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

A THESIS PRESENTED AT

SORBONNE UNIVERSITY

DOCTORAL SCHOOL MATHEMATICAL SCIENCES OF CENTRAL PARIS (ED 386)

JAD DABAGHI

Thesis advisor: Martin Vohralík

Thesis co-advisor: Vincent Martin

INRIA Paris & Sorbonne University

Paris, June 3rd 2019

Outline

Motivation

Study a simplified mathematical model for the storage of radioactive waste

Potential serious environmental hazard. Need for accurate simulation.

Quantify the error, propose robust algorithms, and save computational time.

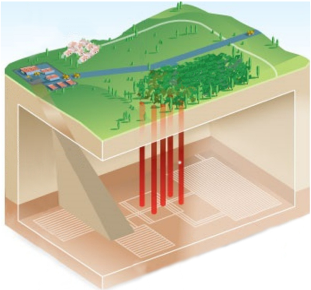
Motivation

Study a simplified mathematical model for the storage of radioactive waste

Potential serious environmental hazard. Need for accurate simulation.

Quantify the error, propose robust algorithms, and save computational time.

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



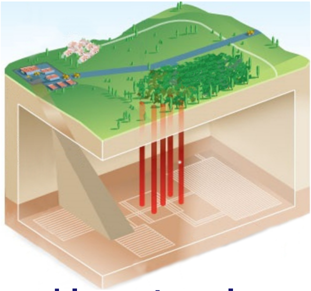
Motivation

Study a simplified mathematical model for the storage of radioactive waste

Potential serious environmental hazard. Need for accurate simulation.

Quantify the error, propose robust algorithms, and save computational time.

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



System of coupled partial differential equations, unsteady problem, strongly nonlinear and degenerate problem, heterogeneous data, phase change: nonlinear complementarity constraints

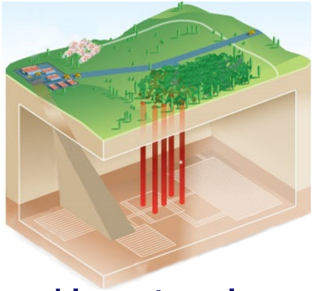
Motivation

Study a simplified mathematical model for the storage of radioactive waste

Potential serious environmental hazard. Need for accurate simulation.

Quantify the error, propose robust algorithms, and save computational time.

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



System of coupled partial differential equations, unsteady problem, strongly nonlinear and degenerate problem, heterogeneous data, phase change: nonlinear complementarity constraints

We study 3 problems of increasing difficulty.

Motivation

Consider the system of PDEs with nonlinear complementarity constraints:

$$\partial_t \left(\varphi(\boldsymbol{u})\right) + \mathcal{A}(\boldsymbol{u}) = \mathcal{F}$$
$$\mathcal{K}(\boldsymbol{u}) \geq 0 \quad \mathcal{G}(\boldsymbol{u}) \geq 0 \quad \mathcal{K}(\boldsymbol{u}) \cdot \mathcal{G}(\boldsymbol{u}) = 0$$

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

Numerical resolution:

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

$$\frac{\varphi(\boldsymbol{u}_h^n) - \varphi(\boldsymbol{u}_h^{n-1})}{t^n - t^{n-1}} + \mathcal{A}(\boldsymbol{u}_h^n) = \mathcal{F}_h^{n-1}$$
$$\mathcal{K}(\boldsymbol{u}_h^n) \geq 0 \quad \mathcal{G}(\boldsymbol{u}_h^n) \geq 0 \quad \mathcal{K}(\boldsymbol{u}_h^n) \cdot \mathcal{G}(\boldsymbol{u}_h^n) = 0$$

- Nonlinear resolution: semismooth Newton algorithm

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

Motivation

Consider the system of PDEs with nonlinear complementarity constraints:

$$\partial_t (\varphi(\boldsymbol{u})) + \mathcal{A}(\boldsymbol{u}) = \mathcal{F}$$
$$\mathcal{K}(\boldsymbol{u}) \geq 0 \quad \mathcal{G}(\boldsymbol{u}) \geq 0 \quad \mathcal{K}(\boldsymbol{u}) \cdot \mathcal{G}(\boldsymbol{u}) = 0$$

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

Numerical resolution:

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

$$\frac{\varphi(\boldsymbol{u}_h^n) - \varphi(\boldsymbol{u}_h^{n-1})}{t^n - t^{n-1}} + \mathcal{A}(\boldsymbol{u}_h^n) = \mathcal{F}_h^{n-1}$$
$$\mathcal{K}(\boldsymbol{u}_h^n) \geq 0 \quad \mathcal{G}(\boldsymbol{u}_h^n) \geq 0 \quad \mathcal{K}(\boldsymbol{u}_h^n) \cdot \mathcal{G}(\boldsymbol{u}_h^n) = 0$$

