Complimentarity constraints with a system of nonlinear PDE's

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Outline

1. Motivation
2. Problem Formulation
3. Discretization and solution method
4. Numerical results
   - Test 1: Homogeneous setting
   - Test 2: Heterogeneous setting
5. Conclusion

- In a deep underground nuclear waste disposal.
- Production of hydrogen from corrosion of waste packages.
- Migration of this hydrogen ?
- Flow can be saturated (only liquid) or unsaturated (liquid/gas).
- Numerical difficulties when gas phase appears/disappears.
- Examples of complementarity problems for porous media flow:
  - Chavent-Jaffré, *Mathematical models and finite elements for reservoir simulation (North-Holland, 1986).*
  - *Jaffré-Sboui. Henrys law and gas phase disappearance.* Transport in Porous Media 12 (2010).
  - Lauser-Hager-Helmig-Wohlmuth. *Advances in Water Resources 34 (2011).*
  - *Buchholzer-Kanzow-Knabner-Kraütle.* Computational Optimization and Applications 50 (2011).

Advantage of formulation with complementarity constraints:
Valid whether the gas phase exists or not.

Goals

- Address numerical difficulties coming from gas phase appearance/disappearance.
- Construct a robust algorithm to resolve these difficulties.
- Develop a solver for nonlinear complementarity problems.

Outline

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

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

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.

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: $c_i = c_w^i + c_h^i = \dfrac{s_i \rho_w^i}{M^w} + \dfrac{s_i \rho_h^i}{M^h}, \quad i = \ell, g.$

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

Physical assumptions :

- Liquid phase contains both components.
- Gas phase contains only hydrogen.
- Gas is compressible $\rho_g = \kappa_g p_g$.
- Liquid incompressible $\rho_w^\ell =$ constant, $c_h^\ell \ll c_{w^\ell}$,

$$\chi_h^\ell \simeq \frac{c_h^\ell}{c_w^\ell} = C_\ell \rho_h^\ell \text{ with } C_\ell = \frac{M^h}{M^w \rho_w^\ell}.$$

χ_h^ℓ is the third main unknown.

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.

- Henry's law is $\widetilde{H}(T)M^h p_g = Hp_g = \rho_h^\ell = C_\ell\,\chi_h^\ell$. 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 $Hp_\ell - C_\ell\,\chi_h^\ell \geq 0$, that is χ_h^ℓ is too small for gas to appear.

Complementarity constraints

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

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

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

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

where

$$j_h^\ell = -\phi \, s_\ell^2 \, C_\ell \, (1 + \chi_h^\ell) \, D_h^\ell \, \vec{\nabla} \chi_h^\ell$$

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

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

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

Outline

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

$$\mathcal{H}(x) = 0,$$

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

Introduce $K = \mathbb{R}^n \times \mathbb{R}^p_+$.

Find $(x, u) \in K$

$$\begin{pmatrix} \mathcal{H}(x) \\ \mathcal{F}(x) - u \\ \mathcal{G}(x) \end{pmatrix}^\top \begin{pmatrix} y - x \\ v - u \end{pmatrix} \geq 0, \quad \forall (y, v) \in K.$$

How to solve this nonlinear complementarity problem ?

Idea: Replace complementarity conditions by equalities.

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

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)

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

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

.

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.

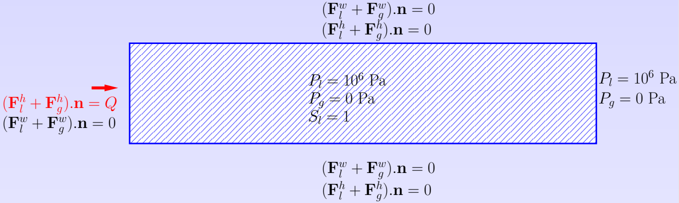
Outline

Outline

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).



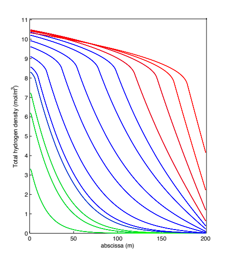
- Van Genuchten-Mualem model for capillary pressure and relative permeabilities.
- Initial conditions: $p_\ell = 10^6$ Pa, $s_\ell = 1$ and $\chi_h^\ell = 0$.

Numerical results - Homogeneous setting

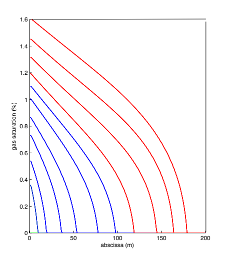
During injection : $0 < t < 5.10^5$ years

- 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 push down the liquid pressure.

