

# A posteriori error estimates for variational inequalities: application to a two-phase flow in porous media

LMAC seminar, UTC

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INRIA Paris & ENPC

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Introduction  
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Stationary variational inequality  
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Two-phase compositional flow  
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Conclusion  
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# Outline

## 1 Introduction

## 2 Stationary variational inequality

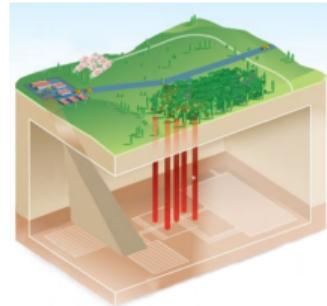
## 3 Two-phase compositional flow

## 4 Conclusion

## Motivation

## **Study a simplified mathematical model for the storage of radioactive waste**

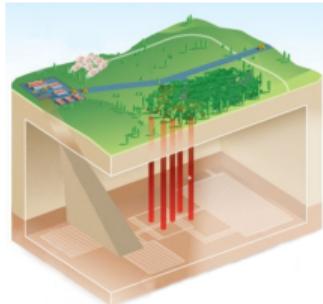
$$\begin{cases} \partial_t l_w(S^l) + \nabla \cdot \Phi_w(S^l, P^l, \chi_h^l) = Q_w \\ \partial_t h(S^l, \chi_h^l) + \nabla \cdot \Phi_h(S^l, P^l, \chi_h^l) = Q_h \\ \mathcal{K}(S^l) \geq 0, \quad \mathcal{G}(S^l, P^l, \chi_h^l) \geq 0, \quad \mathcal{K}(S^l) \cdot \mathcal{G}(S^l, P^l, \chi_h^l) = 0 \end{cases}$$



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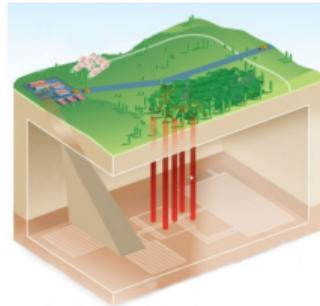
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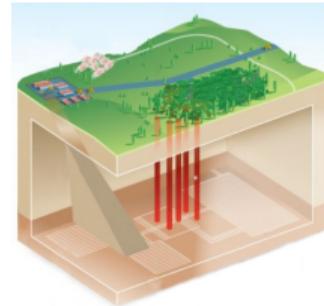
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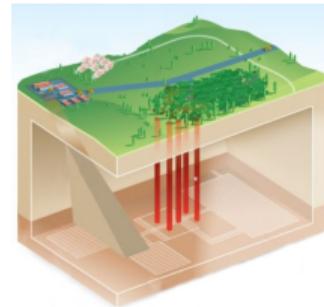
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**Strongly non linear problem, an incomplete mathematical analysis, very complicated problem...**

**We study 2 problems of increasing difficulty.**

## Motivation

Consider the system of PDEs with nonlinear complementarity constraints:

$$\partial_t(\varphi(\mathbf{u})) + \mathcal{A}(\mathbf{u}) = \mathcal{F}$$

This model is used in various physical phenomena: economy, fluid mechanics, elasticity, multiphase flow.

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## Numerical resolution:

- Discretization: Finite elements /finite volumes + backward Euler scheme in time

$$\frac{\varphi(\mathbf{u}_h^n) - \varphi(\mathbf{u}_h^{n-1})}{t^n - t^{n-1}} + \mathcal{A}(\mathbf{u}_h^n) = \mathcal{F}_h^{n-1}$$

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- Nonlinear resolution: inexact semismooth Newton algorithm

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

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## A posteriori error estimate:

$$\left\| \mathbf{u} - \mathbf{u}_h^{n,k,i} \right\| \leq \eta(\mathbf{u}_h^{n,k,i}) \quad \text{where} \quad \|\cdot\| \quad \text{is some norm}$$

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## Three components of the error:

- discretization error: numerical scheme (finite elements, finite volumes...)
  - linearization error: semismooth Newton method ( $k$ )
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## Questions:

Can we estimate each component of the error? **yes!**

- $\| \mathbf{u} - \mathbf{u}_h^{n,k,i} \| \leq \eta_{\text{disc}}^{n,k,i} + \eta_{\text{lin}}^{n,k,i} + \eta_{\text{alg}}^{n,k,i}$

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- $$\bullet \quad \left\| \mathbf{u} - \mathbf{u}_h^{n,k,i} \right\| \leq \eta_{\text{disc}}^{n,k,i} + \eta_{\text{lin}}^{n,k,i} + \eta_{\text{alg}}^{n,k,i}$$

Can we reduce the number of iterations? **yes!**

- Adaptive stopping criterion: semismooth linearization:  $\eta_{\text{lin}}^{n,k,i} \leq \gamma_{\text{lin}} \eta_{\text{disc}}^{n,k,i}$
  - Adaptive stopping criterion: algebraic:  $\eta_{\text{alg}}^{n,k,i} \leq \gamma_{\text{alg}} \left\{ \eta_{\text{disc}}^{n,k,i}, \eta_{\text{lin}}^{n,k,i} \right\}$



## Two-phase compositional flow in porous media

Find  $S^l, P^l, \chi_h^l$   $\left\{ \begin{array}{l} \partial_t l_w(S^l) + \nabla \cdot \Phi_w(S^l, P^l, \chi_h^l) = Q_w, \\ \partial_t l_h(S^l, \chi_h^l) + \nabla \cdot \Phi_h(S^l, P^l, \chi_h^l) = Q_h, \\ \mathcal{K}(S^l) \geq 0, \mathcal{G}(S^l, P^l, \chi_h^l) \geq 0, \mathcal{K}(S^l) \cdot \mathcal{G}(S^l, P^l, \chi_h^l) = 0 \end{array} \right.$



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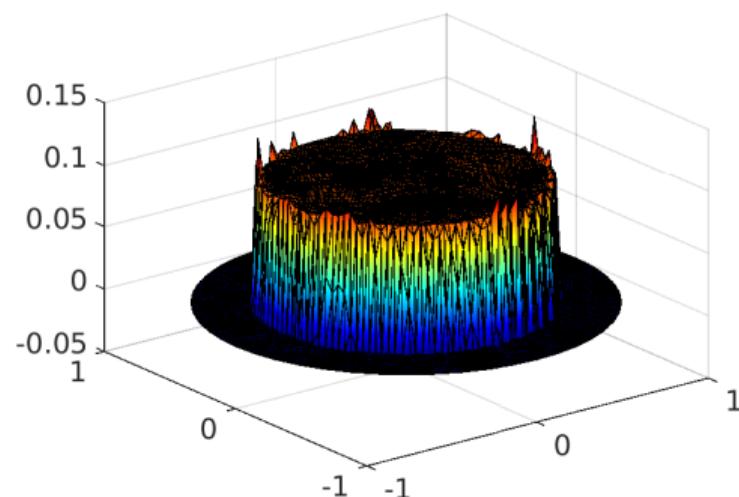
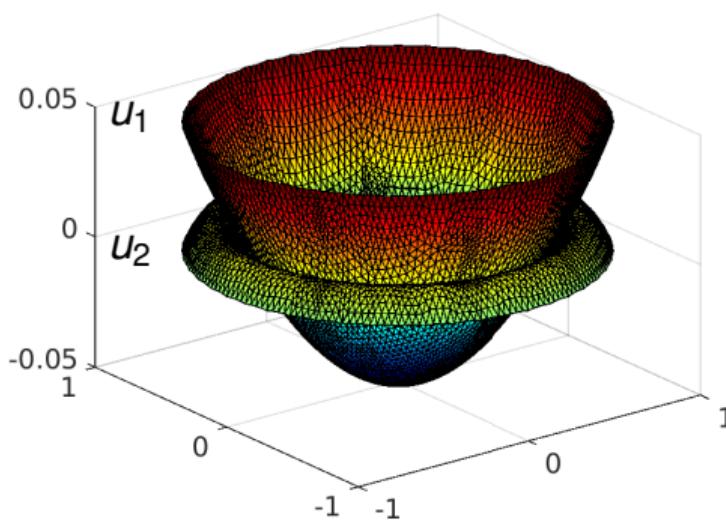
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## Model problem and settings: contact between two membranes

Find  $u_1, u_2, \lambda$  such that

$$\begin{cases} -\mu_1 \Delta u_1 - \lambda = f_1 & \text{in } \Omega, \\ -\mu_2 \Delta u_2 + \lambda = f_2 & \text{in } \Omega, \\ (u_1 - u_2)\lambda = 0, \quad u_1 - u_2 \geq 0, \quad \lambda \geq 0 & \text{in } \Omega, \\ u_1 = g > 0 & \text{on } \partial\Omega, \\ u_2 = 0 & \text{on } \partial\Omega. \end{cases}$$



## Continuous problem

- $$\bullet \quad H_g^1(\Omega) = \{u \in H^1(\Omega), \ u = g \text{ on } \partial\Omega\} \quad \Lambda = \{\chi \in L^2(\Omega), \ \chi \geq 0 \text{ on } \Omega\}$$

**Saddle point type weak formulation:** For  $(f_1, f_2) \in [L^2(\Omega)]^2$  and  $g > 0$  find  $(u_1, u_2, \lambda) \in H_g^1(\Omega) \times H_0^1(\Omega) \times \Lambda$  such that

$$\begin{cases} \sum_{\alpha=1}^2 \mu_\alpha (\nabla u_\alpha, \nabla v_\alpha)_\Omega - (\lambda, v_1 - v_2)_\Omega = \sum_{\alpha=1}^2 (f_\alpha, v_\alpha)_\Omega & \forall (v_1, v_2) \in [H_0^1(\Omega)]^2 \\ (\chi - \lambda, u_1 - u_2)_\Omega \geq 0 & \forall \chi \in \Lambda \end{cases} \quad (\text{S})$$

**equivalent to**

## Variational inequality:

- $\mathcal{K}_g = \{(v_1, v_2) \in H_q^1(\Omega) \times H_0^1(\Omega), v_1 - v_2 \geq 0 \text{ on } \Omega\}$

$$\sum_{\alpha=1}^2 \mu_\alpha (\nabla u_\alpha, \nabla (v_\alpha - u_\alpha))_\Omega \geq \sum_{\alpha=1}^2 (f_\alpha, v_\alpha - u_\alpha)_\Omega \quad \forall \mathbf{v} = (v_1, v_2) \in \mathcal{K}_g \quad (\text{R})$$

## Discretization by finite elements

**For any  $p \geq 1$**

### **Spaces for the discretization:**

$$X_{gh}^p = \{v_h \in \mathcal{C}^0(\bar{\Omega}), v_{h|K} \in \mathbb{P}_p(K), \forall K \in \mathcal{T}_h, \quad v_h = g \text{ on } \partial\Omega\}$$

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**Resolution techniques:** Projected Newton methods (Bertsekas 1982), Active set Newton method (Kanzow 1999), Primal-dual active set strategy (Hintermüller 2002).

