A posteriori error estimates and stopping criteria for a two-phase flow with nonlinear complementarity constraints

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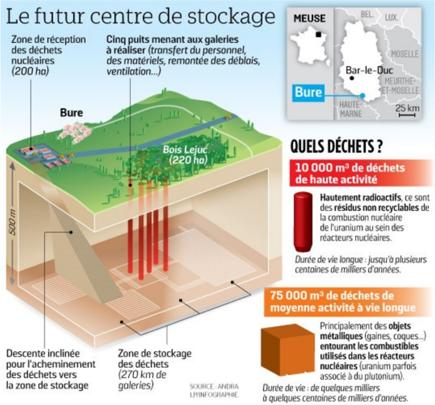
informatics mathematics

École des Ponts ParisTech

Outline

Introduction

Storage of radioactive wastes



Can we estimate each error component?
Can we reduce the computational cost?

Model: System of PDE's with complementarity constraints

$$\mathcal{A}(\boldsymbol{U}) = 0$$

$$\mathcal{K}(\boldsymbol{U}) \geq 0, \quad \mathcal{G}(\boldsymbol{U}) \geq 0, \quad \mathcal{K}(\boldsymbol{U})^T \mathcal{G}(\boldsymbol{U}) = 0.$$

Space/Time discretisation: Finite volumes/Backward Euler scheme

$$S^n(\boldsymbol{U}_h^n) = 0 \qquad \boldsymbol{U}_h^n : \text{unknowns}$$

Resolution: semismooth Newton

$$\mathbb{A}^{n,k-1} \boldsymbol{U}_h^{n,k,i} + \boldsymbol{R}_h^{n,k,i} = \mathbb{F}^{n,k-1}$$

$\Rightarrow$ **A posteriori error estimates**

Outline

Compositional two-phase flow with phase transition

$$\begin{cases} \partial_t l_{\mathrm{w}} + \boldsymbol{\nabla}\cdot(\rho_{\mathrm{w}}^{\mathrm{l}}\mathbf{q}^{\mathrm{l}} - \mathbf{J}_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}} + \boldsymbol{\nabla}\cdot(\rho_{\mathrm{h}}^{\mathrm{l}}\mathbf{q}^{\mathrm{l}} + \rho_{\mathrm{h}}^{\mathrm{g}}\mathbf{q}^{\mathrm{g}} + \mathbf{J}_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0,\ HP^{\mathrm{g}} - \beta^{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0,\ \left(1 - S^{\mathrm{l}}\right)^T \left(HP^{\mathrm{g}} - \beta^{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right) = 0 \end{cases}$$

Unknowns: $S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}$

Darcy's law: $\mathbf{q}^{\mathrm{l}} = -\underline{\mathbf{K}}\dfrac{k_{r\mathrm{l}}(S^{\mathrm{l}})}{\mu_{\mathrm{l}}}\left[\boldsymbol{\nabla}P^{\mathrm{l}} - \rho^{\mathrm{l}}g\boldsymbol{\nabla}z\right]$, $\mathbf{q}^{\mathrm{g}} = -\underline{\mathbf{K}}\dfrac{k_{r\mathrm{g}}(S^{\mathrm{g}})}{\mu_{\mathrm{g}}}\left[\boldsymbol{\nabla}P^{\mathrm{g}} - \rho^{\mathrm{g}}g\boldsymbol{\nabla}z\right]$

Amount of components: $l_{\mathrm{w}} = \phi\rho_{\mathrm{w}}^{\mathrm{l}}S^{\mathrm{l}} + \phi\rho_{\mathrm{w}}^{\mathrm{g}}S^{\mathrm{g}}, \quad l_{\mathrm{h}} = \phi\rho_{\mathrm{h}}^{\mathrm{l}}S^{\mathrm{l}} + \phi\rho_{\mathrm{h}}^{\mathrm{g}}S^{\mathrm{g}}$

Fick flux: $\mathbf{J}_{\mathrm{h}}^{\mathrm{l}} = -\phi M_{\mathrm{h}}S^{\mathrm{l}}C_{\mathrm{l}}D_{\mathrm{h}}^{\mathrm{l}}\boldsymbol{\nabla}\chi_{\mathrm{h}}^{\mathrm{l}}$

Capillary pressure: $P^{\mathrm{g}} = P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})$

Algebraic closure: $S^{\mathrm{l}} + S^{\mathrm{g}} = 1, \quad \chi_{\mathrm{h}}^{\mathrm{l}} + \chi_{\mathrm{w}}^{\mathrm{l}} = 1, \quad \chi_{\mathrm{h}}^{\mathrm{g}} = 1$

Assumption

The water is incompressible and is only present in liquid phase and the gas is slightly compressible

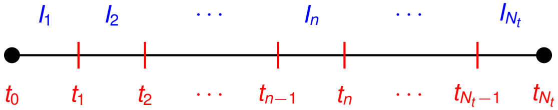
$$\rho_{\mathrm{w}}^{\mathrm{l}} = \mathrm{cst}, \quad \rho_{\mathrm{w}}^{\mathrm{g}} = 0, \quad \rho^{\mathrm{g}} = \beta^{\mathrm{g}}P^{\mathrm{g}}, \quad \rho_{\mathrm{h}}^{\mathrm{l}} = \beta^{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}, \quad \chi_{\mathrm{h}}^{\mathrm{g}} = 1, \quad \chi_{\mathrm{w}}^{\mathrm{g}} = 0.$$

