Flow and trasnsport of pollutants in the subsurface : coupled models and numerical methods

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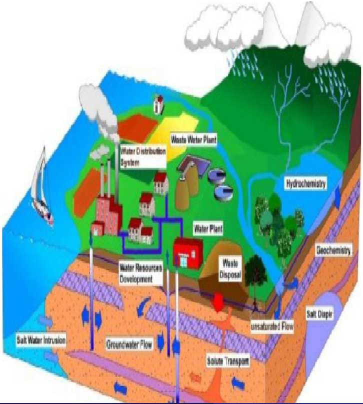
Outline

Plan

1. Motivations
2. Basic models and methods
   - Flow model
   - Transport model
   - Chemistry
3. Coupled models
   - Densisty driven flow
   - Reactive transport

Underground water

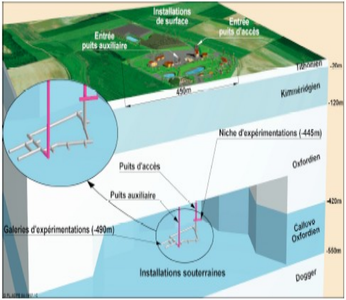
- 22% of all natural water resources
- 51% of all drinking water
- 37% of agricultural water



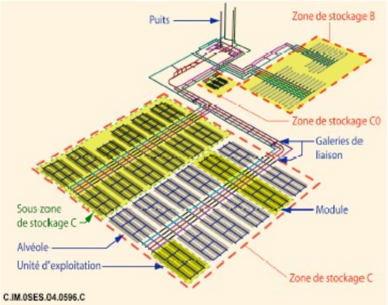
- Possible contamination of groundwater by industrial waste
- Microbial remediation
- Variant : saltwater intrusion : coupling to flow

Nuclear waste storage

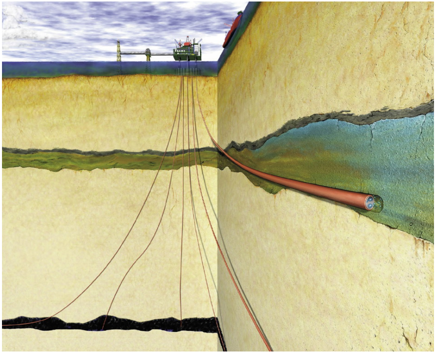
- Assess safety of deep geological nuclear waste storage (clay layer)
- Long term simulation of radionuclide transport
- Wide variation of scales : from package (meter) to regional (kilometers)
- Geochemistry: large number of species



ANDRA



CO_2 sequestration



Sleipner project, Norway

- Long term capture of CO_2 in saline aquifer
- Simulation to understand CO_2 migration through salt
- Coupling of liquid and gas phase, reactive transport

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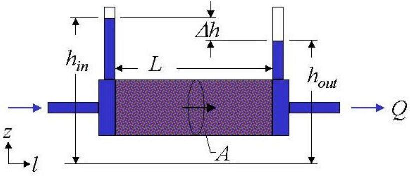
Flow : Darcy's law

Henry Philibert Gaspard Darcy, (1803-1858) French engineer

Darcy's law

$$Q = AK\frac{\Delta h}{L}$$



- Q flow $(\mathrm{m}^3/\mathrm{s})$
- K Hydraulic conductivity (m/s)
- h Piezometric head (m)
  $(h = p/\rho g + z)$

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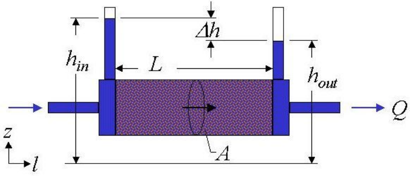

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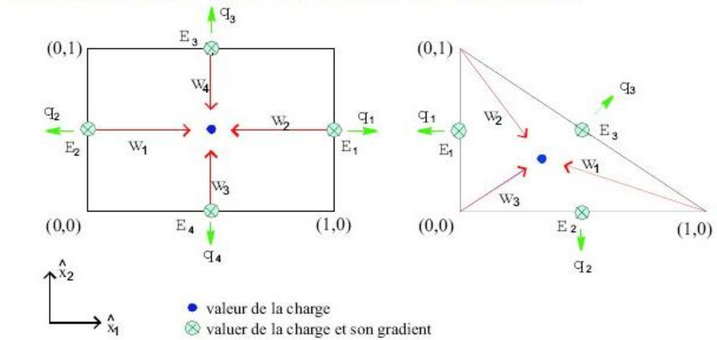
Modern, differential version $q = -K\nabla h$, q Darcy velocity