## Saddle point formulation

**Characterization of the discrete lagrange multiplier:** Define  $\lambda_{1h}$  and  $\lambda_{2h}$  in  $X_h^P$  by

$$\left\{ \begin{array}{lcl} \langle \lambda_{1h}, z_{1h} \rangle_h & := & \mu_1 (\nabla u_{1h}, \nabla z_{1h})_\Omega - (f_1, z_{1h})_\Omega & \forall z_{1h} \in X_{0h}^p, \\ \langle \lambda_{2h}, z_{2h} \rangle_h & := & -\mu_2 (\nabla u_{2h}, \nabla z_{2h})_\Omega + (f_2, z_{2h})_\Omega & \forall z_{2h} \in X_{0h}^p, \\ \langle \lambda_{1h}, \psi_{h,\mathbf{x}_I} \rangle_h & := & \langle \lambda_{2h}, \psi_{h,\mathbf{x}_I} \rangle_h = 0 & \forall \mathbf{x}_I \in \mathcal{V}_{\text{d}}^{p,\text{ext}}, \end{array} \right.$$

where for all  $(w_h, v_h) \in X_h^p \times X_h^p$

$$\langle w_h, v_h \rangle_h := \sum_{\mathbf{a} \in \mathcal{V}_h} w_h(\mathbf{a}) v_h(\mathbf{a}) M_{\mathbf{a}} \quad \text{if } p = 1 \quad \text{and} \quad \langle w_h, v_h \rangle_h := (w_h, v_h)_{\Omega} \quad \text{if } p \geq 2$$

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$p = 1$ :  $\Lambda_h^1 := \left\{ v_h \in X_{0h}^1 \mid v_h(\mathbf{a}) \geq 0 \quad \forall \mathbf{a} \in \mathcal{V}_d^{p,\text{int}} \right\}$  Ben Belgacem, Bernardi, Blouza, and Vohralík (2008)

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$$p \geq 2 \text{ (new): } \Lambda_h^p := \left\{ v_h \in X_h^p \mid \langle v_h, \psi_{h,\mathbf{x}_I} \rangle_h \geq 0 \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \langle v_h, \psi_{h,\mathbf{x}_I} \rangle_h = 0 \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{ext}} \right\} \not\subset \Lambda$$

**Discrete saddle point type formulation** Find  $(u_{1h}, u_{2h}, \lambda_h) \in X_{gh}^p \times X_{0h}^p \times \Lambda_h^p$  such that

$$\forall (z_{1h}, z_{2h}) \in [X_{0h}^p]^2$$

$$\begin{aligned} \sum_{\alpha=1}^2 \mu_\alpha (\nabla u_{\alpha h}, \nabla z_{\alpha h})_\Omega - \langle \lambda_h, z_{1h} - z_{2h} \rangle_h &= \sum_{\alpha=1}^2 (f_\alpha, z_{\alpha h})_\Omega \quad (\text{DS}), \\ \langle \chi_h - \lambda_h, u_{1h} - u_{2h} \rangle_h &\geq 0 \quad \forall \chi_h \in \Lambda_h^p. \end{aligned}$$

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## Lemma

(DR) ***equivalent to*** (DS)

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## Lemma

(DR) ***equivalent to*** (DS)

- $p = 1$ : Ben Belgacem, Bernardi, Blouza, and Vohralík (2008)

**Discrete saddle point type formulation** Find  $(u_{1h}, u_{2h}, \lambda_h) \in X_{gh}^p \times X_{0h}^p \times \Lambda_h^p$  such that

$$\forall (z_{1h}, z_{2h}) \in [X_{0h}^p]^2$$

$$\begin{aligned} \sum_{\alpha=1}^2 \mu_\alpha (\nabla u_{\alpha h}, \nabla z_{\alpha h})_\Omega - \langle \lambda_h, z_{1h} - z_{2h} \rangle_h &= \sum_{\alpha=1}^2 (f_\alpha, z_{\alpha h})_\Omega \quad (\text{DS}), \\ \langle \chi_h - \lambda_h, u_{1h} - u_{2h} \rangle_h &\geq 0 \quad \forall \chi_h \in \Lambda_h^p. \end{aligned}$$

## Lemma

(DR) ***equivalent to*** (DS)

- $p = 1$ : Ben Belgacem, Bernardi, Blouza, and Vohralík (2008)
  - $p \geq 2$ : New → Construction of the basis  $(\Theta_{h,\mathbf{x}_I})_{1 \leq I \leq N_d^p}$  of  $X_h^p$ , dual to  $(\psi_{h,\mathbf{x}_I})_{1 \leq I \leq N_d^p}$ .

$$\langle \Theta_{h,\mathbf{x}_I}, \psi_{h,\mathbf{x}_{I'}} \rangle_h = \delta_I^{I'}$$

$(u_{1h}, u_{2h}, \lambda_h)$  solution of (DS)  $\Rightarrow \langle \chi_h, u_{1h} - u_{2h} \rangle_h \geq 0 \ \forall \chi_h \in \Lambda_h^p$ . Take  $\chi_h = \Theta_{h, \mathbf{x}_I}$ ,  $\mathbf{x}_I \in \mathcal{V}_d^{p, \text{int}}$

$$\sum_{\mathbf{x}'_I \in \mathcal{V}_d^p} (u_{1h} - u_{2h})(\mathbf{x}'_I) \langle \Theta_{h,\mathbf{x}_I}, \psi_{h,\mathbf{x}'_I} \rangle_h = (\textcolor{red}{u_{1h} - u_{2h}})(\mathbf{x}'_I) \geq 0 \Rightarrow \mathbf{u}_h \in \mathcal{K}_{gh}^p$$

## Discrete complementarity problems

$$\sum_{\alpha=1}^2 \mu_\alpha (\nabla u_{\alpha h}, \nabla z_{\alpha h})_\Omega - \langle \lambda_h, z_{1h} - z_{2h} \rangle_h = \sum_{\alpha=1}^2 (f_\alpha, z_{\alpha h})_\Omega \quad \forall (z_{1h}, z_{2h}) \in [X_{0h}^p]^2,$$

$$(u_{1h} - u_{2h})(\mathbf{x}_I) \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, \psi_{h,\mathbf{x}_I} \rangle_h \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, u_{1h} - u_{2h} \rangle_h = 0.$$

### **Expression of the discrete problem in the Lagrange basis and in the dual basis:**

**$p = 1$ : Lagrange basis:**  $u_{1h} = u_{1h}^* + g$  where  $u_{1h}^* \in X_{0h}^p$  and  $g > 0$ .

$$u_{1h} = \sum_{l=1}^{\mathcal{N}_h^{\text{int}}} (\mathbf{X}_{1h})_l \psi_{h,\mathbf{x}_l} + g, \quad u_{2h} = \sum_{l=1}^{\mathcal{N}_h^{\text{int}}} (\mathbf{X}_{2h})_l \psi_{h,\mathbf{x}_l} \in X_{0h}^p \quad \lambda_h = \sum_{l=1}^{\mathcal{N}_h^{\text{int}}} (\mathbf{X}_{3h})_l \psi_{h,\mathbf{a}_l} \in X_{0h}^p,$$

$$\mathbb{E}_1 \mathbf{X}_h = \mathbf{F}, \quad \mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h} \geq 0, \quad \mathbf{X}_{3h} \geq 0, \quad (\mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h}) \cdot \mathbf{X}_{3h} = 0. \quad \mathbb{E}_1 := \begin{bmatrix} \mu_1 \mathbb{S} & \mathbf{0} & -\mathbb{D} \\ \mathbf{0} & \mu_2 \mathbb{S} & +\mathbb{D} \end{bmatrix}$$

## Discrete complementarity problems

$$\sum_{\alpha=1}^2 \mu_\alpha (\nabla u_{\alpha h}, \nabla z_{\alpha h})_\Omega - \langle \lambda_h, z_{1h} - z_{2h} \rangle_h = \sum_{\alpha=1}^2 (f_\alpha, z_{\alpha h})_\Omega \quad \forall (z_{1h}, z_{2h}) \in [X_{0h}^p]^2,$$

$$(u_{1h} - u_{2h})(\mathbf{x}_I) \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, \psi_{h,\mathbf{x}_I} \rangle_h \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, u_{1h} - u_{2h} \rangle_h = 0.$$

### **Expression of the discrete problem in the Lagrange basis and in the dual basis:**

**$p \geq 2$ : Lagrange basis:** The discrete lagrange multiplier  $\lambda_h$  is decomposed in the full space  $X_h^p$  as

$$\lambda_h = \sum_{l=1}^{\mathcal{N}_d^p} \left( \tilde{\mathbf{X}}_{3h} \right)_l \psi_{h,\mathbf{x}_l} \quad \text{with} \quad \tilde{\mathbf{X}}_{3h} \in \mathbb{R}^{\mathcal{N}_d^p}.$$

$$\tilde{\mathbb{E}}_p \mathbf{X}_h = \mathbf{F},$$

$$\mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h} \geq 0, \quad \widehat{\mathbb{M}}\widetilde{\mathbf{X}}_{3h} \geq 0, \quad (\mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h}) \cdot \widehat{\mathbb{M}}\widetilde{\mathbf{X}}_{3h} = 0.$$

## Discrete complementarity problems

$$\begin{aligned} \sum_{\alpha=1}^2 \mu_\alpha (\nabla u_{\alpha h}, \nabla z_{\alpha h})_\Omega - \langle \lambda_h, z_{1h} - z_{2h} \rangle_h &= \sum_{\alpha=1}^2 (f_\alpha, z_{\alpha h})_\Omega \quad \forall (z_{1h}, z_{2h}) \in [X_{0h}^p]^2, \\ (u_{1h} - u_{2h})(\mathbf{x}_I) &\geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, \psi_{h,\mathbf{x}_I} \rangle_h \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, u_{1h} - u_{2h} \rangle_h = 0. \end{aligned}$$

### **Expression of the discrete problem in the Lagrange basis and in the dual basis:**

**$p \geq 2$ : Dual basis:** The discrete Lagrange multiplier  $\lambda_h$  is decomposed in the basis  $\Theta_{h,\mathbf{x}_l}$  as

$$\lambda_h = \sum_{l=1}^{\mathcal{N}_d^{p,\text{int}}} (\boldsymbol{X}_{3h})_l \Theta_{h,\boldsymbol{x}_l}, \quad \text{with} \quad \boldsymbol{X}_{3h} \in \mathbb{R}^{\mathcal{N}_d^{p,\text{int}}}.$$

$$\mathbb{E}_p \mathbf{X}_h = \mathbf{F},$$

$$\mathbf{x}_{1h} + g\mathbf{1} - \mathbf{x}_{2h} \geq 0, \quad \mathbf{x}_{3h} \geq 0, \quad (\mathbf{x}_{1h} + g\mathbf{1} - \mathbf{x}_{2h}) \cdot \mathbf{x}_{3h} = 0.$$

$$\mathbb{E}_p := \begin{bmatrix} \mu_1 \mathbb{S} & \mathbf{0} & -\mathbb{I}_d \\ \mathbf{0} & \mu_2 \mathbb{S} & +\mathbb{I}_d \end{bmatrix}$$

Introduction  
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Stationary variational inequality  
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Two-phase compositional flow  
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Conclusion  
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# Resolution

## C-functions

## Definition

$f : (\mathbb{R}^m)^2 \rightarrow \mathbb{R}^m$  ( $m \geq 1$ ) is a  $C$ -function or a complementarity function if

$$\forall (\mathbf{x}, \mathbf{y}) \in (\mathbb{R}^m)^2 \quad f(\mathbf{x}, \mathbf{y}) = \mathbf{0} \iff \mathbf{x} \geq \mathbf{0}, \quad \mathbf{y} \geq \mathbf{0}, \quad \mathbf{x} \cdot \mathbf{y} = 0.$$

Examples of C-functions are the min function

$$(\min\{\mathbf{x}, \mathbf{y}\})_l := \min\{\mathbf{x}_l, \mathbf{y}_l\} \quad l = 1, \dots, m,$$

## the Fischer–Burmeister function

$$(f_{\text{FB}}(\mathbf{x}, \mathbf{y}))_l := \sqrt{\mathbf{x}_l^2 + \mathbf{y}_l^2} - (\mathbf{x}_l + \mathbf{y}_l) \quad l = 1, \dots, m,$$

or the Mangasarian function

$$(f_M(\mathbf{x}, \mathbf{y}))_l := \xi(|\mathbf{x}_l - \mathbf{y}_l|) - \xi(\mathbf{y}_l) - \xi(\mathbf{x}_l) \quad l = 1, \dots, m,$$

where  $\xi : \mathbb{R} \mapsto \mathbb{R}$  is an increasing function satisfying  $\xi(\mathbf{0}) = \mathbf{0}$ .

Let  $\tilde{\mathbf{C}}$  be any C-function, i.e., satisfying (for  $m = \mathcal{N}_d^{p,\text{int}}$ )

$$\tilde{\mathbf{C}}(\mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h}, \mathbf{X}_{3h}) = 0 \iff \mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h} \geq 0, \mathbf{X}_{3h} \geq 0, (\mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h}) \cdot \mathbf{X}_{3h} = 0.$$

Then, introducing the function  $\mathbf{C} : \mathbb{R}^{3\mathcal{N}_d^{p,\text{int}}} \rightarrow \mathbb{R}^{\mathcal{N}_d^{p,\text{int}}}$  defined as

$$\mathbf{C}(\mathbf{X}_h) = \tilde{\mathbf{C}}(\mathbf{X}_{1h} + g\mathbf{1} - \mathbf{X}_{2h}, \mathbf{X}_{3h})$$

Our problem can be equivalently rewritten as

$$\begin{cases} \mathbb{E}_p \mathbf{X}_h &= \mathbf{F}, \\ \mathbf{C}(\mathbf{X}_h) &= \mathbf{0}. \end{cases}$$

The C-function is not Fréchet differentiable.

How can we solve the nonlinear problem?