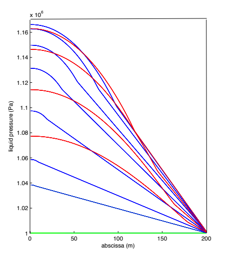
H_2 density



Gas saturation



Liquid pressure

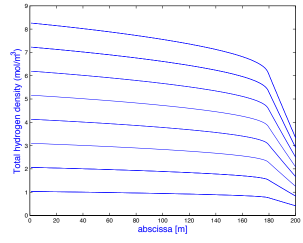


Numerical results - Homogeneous setting

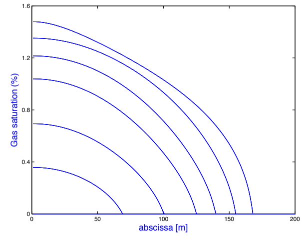
After injection is stopped : $t > 5.10^5$ years

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

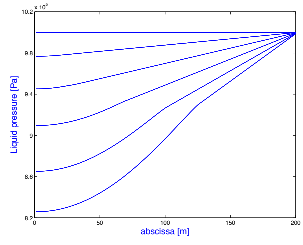
H_2 density



Gas saturation

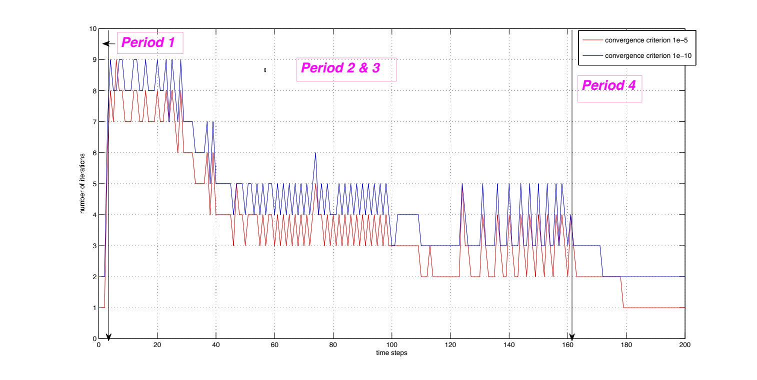


Liquid pressure



Numerical results - Homogeneous setting

Quadratic convergence

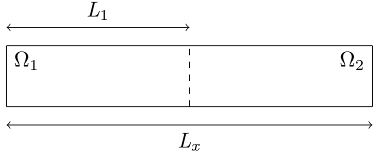


I. Ben Gharbia and J. Jaffré, Gas phase appearance and disappearance as a problem with complementarity constraints, *Mathematics and Computers in Simulation* (submitted).

Outline

▷ 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

- 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 : $p_c^{(1)}(s^{(1)}) = p_c^{(2)}(s^{(2)})$.

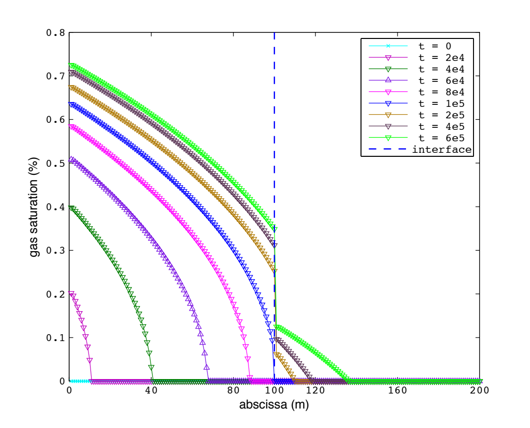
▷ Meshes

- Uniform in space : $\Delta x = 1$m in each subdomain.
- In time : $\Delta t = 2000$ years.

▷ Convergence criterion : 10^{-8}.

Numerical results - Heterogeneous setting

Gas saturation at several times (in years)



Outline

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

F. Clément, J. Ch. Gilbert, M. Kern, J. E. Roberts, M. Vohralik, P. Weis, G. Chavent.

- Mixed finite elements on meshes of deformed cubes.
- A posteriori error estimates.
- Time-space domain decomposition.
- Discrete fracture flow models with matrix-fracture interaction: fractures are modeled as $n-1$ dimensional interfaces.
- Solvers and HPC.
- Some inverse problems from hydrogeology.
- Safe scientific computing using Ocaml.