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

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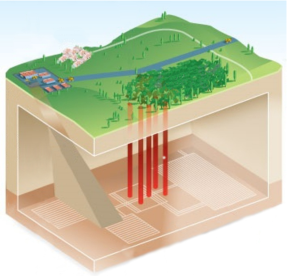
informatics mathematics

École des Ponts ParisTech

Outline

Introduction

Storage of radioactive wastes



Model: System of PDE's with complementarity constraints

$$\partial_t \boldsymbol{U} + \mathcal{A}(\boldsymbol{U}) = 0$$
$$\mathcal{K}(\boldsymbol{U}) \geq 0, \ \ \mathcal{G}(\boldsymbol{U}) \geq 0, \ \ \mathcal{K}(\boldsymbol{U}) \cdot \mathcal{G}(\boldsymbol{U}) = 0.$$

Space/Time discretisation

$$S^n(\boldsymbol{U}_h^n) = 0$$
$$\mathcal{K}(\boldsymbol{U}_h^n) \geq 0 \ \ \mathcal{G}(\boldsymbol{U}_h^n) \geq 0 \ \ \mathcal{K}(\boldsymbol{U}_h^n) \cdot \mathcal{G}(\boldsymbol{U}_h^n) = 0$$

Resolution: semismooth Newton

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

Can we estimate each error components (discretization, linearization, algebraic)?
Can we reduce the computational cost?

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

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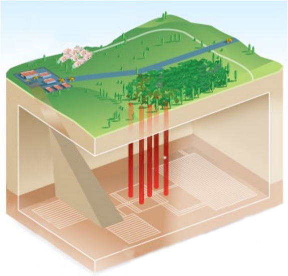

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Outline

Compositional two-phase flow with phase transition

$$\begin{cases} \partial_t l_{\mathrm{w}} + \nabla \cdot \mathbf{\Phi}_{\mathrm{w}} = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}} + \nabla \cdot \mathbf{\Phi}_{\mathrm{h}} = Q_{\mathrm{h}}, \\ \mathcal{K}(S^{\mathrm{l}}) \geq 0, \ \mathcal{G}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) \geq 0, \ \mathcal{K}(S^{\mathrm{l}}) \cdot \mathcal{G}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = 0 \end{cases}$$

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

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

Fluxes: $\mathbf{\Phi}_{\mathrm{w}} := \rho_{\mathrm{w}}^{\mathrm{l}} \mathbf{q}^{\mathrm{l}} - \mathbf{J}_{\mathrm{h}}^{\mathrm{l}}, \quad \mathbf{\Phi}_{\mathrm{h}} := \rho_{\mathrm{h}}^{\mathrm{l}} \mathbf{q}^{\mathrm{l}} + \rho_{\mathrm{h}}^{\mathrm{g}} \mathbf{q}^{\mathrm{g}} + \mathbf{J}_{\mathrm{h}}^{\mathrm{l}}$

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

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

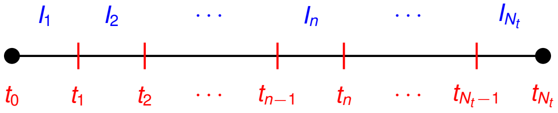
Boundary conditions: $\mathbf{\Phi}_{\mathrm{w}} \cdot \boldsymbol{n}_{\Omega} = 0, \quad \mathbf{\Phi}_{\mathrm{h}} \cdot \boldsymbol{n}_{\Omega} = 0.$

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**

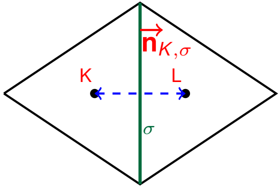
Time discretization: Consider: $t_0 = 0 < t_1 < \cdots < t_{N_t} = t_{\mathrm{F}}$.



