A NUMERICAL METHOD FOR AN UNDERGROUND WASTE REPOSITORY PROBLEM WITH NON STANDART INTERFACE CONDITION

O. Gipouloux

In Collaboration with A. Agouzal and N. Debit

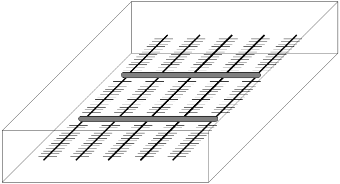
Institut Camill Jordan
CNRS UMR 5208
University of Lyon
France

October 13 2008

Contents

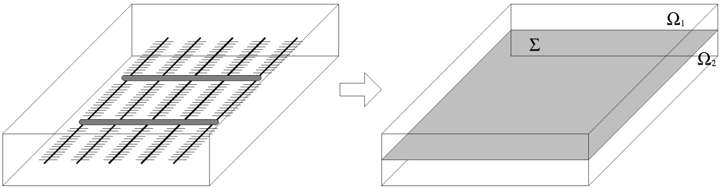
O. Gipouloux

Physical problem



- Convection diffusion problem
- A high number of small sources lying on hyperplan Σ..
- Very small size details ($<$ one meter).
- Very large domain ($>$ few kilometers).
- Long time study ($> 10^6$ years).
- $\Rightarrow$ Direct numerical simulations for performance assesment not realistic.

Homogenization Process



- Separate the domain into two domains Ω_1 and Ω_2 ($\Sigma = \Omega_1 \cap \Omega_2$).
- Reduce the sources to only one on Σ.
- Coupling the problems in Ω_1 and Ω_2 by an interface condition on Σ, depending on physical parameters :
  - More simple case : Flux Jump on Σ.
  - More interesting case : differential problem on Σ.

The non standart interface condition Problem

For sake of Simplicity, whithout transport :

$$\frac{\partial \phi}{\partial t} - \Delta\phi + \gamma\phi = f \quad \text{in } (\Omega_1 \cup \Omega_2),\ 0 < t \leq T \quad (1a)$$

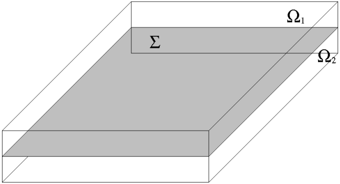
$$\phi = 0, \quad \text{on } (\Gamma \setminus \Sigma),\ 0 < t \leq T, \quad (1b)$$

$$\left[\frac{\partial \phi}{\partial n}\right]_\Sigma - \Delta_\Sigma \phi = g \quad \text{on } \Sigma,\ 0 < t \leq T, \quad (1c)$$

$$[\phi]_\Sigma = 0 \quad \text{on } \Sigma,\ 0 < t \leq T \quad (1d)$$

$$\phi(t = 0, .) = \phi_0 \quad \text{in } (\Omega_1 \cup \Omega_2) \quad (1e)$$

Where $[\cdot]$ denotes the jump through the interface Σ.



Stationary problem

Let consider first the stationary case
(Coming from, for example, the implicit time discretization of the above problem)

$$-\Delta\phi + \phi = f \quad \text{in } (\Omega_1 \cup \Omega_2), \tag{2a}$$

$$\phi = 0, \quad \text{on } (\Gamma \setminus \Sigma), \tag{2b}$$

$$\left[\frac{\partial\phi}{\partial n}\right]_\Sigma - \Delta_\Sigma \phi = g \quad \text{on } \Sigma, \tag{2c}$$

$$[\phi]_\Sigma = 0 \quad \text{on } \Sigma \tag{2d}$$

Equilibrium Formulation

Mixed Formulation for problems in $\Omega_i = 1, 2$.

$$p_i = \nabla\phi \quad \text{in } \Omega_i, i = 1, 2 \tag{3a}$$

$$-\operatorname{div}\ p_i + \phi = f \quad \text{in } \Omega_i, i = 1, 2 \tag{3b}$$

$$[p \cdot n] - \Delta_\Sigma \phi = g \quad \text{on } \Sigma \tag{3c}$$

$$\phi = 0, \quad \text{on } \Gamma \setminus \Sigma \tag{3d}$$

- Let us introduce the product space :
$$W = \prod_{i=1}^{2} H(\operatorname{div}, \Omega_i) \text{ with } \|.\|_W = (\sum_{i=1}^{2} \|.\|^2_{H(\operatorname{div},\Omega_i)})^{1/2}$$
- We denote by λ the trace of ϕ on Σ, $\lambda = \phi_{|\Sigma} \in H^1_0(\Sigma)$.
$$\forall q \in W, \sum_{i=1}^{2} < p_i, q_i >_{0,\Omega_i} + < \operatorname{div}\ p_i, \operatorname{div}\ q_i >_{0,\Omega_i}$$
$$- < \lambda, [q, n] >_\Sigma = -\sum_{i=1}^{2} < f, \operatorname{div} q_i >_{0,\Omega_i} \tag{4a}$$
$$\forall \psi \in H^1_0(\Sigma), < \nabla_\Sigma \phi, \nabla_\Sigma \psi >_{0,\Sigma} + < [p.n], \psi >_\Sigma = < g, \psi >_\Sigma \tag{4b}$$