Inexact semismooth Newton method

**Newton initial vector:**  $\mathbf{X}_h^0 := (\mathbf{X}_{1h}^0, \mathbf{X}_{2h}^0, \mathbf{X}_{3h}^0)^T \in \mathbb{R}^{3N_d^{p,\text{int}}}$ , on step  $k \geq 1$ , one looks for  $\mathbf{X}_h^k \in \mathbb{R}^{3N_d^{p,\text{int}}}$  such that

$$\mathbb{A}^{k-1} \mathbf{x}_h^k = \mathbf{B}^{k-1},$$

where

$$\mathbb{A}^{\textcolor{blue}{k-1}} := \begin{bmatrix} \mathbb{E}_p \\ \mathbf{J}_\mathbf{C}(\mathbf{X}_h^{\textcolor{blue}{k-1}}) \end{bmatrix}, \quad \boldsymbol{B}^{\textcolor{blue}{k-1}} := \begin{bmatrix} \boldsymbol{F} \\ \mathbf{J}_\mathbf{C}(\mathbf{X}_h^{\textcolor{blue}{k-1}})\mathbf{X}_h^{\textcolor{blue}{k-1}} - \mathbf{C}(\mathbf{X}_h^{\textcolor{blue}{k-1}}) \end{bmatrix}.$$

# Inexact semismooth Newton method

**Newton initial vector:**  $\mathbf{X}_h^0 := (\mathbf{X}_{1h}^0, \mathbf{X}_{2h}^0, \mathbf{X}_{3h}^0)^T \in \mathbb{R}^{3\mathcal{N}_d^{p,\text{int}}}$ , on step  $k \geq 1$ , one looks for  $\mathbf{X}_h^k \in \mathbb{R}^{3\mathcal{N}_d^{p,\text{int}}}$  such that

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where

$$\mathbb{A}^{k-1} := \begin{bmatrix} \mathbb{E}_p \\ \mathbf{J}_c(\mathbf{X}_h^{k-1}) \end{bmatrix}, \quad \mathbf{B}^{k-1} := \begin{bmatrix} \mathbf{F} \\ \mathbf{J}_c(\mathbf{X}_h^{k-1})\mathbf{X}_h^{k-1} - \mathbf{C}(\mathbf{X}_h^{k-1}) \end{bmatrix}.$$

**Inexact solver initial vector:**  $\mathbf{X}_h^{k,0} \in \mathbb{R}^{3\mathcal{N}_d^{p,\text{int}}}$ , often taken as  $\mathbf{X}_h^{k,0} = \mathbf{X}_h^{k-1}$ , this yields on step  $i \geq 1$  an approximation  $\mathbf{X}_h^{k,i}$  to  $\mathbf{X}_h^k$  satisfying

$$\mathbb{A}^{k-1} \mathbf{X}_h^{k,i} = \mathbf{B}^{k-1} - \mathbf{R}_h^{k,i},$$

where  $\mathbf{R}_h^{k,i} \in \mathbb{R}^{3\mathcal{N}_d^{p,\text{int}}}$  is the algebraic residual vector.

## Inexact semismooth Newton method

A posteriori error estimates

## A posteriori analysis

$$\left\| \left\| \boldsymbol{u} - \boldsymbol{u}_h^{k,i} \right\| \right\|_{\Omega} := \left( \sum_{\alpha=1}^2 \mu_{\alpha} \left\| \nabla \left( u_{\alpha} - u_{\alpha h}^{k,i} \right) \right\|_{\Omega}^2 \right)^{\frac{1}{2}} \leq \eta^{k,i} := \left( \sum_{K \in Th} \left[ \eta_K (\boldsymbol{u}_h^{k,i})^2 \right]^2 \right)^{\frac{1}{2}}$$

- $\eta_K(\mathbf{u}_h^{k,i})$  local estimator depending on the approximate solution
  - $\eta^{k,i} \leq \eta_{\text{disc}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i}$ : identification of the error components
  - $\eta_K(\mathbf{u}_h^{k,i}) \leq \left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\|_{\zeta_K}$ : local efficiency
  - adaptive inexact stopping criteria based on the error components

# A posteriori analysis

$$\left\| \left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\| \right\|_{\Omega} := \left( \sum_{\alpha=1}^2 \mu_{\alpha} \left\| \nabla \left( u_{\alpha} - u_{\alpha h}^{k,i} \right) \right\|_{\Omega}^2 \right)^{\frac{1}{2}} \leq \eta^{k,i} := \left( \sum_{K \in Th} \left[ \eta_K (\mathbf{u}_h^{k,i})^2 \right]^2 \right)^{\frac{1}{2}}$$

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- adaptive inexact stopping criteria based on the error components

We employ the methodology of equilibrated flux reconstruction to obtain local error estimators.

Destuynder & Métivet (1999) Braess & Schöberl (2008), Ern & Vohralík (2013)

## Component flux reconstruction

## Motivation:

$$-\mu_\alpha \nabla u_\alpha \in \mathbf{H}(\text{div}, \Omega), \quad -\mu_\alpha \nabla u_{\alpha h}^{\textcolor{blue}{k}, \textcolor{red}{i}} \notin \mathbf{H}(\text{div}, \Omega), \quad \nabla \cdot (-\mu_\alpha \nabla u_{\alpha h}^{\textcolor{blue}{k}, \textcolor{red}{i}}) \neq f_\alpha - (-1)^\alpha \lambda_h^{\textcolor{blue}{k}, \textcolor{red}{i}}$$

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## Flux reconstruction:

$$\sigma_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}} \in \mathbf{H}(\text{div}, \Omega) \quad \left( \nabla \cdot \sigma_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}}, 1 \right)_K = \left( f_\alpha - (-1)^\alpha \lambda_h^{\textcolor{blue}{k}, \textcolor{orange}{i}}, 1 \right)_K$$

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## Decomposition of the flux:

$$\sigma_{\alpha h}^{k,i} = \sigma_{\alpha h, \text{alg}}^{k,i} + \sigma_{\alpha h, \text{disc}}^{k,i}$$

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$$\boldsymbol{\sigma}_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}} \in \mathbf{H}(\text{div}, \Omega) \quad \left( \nabla \cdot \boldsymbol{\sigma}_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}}, 1 \right)_K = \left( f_\alpha - (-1)^\alpha \lambda_h^{\textcolor{blue}{k}, \textcolor{orange}{i}}, 1 \right)_K$$

## Decomposition of the flux

$$\sigma_{\alpha h}^{k,i} = \sigma_{\alpha h, \text{alg}}^{k,i} + \sigma_{\alpha h, \text{disc}}^{k,i}$$

## Algebraic flux reconstruction

$\sigma_{\alpha h, \text{alg}}^{k,i} \in \mathbf{H}(\text{div}, \Omega) \quad \nabla \cdot \sigma_{\alpha h, \text{alg}}^{k,i} = r_{\alpha h}^{k,i} \quad \text{where} \quad r_{\alpha h}^{k,i} \quad \text{is the functional representation of} \quad R_{\alpha h}^{k,i}$

Papež, Rüde, Vohralík and Wohlmuth. Submitted for publication (2017).

## Component flux reconstruction

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$$-\mu_\alpha \nabla u_\alpha \in \mathbf{H}(\text{div}, \Omega), \quad -\mu_\alpha \nabla u_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}} \notin \mathbf{H}(\text{div}, \Omega), \quad \nabla \cdot (-\mu_\alpha \nabla u_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}}) \neq f_\alpha - (-1)^\alpha \lambda_h^{\textcolor{blue}{k}, \textcolor{orange}{i}}$$

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## Discretization flux reconstruction

$$\sigma_{\alpha h, \text{disc}}^{k,i} \in \mathbf{H}(\text{div}, \Omega) \quad \left( \nabla \cdot \sigma_{\alpha h, \text{disc}}^{k,i}, 1 \right)_K = \left( f_\alpha - (-1)^\alpha \lambda_h^{k,i} - r_{\alpha h}^{k,i}, 1 \right)_K$$

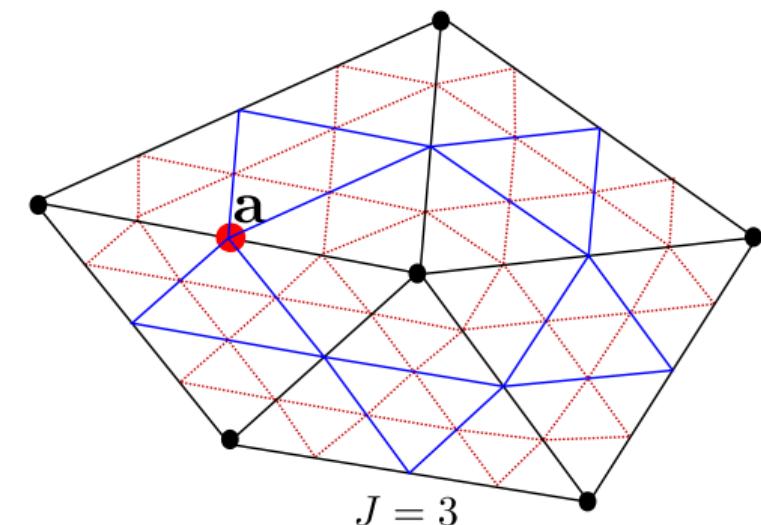
## Discretization flux reconstruction

$$\begin{aligned} \left( \sigma_{\alpha h, \text{disc}}^{\textcolor{blue}{k}, \textcolor{orange}{i}, \textcolor{red}{a}}, \tau_h \right)_{\omega_h^{\textcolor{red}{a}}} - \left( \gamma_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}, \textcolor{red}{a}}, \nabla \cdot \tau_h \right)_{\omega_h^{\textcolor{red}{a}}} &= - \left( \mu_\alpha \psi_{h, \textcolor{red}{a}} \nabla u_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}, \textcolor{red}{a}}, \tau_h \right)_{\omega_h^{\textcolor{red}{a}}} \quad \forall \tau_h \in \mathbf{V}_h^{\textcolor{red}{a}}, \\ \left( \nabla \cdot \sigma_{\alpha h, \text{disc}}^{\textcolor{blue}{k}, \textcolor{orange}{i}, \textcolor{red}{a}}, q_h \right)_{\omega_h^{\textcolor{red}{a}}} &= \left( \tilde{g}_{\alpha h}^{\textcolor{blue}{k}, \textcolor{orange}{i}, \textcolor{red}{a}}, q_h \right)_{\omega_h^{\textcolor{red}{a}}} \quad \forall q_h \in Q_h^{\textcolor{red}{a}}, \end{aligned}$$

$$\mathbf{a} \in \mathcal{V}_h^{\text{int}}$$

$$\mathbf{V}_h^{\mathbf{a}} := \left\{ \boldsymbol{\tau}_h \in \mathbf{RT}_p(\omega_h^{\mathbf{a}}), \boldsymbol{\tau}_h \cdot \mathbf{n}_{\omega_h^{\mathbf{a}}} = 0 \text{ on } \partial\omega_h^{\mathbf{a}} \right\}$$

$$Q_h^a := \mathbb{P}_p^0(\omega_h^a)$$



## Discretization flux reconstruction

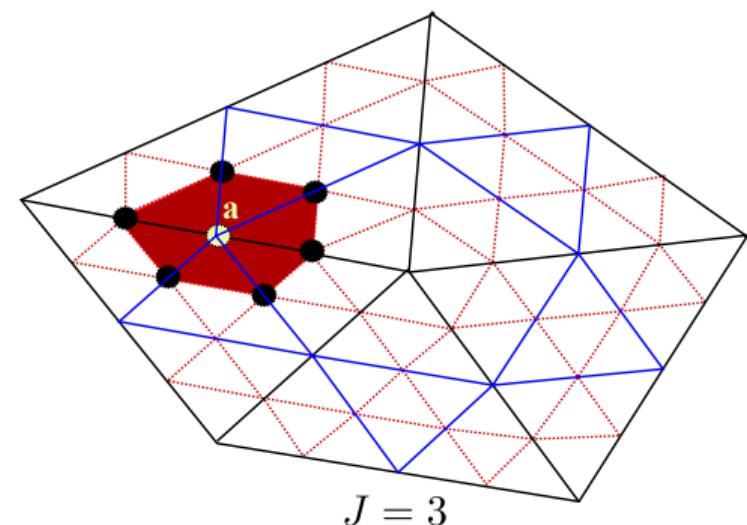
$$\begin{aligned} \left( \sigma_{\alpha h, \text{disc}}^{k, i, a}, \tau_h \right)_{\omega_h^a} - \left( \gamma_{\alpha h}^{k, i, a}, \nabla \cdot \tau_h \right)_{\omega_h^a} &= - \left( \mu_\alpha \psi_{h, a} \nabla u_{\alpha h}^{k, i, a}, \tau_h \right)_{\omega_h^a} \quad \forall \tau_h \in \mathbf{V}_h^a, \\ \left( \nabla \cdot \sigma_{\alpha h, \text{disc}}^{k, i, a}, q_h \right)_{\omega_h^a} &= \left( \tilde{g}_{\alpha h}^{k, i, a}, q_h \right)_{\omega_h^a} \quad \forall q_h \in Q_h^a, \end{aligned}$$

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$$Q_h^a := \mathbb{P}_p^0(\omega_h^a)$$

$$\sigma_{\alpha h, \text{disc}}^{k,i} := \sum_{\mathbf{a} \in \mathcal{V}_h} \sigma_{\alpha h, \text{disc}}^{k,i,\mathbf{a}}$$



