g\,\vec{n}_z)$$

- ε : porosity
- ρ : fluid density
- $\vec{V}$: Darcy rate
- Q_S : source term
- $\mathbb{k}$: permeability tensor
- P : pressure
- μ : viscosity
- g : gravity

Density-driven flow

State equations

$$\varepsilon = \varepsilon(P),\ \rho = \rho(P, C),\ \mu = \mu(C),$$
$$S = \frac{\partial \varepsilon}{\partial P} + \frac{\varepsilon}{\rho}\frac{\partial \rho}{\partial P} = (1 - \varepsilon)\,\alpha + \varepsilon\beta$$

- C : salt concentration (fraction)
- S : storativity

Mass conservation

$$\rho S \frac{\partial P}{\partial t} + \varepsilon \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} + \nabla.\left(\varepsilon \rho \vec{V}\right) = \rho Q_S\,.$$

$\alpha \simeq 4,4\,10^{-10}\ m^2/N$, $\beta \simeq$ 10^{-7}to10^{-9} m^2/N, then $S << 1$

Density-driven flow

Hydraulic head

$$h = \frac{P}{\rho_0 g} + y$$
$$\nabla h = \frac{\nabla P}{\rho_0 g} + \nabla z$$
$$\varepsilon \vec{V} = -\frac{\mathbb{K} \rho_0 g}{\mu} (\nabla h + \frac{\rho - \rho_0}{\rho_0} \nabla z)$$

- ρ_0 : density of pure water

Mass conservation

$$\rho_0 g \rho S \frac{\partial h}{\partial t} + \varepsilon \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} + \nabla . \left(\varepsilon \rho \vec{V} \right) = \rho Q_S \, .$$

Boundary Conditions

Dirichlet or Neumann

Transport by dispersion and convection

Mass conservation

$$\frac{\partial\left(\varepsilon\rho C\right)}{\partial t} + \nabla\left(\varepsilon\rho C\vec{V}\right) = \nabla.\left(\varepsilon\rho\mathbb{D}(\vec{V})\nabla C\right) + Q_c,$$

$$\mathbb{D}(\vec{V}) = D_m I + (\alpha_L - \alpha_T)\frac{\vec{V}\otimes\vec{V}}{\left|\vec{V}\right|} + \alpha_T\left|\vec{V}\right| I$$: dispersion

- D_m : molecular diffusion
- α_L (resp. α_T) : longitudinal(resp. transverse) dispersivity

if $\alpha_L = \alpha_T = 0$ then $\mathbb{D} = D_m I$ is constant

Transport by dispersion and convection

Mass conservation : non conservative form

$$\varepsilon\rho\frac{\partial C}{\partial t} + \varepsilon\rho\,\vec{V}.\nabla C = \nabla.\left(\varepsilon\rho\mathbb{D}(\vec{V})\nabla C\right),$$

Boussineq approximation

$$\frac{\partial C}{\partial t} + \vec{V}\nabla C = \nabla.\left(\mathbb{D}(\vec{V})\nabla C\right)$$

Boundary Conditions

Dirichlet and Neumann

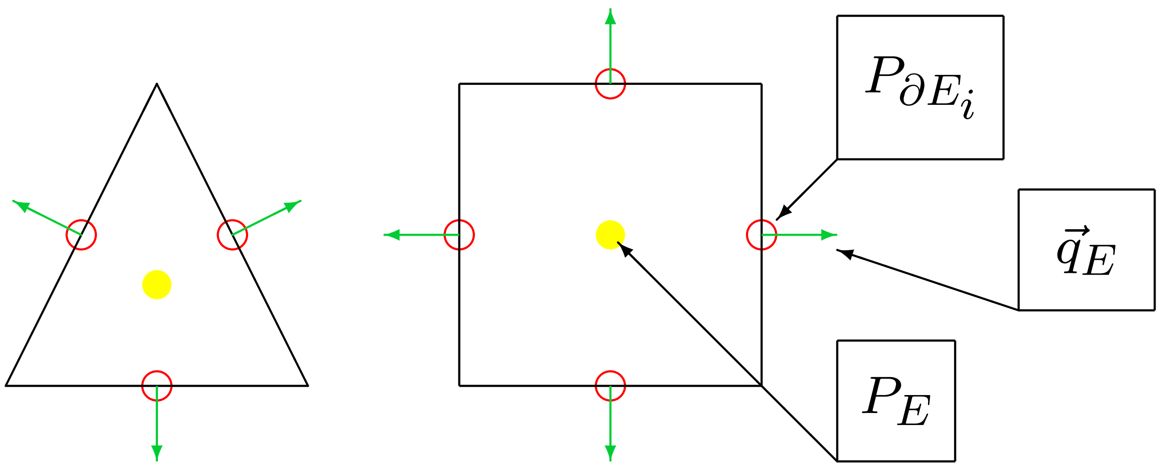
Coupled density-driven flow and transport

