Plan:

PART I
- The situation in the World
- The numerical challenge
- The couplex test case.
- Solution by Domain Decomposition

PART II • Inverse Problems
N-waste in the World

- There is 100 to 400 years of Nuclear electricity depending upon, recycling (MOX) and 3rd generation reactor, use of tritium.
- Waste is dangerous and accumulates at power plant sites. It it is hot and radioactive, it must be stored, usually in water or air cooling pools for 20 to 40 years, possibly chemically processed and concentrated (La Hague plant) and later disposed off.
- Very many disposal solutions have been proposed: sending them into the sun or inside the earth mantle is not yet feasible. An international rule forbids export of N-waste.
- Recycling and processing makes a lot of progress but it is controversial.
- Burial is somewhat inevitable and studied by most country, but deep into the ground or in tunnels? The half life of $^{242}$Pu is $3.46 \times 10^5$. It can be reused for bombs.
- N-waste requires cooling before burial ($\sim 50$Kwatt per canister)
- Burial has been studied in salt (WIP, Germany), granite (Canada & Sweden), clay (Belgium, Switzerland, France, Finlande?)
• Yucca-Mountain in the USA (Los Alamos, LLNL, Berkeley-Lab) has recently been OKayed.
• Canada Sweden (SKB, Aspo) and Finland are about to select their granite sites; they will use luxurious copper canisters. • France (Andra) Spain (Enresa), Belgium (Mol), Switzerland (Nagra, Grimsel) will most likely use a clay site.
• France and Japan will recycle and process (chemically at least) putting the waste into glass.
The French Site at Bure
The Topology
Inside the container there may be glass (C-waste) or mud or concrete surrounding the waste.
The Desired Results

- Concentration at $\{x_i\}_i$ vs $t$
- For all dangerous radionuclides
- Normal and alternate scenarios
- Probabilities are necessary (mean failure for canister industry)
- Because industrial quality
- Because of natural disasters
- Because of human mistakes
Modelling differs in granite and clay

**Normal Scenario:** Canisters don’t break for 10,000 years, then the radionuclides diffuse slowly into the water and convection diffusion takes place.

- Saturated / Unsaturated flow through porous media
- Heat affects geological constants
- Cracks are important, forcing the well disrupt the ground (ETZ).

*Thermo-Hydro-Mecano-chemical (THMC) problem.*
Simplification TH(M) in the near field, HC in the far field
The Near Field

- Modelling of the source terms is very complex but well studied. The idea is that once water is in contact with glass, there is a dissolution of glass proportional to the surface hence a velocity of escape of radio-nucleides: everything is dissolved in 1000 to 5000 years.
- Modelling of the concrete and clay for more than 500 years is a big issue
- Nuclear reactions and metal corrosion produce a small amount of gas (Argon and H)
- The Ph is important, microbes play a role

Saturated zone

The hydrostatic pressure $H$ verifies Darcy’s law

$$\vec{u} = -K \nabla H \quad \nabla \cdot \vec{u} = 0 \quad \Leftrightarrow \quad \nabla \cdot (K \nabla H) = 0$$

Subject to known inflow conditions (?) $H$ or $(K \nabla H) \cdot n$.

Proper values for $K$ is a major problem: double porosity...
The COUPLEX Test Case

Done with freefem+1.10 available at http://www.freefem.org

Fig 1: No Scaling

Fig 2: Scaled, with and without the repository
The Geometry

- **dogger**: $(0 < x < 25000) \times (0 < y < 200)$
- **clay**: Quadrangle: $(0, 200), (0, 295), (25000, 200), (25000, 350)$
- **limestone**: above clay and limited by the line $y = 595$
- **marl**: $(0 < x < 25000) \times (595 < y < 695)$

The vault $R = (18440, 21680) \times (244, 250) \times (100, 200)$

Darcy's law: $\vec{u} = K\nabla H \quad \nabla \cdot \vec{u} = 0.$

- $K_{marl} = 3.15 \times 10^{-5}$
- $K_{lime} = 6.31$
- $K_{clay} = 3.15 \times 10^{-6}$
- $K_{dog} = 25.23$

- On the soil surface (to boundary of marl): $H = 180 + 160x$.
- On right (resp left) bdy of limestone: $H = 310$ (resp 200)
- On right (resp left) bdy of dogger: $H = 289$ (resp 286)
- Homogeneous Neumann conditions on other boundaries.
Darcy Flow by freefem++

\[
\begin{align*}
xL &:= 1.0/25000; \
yL &:= 1.0/1400; \\
\text{border } a(t=0, 25000) & \{ x = t*xL; y = 0 \}; \quad \text{// bottom dogger bdy} \\
\text{... mesh } th = \text{buildmesh}( a(50*n) + \ldots ); \\
K & = 3.153e-5*\text{marl} + 6.3072*\text{limestone} + 3.153e-6*\text{clay} + 25.2288*\text{dogger}; \\
\text{solve(H1)} & \{ \text{pde(H1)} -dyy(H1)*K*xL^2-dxx(H1)*K*yL^2 = 0; \\
& \quad \text{on(b0)} H1=289; \quad \text{on(b2)} H1=310; \quad \text{on(c)} \quad H1 = 180 + 160*x/(25000*xL); \\
& \quad \text{on(d2)} H1=200; \quad \text{on(d0)} H1=286; \}
\end{align*}
\]
Zoom Near the Repository