- Inexact semismooth Newton algorithm

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

Motivation

A posteriori error estimate:

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

Motivation

A posteriori error estimate:

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

Three components of the error:

- discretization error: numerical scheme (finite elements, finite volumes...) (h, τ)
- linearization error: semismooth Newton method (k)
- algebraic error: iterative algebraic solver (i)

Motivation

A posteriori error estimate:

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

Three components of the error:

- discretization error: numerical scheme (finite elements, finite volumes...) (h, τ)
- linearization error: semismooth Newton method (k)
- algebraic error: iterative algebraic solver (i)

Questions:

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

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

Motivation

A posteriori error estimate:

$$\left|\kern-0.25ex\left|\kern-0.25ex\left| \boldsymbol{u} - \boldsymbol{u}_h^{n,k,i} \right|\kern-0.25ex\right|\kern-0.25ex\right| \le \eta(\boldsymbol{u}_h^{n,k,i}) \quad \text{where} \quad |||\cdot||| \quad \text{is some norm}$$

Three components of the error:

- discretization error: numerical scheme (finite elements, finite volumes...) (h, τ)
- linearization error: semismooth Newton method (k)
- algebraic error: iterative algebraic solver (i)

Questions:

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

- $\left|\kern-0.25ex\left|\kern-0.25ex\left| \boldsymbol{u} - \boldsymbol{u}_h^{n,k,i} \right|\kern-0.25ex\right|\kern-0.25ex\right| \le \eta_{\mathrm{disc}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}$

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

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

Chapter 1: Stationary linear variational inequality

$$\text{Find} \quad \boldsymbol{u} \in \mathcal{K}_g \quad a(\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{u}) \geq (\boldsymbol{f}, \boldsymbol{v} - \boldsymbol{u}) \quad \forall \boldsymbol{v} \in \mathcal{K}_g$$

BREZZI HAGGER RAVIART
Error estimates for the finite element solution of variational inequalities. Numer.Math (1977)

AINSWORTH ODEN LEE
Local a posteriori error estimates for variational inequalities Numer.Methods Partial Differential Equations (1993)

KORNHUBER
A posteriori error estimates for elliptic variational inequalities, Comput.Math.Appl (1996)

1975-1995

CHEN NOCHETTO
Residual type a posteriori error estimates for elliptic obstacle problems. Numer.Math (2000)

BRAESS
A posteriori error estimators for obstacle problems-another look- Numer.Math (2005)

VEESER
Efficient and reliable a posteriori error estimators for elliptic obstacle problems. SIAM J. Numer. Anal (2001)

2000-2005

BEN BELGACEM BERNARDI BLOUZA VOHRALIK
On the unilateral contact between two membranes. Part 2. IMA Journal of Numerical Analysis (2012)

CHOULY FABRE HILD POUSIN RENARD
Residual based a posteriori error estimation for contact problems approximated by Nitsche's method IMA J. Numer. Anal (2018)

BURG SCHRODER
A posteriori error control of hp-finite elements for variational inequalities of the first and second kind. Comput. Math.Appl (2015) IMA J. Numer. Anal (2018).

2007-2019

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

Chapter 2: Parabolic linear variational inequality

$$\text{Find} \quad \boldsymbol{u} \in \mathcal{K}_g^{\mathrm{t}} \quad \langle \partial_t \boldsymbol{u}, \boldsymbol{v} - \boldsymbol{u} \rangle + a(\boldsymbol{u}, \boldsymbol{v} - \boldsymbol{u}) \geq (\boldsymbol{f}, \boldsymbol{v} - \boldsymbol{u}) \quad \forall \boldsymbol{v} \in \mathcal{K}_g^{\mathrm{t}}$$

1980-1985

BENSOUSSAN LIONS
Applications of variational inequalities in stochastic control. Studies in Mathematics and its Applications (1982)

GLOWINSKI LIONS TREMOLIERES
Numerical analysis of variational inequalities. Studies in Mathematics and its Applications (1981)

2000-2007

NICAISE SOUALEM
A posteriori error estimates for a nonconforming finite element discretization of the heat equation. M2AN (2005)

MOON NOCHETTO PETERSDORFF ZHANG
A posteriori error analysis for parabolic variational inequalities
ESAIM: Mathematical Modelling and Numerical Analysis (2007)

2007-2019

ACHDOU HECHT POMMIER
A posteriori error estimates for parabolic variational inequalities
J.Sci.Comput (2008)