$$\begin{cases} \rho_0 g \rho S \dfrac{\partial h}{\partial t} + \varepsilon \dfrac{\partial \rho}{\partial C}\dfrac{\partial C}{\partial t} + \nabla.\left(\varepsilon \rho \vec{V}\right) = \rho Q_S \\ \dfrac{\partial C}{\partial t} + \vec{V}\nabla C = \nabla.\left(\mathbb{D}(\vec{V})\nabla C\right) \\ \text{Boundary Conditions} \\ \text{Initial Conditions} \\ \text{Darcy law} \\ \text{State laws} \end{cases}$$

if $S = 0$ then the mass matrix is singular

Mixed Finite Elements : Raviart-Thomas elements

$$\int_{\partial E_j} \vec{w}_i . \vec{n}_{\partial E_j} = \delta_{ij} \qquad \Rightarrow \int_E \nabla . \vec{w}_i = 1 .$$



DOF $\vec{q}_E = \Sigma_{\partial E_j \subset \partial E} Q_j \vec{w}_j$ • DOF for P_E ○ DOF for $P_{\partial E_i}$

Discretised flow equations with Hybrid MFE

$$\begin{cases} A_1 \frac{dP}{dt} + A_2 \frac{dC}{dt} + \Delta_p P - N_p T = F_1 \\ R_p^T P - M_p T = F_2 \\ \vec{V} = \vec{Q}(P,T)/\varepsilon \end{cases}$$

P : head in each element (order nm)
T : head through each edge (order nf)
F_1 : source, Boundary Condition and term with $\rho g n_z$ (order nm)
F_2 : BC and term with $\rho g n_z$ (order nf)
A_1 : diagonal matrix of order nm
A_2 : diagonal matrix of order nm
Δ_p : diagonal matrix d'ordre nm
N_p : sparse matrix of dimensions $nm \times nf$
R_p : sparse matrix of dimensions $nm \times nf$
M_p : sparse matrix of order nf (SPD matrix)

Time discretisation - Implicit Euler - one time step

State laws ε and μ are constant,

ρ is a linear function of C

$$\begin{cases} \rho^{n+1} = \rho(C^{n+1}), \\ A_1(\rho^{n+1})\frac{P^{n+1}-P^n}{\Delta t} + A_2\frac{C^{n+1}-C^n}{\Delta t} + \ldots \\ \quad \Delta_p(\rho^{n+1})P^{n+1} - N_p(\rho^{n+1})T = F_1(\rho^{n+1}) \\ R_p^T P^{n+1} - M_p T = F_2(\rho^{n+1}) \\ \varepsilon\vec{V}^{n+1} = \vec{Q}(P^{n+1}, T) \end{cases}$$

Discrete Flow equation

Case $D(C)$ non singular

$$D(C)\frac{dP}{dt} + \frac{dC}{dt} + M(C)P = F(C)$$
$$\vec{V} = \vec{Q}(P)$$

case $S = 0$

$$\frac{dC}{dt} + M(C)P = F(C)$$
$$\vec{V} = \vec{Q}(P)$$

Transport - Operator splitting

Spatial discretisation

Discontinuous Finite Element Method for advection

Upwinding and Slope Limiting techniques

Mixed Hybrid Finite Element Method for dispersion

Time discretisation

Explicit scheme for advection

Implicit scheme for dispersion

Transport - Operator splitting

One time step

$$C_K^{n+1/2} = C_K^n + \Delta t \mathcal{A}(C_K^n, \vec{V}^n)$$
$$C^{n+1/2} = moy(C_K^{n+1/2})$$