# Estimators

## Violations of physical properties of the numerical solution

$$\sigma_{\alpha h}^{k,i} \neq -\nabla u_{\alpha h}^{k,i} \quad \nabla \cdot \left( -\mu_\alpha \nabla u_{\alpha h}^{k,i} \right) \neq f_\alpha - (-1)^\alpha \lambda_h^{k,i}$$

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Flux estimator:

$$\eta_{F,K,\alpha}^{k,i} := \left\| \mu_\alpha^{\frac{1}{2}} \nabla u_{\alpha h}^{k,i} + \mu_\alpha^{-\frac{1}{2}} \boldsymbol{\sigma}_{\alpha h}^{k,i} \right\|_K,$$

Residual estimator:

$$\eta_{R,K,\alpha}^{k,i} := \frac{h_K}{\pi} \mu_\alpha^{-\frac{1}{2}} \left\| f_\alpha - \nabla \cdot \boldsymbol{\sigma}_{\alpha h}^{k,i} - (-1)^\alpha \lambda_h^{k,i} \right\|_K,$$

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## Violations of the complementarity constraints

$$p=1 : (u_{1h}^{k,i} - u_{2h}^{k,i})(\mathbf{a}) \geqslant 0 \quad \lambda_h^{k,i}(\mathbf{a}) \geqslant 0 \quad \lambda_h^{k,i}(\mathbf{a}) \cdot (u_{1h}^{k,i} - u_{2h}^{k,i})(\mathbf{a}) \neq 0 \quad \forall \mathbf{a} \in \mathcal{V}_h^{\text{int}}$$

$$p \geq 2 : (u_{1h}^{k,i} - u_{2h}^{k,i})(\mathbf{x}_l) \not\geq 0 , \quad \left( \lambda_h^{k,i}, \psi_{h,\mathbf{x}_l} \right)_\Omega \not\geq 0 \quad \forall \mathbf{x}_l \in \mathcal{V}_d^{p,\text{int}} \quad \left( \lambda_h^{k,i}, u_{1h}^{k,i} - u_{2h}^{k,i} \right)_\Omega \neq 0$$

## Strategy for constructing the estimators

$$\lambda_h^{k,i} := \lambda_h^{k,i,\text{pos}} + \lambda_h^{k,i,\text{neg}}, \quad \tilde{\mathcal{K}}_{gh}^p := \left\{ (\nu_{1h}, \nu_{2h}) \in X_{gh}^p \times X_{0h}^p, \ \nu_{1h} - \nu_{2h} \geq 0 \right\} \subset \mathcal{K}_g.$$

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Contact estimator:

$$\eta_{C,K}^{k,i,\text{pos}} := 2 \left( \lambda_h^{k,i,\text{pos}}, u_{1h}^{k,i} - u_{2h}^{k,i} \right)_K,$$

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Nonconformity estimator 1:

$$\eta_{\text{nonc},1,K}^{k,i} := \left\| \mathbf{s}_h^{k,i} - \mathbf{u}_h^{k,i} \right\|_K,$$

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$$\eta_{\text{nonc},2,K}^{k,i} := h_\Omega C_{\text{PF}} \left( \frac{1}{\mu_1} + \frac{1}{\mu_2} \right)^{\frac{1}{2}} \left\| \lambda_h^{k,i,\text{neg}} \right\|_K,$$

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$$\lambda_h^{k,i} := \lambda_h^{k,i,\text{pos}} + \lambda_h^{k,i,\text{neg}}, \quad \tilde{\mathcal{K}}_{gh}^p := \left\{ (\nu_{1h}, \nu_{2h}) \in X_{gh}^p \times X_{0h}^p, \quad \nu_{1h} - \nu_{2h} \geq 0 \right\} \subset \mathcal{K}_g.$$

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**Nonconformity estimator 3:**

$$\eta_{\text{nonc},3,K}^{k,i} := 2h_\Omega C_{\text{PF}} \left( \frac{1}{\mu_1} + \frac{1}{\mu_2} \right)^{\frac{1}{2}} \left\| \lambda_h^{k,i,\text{pos}} \right\|_\Omega \left\| \mathbf{s}_h^{k,i} - \mathbf{u}_h^{k,i} \right\|_K.$$

## Theorem (A posteriori error estimate)

$$\|\| \mathbf{u} - \mathbf{u}_h^{k,i} \| \| \leq \left\{ \left( \left( \sum_{K \in \mathcal{T}_h} \sum_{\alpha=1}^2 \left( \eta_{F,K,\alpha}^{k,i} + \eta_{R,K,\alpha}^{k,i} \right)^2 \right)^{\frac{1}{2}} + \eta_{\text{nonc},1}^{k,i} + \eta_{\text{nonc},2}^{k,i} \right)^2 + \eta_{\text{nonc},3}^{k,i} + \sum_{K \in \mathcal{T}_h} \eta_{C,K}^{k,i,\text{pos}} \right\}^{\frac{1}{2}}$$

## Theorem (A posteriori error estimate)

$$\left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\| \leq \left\{ \left( \left( \sum_{K \in \mathcal{T}_h} \sum_{\alpha=1}^2 \left( \eta_{F,K,\alpha}^{k,i} + \eta_{R,K,\alpha}^{k,i} \right)^2 \right)^{\frac{1}{2}} + \eta_{\text{nonc},1}^{k,i} + \eta_{\text{nonc},2}^{k,i} \right)^2 + \eta_{\text{nonc},3}^{k,i} + \sum_{K \in \mathcal{T}_h} \eta_{C,K}^{k,i,\text{pos}} \right\}^{\frac{1}{2}}$$

## Corollary (Distinction of the error components)

$$\left\| \mathbf{u} - \mathbf{u}_h^{k,i} \right\| \leq \eta_{\text{disc}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i}$$

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$$\|\| \mathbf{u} - \mathbf{u}_h^{k,i} \| \| \leq \eta_{\text{disc}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i}$$

## Adaptive algorithm

If  $\eta_{\text{alg}}^{k,i} \leq \gamma_{\text{alg}} \max \left\{ \eta_{\text{disc}}^{k,i}, \eta_{\text{lin}}^{k,i} \right\}$

**Stop linear solver**

If  $\eta_{\text{lin}}^{k,i} \leq \gamma_{\text{lin}} \eta_{\text{disc}}^{n,k,i}$

**Stop nonlinear solver**

## Theorem (A posteriori error estimate)

$$\|\| \mathbf{u} - \mathbf{u}_h^{k,i} \| \| \leq \left\{ \left( \left( \sum_{K \in \mathcal{T}_h} \sum_{\alpha=1}^2 \left( \eta_{F,K,\alpha}^{k,i} + \eta_{R,K,\alpha}^{k,i} \right)^2 \right)^{\frac{1}{2}} + \eta_{\text{nonc},1}^{k,i} + \eta_{\text{nonc},2}^{k,i} \right)^2 + \eta_{\text{nonc},3}^{k,i} + \sum_{K \in \mathcal{T}_h} \eta_{C,K}^{k,i,\text{pos}} \right\}^{\frac{1}{2}}$$

## Corollary (Distinction of the error components)

$$\|\| \mathbf{u} - \mathbf{u}_h^{k,i} \| \| \leq \eta_{\text{disc}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i}$$

## Adaptive algorithm

If  $\eta_{\text{alg}}^{k,i} \leq \gamma_{\text{alg}} \max \left\{ \eta_{\text{disc}}^{k,i}, \eta_{\text{lin}}^{k,i} \right\}$  p=1:

**Stop linear solver**

If  $\eta_{\text{lin}}^{k,i} \leq \gamma_{\text{lin}} \eta_{\text{disc}}^{n,k,i}$

**Stop nonlinear solver**

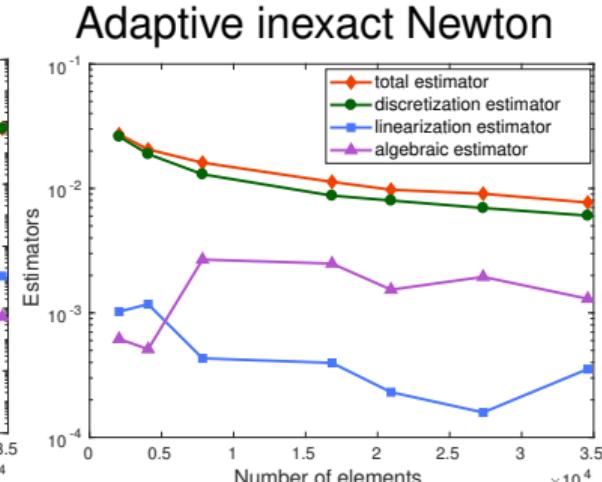
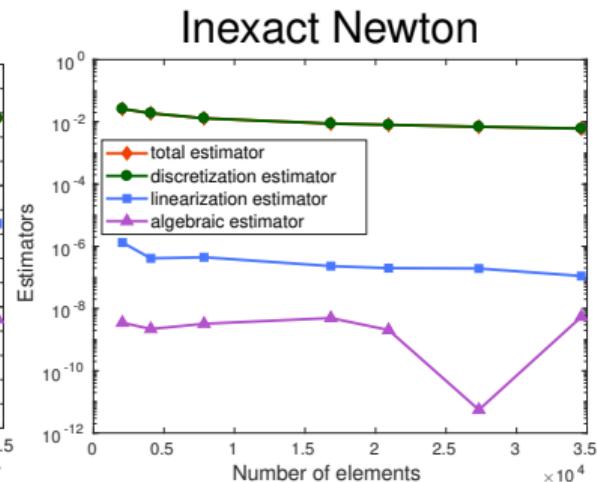
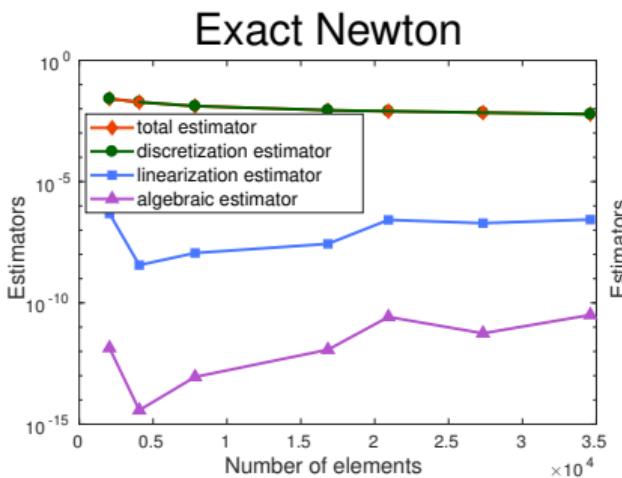
## Local efficiency (shown only for

$$\eta_{\text{disc},K}^{k,i} \lesssim \sum_{\mathbf{a} \in \mathcal{V}_h} \left( \left\| \mu_\alpha^{\frac{1}{2}} \nabla \left( u_\alpha - u_{\alpha h}^{k,i} \right) \right\|_{\omega_h^\mathbf{a}} + \left\| \lambda - \lambda_h^{k,i}(\mathbf{a}) \right\|_{H_*^{-1}(\omega_h^\mathbf{a})} \right)$$

# Numerical experiments

# Numerical experiments

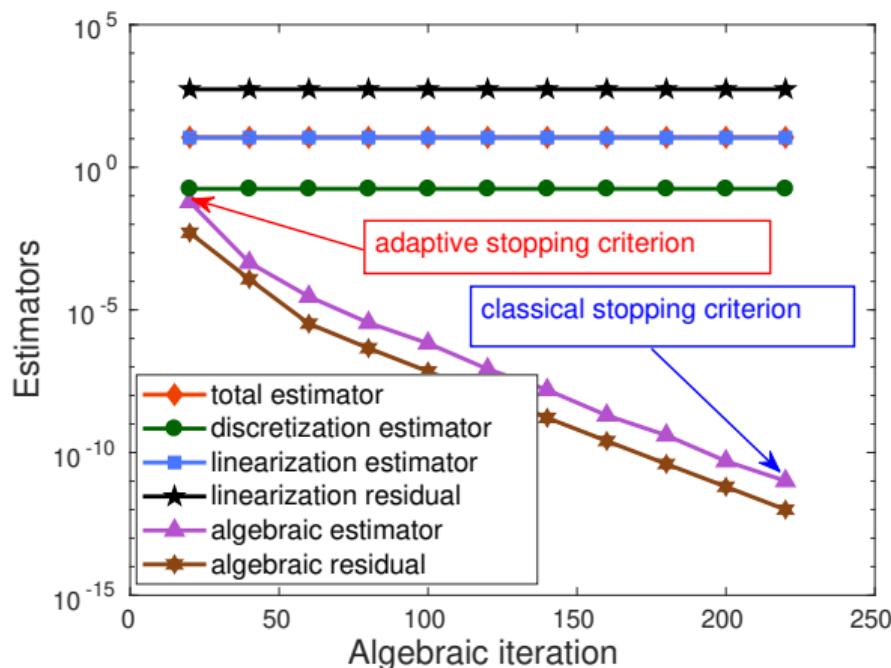
- $\Omega = \text{unit disk}$ ,  $J = 3$ ,  $\mu_1 = \mu_2 = 1$ ,  $g = 0.05$ ,  $\gamma_{\text{lin}} = 0.3$   $\gamma_{\text{alg}} = 0.3$
- semismooth solver: **Newton-min.** Linear solver: **GMRES** with ILU preconditioner.