Equilibrium Formulation

Find $(p, \lambda) \in W \times H_0^1(\Sigma)$ such that, $\forall (q, \psi) \in W \times H_0^1(\Sigma)$:

$$A((p,\lambda),(q,\psi)) = -\sum_{i=1}^{2} < f, \mathrm{div}\, q_i >_{0,\Omega_i} + < g, \psi >_\Sigma \quad (5)$$

where the bilinear form $A(.,.)$ is defined by

$$\begin{aligned} A((p,\lambda),(q,\psi)) &= \sum_{i=1}^{2} < p_i, q_i >_{0,\Omega_i} + < \mathrm{div}\, p_i, \mathrm{div}\, q_i >_{0,\Omega_i} \\ &- < \lambda, [q.n] >_\Sigma \\ &+ < \nabla_\Sigma \phi, \nabla_\Sigma \psi >_{0,\Sigma} + < [p.n], \psi >_\Sigma . \quad (6) \end{aligned}$$

Theorem

There exists a unique solution (p, λ) of the weak formulation (5). Moreover ϕ is the weak solution of the problem (2).

The Approximate Problem

Let us introduce finite dimensional subspaces

$$W_i^h \subset H(\mathrm{div}, \Omega_i),\ W_h = \prod_{i=1}^{2} W_i^h, \text{ and } M_H \subset H_0^1(\Sigma).$$

the abstract discrete formulation of (5) is given by :

$$\text{Find } (p_h, \lambda_H) \in W_h \times M_H \text{ such that, } \forall (q_h, \psi_H) \in W_h \times M_H,$$

$$A((p_h, \lambda_H), (q_h, \psi_H)) = -\sum_{i=1}^{2} < f, \mathrm{div}\, q_h >_{0,\Omega_i} + < g, \psi_H >_{\Sigma} \quad (7)$$

The Approximate Problem

Using Lax-Milgram theorem and Céa Lemma leads to the following approximation result

Theorem

Let $(p, \lambda) \in W \times H_0^1(\Sigma)$ be the solution of the continuous problem (5). The problem (7) admits a unique solution $(p_h, \lambda_H) \in W_h \times M_H$ and there exists a constant C independent of h and H such that

$$\|p - p_h\|_W + \|\lambda - \lambda_H\|_{1,\Sigma} \leq C \inf_{(q_h, \psi_H) \in W_h \times M_H} \{ \|p - q_h\|_W + \|\lambda - \psi_H\|_{1,\Sigma} \} \quad (8)$$

Finite Element Discretization

Basic finite element Choice of W_i^h and M_H :

- regular triangulations $\mathcal{T}_h$ of the domain Ω with triangular ($d = 2$) and tetrahedral ($d = 3$) finite elements whose diameters are less or equal than h, and

$$W_i^h = \{q_h \in H(\mathrm{div}, \Omega_i); \forall T \in \mathcal{T}_h, q_{h_{|T}} \in RT_k(T)\}$$

  where $RT_k(T)$ is the Raviart-Thomas finite element space

- a regular subdivision $\mathcal{S}_H$ of Σ with intervals ($d = 2$) or triangles ($d = 3$) with diameters less or equal than H, and

$$M_H = \{\psi_H \in H_0^1(\Sigma);\ \forall S \in \mathcal{S}_H, \psi_{H_{|S}} \in P_l(S)\}$$

  l being a given positive integer.