$$D^{n+1} = D(\vec{V}^{n+1})$$

$$\frac{C^{n+1} - C^{n+1/2}}{\Delta t} + \Delta_c(D^{n+1})C^{n+1} - R_c(D^{n+1})X = G_1(D^{n+1})$$
$$R_c^T(D^{n+1})C^{n+1} - M_c(D^{n+1})X = G_2(D^{n+1})$$

$$C_K^* = C_K^n + C^{n+1} - C^n$$
$$C_K^{n+1} = \mathcal{L}(C_K^*)$$

Discrete transport equation

Not really correct but...

$$\frac{dC}{dt} = A_c(C, \vec{V}) + A_d(\vec{V})C + G(\vec{V})$$

- A_c discrete advection operator using DFE
- A_d discrete dispersion operator using MHFE

Coupled Density driven flow and transport

Coupled equations

$$\begin{cases} \frac{dC}{dt} = A_c(C, \vec{V}) + A_d(\vec{V})C + G(\vec{V}) \\ \frac{dC}{dt} + D(C)\frac{dP}{dt} = M(C)P + F(C) \\ \vec{V} = \vec{Q}(P) \end{cases}$$

ODE if $D(C)$ non singular, DAE if $D(C)$ singular ($S = 0$)

Operator splitting

Advection and dispersion+flow

Coupling flow and transport - one time step

Operator splitting if $D(C)$ is non singular

$$
\begin{cases}
C_K^{n+1/2} = C_K^n + \Delta t A_c(C_K^n, \vec{V}^n) \\
C^{n+1/2} = moy(C_K^{n+1/2}) \\
C^{n+1} = C^{n+1/2} + \Delta t A_d(\vec{V}^{n+1}) C^{n+1} + \Delta t G(\vec{V}^{n+1}) \\
D(C^n)(P^{n+1/2} - P^n) = -(C^{n+1/2} - C^n) \\
D(C^{n+1})(P^{n+1} - P^{n+1/2}) = -(C^{n+1} - C^{n+1/2}) + \ldots \\
\Delta t M(C^{n+1}) P^{n+1} + \Delta t F(C^{n+1}) \\
C_K^* = C_K^n + C^{n+1} - C^n \\
C_K^{n+1} = \mathcal{L}(C_K^*)
\end{cases}
$$

Coupling flow and transport - one time step

Approximate scheme if $D(C)$ is non singular

$A_d(\vec{V}^{n+1}) \approx A_d(\vec{V}^n)$

$G(\vec{V}^{n+1}) \approx G(\vec{V}^n)$

Decoupled linear transport and linear flow equations

Coupling flow and transport - one time step

Operator splitting if $D(C)$ is singular

$$\begin{cases} C_K^{n+1/2} = C_K^n + \Delta t A_c(C_K^n, \vec{V}^n) \\ C^{n+1/2} = moy(C_K^{n+1/2}) \\ C^{n+1} = C^{n+1/2} + \Delta t A_d(\vec{V}^n) C^{n+1} + \Delta t G(\vec{V}^n) \\ A_c(C_K^{n+1}, \vec{V}^{n+1}) + \frac{C^{n+1} - C^{n+1/2}}{\Delta t} = M(C^{n+1}) P^{n+1} + F(C^{n+1}) \\ C_K^* = C_K^n + C^{n+1} - C^n \\ C_K^{n+1} = \mathcal{L}(C_K^*) \end{cases}$$

Decoupled linear transport and nonlinear flow equations

Coupling flow and transport - one time step

Current implementation if $D(C)$ is singular

$$\begin{cases} C_K^{n+1/2} = C_K^n + \Delta t A_c(C_K^n, \vec{V}^{n+1}) \\ C^{n+1/2} = moy(C_K^{n+1/2}) \\ C^{n+1} = C^{n+1/2} + \Delta t A_d(\vec{V}^n) C^{n+1} + \Delta t G(\vec{V}^n) \\ \frac{C^{n+1} - C^n}{\Delta t} = M(C^{n+1}) P^{n+1} + F(C^{n+1}) \\ C_K^* = C_K^n + C^{n+1} - C^n \\ C_K^{n+1} = \mathcal{L}(C_K^*) \end{cases}$$