**Quality and precision are preserved for adaptive inexact semismooth Newton method.**

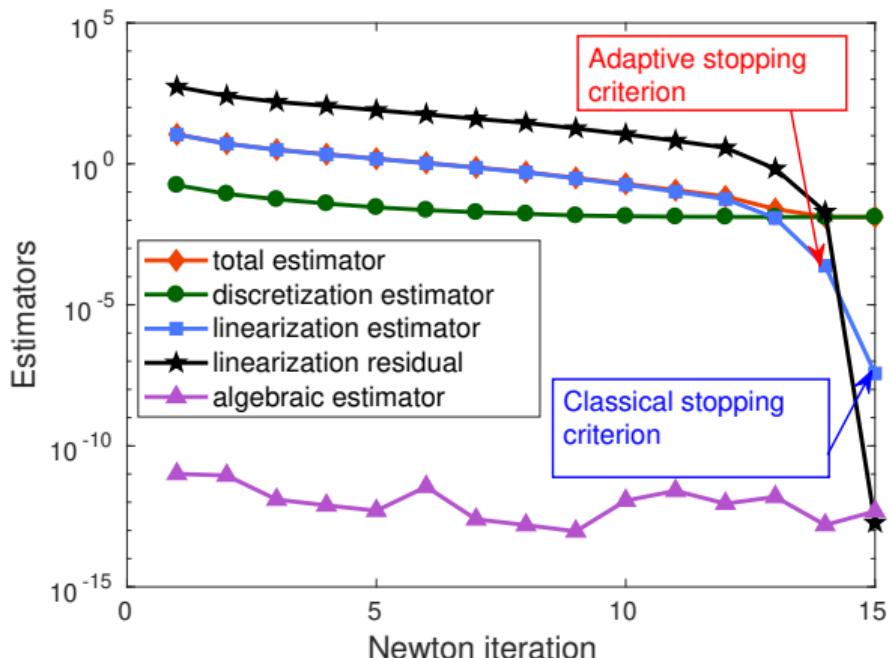
# GMRES adaptivity

Exact/Adapt inexact Newton

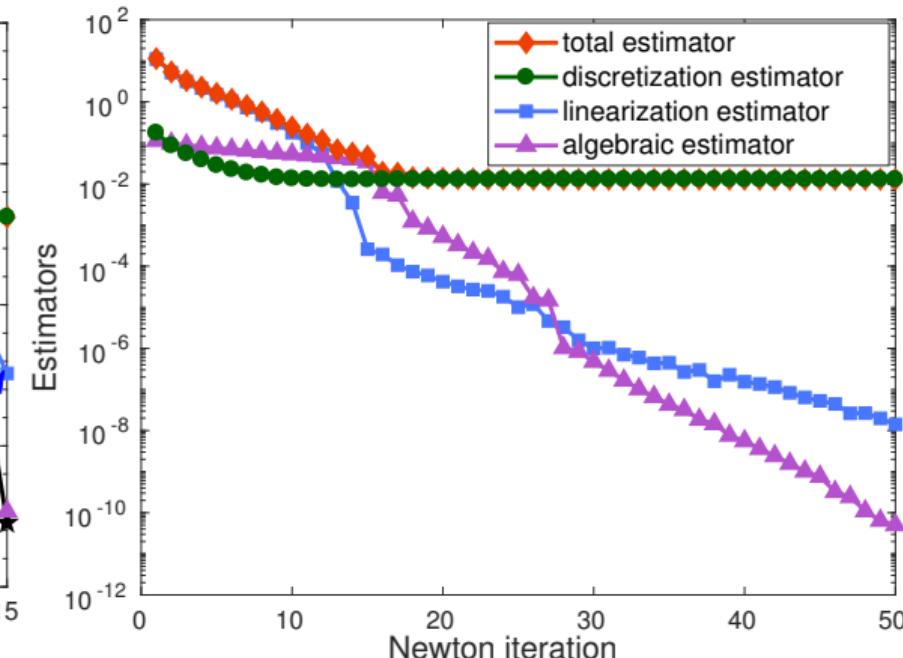


# Newton-min adaptivity

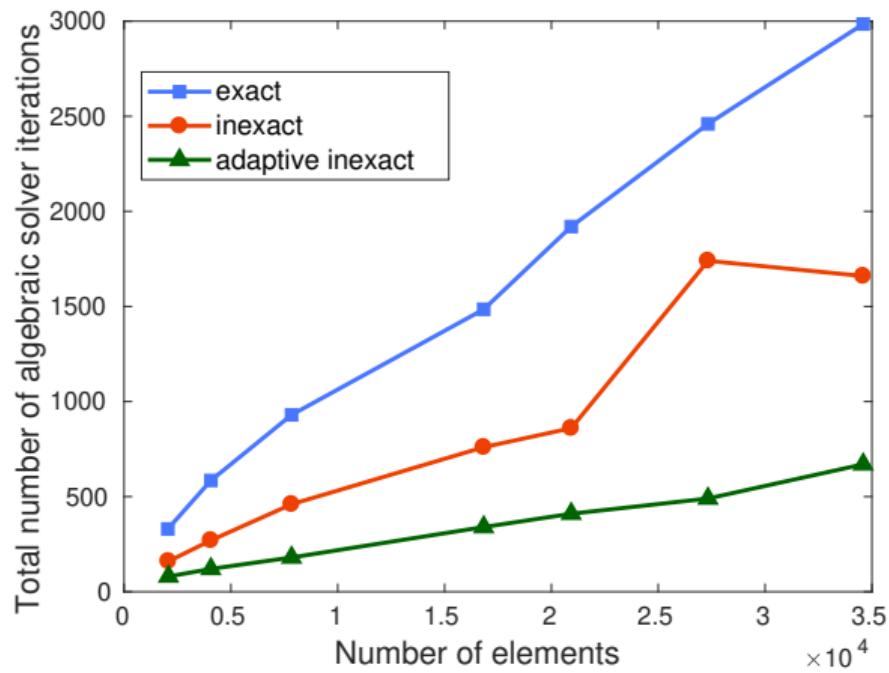
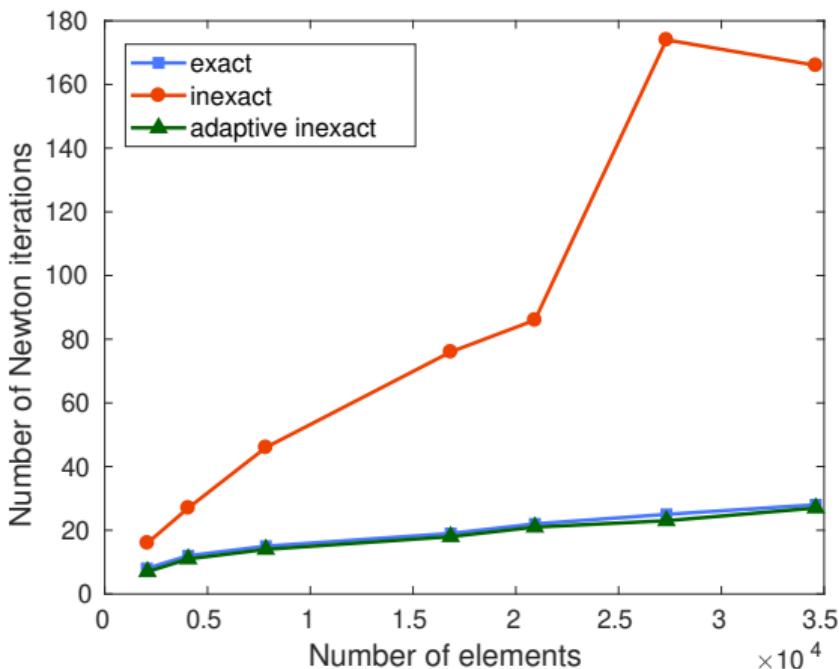
Exact/Adapt inexact Newton



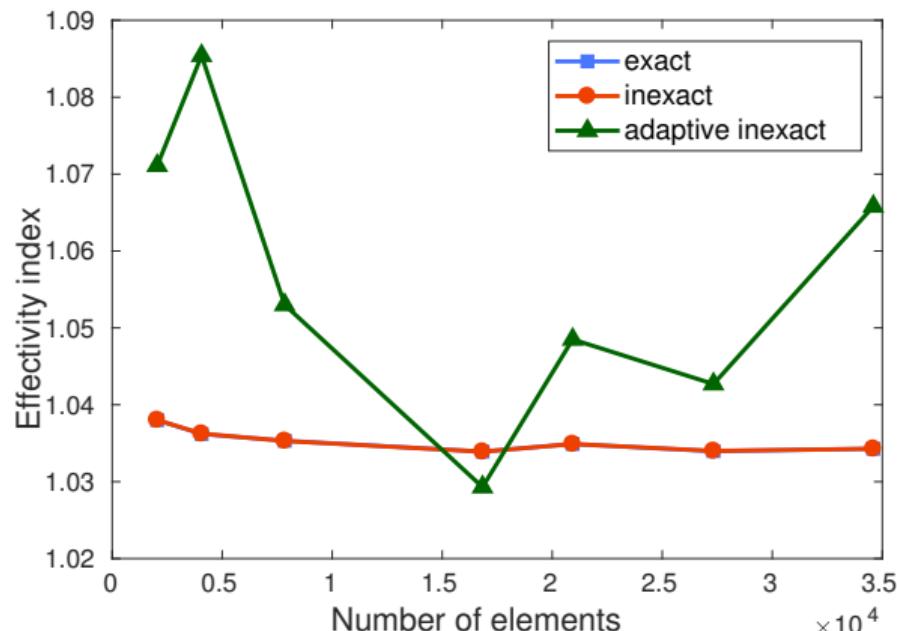
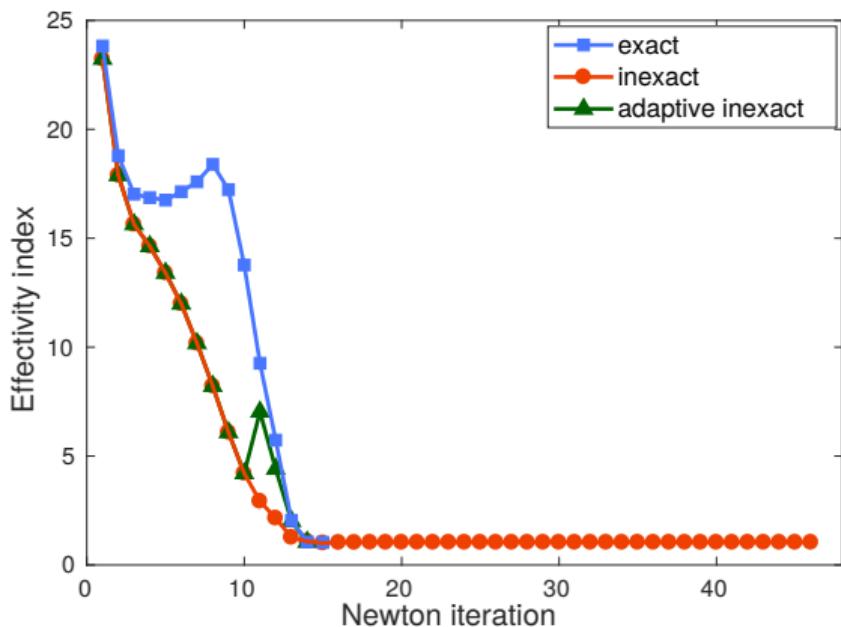
Inexact Newton