Finite Element Discretization

For such a choice of discretizations, one can state the following error estimate,

Theorem

Assuming the solution (p, λ) of (5) is such that $p \in \prod_{i=1}^{2}(H^{\sigma}(\Omega_i))^d$, and $\operatorname{div} p \in \prod_{i=1}^{2}(H^{\sigma}(\Omega_i))^d, 0 < \sigma \leq k+1$, and $\lambda \in H^s(\Sigma)$ with $1 < s < l+1$, there exists a positive constant C independent of discretization parameters such that

$$\|p - p_h\|_W + \|\lambda - \lambda_H\|_{1,\Sigma} \leq C\{\mathcal{O}(h^{\sigma}) + \mathcal{O}(H^{s-1})\}$$

NonStationary problem

Let us introduce a discrete equilibrium formulation of the implicit non stationary problem :

$$(7)\left\{\begin{array}{rcl} \left(\dfrac{\phi_h^{k+1}-\phi_h^k}{\Delta t},\mu_h\right)-(\mathrm{div}\, p_h^{k+1},\mu_h) & = & (f,\mu_h) \\ (p_h^{k+1},q_h)+(\mathrm{div}\, q_h,\phi_h^{k+1}) & = & <[q_h.n],\lambda_h^{k+1}> \\ <\nabla_\Sigma\lambda_h^{k+1},\nabla_\Sigma\alpha_h> & = & -<[p_h^{k+1}.n],\alpha_h> \\ & & +<g,\alpha_h> \end{array}\right.$$

Theorem

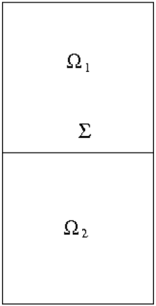
This scheme (7) is proved to be stable. Moreover if $p \in L^\infty(\prod_{i=1}^2 (H^{\sigma_2}(\Omega_i))^d)$, $1/2 < \sigma_2 \le 1$, $\phi \in H^{1+\sigma}(L^2(\Omega)), \lambda \in L^\infty(H^{1+\sigma_1}(\Sigma))$, *with,* $0 < \sigma, \sigma_1 \le 1$, *the solution satisfies the following error estimate,*

$$\left(\sup_{1\le k\le N} \|\phi^k-\phi_h^k\|_{0,\Omega}\right)+\Delta t\,\|p^k-p_h^k\|_{0,\Omega}+\Delta t\,|\lambda^k-\lambda_H^k|_{1,\Sigma} \le$$

$$C\left(|\phi|_{H^{1+\sigma}(L^2(\Omega))}+|p|_{L^\infty(\Pi_{i=1}^2(H_2^\sigma(\Omega_i))^d)}+|\lambda|_{L^\infty(H^{1+\sigma_1}(\Sigma))}\right)[H^{\sigma_1}+h^{\sigma_2}+|\Delta t|^{\sigma+1/2}]$$

Numerical Tests

- 2 dimensional geometry



- Stationary Case.

Domain Decomposition Algorithm

Let consider $(p_{h,i})$, $i = 1, 2$ the restriction of (p_h) to the domain Ω_i. let denote

$$a_i(p_{h,i}, q_{h,i}) = \langle p_{h,i}, q_{h,i} \rangle_{0,\Omega_i} + \langle \text{div } p_{h,i}, \text{div } q_{h,i} \rangle_{0,\Omega_i} \quad i = 1,2 \qquad (9)$$

$$b_i(\lambda_h, q_{h,i}) = \langle \lambda_h, [q_{h,i} \cdot n] \rangle_\Sigma - \langle f_{h,i}, \text{div } q_{h,i} \rangle_{0,\Omega_i} \quad i = 1,2 \qquad (10)$$

$$a_\Sigma(\phi_H, \psi_H) = \langle \nabla_\Sigma \phi_H, \nabla_\Sigma \psi_H \rangle_\Sigma \qquad (11)$$

$$b_\Sigma(p_h, \psi_H) = \langle g_H - [p_h \cdot n], \psi_H \rangle_\Sigma \qquad (12)$$

Domain décomposition :

1. solving in // two uncoupled problems in Ω_1 and Ω_2,
2. Solving the coupling problem on Σ

Let denote$(p^n_{h,i}, \lambda^n_h, \phi^n_H)$ the $n - th$ decomposition domain iteration values of $(p_{h,i}, \lambda_h, \phi_H)$

Decomposition Domain Algorithm

Algorithm 1 Domain decomposition algorithm

λ^0 given, $n = 1$;
$\varepsilon \ll 1$ given, $error = 1$;
while $error \geq \varepsilon$ **do**
  Solve $a_i(p^n_{h,i}, q_{h,i}) = b_i(\lambda^{n-1}, q_{h,i}),\ i = 1, 2$
  Solve $a_\Sigma(\phi^n, \psi) = b_\Sigma(p^n_{h,i}, \psi)$,
  $\lambda^n := \phi^n_{|\Sigma}$;
  $n := n + 1$

$$error = \left(\sum_{i=1,2} \| p^n_{h,i} - p^{n-1}_{h,i} \|^2_{0,\Omega_i} \right)^{1/2}$$