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

Space discretization: $\mathcal{T}_h$ a superadmissible family of conforming simplicial meshes of the space domain Ω. Number of cells : N_{sp}

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



Discretization of the 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

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

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At each time step, for each components, we obtain the nonlinear system of algebraic equations

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Discrete complementarity problem

Discretization of the nonlinear complementarity constraints

$$\mathcal{K}(\boldsymbol{U}_K^n) := 1 - S_K^n \quad \mathcal{G}(\boldsymbol{U}_K^n) := H(P_K^n + P_{\mathrm{cp}}(S_K^n)) - \beta^{\mathrm{l}} \chi_K^n$$

The discretization reads

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Can we reformulate the complementarity constraints?

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Semismoothness

To reformulate the discrete constraints:

Definition (C-function)

$$\forall (\boldsymbol{a}, \boldsymbol{b}) \in \mathbb{R}^{N_{\mathrm{sp}}} \times \mathbb{R}^{N_{\mathrm{sp}}},\ f(\boldsymbol{a}, \boldsymbol{b}) = 0 \iff \boldsymbol{a} \geq 0,\ \boldsymbol{b} \geq 0,\ \boldsymbol{a} \cdot \boldsymbol{b} = 0$$

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

Application: complementarity constraints for the two-phase model

$$\underbrace{1 - S_K^n}_{\mathcal{K}(S_K^n)} \geq 0 \qquad \underbrace{H(P_K^n + P_{\mathrm{cp}}(S_K^n)) - \beta^{\mathrm{l}} \chi_K^n}_{\mathcal{G}(P_K^n, S_K^n, \chi_K^n)} \geq 0$$

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Inexact semismooth Newton method

Semismooth Newton linearization: Given an initial guess $\boldsymbol{U}^{n,0} \in \mathbb{R}^{3N_{\rm sp}}$, consider:

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

Inexact Semismooth Newton linearization: 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

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Can we estimate the semismooth linearization error?

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Outline

1. Introduction
2. Model problem and its discretization
3. A posteriori analysis
4. Numerical experiments
5. Conclusion

Weak solution

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

Assumption (Weak formulation)

$$S^{\mathrm{l}} \in \widehat{Y}, \quad 1 - S^{\mathrm{l}} \in Z, \quad l_{\mathrm{w}} \in Y, \quad l_{\mathrm{h}} \in Y, \quad P^{\mathrm{l}} \in X, \quad \chi_{\mathrm{h}}^{\mathrm{l}} \in X,$$
$$(\boldsymbol{\Phi}_{\mathrm{w}}, \boldsymbol{\Phi}_{\mathrm{h}}) \in \left[L^2((0,t_{\mathrm{F}}); \mathbf{H}(\mathrm{div},\Omega))\right]^2,$$
$$\int_0^{t_{\mathrm{F}}} (\partial_t l_c, \varphi)_\Omega (t)\,\mathrm{d}t - \int_0^{t_{\mathrm{F}}} (\boldsymbol{\Phi}_c, \nabla\varphi)_\Omega (t)\,\mathrm{d}t = \int_0^{t_{\mathrm{F}}} (Q_c, \varphi)_\Omega (t)\,\mathrm{d}t \quad \forall \varphi \in X,$$
$$\int_0^{t_{\mathrm{F}}} \left(\lambda - (1 - S^{\mathrm{l}}), H[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})] - \beta^{\mathrm{l}} \chi_{\mathrm{h}}^{\mathrm{l}}\right)_\Omega (t)\,\mathrm{d}t \geq 0 \quad \forall \lambda \in Z,$$

the initial condition holds.

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

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Approximate solution

$$S_K^{n,k,i} \in \mathbb{P}_0^{\mathrm{d}}(\mathcal{T}_h) \quad P_K^{n,k,i} \in \mathbb{P}_0^{\mathrm{d}}(\mathcal{T}_h) \quad \chi_K^{n,k,i} \in \mathbb{P}_0^{\mathrm{d}}(\mathcal{T}_h)$$

The discrete liquid pressure and discrete molar fraction do not belong to $H^1(\Omega)$