Discretization by the finite volume method

Numerical solution:

$$\boldsymbol{U}^n := (\boldsymbol{U}_K^n)_{K\in\mathcal{T}_h}, \qquad \boldsymbol{U}_K^n := (S_K^n, P_K^n, \chi_K^n)$$ **one value per cell and time step**

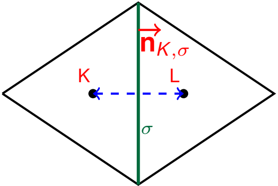
Time discretization: Consider: $t_0 = 0 < t_1 < \cdots < t_{N_t} = t_{\mathrm{F}} = N_t \Delta t$ with constant time step Δt.



$$\partial_t^n v_K := \frac{v_K^n - v_K^{n-1}}{\Delta t}$$

Space discretization: $\mathcal{T}_h$ a superadmissible family of conforming simplicial meshes (Ciarlet) of the space domain Ω.

$$(\nabla v \cdot \boldsymbol{n}_{K,\sigma}, 1)_\sigma := |\sigma| \frac{v_L - v_K}{d_{KL}} \quad \sigma = \overline{K} \cap \overline{L},$$



Discretization of water equation

$$S^n_{\mathrm{w},K}(\boldsymbol{U}^n) := |K|\partial^n_t l_{\mathrm{w},K} + \sum_{\sigma\in\mathcal{E}_K} F_{\mathrm{w},K,\sigma}(\boldsymbol{U}^n) - |K|Q^n_{\mathrm{w,K}} = 0,$$

Total flux

$$F_{\mathrm{w},K,\sigma}(\boldsymbol{U}^n) := \rho^{\mathrm{l}}_{\mathrm{w}}(\mathfrak{M}^{\mathrm{l}})^n_\sigma(\psi^{\mathrm{l}})^n_\sigma - (\mathrm{j}^{\mathrm{l}}_{\mathrm{h}})^n_\sigma \quad \sigma\in\mathcal{E}^{\mathrm{int}}_K \quad \overline{\sigma} = \overline{K}\cap\overline{L}.$$

Discretization of hydrogen equation

$$S^n_{\mathrm{h},K}(\boldsymbol{U}^n) := |K|\partial^n_t l_{\mathrm{h},K} + \sum_{\sigma\in\mathcal{E}_K} F_{\mathrm{h},K,\sigma}(\boldsymbol{U}^n) - |K|Q^n_{\mathrm{h,K}} = 0,$$

Total flux

$$F_{\mathrm{h},K,\sigma}(\boldsymbol{U}^n) := \beta^{\mathrm{l}}\chi^n_\sigma(\mathfrak{M}^{\mathrm{l}})^n_\sigma(\psi^{\mathrm{l}})^n_\sigma + (\psi^{\mathrm{g}})^n_\sigma(\mathfrak{M}^{\mathrm{g}})^n_\sigma(\rho^{\mathrm{g}})^n_\sigma + (\mathrm{j}^{\mathrm{l}}_{\mathrm{h}})^n_\sigma, \quad \sigma\in\mathcal{E}^{\mathrm{int}}_K \quad \overline{\sigma} = \overline{K}\cap\overline{L}.$$

- $\mathfrak{M}^{\mathrm{l}}$: mobility of liquid phase (upwind approx)
- $\mathfrak{M}^{\mathrm{g}}$: mobility of gas phase (upwind approx)
- ψ^{l}: potential of liquid phase
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- $\mathrm{j}^{\mathrm{l}}_{\mathrm{h}}$: discrete Fick term
- $Q^n_{\mathrm{w,K}}$, $Q^n_{\mathrm{h,K}}$: source term constant in space and time

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Discrete complementarity problem

To reformulate the discrete constraints:

Definition (C-function)

$$\forall(\boldsymbol{a},\boldsymbol{b}) \in \mathbb{R}^n \times \mathbb{R}^n,\ f(\boldsymbol{a},\boldsymbol{b}) = 0 \iff \boldsymbol{a} \geq 0,\ \boldsymbol{b} \geq 0,\ \boldsymbol{a}^T\boldsymbol{b} = 0$$

min-function: $\min(\boldsymbol{a},\boldsymbol{b}) = 0 \iff \boldsymbol{a} \geq 0,\ \boldsymbol{b} \geq 0,\ \boldsymbol{a}^T\boldsymbol{b} = 0.$

Application: complementarity constraints for the two-phase model

$$1 - S_K^n \geq 0,\ H(P_K^n + P_{\mathrm{cp}}(S_K^n)) - \beta^{\mathrm{l}}\chi_K^n \geq 0,\ (1 - S_K^n)^T(H(P_K^n + P_{\mathrm{cp}}(S_K^n)) - \beta^{\mathrm{l}}\chi_K^n) = 0$$

$$\Updownarrow$$

$$\min\left(1 - S_K^n, H(P_K^n + P_{\mathrm{cp}}(S_K^n)) - \beta^{\mathrm{l}}\chi_K^n\right) = 0$$

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$$\Updownarrow$$

$$\min\left(1 - S_K^n, H(P_K^n + P_{\mathrm{cp}}(S_K^n)) - \beta^{\mathrm{l}} \chi_K^n\right) = 0$$

Inexact semismooth Newton method

For $1 \leq n \leq N_t$ and $\boldsymbol{U}^{n,0} \in \mathbb{R}^{3N_{\rm sp}}$ fixed, the semismooth Newton algorithm generates a sequence $(\boldsymbol{U}^{n,k})_{k\geq 1} \in \mathbb{R}^{3N_{\rm sp}}$ satisfying:

$$\mathbb{A}^{n,k-1}\boldsymbol{U}^{n,k} = \boldsymbol{B}^{n,k-1},$$

- $\mathbb{A}^{n,k-1} \in \mathbb{R}^{3N_{\rm sp}\times 3N_{\rm sp}}$: Jacobian matrix "in the sense of Clarke" at step $k-1$
- $\boldsymbol{B}^{n,k-1} \in \mathbb{R}^{3N_{\rm sp}}$: right hand side vector at step $k-1$

