Conditions de complémentarité pour un écoulement diphasique dans un milieu poreux avec échange entre les phases

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Plan

Complementarity conditions

Goal:

Resolve for $x \in \mathbb{R}^n$:

$$0 \leq F(x) \perp G(x) \geq 0$$

$\Longleftrightarrow$

$$F(x) \geq 0, \qquad G(x) \geq 0 \qquad \text{and} \qquad F(x)^\top G(x) = 0.$$

where $F : \mathbb{R}^n \to \mathbb{R}^p$, $G : \mathbb{R}^n \to \mathbb{R}^p$ (Combinatorics: 2^p).

Applications:

- Dissolution-Precipitation phenomena.
- Phase appearance-disappearance phenomena.
- Contact problems.
- ...

The problem

M is a real matrix of order n, q is a vector in $\mathbb{R}^n$. Find $x \in \mathbb{R}^n$:

$$\mathrm{LCP}(M, q) : \qquad 0 \leq x \perp (Mx + q) \geq 0.$$

$\Longleftrightarrow$

$$x \geq 0, \qquad Mx + q \geq 0 \qquad \text{and} \qquad x^\top (Mx + q) = 0.$$

Properties of the matrix M

- P-matrice: A matrix with positive principal minors, i.e, $\det M_{II} > 0$ for all nonempty $I \subset \{1, \ldots, n\}$.
  $\rightarrow$ Ensure existence and uniqueness of the solution to the LCP for arbitrary q.
- M-matrice: A P-matrix having nonpositive off-diagonal elements, i.e, $M_{ij} \leq 0$ for all $i \neq j$.
  $\rightarrow$ Ensure convergence of some algorithms.

Outline

Linear Complementarity Problem
Algorithmics

I. Pivoting methods (Lemke's Algorithm)

II. Interior point methods

III. Nonsmooth method

- Reformulation of the Complementarity Conditions using a C-function $\varphi : \mathbb{R}^2 \to \mathbb{R}$ that satisfies

$$\varphi(a, b) = 0 \iff a \geq 0, \quad b \geq 0, \quad ab = 0 \iff 0 \leq a \perp b \geq 0.$$

  - *Minimum Function*

$$\varphi(a, b) = \min(a, b) = 0.$$

  - *Fischer-Burmeister Function*

$$\varphi(a, b) = \sqrt{a^2 + b^2} - (a + b) = 0.$$

Outline

Newton-min

- An efficient choice is the minimum function.
- The system $\min(x, Mx + q) = 0$ is nonsmooth due to the min function.
- Apply Newton-min, a nonsmooth Newton method.
- The Newton-min method can be regarded as an Active Set Strategy.

Newton-min algorithm

Let $x^1 \in \mathbb{R}^n$. For $k = 1, 2 \ldots$, do the following

- Choose complementary index sets A_k and A_k^c, where

$$A_k := \{i : x_i^k \leq (Mx^k + q)_i\},$$
$$A_k^c := \{i : x_i^k > (Mx^k + q)_i\}.$$

$$\varphi(x^k) = min\{x^k, Mx^k + q\} = \begin{cases} x_i^k & \text{if } i \in A_k \\ (Mx^k + q)_i & \text{if } i \in A_k^c. \end{cases}$$

- Select an element $\mathcal{J}_{x^k}^k \in \partial\varphi(x^k)$ such that

$$(\mathcal{J}_x^k)_i = \begin{cases} I_i & \text{if } i \in A_k \\ M_i & \text{if } i \in A_k^c. \end{cases}$$

- Let x^{k+1} be a solution to

$$\varphi(x^k) + \mathcal{J}_{x^k}^k(x^{k+1} - x^k) = 0, \qquad \mathcal{J}_{x^k}^k \in \partial\varphi(x^k).$$

Convergence Results

- When $M \in \mathbf{M}$:
  - Global convergence.
  - Convergence in at most n iterations.
- When $M \in \mathbf{M}_{\varepsilon} := \{M : M \text{ is near an } \mathbf{M}\text{-matrix}\}$:
  - Global convergence.
- When $M \in \mathbf{P}$:
  - Local superlinear convergence.
  - Global convergence for $n = 1$ ou 2.
  - May fail to converge for $n \geq 3$ (counterexamples).