We construct a conforming solution:

$$\begin{tikzcd}
\mathbb{P}_0^{\mathrm{d}}(\mathcal{T}_h) \arrow[r, bend right, "\text{solving local problems in each cell}"'] & \mathbb{P}_2^{\mathrm{d}}(\mathcal{T}_h) \arrow[r, bend right, "\text{Oswald interpolation operator}"'] & \mathbb{P}_2^{\mathrm{c}}(\mathcal{T}_h)
\end{tikzcd}$$

Space-time functions:

$$S_{h\tau}^{n,k,i} \in Y, \quad P_{h\tau}^{n,k,i} \in \mathbb{P}_2^{\mathrm{d}}(\mathcal{T}_h) \notin X, \quad \chi_{h\tau}^{n,k,i} \in \mathbb{P}_2^{\mathrm{d}}(\mathcal{T}_h) \notin X$$

$$\tilde{P}_{h\tau}^{n,k,i} \in \mathbb{P}_2^{\mathrm{c}}(\mathcal{T}_h) \in X,$$
$$\tilde{\chi}_{h\tau}^{n,k,i} \in \mathbb{P}_2^{\mathrm{c}}(\mathcal{T}_h) \in X.$$

Error measure

Dual norm of the residual for the components

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

Residual for the constraints

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

Error measure for the nonconformity of the pressure

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

Error measure for nonconformity of the molar fraction

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

Error measure

Dual norm of the residual for the components

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

Residual for the constraints

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

Error measure for the nonconformity of the pressure

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

Error measure for nonconformity of the molar fraction

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

Error measure

Dual norm of the residual for the components

$$\left\|\mathcal{R}_c(S_{h\tau}^{n,k,i}, P_{h\tau}^{n,k,i}, \chi_{h\tau}^{n,k,i})\right\|_{X_n'} := \sup_{\substack{\varphi\in X_n\\ \|\varphi\|_{X_n}=1}} \int_{I_n} \left(Q_c - \partial_t l_{c,h\tau}^{n,k,i}, \varphi\right)_\Omega (t) + \left(\mathbf{\Phi}_{c,h\tau}^{n,k,i}, \boldsymbol{\nabla}\varphi\right)_\Omega (t)\, \mathrm{dt}$$

Residual for the constraints

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

Error measure for the nonconformity of the pressure

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

Error measure for nonconformity of the molar fraction

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

Error measure

Dual norm of the residual for the components

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

Residual for the constraints

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

Error measure for the nonconformity of the pressure

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

Error measure for nonconformity of the molar fraction

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

Definition (Error measure)

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

Theorem

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

How do we construct each error estimators?

Component flux reconstructions

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

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

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:

$$\boldsymbol{\Theta}_{c,h}^{n,k,i,\nu} := \boldsymbol{\Theta}_{c,h,\mathrm{disc}}^{n,k,i} + \boldsymbol{\Theta}_{c,h,\mathrm{lin}}^{n,k,i} + \boldsymbol{\Theta}_{c,h,\mathrm{alg}}^{n,k,i,\nu} \in \mathbf{H}(\mathrm{div}, \Omega)$$

Error estimators

- $\partial_t l_c + \nabla \cdot \boldsymbol{\Theta}^{n,k,i,\nu}_{c,h} \neq Q_c \qquad \boldsymbol{\Theta}^{n,k,i,\nu}_{c,h} \neq \boldsymbol{\Phi}^{n,k,i}_{c,h\tau}(t^n)$
- $1 - S^{n,k,i}_{h\tau} \ngeq 0 \qquad H\left[P^{n,k,i}_{h\tau} + P_{\mathrm{cp}}\left(S^{n,k,i}_{h\tau}\right)\right] - \beta^{\mathrm{l}}\chi^{n,k,i}_{h\tau} \ngeq 0$
- $P^{n,k,i}_{h\tau} \notin X \qquad \chi^{n,k,i}_{h\tau} \notin X$