Next, we use an iterative algebraic solver at the semismooth Newton step $k \geq 1$, starting from an initial guess $\boldsymbol{U}^{n,k,0}$ generating a sequence $(\boldsymbol{U}^{n,k,i})_{i\geq 1}$ satisfying

$$\mathbb{A}^{n,k-1}\boldsymbol{U}^{n,k,i} = \boldsymbol{B}^{n,k-1} - \boldsymbol{R}^{n,k,i}$$

- $\boldsymbol{R}^{n,k,i} \in \mathbb{R}^{3N_{\rm sp}}$: algebraic residual vector.

Can we estimate the semismooth linearization error?

Can we estimate the iterative algebraic error?

Outline

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Global overview

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Weak solution

$$X := L^2((0,t_{\mathrm{F}}); H^1(\Omega)), \quad Y := H^1((0,t_{\mathrm{F}}); L^2(\Omega)), \quad \widehat{Y} := H^1((0,t_{\mathrm{F}}); L^\infty(\Omega)),$$
$$Z := \left\{ v \in L^2((0,t_{\mathrm{F}}); L^\infty(\Omega)),\ v \geq 0 \text{ on } \Omega \times (0,t_{\mathrm{F}}) \right\}.$$

Assumption (Weak formulation)

$S^{\mathrm{l}} \in \widehat{Y}, \quad 1 - S^{\mathrm{l}} \in Z, \quad l_{\mathrm{w}} \in Y, \quad l_{\mathrm{h}} \in Y, \quad P^{\mathrm{l}} \in X, \quad \chi_{\mathrm{h}}^{\mathrm{l}} \in X,$

$\left(\boldsymbol{\Phi}_{\mathrm{w}} := \rho_{\mathrm{w}}^{\mathrm{l}} \mathbf{q}^{\mathrm{l}} - \mathbf{J}_{\mathrm{h}}^{\mathrm{l}}, \boldsymbol{\Phi}_{\mathrm{h}} := \rho_{\mathrm{h}}^{\mathrm{l}} \mathbf{q}^{\mathrm{l}} + \rho_{\mathrm{h}}^{\mathrm{g}} \mathbf{q}^{\mathrm{g}} + \mathbf{J}_{\mathrm{h}}^{\mathrm{l}}\right) \in \left[L^2((0,t_{\mathrm{F}}); \mathbf{H}(\mathrm{div},\Omega))\right]^2,$

$$\int_0^{t_{\mathrm{F}}} (\partial_t l_c, \varphi)_\Omega(t)\,\mathrm{d}t - \int_0^{t_{\mathrm{F}}} (\boldsymbol{\Phi}_c, \nabla\varphi)_\Omega(t)\,\mathrm{d}t = \int_0^{t_{\mathrm{F}}} (Q_c, \varphi)_\Omega(t)\,\mathrm{d}t \ \forall \varphi \in X, \ \forall c \in \{\mathrm{w}, \mathrm{h}\}$$

$$\int_0^{t_{\mathrm{F}}} \left(\lambda - (1 - S^{\mathrm{l}}), H[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})] - \beta^{\mathrm{l}} \chi_{\mathrm{h}}^{\mathrm{l}}\right)_\Omega(t)\,\mathrm{d}t \geq 0 \quad \forall \lambda \in Z,$$

the initial condition holds.

$\|\varphi\|_X^2 := \sum_{n=1}^{N_t} \|\varphi\|_{X_n}^2\,\mathrm{d}t, \quad \|\varphi\|_{X_n} := \int_{I_n} \sum_{K \in \mathcal{T}_h} \|\varphi\|_{X,K}^2\,\mathrm{d}t,$

Define space-time functions:

$P_{h\tau}^{n,k,i}(t^n) = P_h^{n,k,i} \in \mathbb{P}_2^{\mathrm{d}}(\mathcal{T}_h), \ \tilde{P}_{h\tau}^{n,k,i}(t^n) = \tilde{P}_h^{n,k,i} \in \mathbb{P}_2^{\mathrm{c}}(\mathcal{T}_h), \ l_{c,h\tau}^{n,k,i}(t^n) = l_{c,h}^{n,k,i} \in \mathbb{P}_0^{\mathrm{d}}(\mathcal{T}_h),$

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Error measure

Dual norm of the residual for the components

$$\|\mathcal{R}_c(S_{h\tau}, P_{h\tau}, \chi_{h\tau})\|_{X_n'} = \sup_{\varphi \in X_n, \|\varphi\|_{X_n}=1} \int_{I_n} (Q_c - \partial_t l_{c,h\tau}, \varphi)_\Omega (t) + (\mathbf{\Phi}_{c,h\tau}, \mathbf{\nabla}\varphi)_\Omega (t)\, \mathrm{dt}.$$

Residual for the constraints

$$\mathcal{R}_{\mathrm{e}}(S_{h\tau}, P_{h\tau}, \chi_{h\tau}) = \int_{I_n} \left(1 - S_{h\tau}, H\left[P_{h\tau} + P_{\mathrm{cp}}(S_{h\tau})\right] - \beta^{\mathrm{l}} \chi_{h\tau}\right)_\Omega (t)\, \mathrm{dt}.$$

