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 intrusion: 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
- \(\bar{S} \in \mathbb{R}^{N_x+N_y,N_c+N_s} = \begin{pmatrix} S & 0 \\ A & B \end{pmatrix}\) : stoechiometric coefficients
Mass conservation

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

- \( W \) 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

\[ F = A^T y + D^T p \]

\[ p \in \mathbb{R}^{N_p} : \text{precipitated species} \]

Mass action laws

\[ \Pi : \text{saturation index} \]

\[ \Pi = \log K_p + D \log c \]

\[ \begin{cases} 
  p_i = 0 & \text{if } \Pi_i < 1 \\
  \Pi_i = 1 & \text{otherwise .} 
\end{cases} \]
Coupled transport and chemistry models

Convection-dispersion

\[ \mathcal{L}C = \nabla (C \vec{V}) - \nabla \cdot (D \nabla C) \]

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)

\[ C = c + S^T x \]
\[ F = A^T y \]
\[ T = C + F \]
\[ W = s + B^T y \]
Sequential Iterative method

Implicit Euler scheme - Formulation TCF

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

SOR-Newton iterations

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

$$
\begin{pmatrix}
M \frac{dX}{dt} + \Phi(X) = 0, \\
MX^{n+1} + \Delta t \Phi(X^{n+1}) = MX^n
\end{pmatrix}
$$
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 $5.5 \times 10^{-4}$ : 4212 CPU seconds
- SI, timestep $10^{-3}$ : 2465 CPU seconds
- DAE, timestep $5.5 \times 10^{-4}$ : 409 CPU seconds
Reactive transport - open questions

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

Salt Water Intrusion in Coastal Areas

Excess pumping of fresh water

Well contaminated with salt water

Lowered water table

Fresh groundwater aquifer

Salt water intrusion

Original salt water interface

Original salt water

Salt Water
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,
Density-driven flow

Mass conservation

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\varepsilon \rho \vec{V}) = \rho Q_S
\]

Generalized Darcy law

\[
\varepsilon \vec{V} = -\frac{1}{\mu} \mathbf{k} (\nabla P + \rho g \vec{n}_z)
\]

- \(\varepsilon\): porosity
- \(\rho\): fluid density
- \(\vec{V}\): Darcy rate
- \(Q_S\): source term
- \(\mathbf{k}\): permeability tensor
- \(P\): pressure
- \(\mu\): viscosity
- \(g\): gravity
Density-driven flow

State equations

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

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

Mass conservation

\[ \rho S \frac{\partial P}{\partial t} + \varepsilon \frac{\partial \rho \partial C}{\partial t} + \nabla \cdot (\varepsilon \rho \vec{V}) = \rho Q_S. \]

\[ \alpha \approx 4 \times 10^{-10} \text{ m}^2/N, \quad \beta \approx 10^{-7} \text{ to } 10^{-9} \text{ m}^2/N, \text{ then } S \ll 1 \]
Density-driven flow

Hydraulic head

\[ h = \frac{P}{\rho_0 g} + y \]
\[ \nabla h = \frac{\nabla P}{\rho_0 g} + \nabla z \]
\[ \varepsilon \vec{V} = -\frac{k}{\mu} \left( \nabla h + \frac{\rho - \rho_0}{\rho_0} \nabla z \right) \]

- \( \rho_0 \) : density of pure water

Mass conservation

\[ \rho_0 g \rho S \frac{\partial h}{\partial t} + \varepsilon \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} + \nabla \cdot (\varepsilon \rho \vec{V}) = \rho Q_S. \]

Boundary Conditions

Dirichlet or Neumann
Transport by dispersion and convection

Mass conservation

\[ \frac{\partial (\varepsilon \rho C)}{\partial t} + \nabla (\varepsilon \rho CV) = \nabla \cdot (\varepsilon \rho \mathbb{D}(\vec{V}) \nabla C) + Q_c, \]

\[ \mathbb{D}(\vec{V}) = D_m I + (\alpha_L - \alpha_T) \frac{\vec{V} \otimes \vec{V}}{|\vec{V}|} + \alpha_T |\vec{V}| I : \text{dispersion} \]