Nonlinear coupled transport and flow equations

Coupling by fixed point iterations

Fixed point loop

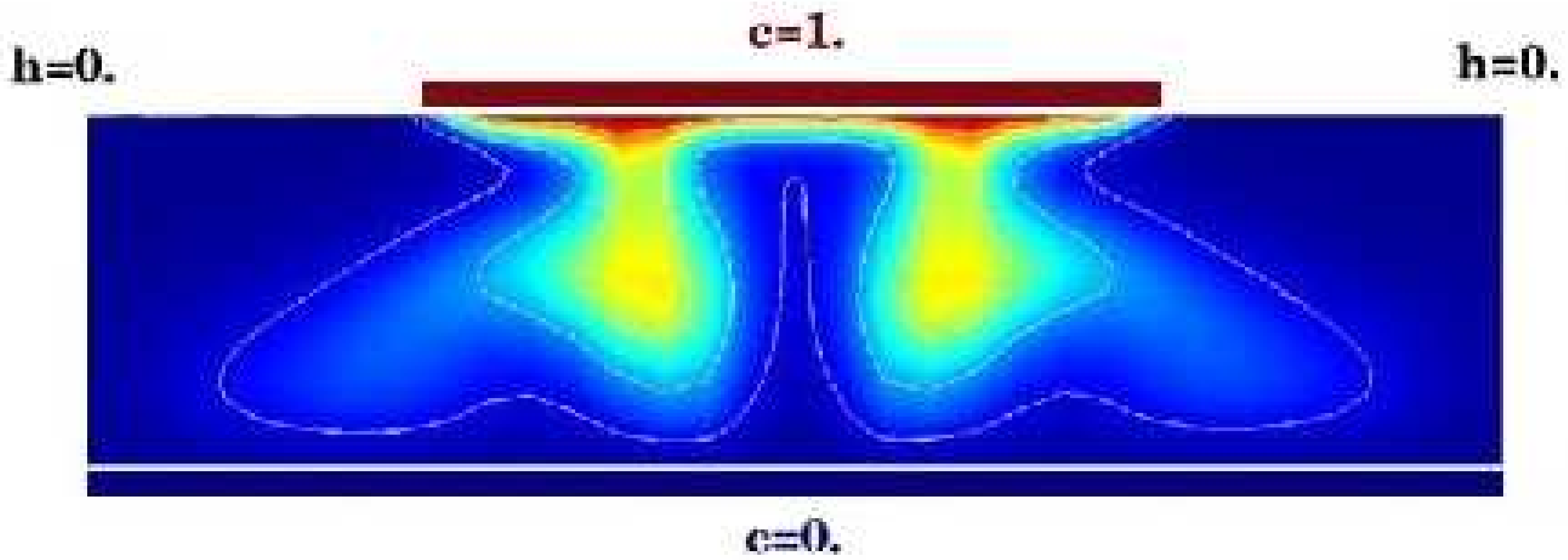
$$
\begin{cases}
C_K^{n+1/2} = C_K^n + \Delta t A_c(C_K^n, \vec{V}^{n+1,k}) \\
C^{n+1/2} = moy(C_K^{n+1/2}) \\
C^{n+1,k+1} = C^{n+1/2} + \Delta t A_d(\vec{V}^n) C^{n+1,k+1} + \Delta t G(\vec{V}^n) \\
\frac{C^{n+1,k+1} - C^n}{\Delta t} = M(C^{n+1,k+1}) P^{n+1,k+1} + F(C^{n+1,k+1}) \\
C_K^* = C_K^n + C^{n+1,k+1} - C^n \\
C_K^{n+1,k+1} = \mathcal{L}(C_K^*)
\end{cases}
$$