Discretization estimator

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

$$\eta^{n,k,i,\nu}_{\mathrm{F},K,c}(t) := \left\| \boldsymbol{\Theta}^{n,k,i,\nu}_{c,h} - \boldsymbol{\Phi}^{n,k,i}_{c,h\tau}(t) \right\|_K$$

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

$$\eta^{n,k,i}_{\mathrm{NC},K,\mathrm{l},c}(t) := \left\| \underline{\mathbf{K}} \frac{k^{\mathrm{l}}_{\mathrm{r}}(S^{n,k,i}_{h\tau})}{\mu^{\mathrm{l}}} \rho^{\mathrm{l}}_c \nabla \left(P^{n,k,i}_{h\tau} - \tilde{P}^{n,k,i}_{h\tau} \right)(t) \right\|_K$$

$$\eta^{n,k,i}_{\mathrm{NC},K,\chi}(t) := \left\| -\phi M_{\mathrm{h}} S^{n,k,i}_{h\tau} \left(\frac{\rho^{\mathrm{l}}_{\mathrm{w}}}{M_{\mathrm{w}}} + \frac{\beta^{\mathrm{l}}}{M_{\mathrm{h}}} \chi^{n,k,i}_{h\tau} \right) D^{\mathrm{l}}_{\mathrm{h}} \nabla \left(\chi^{n,k,i}_{h\tau} - \tilde{\chi}^{n,k,i}_{h\tau} \right)(t) \right\|_K$$

Error estimators

- $\partial_t l_c + \nabla \cdot \boldsymbol{\Theta}_{c,h}^{n,k,i,\nu} \neq Q_c \quad \boldsymbol{\Theta}_{c,h}^{n,k,i,\nu} \neq \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t^n)$
- $1 - S_{h\tau}^{n,k,i} \not\geq 0 \quad H\left[P_{h\tau}^{n,k,i} + P_{\mathrm{cp}}\left(S_{h\tau}^{n,k,i}\right)\right] - \beta^{\mathrm{l}}\chi_{h\tau}^{n,k,i} \not\geq 0$
- $P_{h\tau}^{n,k,i} \notin X \quad \chi_{h\tau}^{n,k,i} \notin X$

Discretization estimator

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

$$\eta_{\mathrm{F},K,c}^{n,k,i,\nu}(t) := \left\| \boldsymbol{\Theta}_{c,h}^{n,k,i,\nu} - \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t) \right\|_K$$

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

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

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

Error estimators

Linearization estimator

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

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

$$\eta^{n,k,i}_{\mathrm{P},K,\mathrm{neg}}(t) := \left(\left\{ 1 - S^{n,k,i}_{h\tau} \right\}^-, \left\{ H \left[P^{n,k,i}_{h\tau} + P_{\mathrm{cp}} \left(S^{n,k,i}_{h\tau} \right) \right] - \beta^1 \chi^{n,k,i}_{h\tau} \right\}^- \right)_K (t)$$

Algebraic estimator

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

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

Remark

$$\eta^{n,k,i}_{\mathrm{lin}} \to 0 \quad \eta^{n,k,i}_{\mathrm{alg}} \to 0 \quad \textit{when} \quad k, i \to \infty$$

Error estimators

Linearization estimator

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

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

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

Algebraic estimator

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

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

Remark

$$\eta_{\mathrm{lin}}^{n,k,i} \to 0 \quad \eta_{\mathrm{alg}}^{n,k,i} \to 0 \quad \textit{when} \quad k, i \to \infty$$

Error estimators

Linearization estimator

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

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

$$\eta^{n,k,i}_{\mathrm{P},K,\mathrm{neg}}(t) := \left(\left\{ 1 - S^{n,k,i}_{h\tau} \right\}^{-}, \left\{ H \left[P^{n,k,i}_{h\tau} + P_{\mathrm{cp}} \left(S^{n,k,i}_{h\tau} \right) \right] - \beta^{1} \chi^{n,k,i}_{h\tau} \right\}^{-} \right)_K (t)$$