- \( D_m \): molecular diffusion
- \( \alpha_L \) (resp. \( \alpha_T \)): 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

\[ \varepsilon \rho \frac{\partial C}{\partial t} + \varepsilon \rho \vec{V} \cdot \nabla C = \nabla \cdot (\varepsilon \rho \mathbb{D}(\vec{V}) \nabla C), \]

Boussineq approximation

\[ \frac{\partial C}{\partial t} + \vec{V} \nabla C = \nabla \cdot (\mathbb{D}(\vec{V}) \nabla C) \]

Boundary Conditions

Dirichlet and Neumann
Coupled density-driven flow and transport

\[
\rho_0 g \rho S \frac{\partial h}{\partial t} + \varepsilon \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} + \nabla \cdot (\varepsilon \rho \vec{V}) = \rho Q_S
\]

\[
\frac{\partial C}{\partial t} + \vec{V} \nabla C = \nabla \cdot (\mathcal{D}(\vec{V}) \nabla C)
\]

Boundary Conditions
Initial Conditions
Darcy law
State laws

if \( S = 0 \) then the mass matrix is singular
Spatial discretisation of flow

Mixed Finite Elements : Raviart-Thomas elements

\[ \int_{\partial E_j} \vec{w}_i \cdot \vec{n}_{\partial E_j} = \delta_{ij} \Rightarrow \int_E \nabla \cdot \vec{w}_i = 1. \]

DOF \( \vec{q}_E = \sum_{\partial E_j \subset \partial E} Q_j \vec{w}_j \)

- DOF for \( P_E \)
- DOF for \( P_{\partial E_i} \)
Discretised flow equations with Hybrid MFE

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

- $P$: 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 $nm$
- $\Delta_p$: 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)
State laws $\varepsilon$ and $\mu$ are constant, 

$\rho$ is a linear function of $C$

\[
\begin{align*}
\rho^{n+1} &= \rho(C^{n+1}), \\
A_1(\rho^{n+1})\frac{P^{n+1} - P^n}{\Delta t} + A_2\frac{C^{n+1} - C^n}{\Delta t} + \ldots \\
\Delta_p(\rho^{n+1})P^{n+1} - N_p(\rho^{n+1})T &= F_1(\rho^{n+1}) \\
R_p^T P^{n+1} - M_p T &= F_2(\rho^{n+1}) \\
\varepsilon \vec{V}^{n+1} &= \vec{Q}(P^{n+1}, T)
\end{align*}
\]
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
One time step

\[ C_{K}^{n+1/2} = C_{K}^{n} + \Delta t A(C_{K}^{n}, \vec{V}^{n}) \]
\[ C^{n+1/2} = \text{moy}(C_{K}^{n+1/2}) \]

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

\[ \frac{C^{n+1}-C^{n+1/2}}{\Delta t} + \Delta c(D^{n+1})C^{n+1} - R_{c}(D^{n+1})X = G_{1}(D^{n+1}) \]
\[ R_{T}(D^{n+1})C^{n+1} - M_{c}(D^{n+1})X = G_{2}(D^{n+1}) \]

\[ C_{K}^{*} = C_{K}^{n} + C^{n+1} - C^{n} \]
\[ C_{K}^{n+1} = \mathcal{L}(C_{K}^{*}) \]
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

\[
\begin{align*}
\frac{dC}{dt} &= A_c(C, \vec{V}) + A_d(\vec{V})C + G(\vec{V}) \\
\frac{dC}{dt} + D(C)\frac{dP}{dt} &= M(C)P + F(C) \\
\vec{V} &= \vec{Q}(P)
\end{align*}
\]