Error measure for the nonconformity of the pressure

$$\mathcal{N}_P(P_{h\tau}) := \inf_{\delta_{\mathrm{l}} \in X_n} \left\{ \sum_{c \in \{\mathrm{w,h}\}} \int_{I_n} \left\| \underline{\mathbf{K}} \frac{k_{\mathrm{r}}^{\mathrm{l}}(S_{h\tau})}{\mu^{\mathrm{l}}} \rho_c^{\mathrm{l}} \mathbf{\nabla} \left(P_{h\tau} - \delta_{\mathrm{l}}\right)(t) \right\|^2 \mathrm{dt} \right\}^{\frac{1}{2}},$$

Error measure for nonconformity of the molar fraction

$$\mathcal{N}_\chi(\chi_{h\tau}) := \inf_{\theta \in X_n} \left\{ \int_{I_n} \left\| -\phi M_{\mathrm{h}} S_{h\tau} \left(\frac{\rho_{\mathrm{w}}^{\mathrm{l}}}{M_{\mathrm{w}}} + \frac{\beta^{\mathrm{l}}}{M_{\mathrm{h}}} \chi_{h\tau} \right) D_{\mathrm{h}}^{\mathrm{l}} \mathbf{\nabla} \left(\chi_{h\tau} - \theta\right)(t) \right\|^2 \mathrm{dt} \right\}^{\frac{1}{2}},$$

Definition (Error measure)

$$\mathcal{N}^n = \left\{ \sum_{c \in \mathcal{C}} \|\mathcal{R}_c(S_{h\tau}, P_{h\tau}, \chi_{h\tau})\|_{X_n'}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{p \in \mathcal{P}} \mathcal{N}_p^2 + \mathcal{N}_\chi^2 \right\}^{\frac{1}{2}} + \mathcal{R}_{\mathrm{e}}(S_{h\tau}, P_{h\tau}, \chi_{h\tau})$$

Finite volume linearization

The finite volume scheme provides

$$|K|\partial_t^n l_{c,K} + \sum_{\sigma\in\mathcal{E}_K} F_{c,K,\sigma}(\boldsymbol{U}^n) = |K|Q_{c,K}^n,$$

Inexact semismooth linearization

$$\frac{|K|}{\Delta t}\left[l_{c,K}\left(\boldsymbol{U}^{n,k-1}\right) - l_{c,K}^{n-1} + \mathcal{L}_{c,K}^{n,k,i}\right] + \sum_{\sigma\in\mathcal{E}_K^{\text{int}}} \mathcal{F}_{c,K,\sigma}^{n,k,i} - |K|Q_{c,K}^n + \boldsymbol{R}_{c,K}^{n,k,i} = 0$$

Linear perturbation in the accumulation

$$\mathcal{L}_{c,K}^{n,k,i} = \sum_{K'\in\mathcal{T}_h} \frac{|K|}{\Delta t}\frac{\partial l_{c,K}^n}{\partial \boldsymbol{U}_{K'}^n}(\boldsymbol{U}_{K'}^{n,k-1})\left[\boldsymbol{U}_{K'}^{n,k,i} - \boldsymbol{U}_{K'}^{n,k-1}\right],$$

Linearized component flux

$$\mathcal{F}_{c,K,\sigma}^{n,k,i} = \sum_{K'\in\mathcal{T}_h} \frac{\partial F_{c,K,\sigma}}{\partial \boldsymbol{U}_{K'}^n}\left(\boldsymbol{U}^{n,k-1}\right)\left[\boldsymbol{U}_{K'}^{n,k,i} - \boldsymbol{U}_{K'}^{n,k-1}\right] + F_{c,K,\sigma}\left(\boldsymbol{U}^{n,k-1}\right).$$

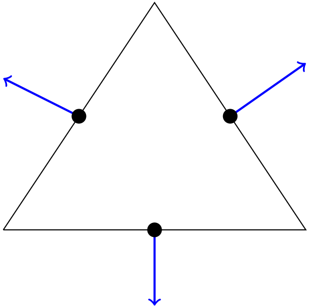
Raviart Thomas spaces

Definition

The lowest-order Raviart–Thomas space is defined by

$$\mathbf{RT}_0(\Omega) = \{\boldsymbol{w}_h \in \mathbf{H}(\mathrm{div}, \Omega), \boldsymbol{w}_h|_K \in \mathbf{RT}_0(K)\ \forall K \in \mathcal{T}_h\}$$

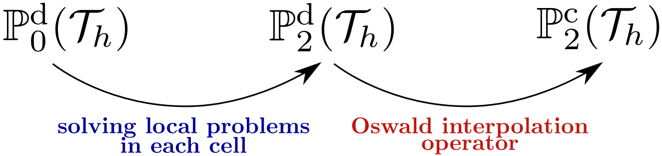
$$\mathbf{RT}_0(K) = [\mathbb{P}_0(K)]^2 + \vec{\boldsymbol{x}} \cdot \mathbb{P}_0(K)$$

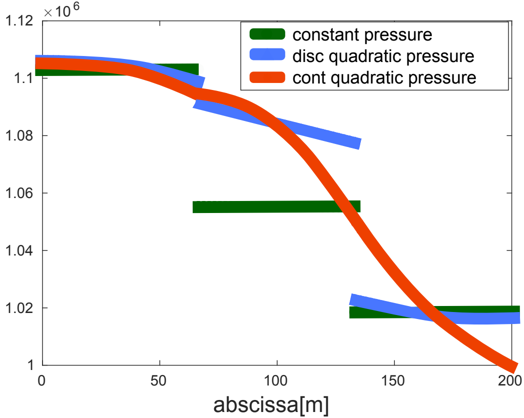


Degrees of freedom $\mathbf{RT}_0$:

$$v_j = (\boldsymbol{v} \cdot \boldsymbol{n}_{e_j}, 1)_{e_j}, \quad e_j \in \partial K, \quad j = \{1, 2, 3\}.$$