Flow equations

$$\nabla \cdot q = 0 \qquad \text{incompressibility}$$

Mixed finite elements

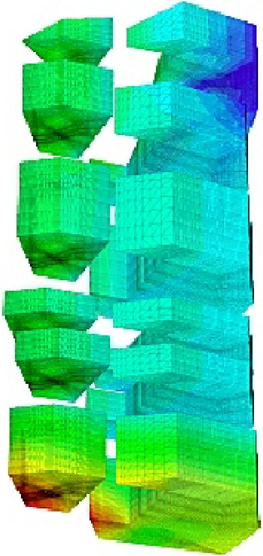
- Approximate both head and Darcy velocity
- Locally mass conservative
- Flux is continuous across element faces
- Allows full diffusion tensor



Raviart-Thomas space

Domain decomposition

- Flow around nuclear waste storage area
- Computed by domain decomposition (Robin–Robin)
- Subdomain code in C++ (LifeV), interface solver in Ocaml
- Parallelism in OcamlP3l (skeleton based)
- F. Clément, V. Martin (thesis), P. Weis (INRIA, Estime)



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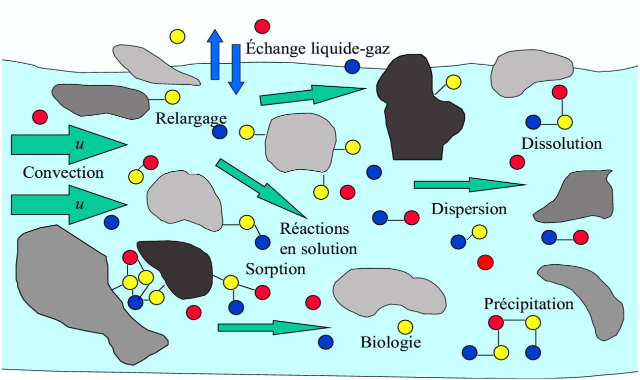
Physics of advection–dispersion



Convection	Transport by velocity field
Diffusion	motion due to concentration gradient
Dispersion	due microscopic velocity heterogeneity
Reaction	between species, interaction with host matrix

Transport model

Convection–diffusion equation

$$\omega \frac{\partial c}{\partial t} - \underbrace{\operatorname{div}(\mathbf{D}\,\mathrm{grad}\,c)}_{\text{dispersion}} + \underbrace{\operatorname{div}(\mathbf{u}c)}_{\text{advection}} + \omega\lambda c = f$$

- c: concentration $[\mathrm{mol}/\mathrm{l}]$
- *omega*: porosity (–)
- λ radioactive decay $[\mathrm{s}^{-1}]$
- $\mathbf{u}$ Darcy velocity $[\mathrm{m}/\mathrm{s}]$

Dispersion tensor

$$\mathbf{D} = d_e\mathbf{I} + |\mathbf{u}|[\alpha_l\mathbf{E}(\mathbf{u}) + \alpha_t(I - \mathbf{E}(\mathbf{u}))], \quad E_{ij}(\mathbf{u}) = \frac{u_i u_j}{|\mathbf{u}|}$$

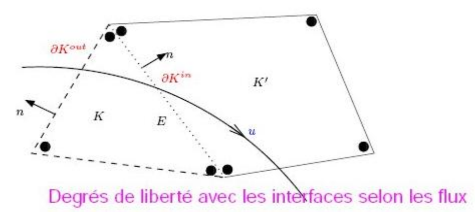
α_l, α_t dispersicity coeff. $[\mathrm{m}]$, d_e molecular diffusion $[\mathrm{m}/\mathrm{s}^2]$

Solution by operator splitting

Advection step

Explicit, finite volumes / discontinuous Galerkine

- Locally mass conservative
- Keeps sharp fronts
- Small numerical diffusion
- Allows unstructured meshes
- CFL condition: use sub–time–steps



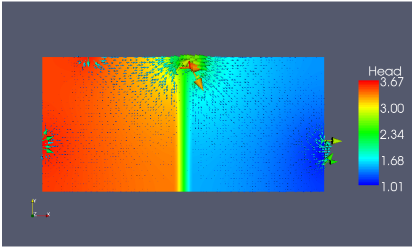
Dispersion step

Like flow equation (time dependant): mixed finite elements (implicit)