Algebraic estimator

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

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

Remark

$$\eta^{n,k,i}_{\mathrm{lin}} \to 0 \quad \eta^{n,k,i}_{\mathrm{alg}} \to 0 \quad \textit{when} \quad k, i \to \infty$$

Adaptivity

Algorithm 1 Adaptive inexact semismooth Newton algorithm

Initialization (semismooth Newton): Choose an initial vector $\boldsymbol{U}^{n,0} := \boldsymbol{U}^{n-1} \in \mathbb{R}^{3N_{\rm sp}}$, $(k = 0)$

Do

$k = k + 1$

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

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

Initialization (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 $\boxed{\eta_{\rm alg}^{n,k,i} \geq \gamma_{\rm alg} \max\left\{\eta_{\rm disc}^{n,k,i}, \eta_{\rm lin}^{n,k,i}\right\}}$

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

End

Outline

Numerical experiments

Ω: one-dimensional core with length $L = 200m$.

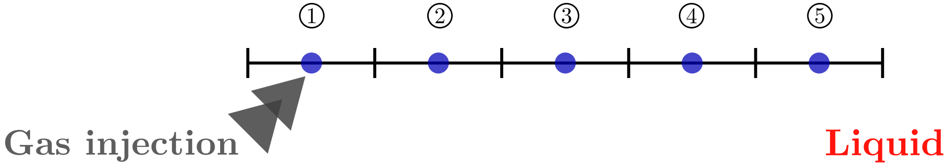
Semismooth solver: Newton-min

Iterative algebraic solver: GMRES.

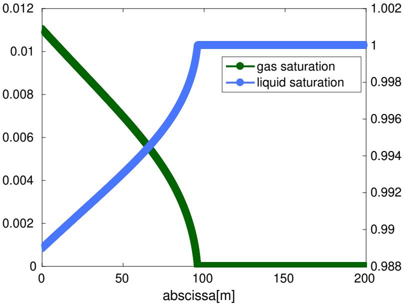
Time step: $\Delta t = 5000$ years,

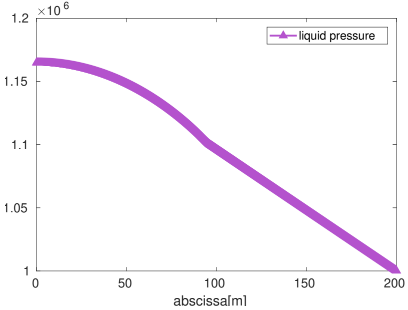
Number of cells: $N_{\rm sp} = 1000$,

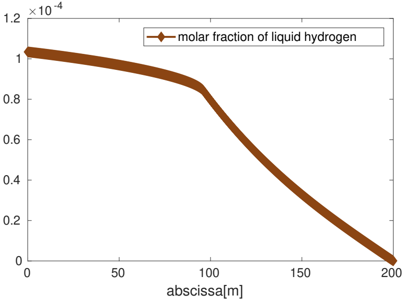
Final simulation time: $t_{\rm F} = 5 \times 10^5$ years.



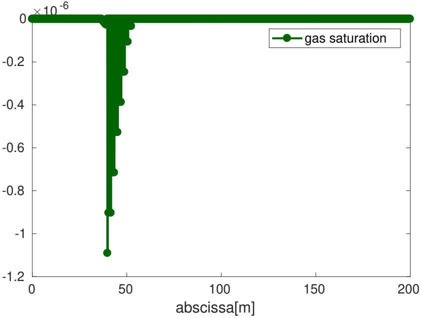
Numerical solution $t = 1.05 \times 10^5$ years

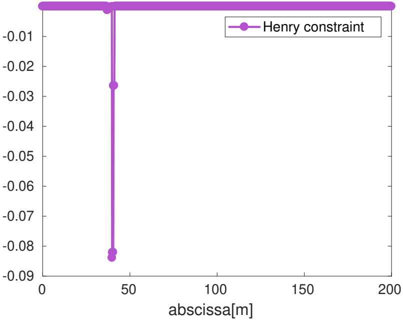






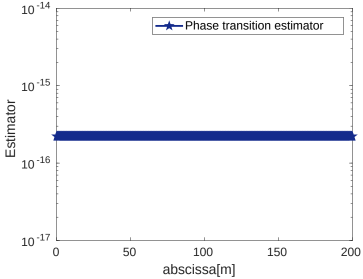
Violation of the complementarity constraints