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IMA 19/11/04
Numerical Simulation in 3D

A 3D version of the same is being developed, called freefem3D. It is based on the fictitious domain embedding finite element method; the geometry is specified by a POV-Ray file, particularly simple here because the computational domain is the fictitious domain itself:

```plaintext
camera {location<-10000,-10000,0> look_at <1900,250,150>}
light_source {<2, 4, -3> color rgb <1,1,0>}
background{color rgb <1,1,1>}
box {<18440,244,2000>, <21680,264,4000>}
   pigment {color rgb <1,0,0>}
```

The mesh is uniform with $240 \times 60 \times 30$ points.

```plaintext
double N = 30; vector n = (8*N, 2*N, N); vector a = (0,0,0); vector b = (25000,695*L,6000); scene
S=pov("dechet2.pov"); mesh Mesh = structured(n,a,b); domain D = domain(S);

function dogger = one(y<=199.99); function clay =
   one(y <= (295.01+ 55.01*x/25000)) * one(y>199.99);
function limestone = one(y<=594.99) * one(y>(295.01+55.01*x/25000));
function marl = one(y>594.99); function K = (3.1536e-5 * marl + 6.3072 * limestone
```

IMA 19/11/04
+ 3.1536e-6*clay + 25.2288*dogger)*(1-one(<1,0,0>));

function penal = 1-one(<1,0,0>);

solve(H) in D by Mesh
    cg(maxiter=900,epsilon=1E-10), krylov(precond=ichol)
{
    pde(H) -div(K*grad(H))=0;
    dnu(H)=0 on <1,0,0>;
    H =289* dogger + 310* limestone
       + clay* (289 + (y-200)*21.0/150)
       + marl * (310 + (y - 595)*0.3) on Mesh xmax;
    H =286*dogger + 200*limestone
       + clay * (286 - (y-200)*86/95)
       + marl * (200 - (y - 595)*0.2) on Mesh xmin;
    H =180 + 160 * x/25000 on Mesh ymax;
}; plot(medit,"H",H*penal,Mesh);
Results

3D Simulation, two views with colored levels of $H$
Asymptotics and Domain Decomposition

Let $\kappa_\varepsilon = \kappa_0 + \varepsilon \kappa_1 + \ldots$ \quad $\nabla \cdot (\kappa \nabla \phi_\varepsilon) = 0 \quad \phi_\varepsilon | \Gamma = \phi_\Gamma$

Assume $\kappa_0 = 0$ in $\Omega_1$, $\kappa_1 = 0$ in $\Omega_0$, $\bar{\Omega} = \bar{\Omega}_0 \cup \bar{\Omega}_1$, $\Gamma_{01} = \bar{\Omega}_0 \cap \bar{\Omega}_1$.

Then \quad $-\nabla \cdot [\kappa_i \nabla \phi_i] = 0$ in $\Omega_i$ \quad $\phi_i | \Gamma \cup \partial \Omega_i = \phi_\Gamma$

and \quad $\phi_0 = \phi_1$ \quad $\kappa_0 \frac{\partial \phi_0}{\partial n} = -\kappa_1 \frac{\partial \phi_1}{\partial n}$ on $\Gamma_{01}$

Therefore if $\kappa_0 >> \kappa_1$ and constant, it decouples

$-\Delta \phi_0 = 0$ in $\Omega_0$ \quad $\frac{\partial \phi_0}{\partial n} | \Gamma_{01} = 0 \quad \Delta \phi_1 = 0$ in $\Omega_1$ \quad $\phi_1 | \Gamma_{01} = \phi_0$

Prop. 1 Let $\phi_c$ be $\phi_i$ in $\Omega_i$, $i = 1, 2$. Let $\phi$ be the exact solution then

\[ \| \phi_c - \phi \| \leq C \left| \frac{\kappa_1}{\kappa_0} \right| \left\| \frac{\partial \phi_1}{\partial n} \right\| \]

Because of the error on the Neuman condition and continuity w/r to data.
Analytical Solution

For a permeable vault to an excellent precision

- In dogger:
  \[ H_d(x, y, z) = 286 + 1.210^{-4}x \]