end while

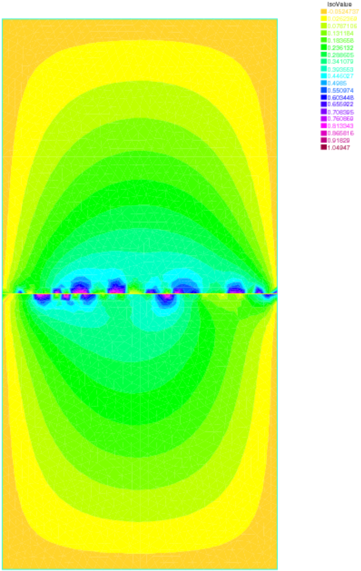
Numerical Results

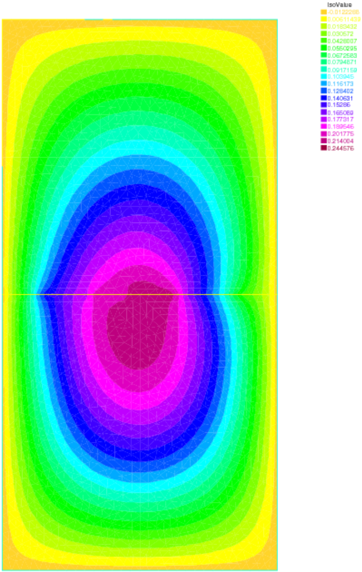
Let consider the analytic test case :

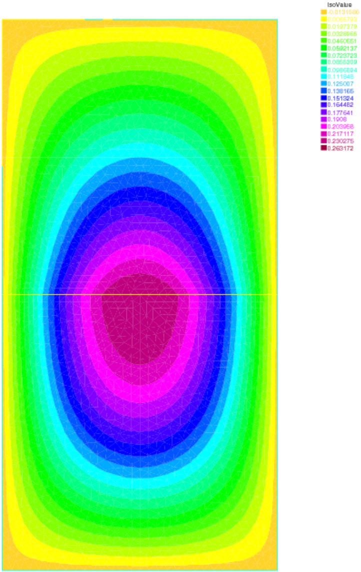
$$\phi(x,y) = \begin{cases} x(1-x)(2-y) & \text{if} \quad (x,y) \in \Omega_1 \\ x(1-x) & \text{if} \quad (x,y) \in \Sigma \\ x(1-x)\sin(\pi/2y) & \text{if} \quad (x,y) \in\in \Omega_2 \end{cases}$$

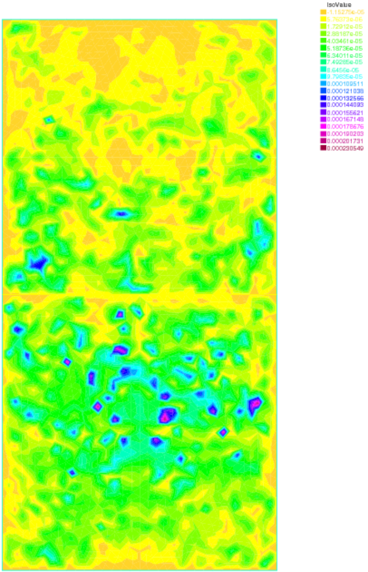
which is solution of the initial problem with source term (f,g) defined by

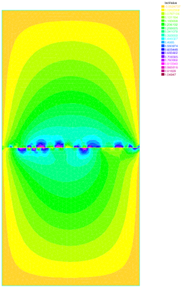
$$\begin{aligned} f(x,y) &= \begin{cases} (2+x(1-x))(2-y) & \text{if} \quad (x,y) \in \Omega_1 \\ \left(x(1-x)(1+\pi^2/4)+2\right)\sin(\pi/2y) & \text{if} \quad (x,y) \in\in \Omega_2 \end{cases} \\ g(x) &= 2 - x(1-x) \end{aligned}$$

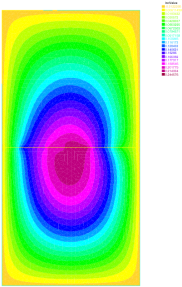

IsoValue
-0.0524737
0.0262369
0.0787106
0.131184
0.183658
0.236132
0.288605
0.341079
0.393553
0.446027
0.4985
0.550974
0.603448
0.655922
0.708395
0.760869
0.813343
0.865816
0.91829
1.04947