I. Ben Gharbia and J. Ch. Gilbert, Nonconvergence of the plain Newton-min algorithm for linear complementarity problems with a P-matrix, *Mathematical Programming. Published Online, (2011).*

Outline

A natural remedy would be to add a globalization technique (line-search) to the Newton-min algorithm in order to force its convergence for **P**-matrices.

Problem:
This globalization is not straightforward since the Newton-min direction is not a descent direction of $x \mapsto \frac{1}{2} \|\min(x, Mx + q)\|^2$.

Idea:
Add the constraint $x \geq 0$ for ensuring descent of the computed directions.

- Solving the linear complementarity problem written as follow

$$\begin{cases} \inf \ \Theta_1(x) \\ x \geq 0 \\ Mx + q \geq 0, \end{cases}$$

where $\Theta_1(x) := \|H(x)\|_1 = e^\top H(x) = \sum_{i=1}^{n} \min(x_i, (Mx+q)_i).$

- Search direction: A direction d is defined as a solution to the linear optimization problem

$$\begin{cases} \inf \ e^\top J d \\ x + d \geq 0 \\ (Mx + q) + Md \geq 0 \end{cases} \tag{2.1}$$

where

$$J_i = \begin{cases} I_i & \text{if } i \in A \\ M_i & \text{if } i \in A^c. \end{cases}$$

Convergent algorithm

The algorithm generates pairs $(x, \mathcal{C})$ *formed of an iterate* $x \in \mathbb{R}^n$ *and a collection of visited pieces* $\mathcal{C} = \{A_1, \ldots, A_m\}$, *where each* $A = A_i$ *is a subset of* $[\![1, n]\!]$ *that refers to the convex polynomial*

$$P_A := \{x \in \mathbb{R}^n : x_A \leq (Mx + q)_A,\ x_{A^c} \geq (Mx + q)_{A^c}\}.$$

At the beginning, the first iterate x *is given and* $\mathcal{C}$ *is set to* $\varnothing$. *One iteration, from* $(x, \mathcal{C})$ *to* $(x^+, \mathcal{C}^+)$, *works as follows.*

1. *If all the sets* A *such that* $x \in P_A$ *are in* $\mathcal{C}$, *exit the solver, otherwise, pick an index set* $A \notin \mathcal{C}$ *such that* $x \in P_A$.
2. *Set* $J_A := I_A$, $J_{A^c} := M_{A^c}$, *and solve* (2.1) *for* d.
3. *If* $e^\top Jd < 0$, *set* $x^+ := x + d$ *and* $\mathcal{C}^+ := \varnothing$ *(the iteration is completed)*
   otherwise, set $\mathcal{C} := \mathcal{C} \cup \{A\}$ *and pursue the iteration at step 1.*

Outline

Theoretical results - Convergence

Proposition (Descent direction)

If M is a **P**-matrix and if x is not a solution to LCP(M, q), then any solution d to the linear optimization problem (2.1) satisfies

$$\Theta_1'(x; d) < 0.$$

Theorem (Convergence of algorithm)

If M is a **P**-matrix, then the algorithm is well defined and generates a sequence that converges to the unique solution in a finite number of iterations.

I. Ben Gharbia and J. Ch. Gilbert, A Convergent algorithm for **P**-matrices, (*In preperation*).

Numerical results - Exponential-Time Examples

Murty example | Fathi example

$$M_1 = \begin{pmatrix} 1 & 2 & 2 & \cdots & 2 \\ 0 & 1 & 2 & \cdots & 2 \\ 0 & 0 & 1 & \cdots & 2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}, \qquad M_2 = \begin{pmatrix} 1 & 2 & 2 & \cdots & 2 \\ 2 & 5 & 6 & \cdots & 6 \\ 2 & 6 & 9 & \cdots & 10 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 2 & 6 & 10 & \cdots & 4(n-1)+1 \end{pmatrix}$$

$$x^0 = 0 \quad \text{and} \quad q = -1.$$

n	M_1	M_2
10	1	2
50	1	2
100	1	2
500	1	2
1000	1	2

Number of iterations for Exponential-Time Examples

Outline

Motivation: Couplex-Gas, an Andra-Momas benchmark

- In a deep underground nuclear waste disposal.
- Production of hydrogen from corrosion of waste packages.
- Migration of this hydrogen ?
- Flow either saturated (liquid) or unsaturated (liquid/gas).
- When there is gas phase appearance/disappearance :
  - Variable switching or substitution (A. Bourgeat et al.).
  - Artificial small non-zero saturation (M. Panfilov et al.).
  - Complementarity formulation (J. Jaffré & A. Sboui; E. Marchand, P. Knabner et al.; B. Wohlmuth et al.).
  - ...