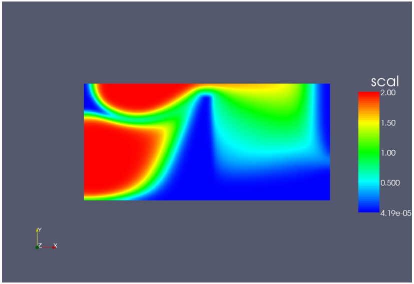
Order 1 method

Example: transport around an obstacle

MoMaS benchmark for reactive transport. Here transport only



Head and velocity

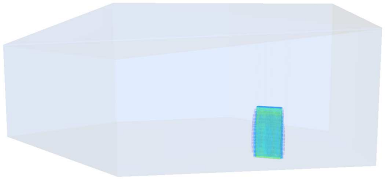


Concentration at $t = 25$

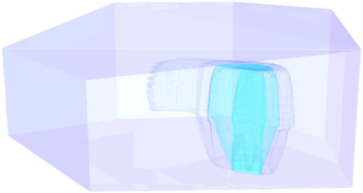
J. B. Apoung, P. Havé, J. Houot, MK, A. Semin

Transport around a nuclear waste storage site

GdR MoMaS benchmark, Andra model



Concentration at 130 000 years



Concentration at 460 000 years

A. Sboui, E. Marchand (INRIA, Estime)

Plan

Classification of chemical reactions

According to nature of reaction

Homogeneous	In the same phase (aqueous, gaseous, ...) Examples: Acid base, oxydo–reduction

According to speed of reaction

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Slow reactions	Irreversible, modeled using kinetic law
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Depends on relative speed of reactions and transport.

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In this talk: Equilibrium reactions, with sorption.

Sorption processes

Definition

Sorption is the accumulation of a fluid on a solid at the fluid–solid interface.

Main mechanism for exchanges between dissolved species and solid surfaces.

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Can be modeled as mass action law

The chemical problem

System of non-linear equations

$$\left.\begin{aligned} c + S^T x + A^T y &= T, \\ \bar{c} + B^T \bar{x} &= W, \end{aligned}\right\} \quad \text{Mass conservation}$$

$$\left.\begin{aligned} \log x &= S \log c + \log K_x, \\ \log \bar{x} &= A \log c + B \log \bar{c} + \log K_y. \end{aligned}\right\} \quad \text{Mass action law}$$

Dissolved total: $C = c + S^T x$, Fixed total: $F = A^T \bar{x}$.

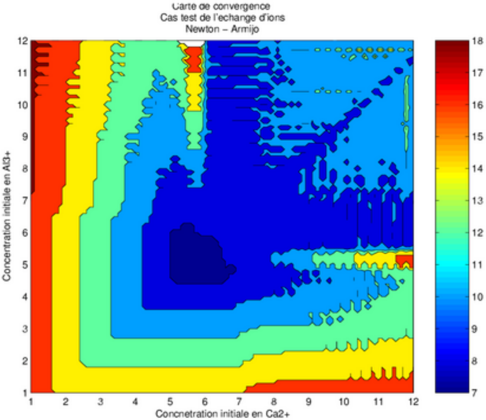
Role of chemical model

Given totals T (and W, known), split into mobile and immobile total concentrations.

$$C = \Phi(T), \qquad F = \Psi(T)$$

Numerical solution of chemical problem

Take concentration logarithms as main unknowns
Use globalized Newton's method (line search, trust region).



Ion exchange: 6 species, 4 components (vary initial guess)

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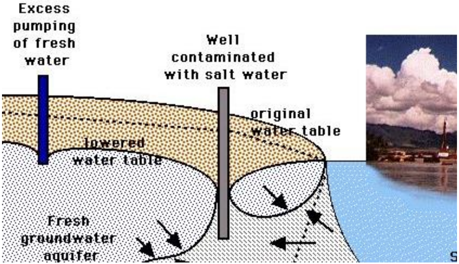
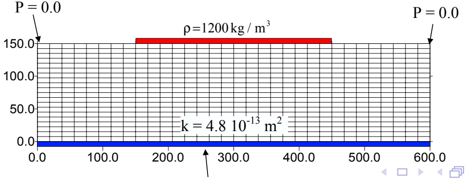
Motivations