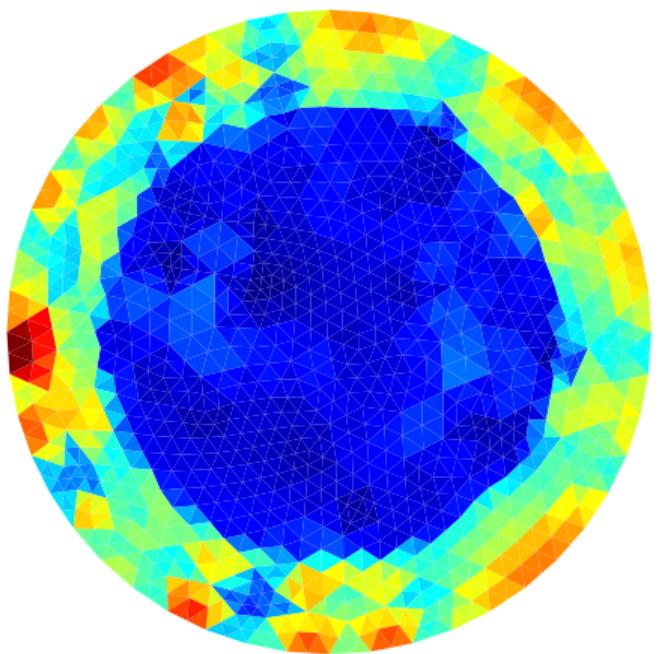
# Overall performance



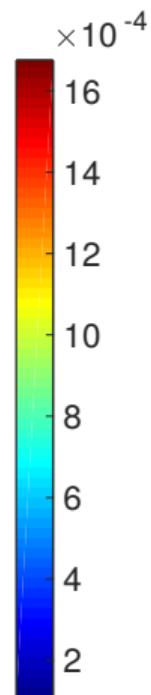
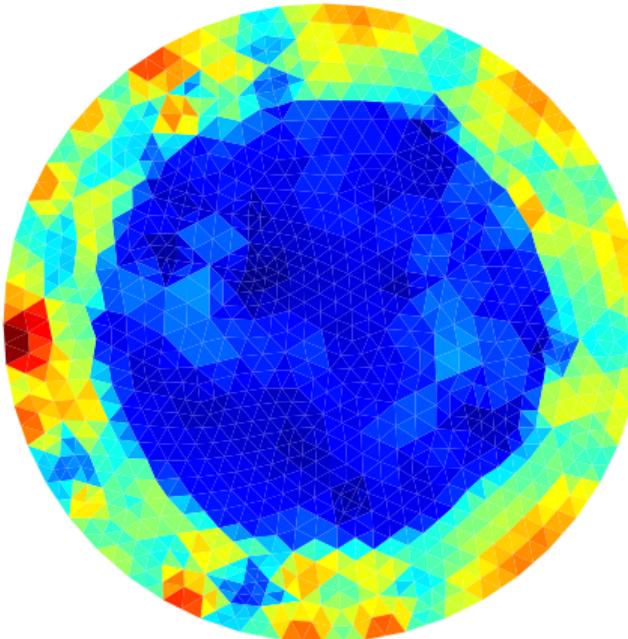
# Effectivity indices



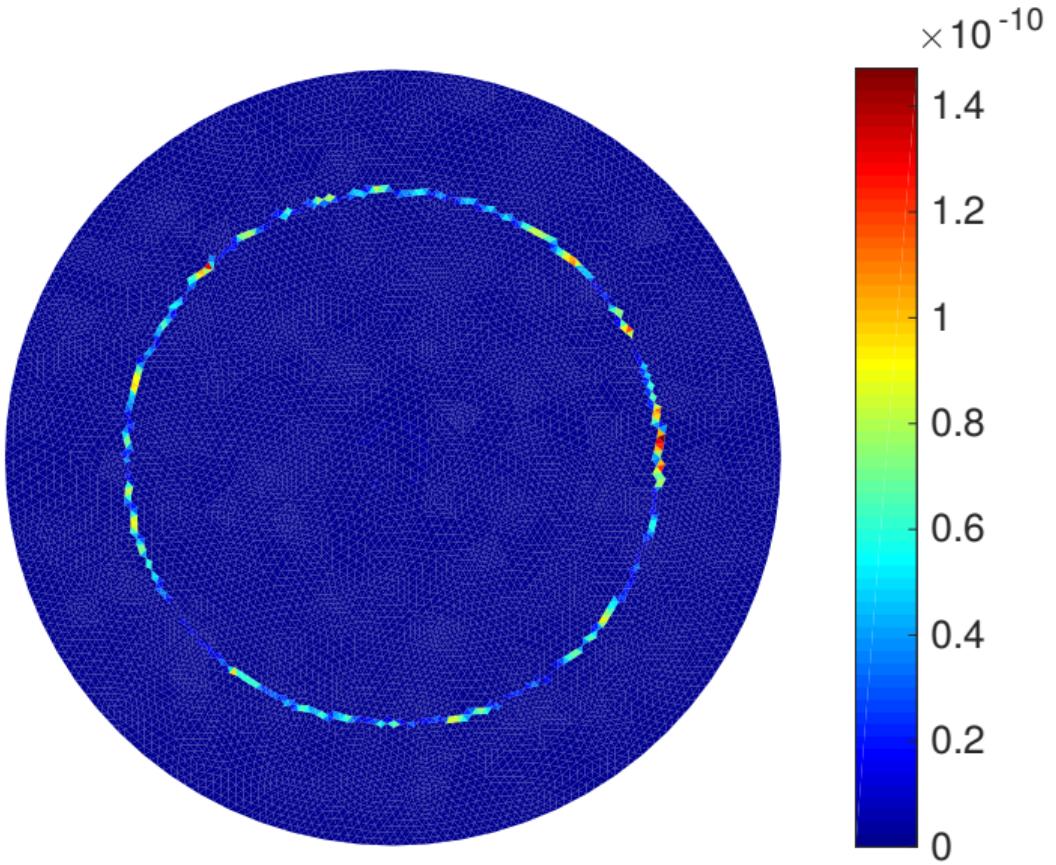
## Local distribution of the error



## Local error estimator



## Contact estimator

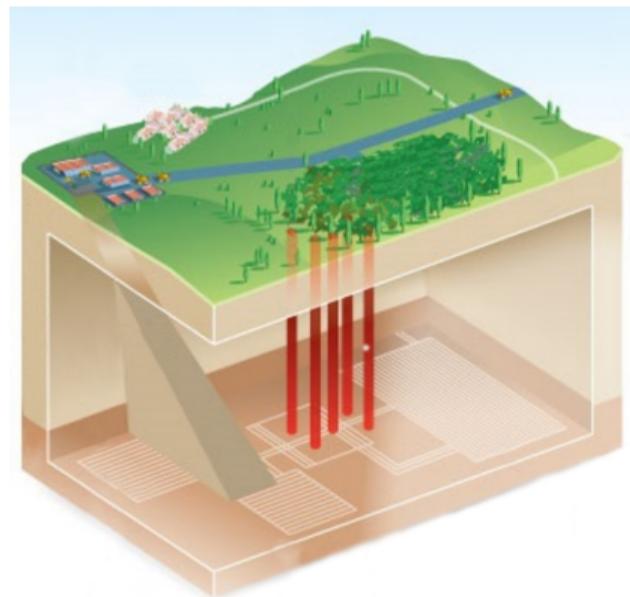
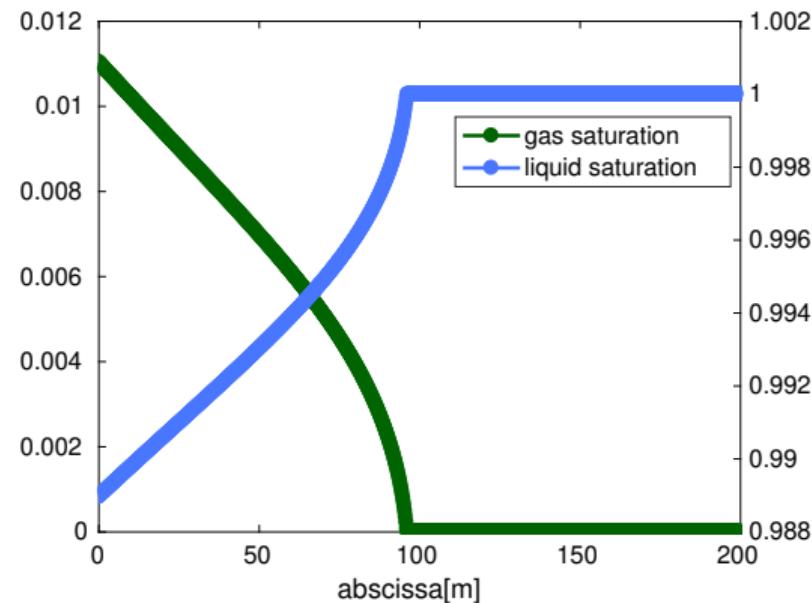


# Outline

- 1 Introduction
- 2 Stationary variational inequality
- 3 Two-phase compositional flow
- 4 Conclusion

# Model problem for the storage of radioactive wastes

$$\begin{cases} \partial_t l_w(\mathbf{S}^l) + \nabla \cdot \Phi_w(\mathbf{S}^l, \mathbf{P}^l, \chi_h^l) = Q_w, \\ \partial_t l_h(\mathbf{S}^l, \mathbf{P}^l, \chi_h^l) + \nabla \cdot \Phi_h(\mathbf{S}^l, \mathbf{P}^l, \chi_h^l) = Q_h, \\ 1 - \mathbf{S}^l \geq 0, \quad H(\mathbf{P}^l + P_{cp}(\mathbf{S}^l)) - \beta_l \chi_h^l \geq 0, \quad (1 - \mathbf{S}^l) \cdot (H(\mathbf{P}^l + P_{cp}(\mathbf{S}^l)) - \beta_l \chi_h^l) = 0 \end{cases}$$



# Discretization by the finite volume method

## Numerical solution:

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

## Discretization of the water equation

$$S_{w,K}^n(\boldsymbol{U}^n) := |K| \partial_t^n l_{w,K} + \sum_{\sigma \in \mathcal{E}_K} F_{w,K,\sigma}(\boldsymbol{U}^n) - |K| Q_{w,K}^n = 0,$$

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## Discretization of the water equation

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

$$S_{c,K}^n(\boldsymbol{U}_h^n) = 0$$

# Discrete complementarity problem and semismoothness

## Discretization of the nonlinear complementarity constraints

$$\mathcal{K}(\mathbf{U}_K^n) := \mathbf{1} - \mathbf{S}_K^n \quad \mathcal{G}(\mathbf{U}_K^n) := \mathbf{H}(\mathbf{P}_K^n + \mathbf{P}_{\text{cp}}(\mathbf{S}_K^n)) - \beta^1 \chi_K^n$$

The discretization reads

$$\mathbf{S}_{c,K}^n(\mathbf{U}_h^n) = 0$$

$$\mathcal{K}(\mathbf{U}_K^n) \geq 0, \quad \mathcal{G}(\mathbf{U}_K^n) \geq 0, \quad \mathcal{K}(\mathbf{U}_K^n) \cdot \mathcal{G}(\mathbf{U}_K^n) = 0$$

- We reformulate the complementarity constraints with C-functions
- We employ inexact semismooth linearization
- Can we estimate each error component?

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# A posteriori error estimates

# Weak solution

**Motivation: Define rigorously the dual norm of the residual**

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

$$X := L^2((0, t_F); H^1(\Omega)), \quad Y := H^1((0, t_F); L^2(\Omega)), \quad Z := L_+^2((0, t_F); L^\infty(\Omega))$$

$$\|\varphi\|_{X_n} := \int_{I_n} \sum_{K \in \mathcal{T}_h} \|\varphi\|_{X,K}^2 dt, \quad \|\varphi\|_{X,K}^2 := \varepsilon h_K^{-2} \|\varphi\|_K^2 + \|\nabla \varphi\|_K^2$$

**Assumption:**

- $1 - S^l \in Z, \quad I_c \in Y, \quad P^l \in X, \quad \chi_h^l \in X, \quad \Phi_c \in L^2((0, t_F); \mathbf{H}(\text{div}, \Omega))$
- $\int_0^{t_F} (\partial_t I_c, \varphi)_\Omega (t) dt - \int_0^{t_F} (\Phi_c, \nabla \varphi)_\Omega (t) dt = \int_0^{t_F} (Q_c, \varphi)_\Omega (t) dt \quad \forall \varphi \in X$
- $\int_0^{t_F} (\lambda - (1 - S^l), H[P^l + P_{cp}(S^l)] - \beta^l \chi_h^l)_\Omega (t) dt \geq 0 \quad \forall \lambda \in Z$
- the initial condition holds

# Weak solution

**Motivation: Define rigorously the dual norm of the residual**

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## Weak solution

**Motivation: Define rigorously the dual norm of the residual**

$$\left\| \mathcal{R}_c(S_{h\tau}^{n,\textcolor{blue}{k},\textcolor{red}{i}}, P_{h\tau}^{n,\textcolor{blue}{k},\textcolor{red}{i}}, \chi_{h\tau}^{n,\textcolor{blue}{k},\textcolor{red}{i}}) \right\|_{X'_n} := \sup_{\substack{\varphi \in X_n \\ \|\varphi\|_{X_n} = 1}} \int_{I_n} \left( Q_c - \partial_t I_{c,h\tau}^{n,\textcolor{blue}{k},\textcolor{red}{i}}, \varphi \right)_\Omega(t) + \left( \Phi_{c,h\tau}^{n,\textcolor{blue}{k},\textcolor{red}{i}}, \nabla \varphi \right)_\Omega(t) dt$$

$$X := L^2((0, t_F); H^1(\Omega)), \quad Y := H^1((0, t_F); L^2(\Omega)), \quad Z := L_+^2((0, t_F); L^\infty(\Omega))$$

$$\|\varphi\|_{X_n} := \int_{I_n} \sum_{K \in \mathcal{T}_h} \|\varphi\|_{X,K}^2 dt, \quad \|\varphi\|_{X,K}^2 := \varepsilon h_K^{-2} \|\varphi\|_K^2 + \|\nabla \varphi\|_K^2$$