Motivation - Goal

- Formulation with complementarity constraints and Henry's law, see J. Jaffré, A. Sboui. Henrys law and gas phase disappearance. *Transport in Porous Media, 12 (2010), 521-526.*

Advantage : Valid whether the gas phase exists or not.

Goals :

- Address difficulties coming from non-standard physical situations : Gas phase Appearance/Disappearance.
- Build a robust algorithm to resolve these difficulties.
- Development of solver for nonlinear complementarity problems.

Outline

Phase equations

2 fluid phases: liquid ($i = \ell$) and gas ($i = g$)

Phases occupy the entire pore space: $s_\ell + s_g = 1$.

Capillary pressure law: $p_c(s_\ell) = p_g - p_\ell \geq 0$, p_c decreasing, $p_c(1) = 0$.

Since liquid phase does not disappear while gas phase may disappear, the main unknowns will be s_ℓ and p_ℓ.

Fluid components

2 components : water ($j = w$) and hydrogen ($j = h$).

Mass density of phase i: $\rho_i = \rho_w^i + \rho_h^i, \quad i = \ell, g$.

Molar concentration of phase i: $c_i = c_w^i + c_h^i = \frac{s_i \rho_w^i}{M^w} + \frac{s_i \rho_h^i}{M^h}, \quad i = \ell, g$.

Molar fractions : $\chi_h^i = \frac{c_h^i}{c_i}, \quad \chi_w^i = \frac{c_w^i}{c_i}, \quad i = \ell, g, \quad (\chi_w^i + \chi_h^i = 1)$.

Physical assumptions :

- Liquid phase contains both components.
- Gas phase contains only hydrogen.
- Gas is compressible $\rho_g = C_g p_g$.
- Liquid is incompressible $\rho_w^\ell =$ constant.

χ_h^ℓ is the third main unknown.

Mass conservation for each component

Water: $$\phi \frac{\partial}{\partial t}(s_\ell \rho_w^\ell) + \mathrm{div}(\rho_w^\ell \mathbf{q}_\ell + j_w^\ell) = Q_w$$

Hydrogen: $$\phi \frac{\partial}{\partial t}(s_\ell \rho_h^\ell + s_g \rho_g) + \mathrm{div}(\rho_h^\ell \mathbf{q}_\ell + \rho_g \mathbf{q}_g + j_h^\ell) = Q_h,$$

where diffusion of the components in the liquid phase is modeled by

$$j_h^\ell = -\phi M^h s_\ell c_\ell D_h^\ell \vec{\nabla} \chi_h^\ell, \quad j_h^\ell + j_w^\ell = 0.$$

ϕ = porosity, D_h^ℓ = molecular diffusion coefficient.

Darcy's law: $\mathbf{q}_i = -K(x) k_i(s_i)(\vec{\nabla} p_i - \rho_i g \vec{\nabla} z), \quad i = \ell, g$

K the absolute permeability
$\mathbf{q}_i$ Darcy velocity, s_i saturation, p_i fluid pressure, k_i mobility

Complementarity equations

- Henry's law is $H(T)M^h p_g = Hp_g = \rho_h^\ell = C_\ell\,\chi_h^\ell$. It is valid when both phases are present.

- To integrate Henry's law into a formulation which includes the case with no gas phase, introduce the liquid pressure $p_\ell = p_g - p_c(s_\ell)$, and
  - either gas phase exists: $1 - s_\ell > 0$ and $H(p_\ell + p_c(s_\ell)) - C_\ell\,\chi_h^\ell = 0$,
  - or gas phase does not exist: $s_\ell = 1, p_c(s_\ell) = 0$ and $Hp_\ell - C_\ell\,\chi_h^\ell \geq 0$.

Complementarity constraints

$$(1 - s_\ell)\big(H(p_\ell + p_c(s_\ell)) - C_\ell\chi_h^\ell\big) = 0, \quad 1 - s_\ell \geq 0, \quad H(p_\ell + p_c(s_\ell)) - C_\ell\,\chi_h^\ell \geq 0.$$

Advantage: Avoid the change of variables and equations in saturated/unsaturated regions.