Seawater intrusion can threaten drinking water resevoir



Synthetic model (Elder): fingering instability



Physical model

Flow

Mass conservation for fluid $\dfrac{\partial(\rho\omega)}{\partial t} + \nabla.\left(\varepsilon\rho\vec{V}\right) = \rho Q_S,$

Generalized Darcy's law $\varepsilon\vec{V} = -\dfrac{1}{\mu}K\left(\nabla P + \rho g\vec{n}_z\right),,$

Equation of state $\rho = \rho_0 + \dfrac{\partial\rho}{\partial C_m}C_m, \quad \rho_0 = 1000, \quad \dfrac{\partial\rho}{\partial C_m} = 200.$

Transport

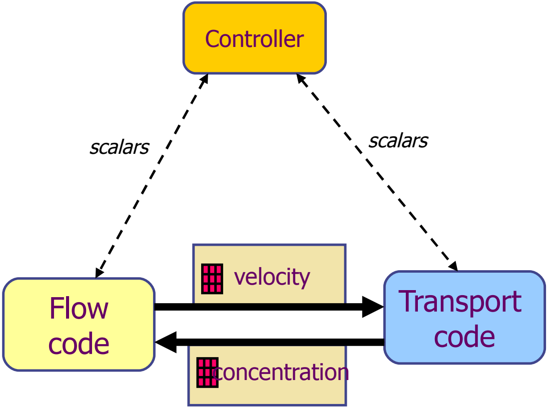
Salt mass conservation

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

Dispersion tensor $D(\vec{V}) = D_m I + (\alpha_L - \alpha_T)\dfrac{\vec{V}\otimes\vec{V}}{\left|\vec{V}\right|} + \alpha_T\left|\vec{V}\right| I$

Distributed implementation

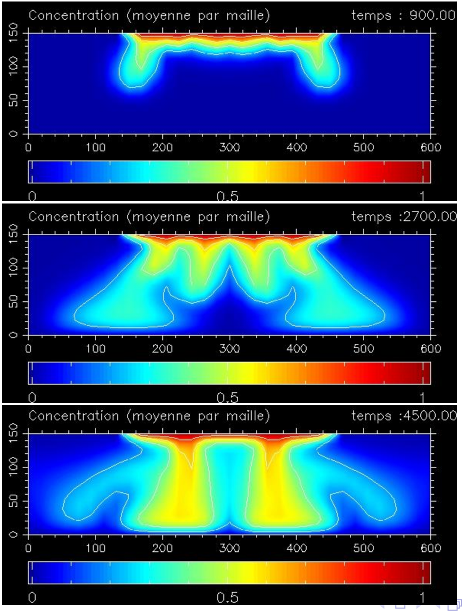
Coupling between flow and transport :



Use Corba for coupling components

Joint work with J. Erhel, Ph. Ackerer, Ch. Perez, M. Mancip

Elder model


Concentration (moyenne par maille)
temps : 900.00
0
50
100
150
0
100
200
300
400
500
600
0
0.5
1
Concentration (moyenne par maille)
temps :2700.00
0
50
100
150
0
100
200
300
400
500
600
0
0.5
1
Concentration (moyenne par maille)
temps :4500.00
0
50
100
150
0
100
200
300
400
500
600
0
0.5
1

Plan

The coupled system

Transport for each species (same dispersion tensor for all species)

$$
\begin{aligned}
\frac{\partial x_i}{\partial t} + L(x_i) &= r_i^x, & \frac{\partial c_j}{\partial t} + L(c_j) &= r_j^c, \\
\frac{\partial y_i}{\partial t} &= r_i^y, & \frac{\partial s_j}{\partial t} &= r_j^s,
\end{aligned}
$$

The coupled system

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$$\frac{\partial x_i}{\partial t} + L(x_i) = r_i^x, \quad \frac{\partial c_j}{\partial t} + L(c_j) = r_j^c,$$
$$\frac{\partial y_i}{\partial t} = r_i^y, \quad \frac{\partial s_j}{\partial t} = r_j^s,$$

Eliminate (unknown) reaction rates by using conservation laws ($T = C + F$)

$$\frac{\partial T^{ic}}{\partial t} + L(C^{ic}) = 0, \quad ic = 1, \dots, N_c$$
$$T_{ix}^{ic} = C_{ix}^{ic} + F_{ix}^{ic} \quad ic = 1, .., N_c \text{ and } ix = 1, .., N_x$$
$$F_{ix} = \Psi(T_{ix}) \quad ix = 1, \dots, N_x.$$