Phase pressure reconstruction





Component flux reconstructions

Discretization error flux reconstruction:

$$\left(\boldsymbol{\Theta}_{c,h,\mathrm{disc}}^{n,k,i} \cdot \boldsymbol{n}_K, 1\right)_\sigma = F_{c,K,\sigma}\left(\boldsymbol{U}^{n,k,i}\right) \quad \forall K \in \mathcal{T}_h$$

Linearization error flux reconstruction:

$$\left(\boldsymbol{\Theta}_{c,h,\mathrm{lin}}^{n,k,i} \cdot \boldsymbol{n}_K, 1\right)_\sigma = \mathcal{F}_{c,K,\sigma}^{n,k,i} - F_{c,K,\sigma}\left(\boldsymbol{U}^{n,k,i}\right) \quad \forall K \in \mathcal{T}_h,$$

Algebraic error flux reconstruction:

$$\boldsymbol{\Theta}_{c,h,\mathrm{alg}}^{n,k,i,\nu} := \boldsymbol{\Theta}_{c,h,\mathrm{disc}}^{n,k,i+\nu} + \boldsymbol{\Theta}_{c,h,\mathrm{lin}}^{n,k,i+\nu} - \left(\boldsymbol{\Theta}_{c,h,\mathrm{disc}}^{n,k,i} + \boldsymbol{\Theta}_{c,h,\mathrm{lin}}^{n,k,i}\right) \quad \forall K \in \mathcal{T}_h$$

Total flux reconstruction:

$$\boldsymbol{\Theta}_{c,h}^{n,k,i,\nu} = \boldsymbol{\Theta}_{c,h,\mathrm{disc}}^{n,k,i} + \boldsymbol{\Theta}_{c,h,\mathrm{lin}}^{n,k,i} + \boldsymbol{\Theta}_{c,h,\mathrm{alg}}^{n,k,i,\nu}$$

Proposition (Equilibration property)

$$\left(Q_{c,K}^n - \frac{l_{c,K}(\boldsymbol{U}^{n,k-1}) - l_{c,K}^{n-1} + \mathcal{L}_{c,K}^{n,k,i+\nu}}{\tau_n} - \boldsymbol{\nabla} \cdot \boldsymbol{\Theta}_{c,h}^{n,k,i,\nu}, 1\right)_K = R_{c,K}^{n,k,i+\nu}$$

Error estimators

Remark

$\partial_t l_c + \nabla \cdot \Theta_{c,h}^{n,k,i,\nu} \neq Q_c$ and $\Theta_{c,h}^{n,k,i,\nu} \neq \Phi_{c,h\tau}^{n,k,i}(t^n)$ and $1 - S_{h\tau}^{n,k,i} \ngeq 0$ and $H\left[P_{h\tau}^{n,k,i} + P_{\mathrm{cp}}\left(S_{h\tau}^{n,k,i}\right)\right] - \beta^{\mathrm{l}}\chi_{h\tau}^{n,k,i} \ngeq 0$ and $P_{h\tau}^{n,k,i} \notin X$ and $\chi_{h\tau}^{n,k,i} \notin X$

Discretization estimator

$$\eta_{\mathrm{R},K,c}^{n,k,i,\nu} = \min\left\{C_{\mathrm{PW}}, \varepsilon^{-\frac{1}{2}}\right\} h_K \left\| Q_{c,h}^n - \frac{l_{c,K}(\boldsymbol{U}^{n,k-1}) - l_{c,K}^{n-1} + \mathcal{L}_{c,K}^{n,k,i}}{\tau_n} - \nabla \cdot \Theta_{c,h}^{n,k,i} \right\|_K$$

$$\eta_{\mathrm{F},K,c}^{n,k,i,\nu}(t) = \left\| \Theta_{c,h}^{n,k,i,\nu} - \Phi_{c,h\tau}^{n,k,i}(t) \right\|_K$$

$$\eta_{\mathrm{P},K,\mathrm{pos}}^{n,k,i}(t) = \left(\left\{1 - S_{h\tau}^{n,k,i}\right\}^+(t), \left\{H\left[P_{h\tau}^{n,k,i} + P_{\mathrm{cp}}\left(S_{h\tau}^{n,k,i}\right)\right] - \beta^{\mathrm{l}}\chi_{h\tau}^{n,k,i}\right\}^+(t) \right)_K$$

$$\eta_{\mathrm{NC},K,\mathrm{l},c}^{n,k,i}(t) = \left\| \underline{\mathbf{K}} \frac{k_{\mathrm{r}}^{\mathrm{l}}(S_{h\tau}^{n,k,i})}{\mu^{\mathrm{l}}} \rho_c^{\mathrm{l}} \nabla \left(P_{h\tau}^{n,k,i} - \tilde{P}_{h\tau}^{n,k,i}\right)(t) \right\|_K$$

$$\eta_{\mathrm{NC},K,\chi}^{n,k,i}(t) = \left\| -\phi M_{\mathrm{h}} S_{h\tau}^{n,k,i} \left(\frac{\rho_{\mathrm{w}}^{\mathrm{l}}}{M_{\mathrm{w}}} + \frac{\beta^{\mathrm{l}}}{M_{\mathrm{h}}} \chi_{h\tau}^{n,k,i} \right) D_{\mathrm{h}}^{\mathrm{l}} \nabla \left(\chi_{h\tau}^{n,k,i} - \tilde{\chi}_{h\tau}^{n,k,i}\right)(t) \right\|_K$$