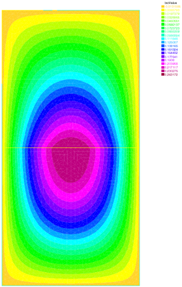

IsoValue
-0.0122268
0.00611439
0.0183432
0.030672
0.0428007
0.0550295
0.0672583
0.0794871
0.0917159
0.103945
0.116173
0.128402
0.140631
0.15286
0.165089
0.177317
0.189546
0.201775
0.214004
0.244576

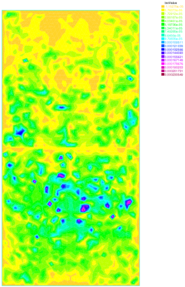

IsoValue
-0.0131586
0.0065793
0.0197379
0.0328965
0.0460551
0.0592137
0.0723723
0.0855309
0.0986894
0.111848
0.125007
0.138165
0.151324
0.164482
0.177641
0.1908
0.203958
0.217117
0.230275
0.263172


IsoValue
-1.15275e-05
5.76373e-06
1.72912e-05
2.88187e-05
4.03461e-05
5.18736e-05
6.34011e-05
7.49285e-05
8.6456e-05
9.79835e-05
0.000109511
0.000121038
0.000132566
0.000144093
0.000155621
0.000167148
0.000178676
0.000190203
0.000201731
0.000230549



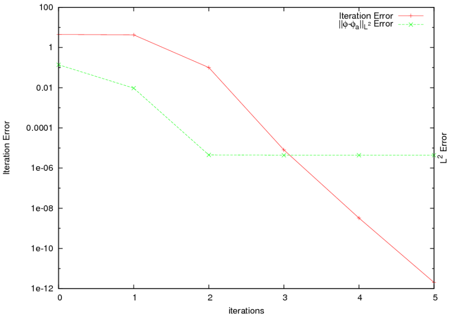


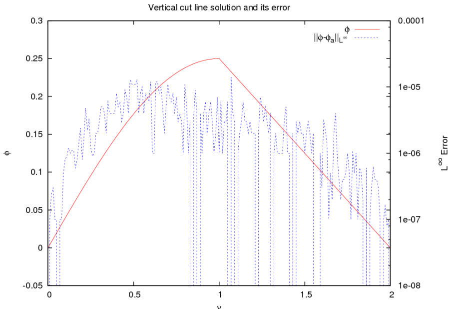


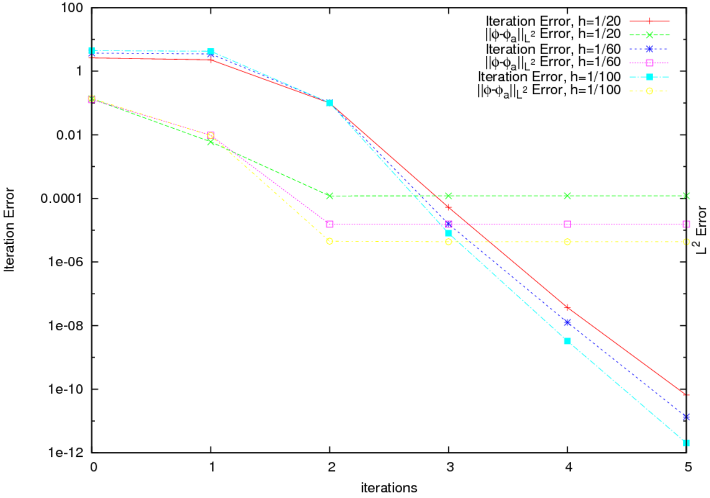


CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE
Lyon

O. Gipouloux


Iteration Error
||φ-φa||L² Error
Iteration Error
L² Error
iterations
100
1
0.01
0.0001
1e-06
1e-08
1e-10
1e-12
0
1
2
3
4
5


Vertical cut line solution and its error
φ
||φ-φa||L∞
φ
L∞ Error
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0.0001
1e-05
1e-06
1e-07
1e-08
0
0.5
1
1.5
2


Iteration Error, h=1/20
||ϕ-ϕa||L2 Error, h=1/20
Iteration Error, h=1/60
||ϕ-ϕa||L2 Error, h=1/60
Iteration Error, h=1/100
||ϕ-ϕa||L2 Error, h=1/100
Iteration Error
L2 Error
iterations
100
1
0.01
0.0001
1e-06
1e-08
1e-10
1e-12
0
1
2
3
4
5

Conclusions

- Conservative method for non standart interface condition
- Coupled system in which all matching conditions remain implicit.
- Numerical scheme and errors estimates.
- Decomposition domain algorithm.
- $\rightarrow$ to be implemented in the underground waste repository situation.