Elder test problem

Parameters for Elder test problem

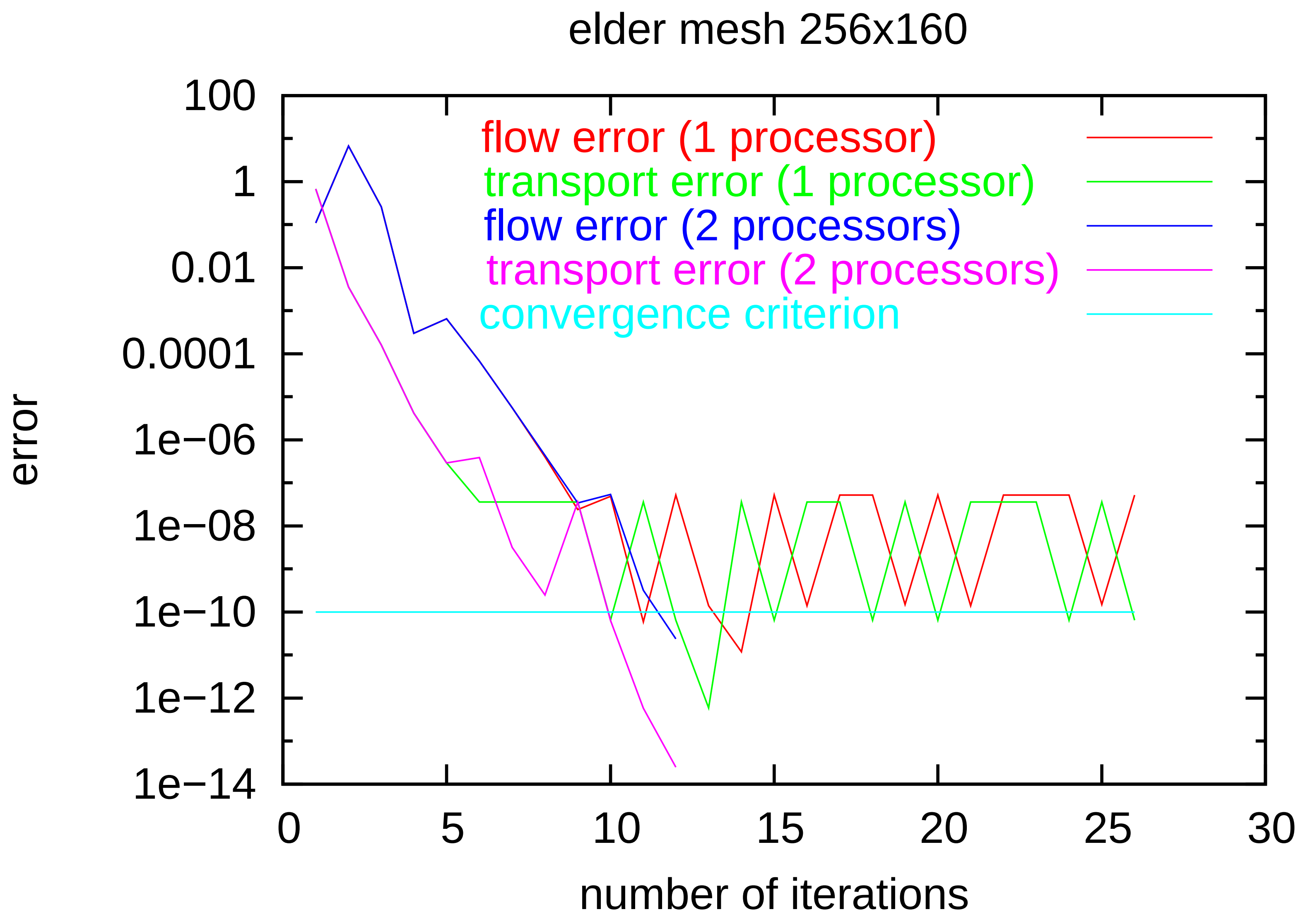
Permeability	$kx = ky = 4.845 \times 10^{-13}\ m^2$
Porosity	$\epsilon = 0.1$
Storativity	$S = 0$
Dispersivity	$\alpha_L = \alpha_T = 0\ m$
Molecular diffusion coefficient	$D_m = 3.565 \times 10^{-6}\ m^2 s^{-1}$
State equations	$\rho = \rho_0 + 200C$
	$\mu = 10^{-3}\ Pa.s$
Domain	$600 \times 150\ m$

Elder test problem - results



t=10 years

Elder test problem - convergence analysis



Saltwater intrusion - open questions

- Which operator splitting formulation if D is singular ?
- Theoretical convergence analysis ?
- Validation of results ?
- Reduced coupled models ?