## Assumption:

- $1 - \mathcal{S}^l \in Z$ ,  $l_c \in Y$ ,  $P^l \in X$ ,  $\chi_h^l \in X$ ,  $\Phi_c \in L^2((0, t_F); \mathbf{H}(\text{div}, \Omega))$
  - $\int_0^{t_F} (\partial_t l_c, \varphi)_\Omega(t) dt - \int_0^{t_F} (\Phi_c, \nabla \varphi)_\Omega(t) dt = \int_0^{t_F} (Q_c, \varphi)_\Omega(t) dt \quad \forall \varphi \in X$
  - $\int_0^{t_F} (\lambda - (1 - \mathcal{S}^l), H[P^l + P_{cp}(\mathcal{S}^l)] - \beta^l \chi_h^l)_\Omega(t) dt \geq 0 \quad \forall \lambda \in Z$
  - the initial condition holds

# Approximate solution

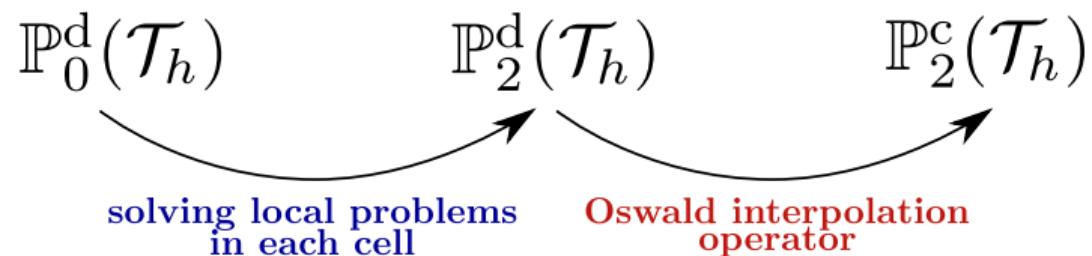
$$S_K^{n,k,i} \in \mathbb{P}_0^d(\mathcal{T}_h) \quad P_K^{n,k,i} \in \mathbb{P}_0^d(\mathcal{T}_h) \quad \chi_K^{n,k,i} \in \mathbb{P}_0^d(\mathcal{T}_h)$$

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

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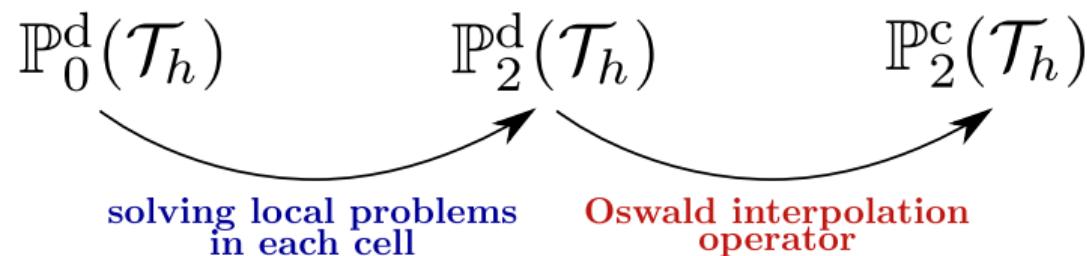
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The discrete liquid pressure and discrete molar fraction do not belong to  $H^1(\Omega)$  **We construct a conforming solution:**



Space-time functions:

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

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

# Error measure

- **Dual norm of the residual for the components**
- Residual for the constraints

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

- Error measure for the nonconformity of the pressure  $\mathcal{N}_P(P_{h\tau}^{n,k,i})$
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$$\mathcal{N}^{n,k,i} := \left\{ \sum_{c \in \mathcal{C}} \left\| \mathcal{R}_c(S_{h\tau}^{n,k,i}, P_{h\tau}^{n,k,i}, \chi_{h\tau}^{n,k,i}) \right\|_{X'_n}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{p \in \mathcal{P}} \mathcal{N}_p^2 + \mathcal{N}_\chi^2 \right\}^{\frac{1}{2}} + \mathcal{R}_e(S_{h\tau}^{n,k,i}, P_{h\tau}^{n,k,i}, \chi_{h\tau}^{n,k,i})$$

## Theorem

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

How do we construct each error estimators?

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How do we construct each error estimators?

## Component flux reconstructions

**The finite volume scheme provides**

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

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Inexact semismooth linearization

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

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Linear perturbation in the accumulation

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

Linearized component flux

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

## Discretization error flux reconstruction:

$$\Theta_{c,h,\text{disc}}^{n,k,i} |_{K \in \mathbf{RT}_0(K)} \quad \left( \Theta_{c,h,\text{disc}}^{n,k,i} \cdot \boldsymbol{n}_K, 1 \right)_\sigma := F_{c,K,\sigma} \left( \boldsymbol{U}^{n,k,i} \right) \quad \forall K \in \mathcal{T}_h$$

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## Linearization error flux reconstruction:

$$\Theta_{c,h,\text{lin}}^{n,k,i}|_K \in \mathbf{RT}_0(K) \quad \left( \Theta_{c,h,\text{lin}}^{n,k,i} \cdot \mathbf{n}_K, 1 \right)_\sigma := \mathcal{F}_{c,K,\sigma}^{n,k,i} - F_{c,K,\sigma}(\mathbf{U}^{n,k,i}) \quad \forall K \in \mathcal{T}_h$$

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## Algebraic error flux reconstruction:

$$\Theta_{c,h,\text{alg}}^{n,k,i,v} := \Theta_{c,h,\text{disc}}^{n,k,i+v} + \Theta_{c,h,\text{lin}}^{n,k,i+v} - \left( \Theta_{c,h,\text{disc}}^{n,k,i} + \Theta_{c,h,\text{lin}}^{n,k,i} \right) \quad \forall K \in \mathcal{T}_h$$

## Discretization error flux reconstruction:

$$\Theta_{c,h,\text{disc}}^{n,k,i}|_K \in \mathbf{RT}_0(K) \quad \left( \Theta_{c,h,\text{disc}}^{n,k,i} \cdot \mathbf{n}_K, 1 \right)_\sigma := F_{c,K,\sigma}(\mathbf{U}^{n,k,i}) \quad \forall K \in \mathcal{T}_h$$

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## Algebraic error flux reconstruction:

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

## Total flux reconstruction:

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

# Error estimators

Violation of physical properties of the approximate solution

$$\partial_t I_c + \nabla \cdot \Theta_{c,h}^{n,k,i,\nu} \neq Q_c \quad \Theta_{c,h}^{n,k,i,\nu} \neq \Phi_{c,h\tau}^{n,k,i}(t^n)$$

Violation of the complementarity constraints

$$1 - S_{h\tau}^{n,k,i} \not\geq 0 \quad H \left[ P_{h\tau}^{n,k,i} + P_{cp} \left( S_{h\tau}^{n,k,i} \right) \right] - \beta^l \chi_{h\tau}^{n,k,i} \not\geq 0$$

Nonconformity of the approximate solution

$$P_{h\tau}^{n,k,i} \notin X \quad \chi_{h\tau}^{n,k,i} \notin X$$

- 1 Discretization estimator
- 2 Linearization estimator
- 3 Algebraic estimator

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- ① Discretization estimator
- ② Linearization estimator
- ③ Algebraic estimator

# Numerical experiments

# Numerical experiments

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

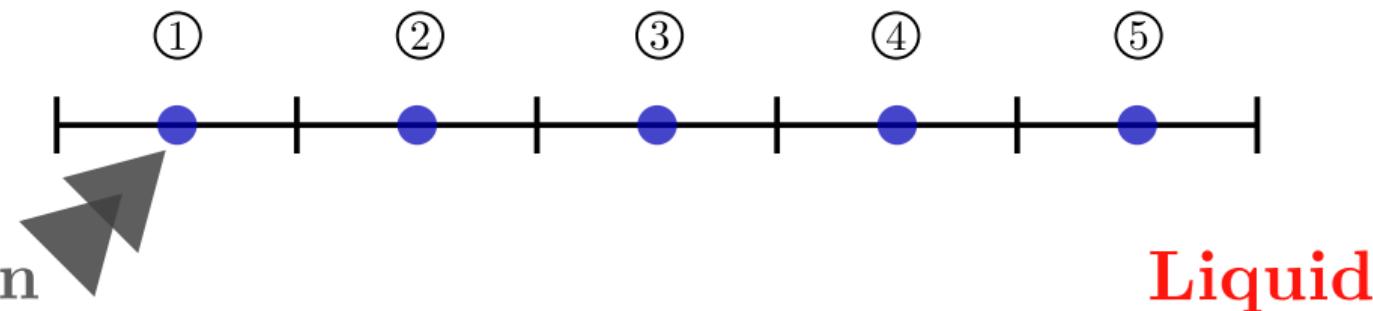
**Semismooth solver:** Newton-min

**Iterative algebraic solver:** GMRES.

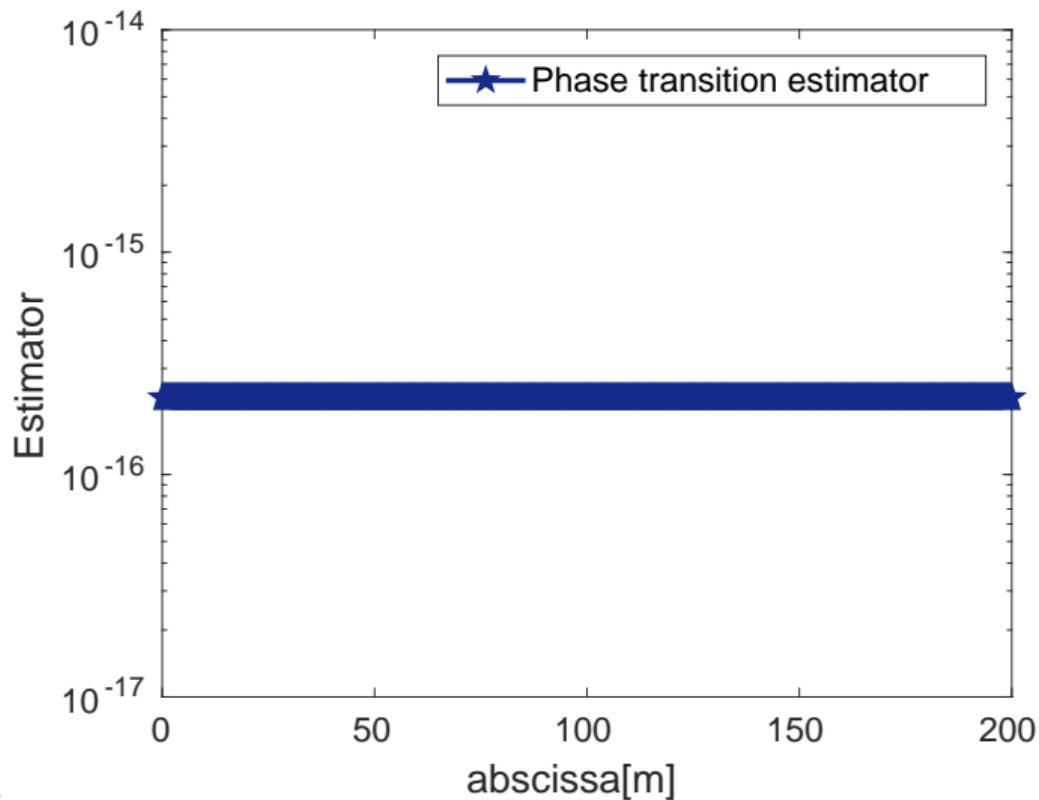
**Time step:**  $\Delta t = 5000$  years,