Error estimators

Linearization estimator

$$\eta_{\mathrm{NA},K,c}^{n,k,i} = \varepsilon^{-\frac{1}{2}} h_K (\tau_n)^{-1} \left\| l_{c,K}(\boldsymbol{U}^{n,k,i}) - l_{c,K}(\boldsymbol{U}^{n,k-1}) - \mathcal{L}_{c,K}^{n,k,i} \right\|_K$$

$$\eta_{\mathrm{P},K,\mathrm{neg}}^{n,k,i}(t) = \left(\left\{ 1 - S_{h\tau}^{n,k,i} \right\}^{-}(t), \left\{ H \left[P_{h\tau}^{n,k,i} + P_{\mathrm{cp}} \left(S_{h\tau}^{n,k,i} \right) \right] - \beta^{\mathrm{l}} \chi_{h\tau}^{n,k,i} \right\}^{-}(t) \right)_K$$

Algebraic estimator

$$\eta_{\mathrm{alg},K,c}^{n,k,i} := \left\| \boldsymbol{\Theta}_{c,h,\mathrm{alg}}^{n,k,i,\nu} \right\|_K$$

$$\eta_{\mathrm{rem},K,c}^{n,k,i,\nu} := h_K |K|^{-1} \varepsilon^{-\frac{1}{2}} \left\| \boldsymbol{R}_{c,K}^{n,k,i+\nu} \right\|_K$$

Theorem

$$\mathcal{N}^{n,k,i} \leq \eta_{\mathrm{disc}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}$$

Adaptivity

Algorithm 1 Adaptive inexact semismooth Newton algorithm

Initialization: Choose an initial vector $\boldsymbol{U}^{n,0} \in \mathbb{R}^{3N_h}$, $(k = 0)$

Do

$k = k + 1$

Compute $\mathbb{A}^{n,k-1} \in \mathbb{R}^{3N_h,3N_h}$, $\quad \boldsymbol{B}^{n,k-1} \in \mathbb{R}^{3N_h}$

Consider the system of linear algebraic equations $\mathbb{A}^{n,k-1}\boldsymbol{U}^{n,k} = \boldsymbol{B}^{n,k-1}$

Initialization for the linear solver: Define $\boldsymbol{U}^{n,k,0} = \boldsymbol{U}^{n,k-1}$, $(i = 0)$ as initial guess for the linear solver

Do

$i = i + 1$

Compute Residual: $\boldsymbol{R}^{n,k,i} = \boldsymbol{B}^{n,k-1} - \mathbb{A}^{n,k-1}\boldsymbol{U}^{n,k,i}$

Compute estimators

While $\eta_{\text{alg}}^{n,k,i} \geq \gamma_{\text{alg}} \max\left\{\eta_{\text{disc}}^{n,k,i}, \eta_{\text{lin}}^{n,k,i}\right\}$

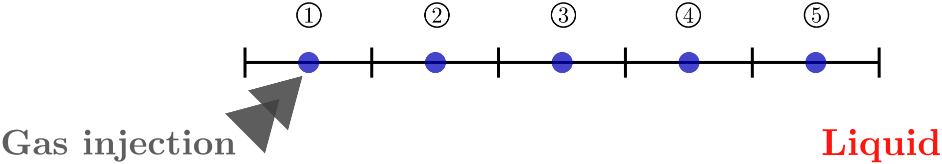
While $\eta_{\text{lin}}^{n,k,i} \geq \gamma_{\text{lin}}\eta_{\text{disc}}^{n,k,i}$

End

Outline

Numerical experiments

Ω: one-dimensional core with length $L = 200m$. We consider the **semismooth Newton-min solver** in combination with the **GMRES** algebraic solver.
$\Delta t = 5000$ years, $N_{\text{sp}} = 1000$ cells, $t_{\text{F}} = 5 \times 10^5$ years.



Van Genuchten–Mualem model:

$$P_{\text{cp}}(S^{\text{l}}) = P_r \left(S_{\text{le}}^{-\frac{1}{m}} - 1 \right)^{\frac{1}{n^*}}$$

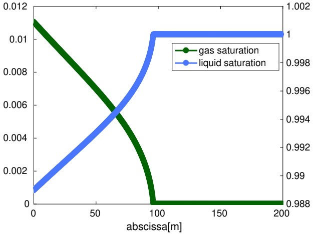
$$k_{\text{r}}^{\text{l}}(S^{\text{l}}) = \sqrt{S_{\text{le}}} \left(1 - (1 - S_{\text{le}}^{\frac{1}{m}})^m \right)^2, \quad k_{\text{r}}^{\text{g}}(S^{\text{l}}) = \sqrt{1 - S_{\text{le}}} \left(1 - S_{\text{le}}^{\frac{1}{m}} \right)^{2m}$$

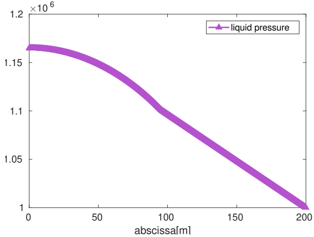
with

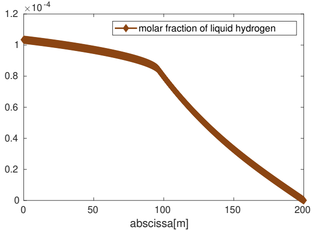
$$S_{\text{le}} = \frac{S^{\text{l}} - S_{\text{lr}}}{1 - S_{\text{lr}} - S_{\text{gr}}} \quad \text{and} \quad m = 1 - \frac{1}{n^*}$$