- In clay:
  \[ H_c = (200 + 4.410^{-3}x) \frac{y - 200}{95 + 0.0393x} - (286 + 1.210^{-4}x) \frac{y - 295 - 0.0393x}{95 + 0.0393x} \]

- In limestone:
  \[ H_l = 200 + 4.410^{-3}x \]

- Marl:
  \[ H_m = (1.8 + 6.410^{-5}x)(y - 595) - (2 + 4.410^{-5}x)(y - 695) \]
Convection - Diffusion of I\textsuperscript{129} and Pu\textsuperscript{242}

\[ R_i \omega_i (\partial_t C_i + \lambda_i C_i) - \nabla \cdot (D_i \nabla C_i) + u \cdot \nabla C_i = 0 \quad \text{in } \Omega \times (0, T) \quad i = 1, 2. \]

- \( R_i = 1 \) except for Pu\textsuperscript{242} in the clay = 10\textsuperscript{5}
- Porosity \( \omega = 0.1 \), but in clay = 0.001 for I\textsuperscript{129}, = 0.2 for Pu\textsuperscript{242}
- \( \lambda_i = \log 2/T_i \), \( T_i = 1.57 \times 10^7 \) for I\textsuperscript{129}, 3.76 \times 10^5 for Pu\textsuperscript{242}

\[ D_i = \begin{pmatrix} D_{Li} & 0 \\ 0 & D_{Ti} \end{pmatrix} \quad \text{with} \quad D_{Mi} = D_{ei} + \alpha_M |u|, \quad M = L, T, \quad i = 1, 2. \]

<table>
<thead>
<tr>
<th></th>
<th>I\textsuperscript{129}</th>
<th>Pu\textsuperscript{242}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>De(m\textsuperscript{2}/y) ( \alpha_L )(m) ( \alpha_T )(m)</td>
<td>De(m\textsuperscript{2}/y) ( \alpha_L )(m) ( \alpha_T )(m)</td>
</tr>
<tr>
<td>Dogger</td>
<td>5.0e-4 \quad 50 \quad 1</td>
<td>5.0e-4 \quad 50 \quad 1</td>
</tr>
<tr>
<td>Clay</td>
<td>9.48e-7 \quad 0 \quad 0</td>
<td>4.42e-4 \quad 0 \quad 0</td>
</tr>
<tr>
<td>lime stone</td>
<td>5.0e-4 \quad 50 \quad 1</td>
<td>5.0e-4 \quad 50 \quad 1</td>
</tr>
<tr>
<td>marl</td>
<td>5.0e-4 \quad 0 \quad 0</td>
<td>5.0e-4 \quad 50 \quad 0</td>
</tr>
</tbody>
</table>
The Iodine Problem

For a permeable vault to an excellent precision

- In dogger: $H_d(x, y, z) = 286 + 1.210^{-4}x$
- In clay: $H_c = (200 + 4.410^{-3}x)\frac{y-200}{95+0.0393x} - (286 + 1.210^{-4}x)\frac{y-295-0.0393x}{95+0.0393x}$
- In limestone: $H_l = 200 + 4.410^{-3}x$
- Marl: $H_m = (1.8 + 6.410^{-5}x) (y-595)-(2 + 4.410^{-5}x) (y-695)$

Iodine transport: $\beta = \frac{K}{\lambda \omega^0} \nabla H \quad \frac{\partial C}{\partial t} - \nabla \cdot (\kappa \nabla C) + \beta \cdot \nabla C + \alpha C = 0$

In clay $\kappa = 9.48 \times 10^{-4}$, $\beta = 3.153 \times 10^{-6} (4.8(y-200), 900 + 0.044x)^T$, $\alpha = 0.44149 \times 10^{-4}$ and a source term in $R$:

\[ t \leq 1115 \ ? \ 0.0001*(t-1100)^+ \ : \ 0.0015*\exp((1115-t)/420); \]
Rescale the problem by $X = x/25000$ and $Y = y/1400 \Rightarrow$

$$\frac{\partial C}{\partial t} - \nabla_X \cdot (\kappa' \nabla_X C) + \beta' \cdot \nabla_X C + \alpha C = 0$$

with $\kappa_{XX} = 5 \times 10^{-12}$, $\kappa_{YY} = 1.6 \times 10^{-9}$ and $\beta' = (O(8 \times 10^{-10}), O(4 \times 10^{-8}))^T$. The $X$-diffusion can be neglected and also $\alpha$. The problem becomes one dimensional in $C'(X, Y, t) = C(X + \beta't, Y + \beta't, t)$:

$$\frac{\partial C'}{\partial t} - \kappa'_{YY} \frac{\partial^2 C'}{\partial Y^2} = 0 \text{ in } \Omega_c \quad C'|_{t=0} = 0.61 \ 1_R, \quad \frac{\partial C'}{\partial Y}|_{\partial \Omega_c} = 0$$