A nonlinear problem with nonlinear complementarity equations

$$\phi \frac{\partial}{\partial t}(\rho_w^\ell \, s_\ell)) + \mathrm{div}\big(\rho_w^\ell \, \mathbf{q}_\ell - j_h^\ell\big) = Q_w$$

$$\phi \frac{\partial}{\partial t}\big(s_\ell C_\ell \, \chi_h^\ell + (1 - s_\ell) C_g (p_\ell + p_c(s_\ell))\big) + \mathrm{div}\big(C_\ell \, \chi_h^\ell \, \mathbf{q}_\ell + C_g (p_\ell + p_c(s_\ell)) \, \mathbf{q}_g + j_h^\ell\big) = Q_h,$$

where $j_h^\ell = -\phi \, s_\ell^2 \, C_\ell \, (1 + \chi_h^\ell) \, D_h^\ell \, \vec{\nabla} \chi_h^\ell$, $\quad C_\ell = \dfrac{M^h}{M^w} \, \rho_w^\ell$

$$\mathbf{q}_\ell = -K(x) k_\ell(s_\ell)(\vec{\nabla} p_\ell - \rho_\ell g \vec{\nabla} z)$$

$$\mathbf{q}_g = -K(x) k_g(1 - s_\ell)(\vec{\nabla}(p_\ell + p_c(s_\ell)) - C_g(p_\ell + p_c(s_\ell)) g \vec{\nabla} z)$$

$$(1 - s_\ell)\big(H(p_\ell + p_c(s_\ell)) - C_\ell \chi_h^\ell\big) = 0, \quad 1 - s_\ell \geq 0, \quad H(p_\ell + p_c(s_\ell)) - C_\ell \, \chi_h^\ell \geq 0.$$

Outline

The discrete problem

Discretized with cell-centered finite volumes : N, the number of cells.

$x \in \mathbb{R}^{3N}$, vector of unknowns for $s_\ell, p_\ell, \chi_h^\ell$

$\mathcal{H} : \mathbb{R}^{3N} \to \mathbb{R}^{2N}$ for discrete conservation equations

$\mathcal{F} : \mathbb{R}^{3N} \to \mathbb{R}^{N}$ for discrete $1 - s_\ell$

$\mathcal{G} : \mathbb{R}^{3N} \to \mathbb{R}^{N}$ for discrete $H(p_\ell + p_c(s_\ell)) - C_\ell \, \chi_h^\ell$

Problem in compact form

$$\mathcal{H}(x) = 0,$$
$$\mathcal{F}(x)^\top \mathcal{G}(x) = 0, \quad \mathcal{F}(x) \geq 0, \quad \mathcal{G}(x) \geq 0.$$

How to solve this nonlinear complementarity problem ?

Idea: Replace complementarity conditions.

Reformulation of the Complementarity Conditions

Introduce a C-function $\varphi : \mathbb{R}^2 \to \mathbb{R}$ that satisfies

$$\varphi(a, b) = 0 \iff a \geq 0, \quad b \geq 0, \quad ab = 0,$$

An efficient choice is the minimum function.

Replace complementarity constraints by $\varphi(x) = \min\{\mathcal{F}(x), \mathcal{G}(x)\} = 0$.

A Nonsmooth system using the Minimum function

The problem is equivalent to

$$\psi(x) = 0, \quad \text{where} \quad \psi(x) := \begin{pmatrix} \mathcal{H}(x) \\ \varphi(x) \end{pmatrix}.$$

- The system is nonsmooth due to the min function.
- Apply Newton-min, a nonsmooth Newton method.
- Local convergence of Newton-min.