Numerical experiments

Solution at $t = 1.05 \times 10^5$ years



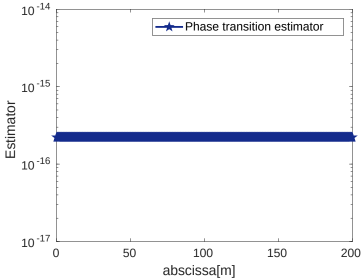




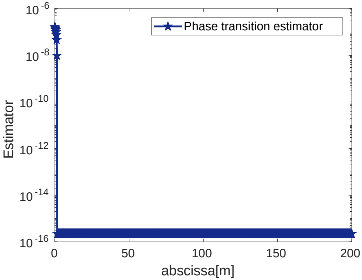
Complementarity constraints at $k = 4$ and $i = 2$

Phase transition estimator

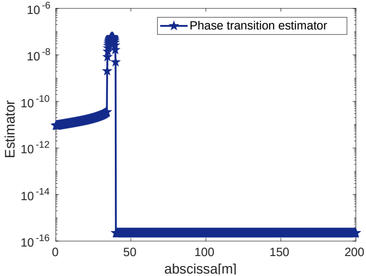
$t = 2500$ years



$t = 1.25 \times 10^4$ years



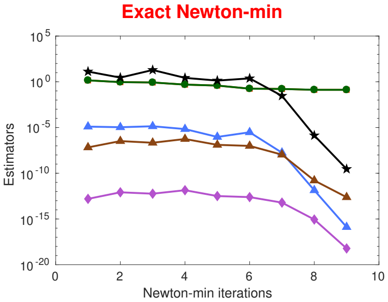
$t = 4.25 \times 10^4$ years

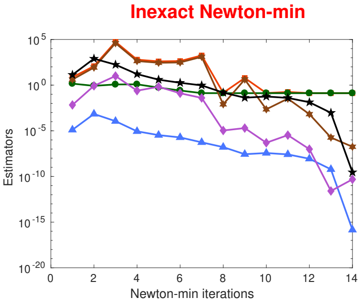


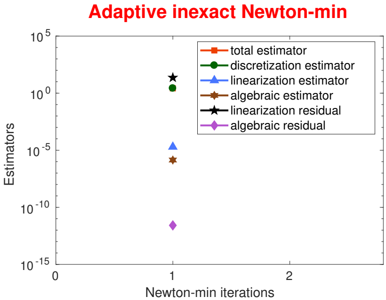
Remark

This estimator detects the error caused by the appearance of the gas phase whenever the gas spreads throughout the domain.