The Green function of the heat equation in 1D is $e^{-\frac{x^2}{4\kappa'_{YY} t}}/\sqrt{\kappa t}$ so the solution is

$$C'(x, y, t) = 0.61 \int_{R \cap \{x\}} e^{-\frac{|z-y|^2}{4\kappa'_{YY} t}} dZ$$
Finally

$$C(x, y, t) = 0.61 \int_{R \cap \{x-\beta_1 t\}} e^{-\frac{|z-y+\beta_2 t|^2}{4\kappa t}} \frac{d\sqrt{\kappa t}}{dz}$$

**LEFT:** level lines of $C$ from the analytical approximation.

**RIGHT:** Simulation by the finite element method of the complete equation; level line of $C$ (iodine). Both plots are for $t=60000$ years.
Iodine in the limestone layer

- Diffusion coeff: \((0.56, 3.54) \times 10^{-3}\) Convective x-velocity \(-0.2\).
- Thus it takes 5 years to cross a distance of order one while the characteristic diffusion lengths for 5 years are \((0.09, 0.23)\).
- Hence all terms are more or less of the same order in PDE.
- The time step should agree with the physics \(\Rightarrow 5\) years!
- Results are requested after a million year while source term (i.e. the boundary condition from the clay) varies very slowly,
- \(\Rightarrow\) the problem is *stationary* at every time step! Same in dogger
Results with UG (P. Bastian)
FULL 3D Solution in Clay Layer

Computed by S. Del Pino
Parallel Computing

Within a single layer $K$ is constant. It is also ideal for DDM and homogenization.
Perspective

- Archimedes force: will the canister sink into the clay?
- Geochemistry is important + micro-organisms?
- Modelling of EDZ (double porosity models...)
- There is an unsaturated zone which cannot be neglected when hot (THMC).
- Outside expertise is not used (UG,NUFT,FEMH, Code-brite...)
- Probability, error bounds, code assessment...
- Andra is very far from a convincing calculation
- Geological parameters are not really known: data assimilation.
Part II: Inverse Problems: Seismic Imaging and Least Squares

- G. Chavent, J. Jaffré...

\[ \rho \partial_{tt} u - \nabla \cdot (\sigma \nabla u) = 0 \quad + \text{B.C.} \]

\[ u = u_d \text{ on } D \times (0, T) \implies \rho? \]
Sensitivity with respect to Discontinuity

- Introduced by Sokolowski, Masmoudi, Feijoo, Allaire.
- It allows for a wide variety of changes in the domain shapes.

Consider another approach

\[ \bar{\Omega} = \bar{\Omega}_1^a \cup \bar{\Omega}_2^a \quad \Omega_1^a \cap \Omega_2^a = \emptyset \quad \Sigma^a = \bar{\Omega}_1^a \cap \bar{\Omega}_2^a. \]

Let \( \kappa(a) \) be piecewise constant \( = \kappa_i \) on \( \Omega_i^a \):

\[-\nabla \cdot (\kappa(a) \nabla u(a)) = f + \text{B.C. on } \Gamma = \partial \Omega.\]

What is \( u' := \frac{\partial u}{\partial a} \) at \( a = 0 \)?

This information is needed to solve inverse problems.
The traditional approach fails

Let \( I_{\Omega_2^a} \) be the characteristic function of \( \Omega_2^a \)

Let \([\kappa]\) be the jump \( \kappa_2 - \kappa_1 \),

\[
\kappa(a) = \kappa_1 + [\kappa]I_{\Omega_2^a}.
\]

In the sense of distribution theory

\[
\frac{d\kappa}{da}(a) = -x' \cdot n[\kappa]\delta_{\Sigma^a}.
\]

where \( s \to x(s; a) \) is \( \Sigma^a \) and \( x' = dx/da \). Ex in 1D:

\[
\kappa(a) = \kappa_1 + [\kappa]I(x > a) \Rightarrow \kappa' = -[\kappa]\delta(x - a)
\]

So it is tempting to write

\[
\int_{\Omega} \kappa(a) \nabla u' \nabla w = - \int_{\Omega} \kappa' \nabla u \nabla w = - \int_{\Sigma} [\kappa]x' \cdot n \nabla u \nabla w
\]

but the last integral makes no sense because \( \nabla u \) is discontinuous across \( \Sigma^a \).
Conclusion

- For nuclear waste repository assessment the direct problem is doable for known geophysical parameters.
- These sites will be experimented with for 50 years so many data can be obtained at some places and at others an inverse procedure can be used.
- The modeling is not completely clear, especially for very small diffusion.
- These problems are of national importance, so the numerical simulations are greatly needed.