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

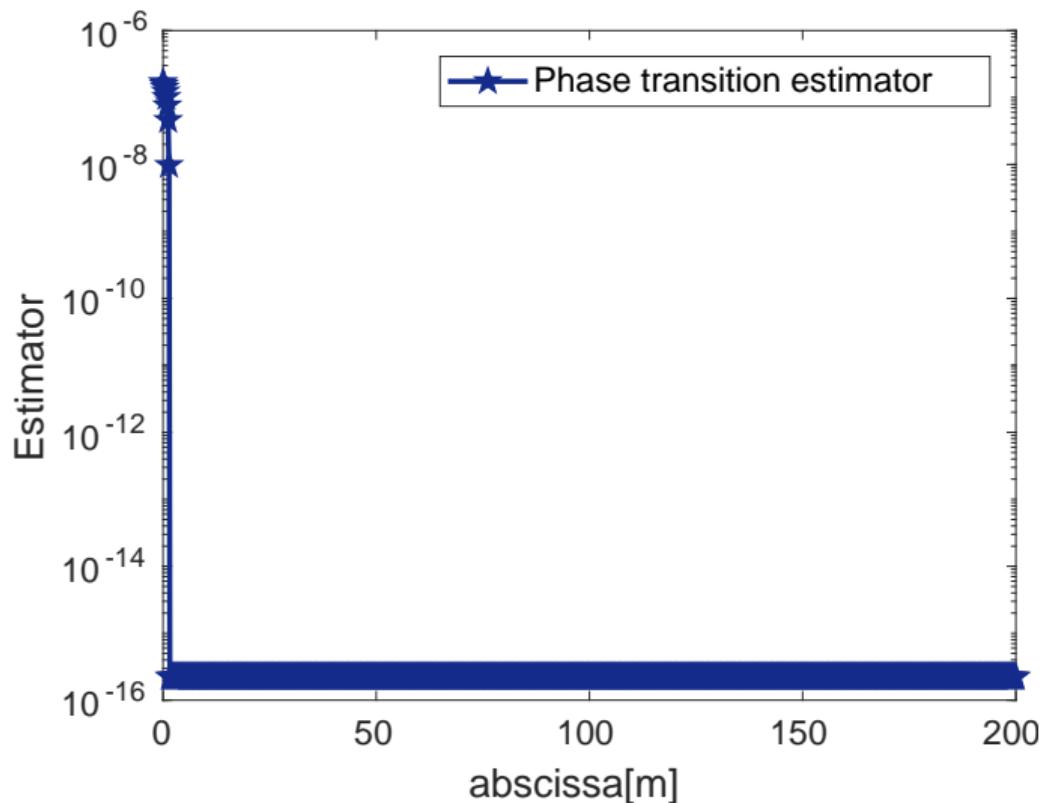
**Final simulation time:**  $t_F = 5 \times 10^5$  years.



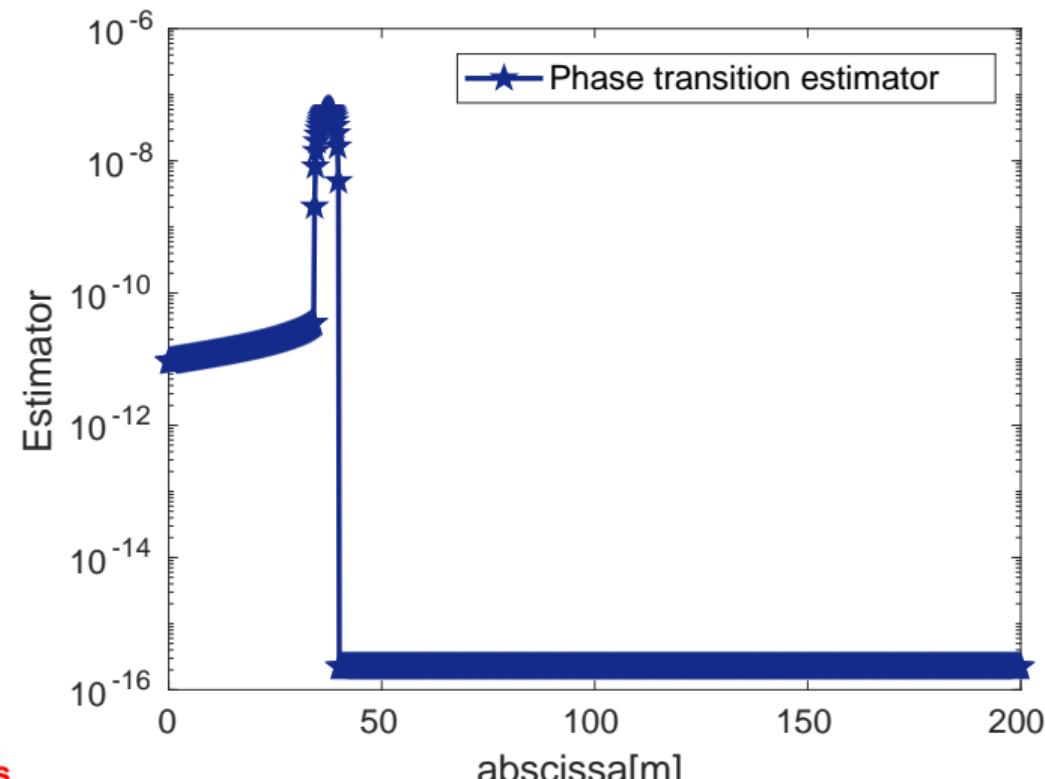
# Phase transition estimator



# Phase transition estimator

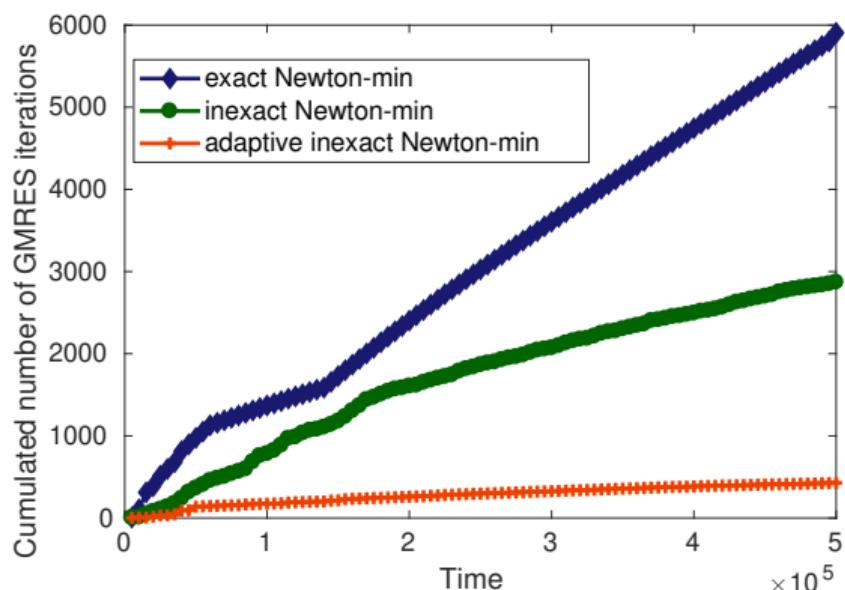
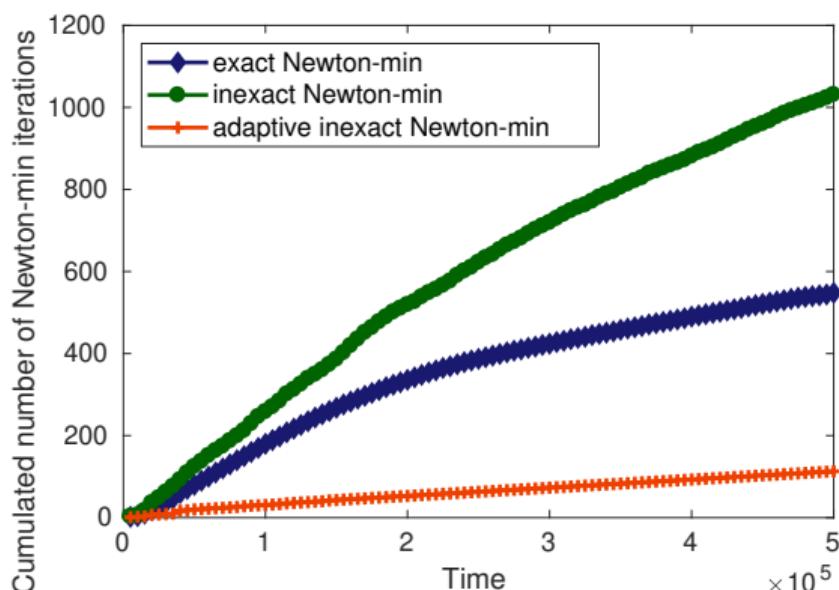


# Phase transition estimator



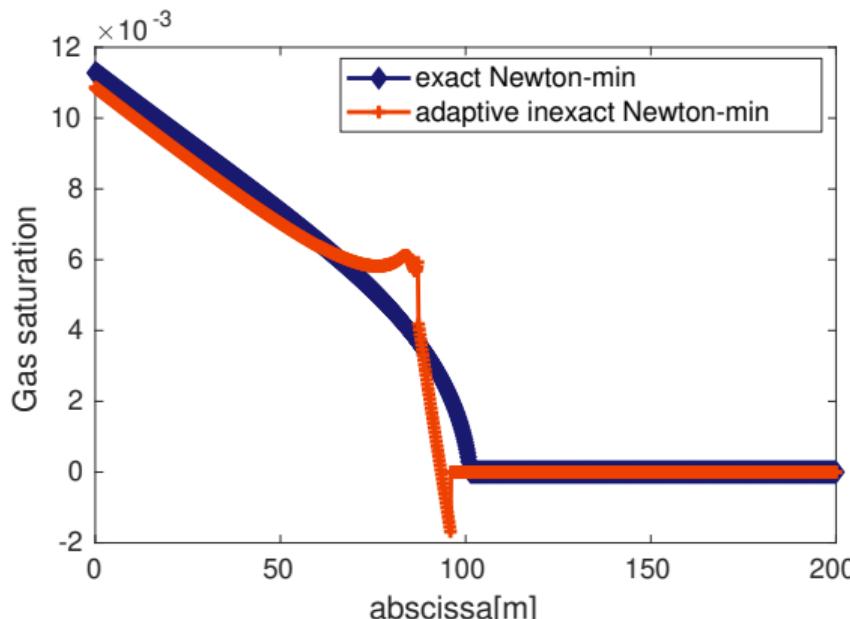
$t = 4.25 \times 10^4$  years

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

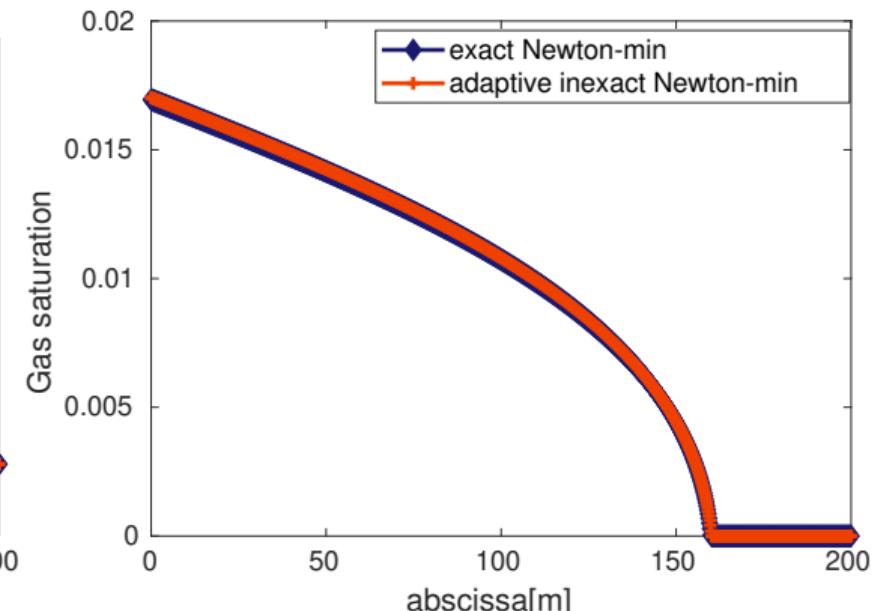


Accuracy  $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

$t = 1.05 \times 10^5$  years



$t = 3.5 \times 10^5$  years



Introduction  
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Stationary variational inequality  
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Two-phase compositional flow  
ooooooooooooooo

Conclusion  
oo

# Outline

1 Introduction

2 Stationary variational inequality

3 Two-phase compositional flow

4 Conclusion

# Conclusion

- Variational inequality: we devised a posteriori error estimates with  $\mathbb{P}_p$  finite elements.
- Two-phase flow with phase transition: a posteriori error estimates for a cell centered finite volume discretization.
- Formulations with complementarity constraints and semismooth algorithms.
- We distinguished the different error components.
- Adaptive stopping criteria  $\Rightarrow$  reduction of the number of iterations.
- Extension of the stationary problem to a parabolic inequality:

J. DABAGHI, V. MARTIN, AND M. VOHRALÍK, *A posteriori error estimate and adaptive stopping criteria for a parabolic variational inequality*. In preparation, 2019

## Implementation

- contact problem between two membranes: MATLAB code. Collaboration with Jan Papež (INRIA Paris).
- Two phase flow: MATLAB code. Collaboration with Ibtihel Ben Ghabria (IFPEN).

# Thank you for your attention