See I. Ben Gharbia & J. Ch Gilbert (2010), S. Kräutle (2011), P. Knabner et al. (2009) , Ito & Kunish (2009) and C. Kanzow (2004)

Newton-min algorithm

For $k = 1, 2 \ldots$, do the following

- Choose complementary index sets A_k and A_k^c, where

$$A_k := \{i : \mathcal{F}_i(x^k) < \mathcal{G}_i(x^k)\},$$
$$A_k^c := \{i : \mathcal{F}_i(x^k) \geq \mathcal{G}_i(x^k)\}.$$

$$\varphi(x^k) = min\{\mathcal{F}(x^k), \mathcal{G}(x^k)\} = \begin{cases} \mathcal{F}_i(x^k) & \text{if } i \in A_k, \\ \mathcal{G}_i(x^k) & \text{if } i \in A_k^c. \end{cases}$$

- Select an element $\mathcal{J}_{x^k}^k \in \partial\varphi(x^k)$ such that

$$(\mathcal{J}_{x^k}^k)_i = \begin{cases} \mathcal{F}_i'(x^k) & \text{if } i \in A_k, \\ \mathcal{G}_i'(x^k) & \text{if } i \in A_k^c. \end{cases}$$

- Let x^{k+1} be a solution to

$$\mathcal{H}(x^k) + \mathcal{H}'(x^k)(x^{k+1} - x^k) = 0,$$
$$\varphi(x^k) + \mathcal{J}_{x^k}^k(x^{k+1} - x^k) = 0, \qquad \mathcal{J}_{x^k}^k \in \partial\varphi(x^k).$$

A theoretical result - Convergence

Theorem:

Let x^* be a solution of the nonlinear system $\psi(x) = 0$ and such that J is nonsingular for all $J \in \partial\psi(x^*)$. Then there exists ϵ such that for every starting point $x^0 \in B_\epsilon(x^*)$:

▷ The Newton-min algorithm is well-defined and produces a sequence $\{x^k\}$ that converges to x^*.

▷ The rate of convergence is quadratic.

Outline

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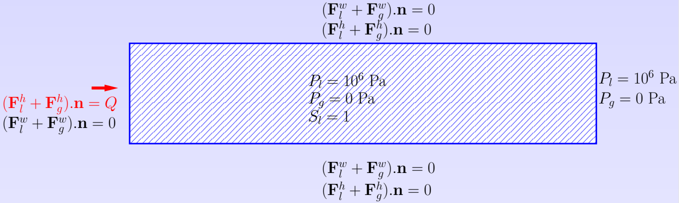
2. Linear Complementarity Problem
   - Algorithmics
   - Local analysis of Newton-min
   - Global convergence
   - Results
3. Nonlinear Complementarity Problem
   - Motivation
   - Problem Formulation
   - Discretization and solution method
   - Numerical results
     - Test 1: Homogeneous setting
     - Test 2: Hetergeneous setting
   - Conclusion

Homogeneous setting

Test inspired from the Couplex Gas benchmark:

- Inject hydrogen gas on the left of a 1-D porous medium saturated at initial time with liquid ($T_{inj} = 5.10^5$ years).
- After a while the hydrogen injection is stopped ($T_{simul} = 10^6$ years).



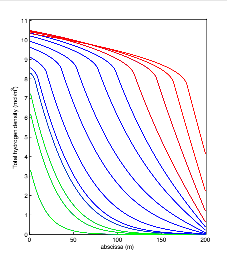
- Van Genuchten-Mualem model for capillary pressure and relative permeabilities.
- Initial conditions: $p_\ell = 10^6$ Pa, $s_\ell = 1$ and $\chi_h^\ell = 0$.

Numerical results - Homogeneous setting

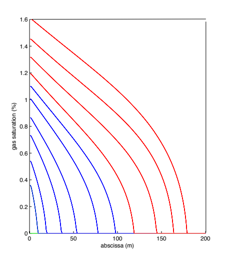
During injection : $0 < t < 5.10^5$ years

- Period 1: Only Hydrogen density increases.
- Period 2: Gas phase appears and liquid pressure increases.
- Period 3: Smaller $\vec{\nabla} p_\ell$ and no water injection slow down the liquid pressure.

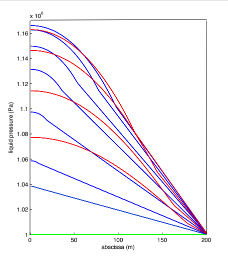
H_2 density



Gas saturation



Liquid pressure

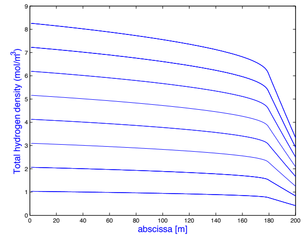


Numerical results - Homogeneous setting

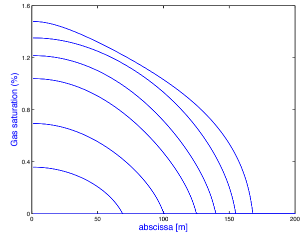
After injection is stopped : $t > 5.10^5$ years

- Gas saturation and H_2 density decrease.
- Liquid pressure increases.
- When $t \to \infty$, gas phase disappears and the system reaches a stationary state.