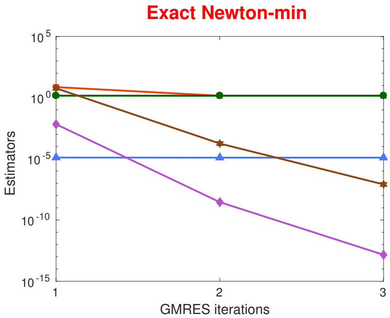
Newton-min adaptivity

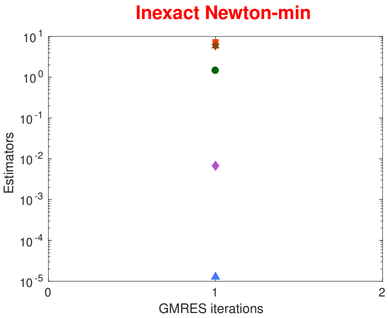


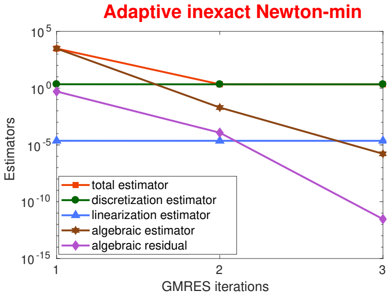




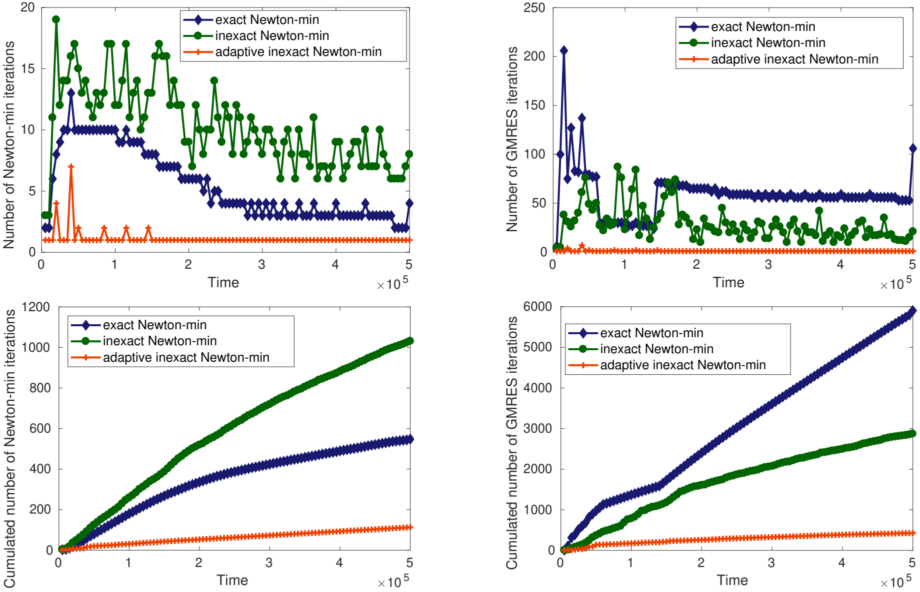
GMRES adaptivity





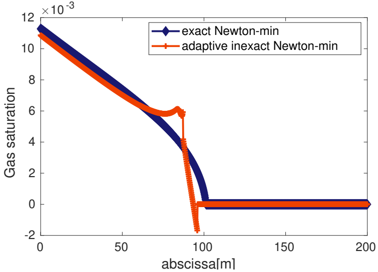


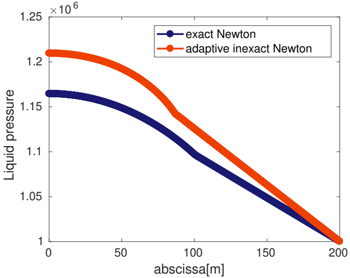
Overall performance



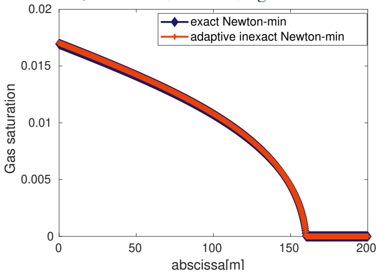
Accuracy

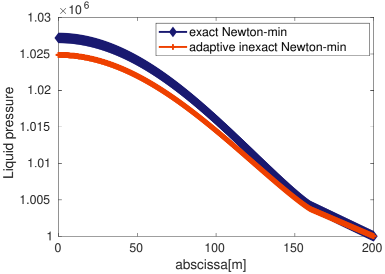
$t = 1.05 \times 10^5$ years, $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$





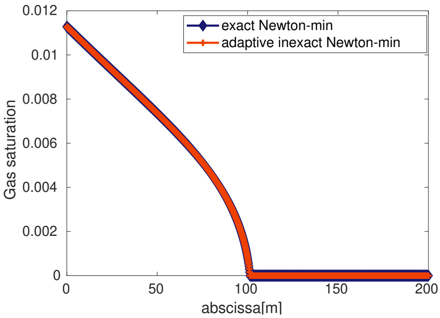
$t = 3.5 \times 10^5$ years, $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

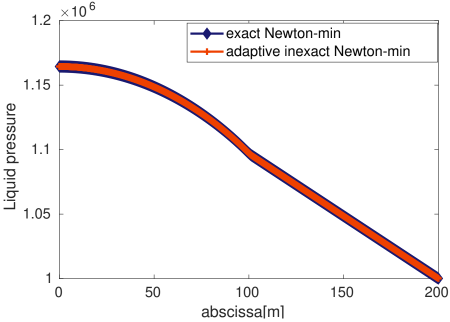




Accuracy

$t = 1.05 \times 10^5$ years, $\gamma_{\text{lin}} = 10^{-6}$, $\gamma_{\text{alg}} = 10^{-3}$





$(\gamma_{\text{alg}}, \gamma_{\text{lin}})$	Cumulated Newton-min iterations	Cumulated GMRES iterations
$(10^{-1}, 10^{-1})$	100	366
$(10^{-3}, 10^{-3})$	113	427
$(10^{-6}, 10^{-3})$	108	967
$(10^{-3}, 10^{-6})$	351	1682
$(10^{-6}, 10^{-6})$	308	2019
Exact resolution	**600**	**6000**

Complements: Newton–Fischer–Burmeister

$$[f_{\mathrm{FB}}(\boldsymbol{a},\boldsymbol{b})]_l = \sqrt{\boldsymbol{a}_l^2 + \boldsymbol{b}_l^2} - (\boldsymbol{a}_l + \boldsymbol{b}_l) \quad l = 1, \dots, N_{\mathrm{sp}}.$$

$(\gamma_{\mathrm{alg}}, \gamma_{\mathrm{lin}})$	Cumulated number of Newton–Fischer–Burmeister iterations	Cumulated number of GMRES iterations
$\left(10^{-1}, 10^{-1}\right)$	100	428
$\left(10^{-3}, 10^{-3}\right)$	119	751
$\left(10^{-3}, 10^{-6}\right)$	482	2074
$\left(10^{-6}, 10^{-3}\right)$	117	1694
Exact resolution	**757**	**10089**

- **Adaptive inexact Newton–Fischer–Burmeister is faster than exact Newton–Fischer–Burmeister. It saves roughly** 90% **of the iterations**
- **Adaptive inexact Newton-min is faster than Adaptive inexact Newton–Fischer–Burmeister. It saves roughly** 40% **of the iterations.**

Outline

Conclusion

- We devised an a posteriori error estimate between the exact and approximate solution for a wide class of semi-smooth Newton methods.

- This estimate distinguishes the error components.

Ongoing work:

- Devise space-time adaptivity
- Optimize the code

I. Ben Gharbia, J. Dabaghi, V. Martin, and M. Vohralík, *A posteriori error estimates and adaptive stopping criteria for a compositional two-phase flow with nonlinear complementarity constraints*. HAL Preprint 01919067, submitted for publication, 2018

J. Dabaghi, V. Martin, and M. Vohralík, *Adaptive inexact semismooth Newton methods for the contact problem between two membranes*. HAL Preprint 01666845, submitted for publication, 2018

J. Dabaghi, V. Martin, and M. Vohralík, *A posteriori error estimate and adaptive stopping criteria for a parabolic variational inequality*. In preparation.

Thank you for your attention!