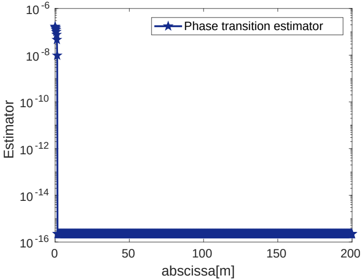


Phase transition estimator

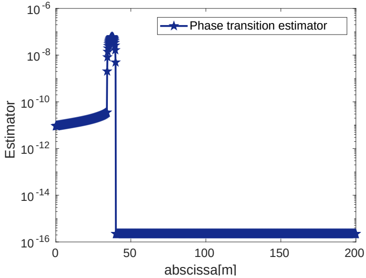
$t = 2500$ years



$t = 1.25 \times 10^4$ years



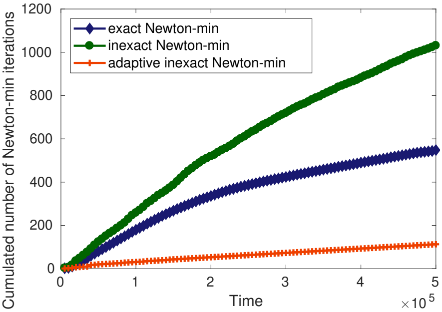
$t = 4.25 \times 10^4$ years

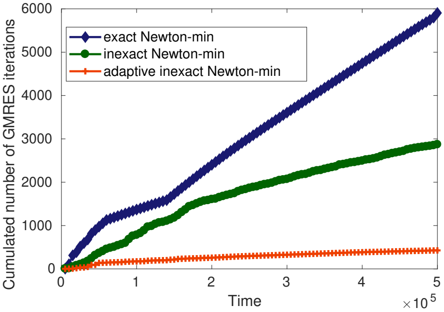


Remark

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

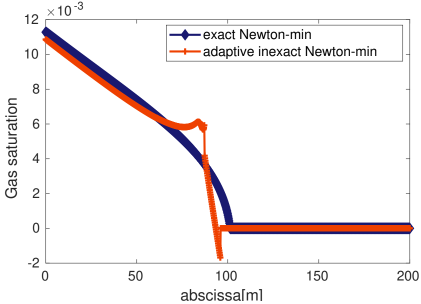
Overall performance $\gamma_{\rm lin} = \gamma_{\rm alg} = 10^{-3}$



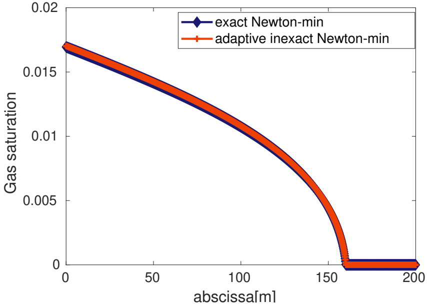


Accuracy $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years



Complements: Newton–Fischer–Burmeister

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

$(\gamma_{\mathrm{alg}}, \gamma_{\mathrm{lin}})$	Cumulated number of Newton–Fischer–Burmeister iterations	Cumulated number of GMRES iterations
$(10^{-1}, 10^{-1})$	100	428
$(10^{-3}, 10^{-3})$	119	751
$(10^{-3}, 10^{-6})$	482	2074
$(10^{-6}, 10^{-3})$	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 for a two-phase flow problem with phase appearance and disappearance an a posteriori error estimate between the exact and approximate solution
- We treat a wide class of semismooth Newton methods
- This estimate distinguishes the error components

Ongoing work:

- Devise space-time adaptivity
- extension to multiphase compositional flow with several phase transitions

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

Thank you for your attention!