Number of transport equations reduced from $N_x + N_y$ to $N_c + N_s$

Coupling formulations and algorithms(1)

CC formulation, explicit chemistry

$$\begin{cases} \dfrac{dC}{dt} + \dfrac{dF}{dt} + LC = 0 \\ H(z) - \begin{pmatrix} C+F \\ W \end{pmatrix} = 0 \\ F - F(z) = 0. \end{cases}$$

- $+$ Explicit Jacobian
- $+$ Chemistry function, no chemical solve
- $-$ Intrusive approach (chemistry not a black box)
- $-$ Precipitation not easy to include

Coupled system is index 1 DAE

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

Use standard DAE software

J. Erhel, C. de Dieuleveult (Andra thesis)

Coupling formulations and algorithms(2)

TC formulation, implicit chemistry

$$\begin{cases} \dfrac{dT}{dt} + LC = 0 \\ T - C - F = 0 \\ F - \Psi(T) = 0 \end{cases}$$

- $+$ Non-intrusive approach (chemistry as black box)
- $+$ Precipitation can (probably) be included
- $-$ One chemical solve for each function evaluation

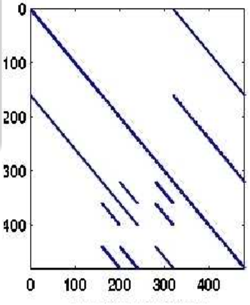
$$\begin{cases} \dfrac{C^{n+1} - C^n}{\Delta t} + \dfrac{F^{n+1} - F^n}{\Delta t} + L(C^{n+1}) = 0 \\ T^{n+1} = C^{n+1} + F^{n+1} \\ F^{n+1} = \Psi(T^{n+1}) \end{cases}$$

Solve by Newton's method

Solution by Newton–Krylov

Structure of Jacobian matrix

$$f'(C,T,F) = \begin{pmatrix} (I+\Delta t L) & 0 & I \\ -I & I & -I \\ 0 & -\Psi'(T) & I \end{pmatrix}$$



- Solve the linear system by an iterative method (GMRES)
- Require only jacobian matrix by vector products.

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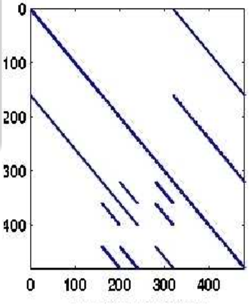

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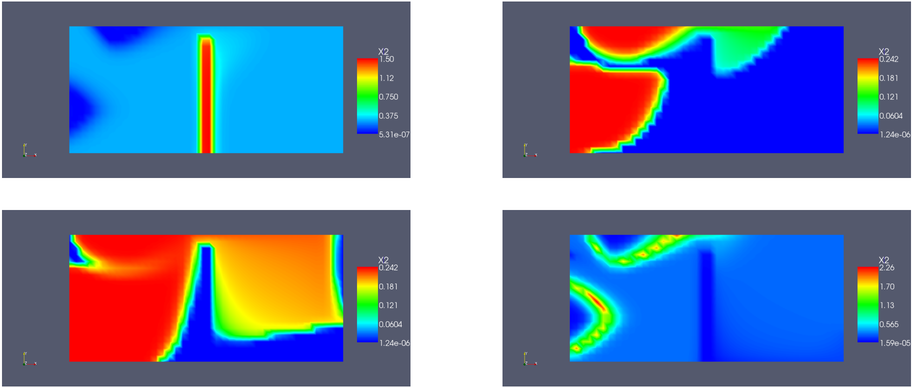
Inexact Newton

- Approximation of the Newton's direction $\|f'(x_k)d + f(x_k)\| \leq \eta \|f(x_k)\|$
- Choice of the forcing term η?
  - Keep quadratic convergence (locally)
  - Avoid oversolving the linear system
- $\eta = \gamma \|f(x_k)\|^2 / \|f(x_{k-1})\|^2$ (Kelley, Eisenstat and Walker)

MoMaS reactive transport benchmark

Numerically difficult tets case, 12 chemical species (J. Carrayrou)

Concentration of species 2 at $t = 50$, $t = 1000$,$t = 2000$, $t = 5010$.



C. de Dieuleveult (Andra Thesis, INRIA, Sage)