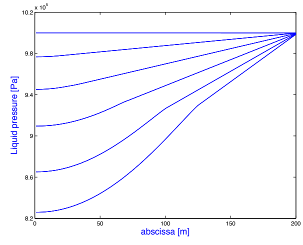
H_2 density



Gas saturation

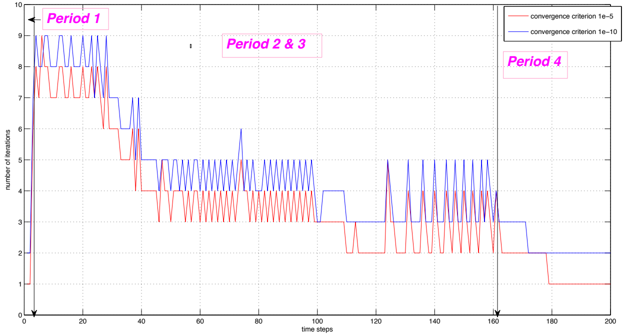


Liquid pressure



Numerical results - Homogeneous setting

Quadratic convergence

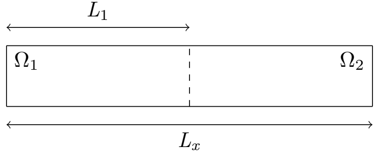


I. Ben Gharbia and J. Jaffré, Gas phase appearance and disappearance as a problem with complementarity constraints, *Mathematics and Computers in Simulation (submitted)*.

Hetergeneous setting

▷ Consider MOMAS heterogeneous benchmark Problem 2.

▷ The porous medium characteristics and the fluids properties are from http://sources.univ-lyon1.fr/cast_test/multi.mat.pdf.



▷ The characteristics of porous medium (in particular capillary pressure) are different in each subdomain. $\mathcal{L}_x = 200$, $\mathcal{L}_1 = 100$.

▷ Boundary and initial conditions

- At $t = 0$: $p_\ell = 10^6$ Pa, $s_\ell = 1$ and $\chi_h^\ell = 0$,
- At $x = 200$: $p_\ell = 10^6$ Pa,
- At $x = 0$: $\text{flux}_{hydrogen} = 5.57$ mg/m^2/yr, $\text{flux}_{water} = 0$.

Interface conditions - Hetergeneous setting

▷ Interface conditions

- Liquid pressure should be continous : $p_\ell^{(1)} = p_\ell^{(2)}$.
- Water flux should be continous : $\mathbf{u}_w^{(1)} = \mathbf{u}_w^{(2)}$.
- Hydrogen flux should be continous : $\mathbf{u}_h^{(1)} = \mathbf{u}_h^{(2)}$.
- Capillary pressure continuity condition : $p_c^{(1)}(s^{(1)}) = p_c^{(2)}(s^{(2)})$.

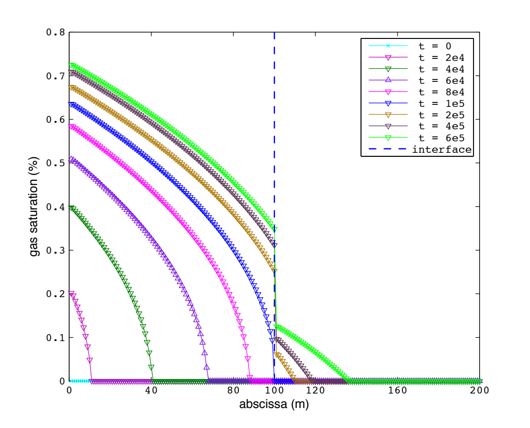
▷ Meshes

- Uniform in space : dx= 1m in each subdomain.
- In time : dt = 2000 years.

▷ Convergence criterion : 10^{-8}.

Numerical results - Hetergeneous setting

Gas saturation at several times (in years)



Outline

Conclusion

- The formulation handles well appearance and disappearance of the gas phase.
- Newton-min is well adapted for our problem.
- Locally quadratic convergence.

THANK YOU !