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

Operator splitting

Advection and dispersion+flow
Operator splitting if \( D(C) \) is non singular

\[
\begin{align*}
C^{n+1/2}_K &= C^n_K + \Delta t A_c(C^n_K, \vec{v}^n) \\
C^{n+1/2} &= \text{moy}(C^{n+1/2}_K) \\
C^{n+1} &= C^{n+1/2} + \Delta t A_d(\vec{v}^{n+1})C^{n+1} + \Delta t G(\vec{v}^{n+1}) \\
D(C^n)(P^{n+1/2} - P^n) &= -(C^{n+1/2} - C^n) \\
D(C^{n+1})(P^{n+1} - P^{n+1/2}) &= -(C^{n+1} - C^{n+1/2}) + \ldots \\
\Delta t M(C^{n+1})P^{n+1} &= \Delta t F(C^{n+1}) \\
C^*_K &= C^n_K + C^{n+1} - C^n \\
C^{n+1}_K &= \mathcal{L}(C^*_K)
\end{align*}
\]
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
Operator splitting if $D(C)$ is singular

\[
\begin{align*}
C_{K}^{n+1/2} &= C_{K}^{n} + \Delta tA_{c}(C_{K}^{n}, \vec{V}^{n}) \\
C^{n+1/2} &= \text{moy}(C_{K}^{n+1/2}) \\
C^{n+1} &= C^{n+1/2} + \Delta tA_{d}(\vec{V}^{n})C^{n+1} + \Delta tG(\vec{V}^{n}) \\
A_{c}(C_{K}^{n+1}, \vec{V}^{n+1}) + \frac{C^{n+1} - C^{n+1/2}}{\Delta t} &= M(C^{n+1})P^{n+1} + F(C^{n+1}) \\
C_{K}^{*} &= C_{K}^{n} + C^{n+1} - C^{n} \\
C_{K}^{n+1} &= \mathcal{L}(C_{K}^{*})
\end{align*}
\]

Decoupled linear transport and nonlinear flow equations
Current implementation if $D(C')$ is singular

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

Nonlinear coupled transport and flow equations
Coupling by fixed point iterations

Fixed point loop

\[
\begin{align*}
C_{K}^{n+1/2} &= C_{K}^{n} + \Delta t A_{c}(C_{K}^{n}, \vec{V}^{n+1,k}) \\
C^{n+1/2} &= \text{moy}(C_{K}^{n+1/2}) \\
C^{n+1,k+1} &= C^{n+1/2} + \Delta t A_{d}(\vec{V}^{n}) C^{n+1,k+1} + \Delta t G(\vec{V}^{n}) \\
\frac{C^{n+1,k+1} - C^{n}}{\Delta t} &= M(C^{n+1,k+1}) P^{n+1,k+1} + F(C^{n+1,k+1}) \\
C_{K}^{*} &= C_{K}^{n} + C^{n+1,k+1} - C^{n} \\
C_{K}^{n+1,k+1} &= \mathcal{L}(C_{K}^{*})
\end{align*}
\]
### Parameters for Elder test problem

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability</td>
<td>$k_x = k_y = 4.845 \times 10^{-13} , m^2$</td>
</tr>
<tr>
<td>Porosity</td>
<td>$\epsilon = 0.1$</td>
</tr>
<tr>
<td>Storativity</td>
<td>$S = 0$</td>
</tr>
<tr>
<td>Dispersivity</td>
<td>$\alpha_L = \alpha_T = 0 , m$</td>
</tr>
<tr>
<td>Molecular diffusion coefficient</td>
<td>$D_m = 3.565 \times 10^{-6} , m^2 s^{-1}$</td>
</tr>
<tr>
<td>State equations</td>
<td>$\rho = \rho_0 + 200 C'$</td>
</tr>
<tr>
<td></td>
<td>$\mu = 10^{-3} , Pa.s$</td>
</tr>
<tr>
<td>Domain</td>
<td>$600 \times 150 , m$</td>
</tr>
</tbody>
</table>
Elder test problem - results

t=10 years
Elder test problem - convergence analysis

elder mesh 256x160

flow error (1 processor)
transport error (1 processor)
flow error (2 processors)
transport error (2 processors)
convergence criterion

error

number of iterations
Saltwater intrusion - open questions

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