ERN SMEARS VOHRALIK
Guaranteed, locally space-time efficient, and polynomial-degree robust a posteriori error estimates for high-order discretizations of parabolic problems.
SIAM J. Numer. Anal (2017)

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

Chapter 3: Two-phase compositional flow with phase change

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

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

1980-2000

CHAVENT JAFFRE
Mathematical models and finite elements for reservoir simulation, North Holland (1986)

HELMIG
Multiphase flow and transport processes in the subsurface-A contribution to the modeling of hydrosystems, Springer-Verlag (1997)

2000-2011

GROSS REUSKEN
Numerical methods for two-phase incompressible flows Springer-Verlag (2011)

RIVIERE
Discontinuous Galerkin methods for solving elliptic and parabolic equations, Frontiers in Applied Mathematics SIAM (2008)

LAUSER HAGER HELMIG WOHLMUTH
A new approach for phase transitions in miscible multiphase flow in porous media Advances in Water Ressources (2011)

2012-2019

VOHRALIK WHEELER
A posteriori error estimates, stopping criteria and adaptivity for two-phase flows, Comput. Geosci (2013)

BEN GHARBIA JAFFRE
Gas phase appearance and disappearance as a problem with complementritty constraints math. Comput. Simulation (2014)

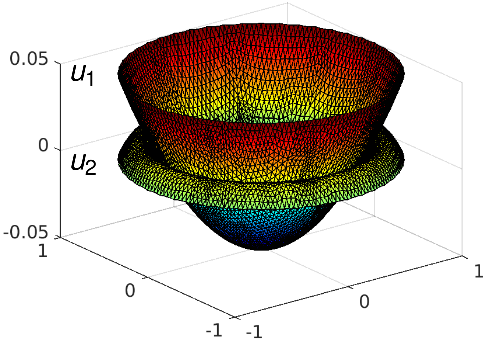
DI PIETRO FLAURAUD VOHRALIK YOUSEF
A posteriori error estimates, stopping criteria, and adaptivity for multiphase compositional Darcy flows in porous media, J. Comput. Phys. (2014)

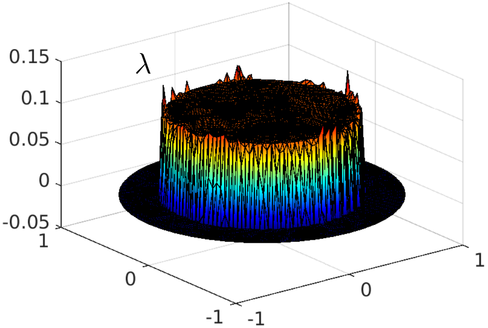
I. BEN GHARBIA, J. DABAGHI, V. MARTIN, AND M. VOHRALÍK, *A posteriori error estimates and adaptive stopping criteria for a compositional two-phase flow with nonlinear complementarity constraints*. HAL Preprint 01919067, In revision, 2019

Outline

Model problem and settings: contact between two membranes

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





Continuous problem

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

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

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

equivalent to

Variational inequality:

- $\mathcal{K}_g = \{(v_1, v_2) \in H_g^1(\Omega) \times H_0^1(\Omega),\ v_1 - v_2 \geq 0 \text{ a.e. in } \Omega\}$ **convex**

Find $\boldsymbol{u} = (u_1, u_2) \in \mathcal{K}_g$ s.t. $\displaystyle\sum_{\alpha=1}^{2} \mu_\alpha (\nabla u_\alpha, \nabla (v_\alpha - u_\alpha))_\Omega \geq \sum_{\alpha=1}^{2} (f_\alpha, v_\alpha - u_\alpha)_\Omega \quad \forall \boldsymbol{v} \in \mathcal{K}_g$ $\quad (\mathrm{R})$

Discretization by finite elements

For any $p \geq 1$

Spaces for the discretization:

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

$$X_{0h}^{p} = \{v_h \in \mathcal{C}^0(\overline{\Omega});\ v_h|_K \in \mathbb{P}_p(K), \ \forall K \in \mathcal{T}_h, \ \ v_h = 0 \ \text{ on } \ \partial\Omega\}$$

$$\mathcal{K}_{gh}^{p} = \left\{(v_{1h}, v_{2h}) \in X_{gh}^{p} \times X_{0h}^{p},\ v_{1h}(\boldsymbol{x}_l) - v_{2h}(\boldsymbol{x}_l) \geq 0 \ \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p}\right\} \not\subset \mathcal{K}_g \quad \forall p \geq 2$$

Discretization by finite elements

For any $p \geq 1$

Spaces for the discretization:

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

$$X_{0h}^p = \left\{ v_h \in \mathcal{C}^0(\overline{\Omega}); \ v_h|_K \in \mathbb{P}_p(K), \ \forall K \in \mathcal{T}_h, \ \ v_h = 0 \ \text{ on } \ \partial\Omega \right\}$$

$$\mathcal{K}_{gh}^p = \left\{ (v_{1h}, v_{2h}) \in X_{gh}^p \times X_{0h}^p, \ v_{1h}(\boldsymbol{x}_l) - v_{2h}(\boldsymbol{x}_l) \geq 0 \ \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^p \right\} \not\subset \mathcal{K}_g \quad \forall p \geq 2$$

Discrete variational inequality: find $\boldsymbol{u}_h = (u_{1h}, u_{2h}) \in \mathcal{K}_{gh}^p$ such that

$$\sum_{\alpha=1}^{2} \mu_\alpha \left(\nabla u_{\alpha h}, \nabla \left(v_{\alpha h} - u_{\alpha h} \right) \right)_\Omega \geq \sum_{\alpha=1}^{2} \left(f_\alpha, v_{\alpha h} - u_{\alpha h} \right)_\Omega \quad \forall \boldsymbol{v}_h = (v_{1h}, v_{2h}) \in \ \mathcal{K}_{gh}^p \qquad \text{(DR)}$$

Well-posed problem (Lions–Stampacchia)

Discretization by finite elements

For any $p \geq 1$

Spaces for the discretization:

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

$$X_{0h}^p = \left\{ v_h \in \mathcal{C}^0(\overline{\Omega}); \ v_h|_K \in \mathbb{P}_p(K), \ \forall K \in \mathcal{T}_h, \ \ v_h = 0 \ \text{ on } \ \partial\Omega \right\}$$

$$\mathcal{K}_{gh}^p = \left\{ (v_{1h}, v_{2h}) \in X_{gh}^p \times X_{0h}^p, \ v_{1h}(\boldsymbol{x}_l) - v_{2h}(\boldsymbol{x}_l) \geq 0 \ \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^p \right\} \not\subset \mathcal{K}_g \quad \forall p \geq 2$$

Discrete variational inequality: find $\boldsymbol{u}_h = (u_{1h}, u_{2h}) \in \mathcal{K}_{gh}^p$ such that

$$\sum_{\alpha=1}^{2} \mu_\alpha \left(\nabla u_{\alpha h}, \nabla \left(v_{\alpha h} - u_{\alpha h} \right) \right)_\Omega \geq \sum_{\alpha=1}^{2} \left(f_\alpha, v_{\alpha h} - u_{\alpha h} \right)_\Omega \quad \forall \boldsymbol{v}_h = (v_{1h}, v_{2h}) \in \ \mathcal{K}_{gh}^p \qquad \text{(DR)}$$

Well-posed problem (Lions–Stampacchia)

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

Saddle point formulation

Recall $\Lambda = \{\chi \in L^2(\Omega),\ \chi \geq 0 \text{ a.e. in } \Omega\}$

$p = 1$: $\Lambda_h^1 := \left\{ v_h \in X_{0h}^1\ v_h(\boldsymbol{a}) \geq 0\ \forall \boldsymbol{a} \in \mathcal{V}_d^{1,\mathrm{int}} \right\} \subset \boldsymbol{\Lambda}$ Ben Belgacem, Bernardi, Blouza, and Vohralík (2012).

$p \geq 2$ **(new)**: $\Lambda_h^p := \left\{ v_h \in X_h^p\ \left(v_h, \psi_{h,\boldsymbol{x}_l}\right)_\Omega \geq 0\ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}\ \left(v_h, \psi_{h,\boldsymbol{x}_l}\right)_\Omega = 0\ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{ext}} \right\} \not\subset \boldsymbol{\Lambda}$

$$\langle w_h, v_h\rangle_h := \sum_{\boldsymbol{a}\in\mathcal{V}_h} w_h(\boldsymbol{a})v_h(\boldsymbol{a}) \left(\psi_{h,\boldsymbol{a}}, 1\right)_{\omega_h^{\boldsymbol{a}}} \quad \text{if} \quad p = 1 \quad \text{and} \quad \langle w_h, v_h\rangle_h := (w_h, v_h)_\Omega \quad \text{if} \quad p \geq 2$$

Saddle point formulation

Recall $\Lambda = \{\chi \in L^2(\Omega),\ \chi \geq 0 \text{ a.e. in } \Omega\}$

$p = 1$**:** $\Lambda_h^1 := \left\{ v_h \in X_{0h}^1\ v_h(\boldsymbol{a}) \geq 0\ \forall \boldsymbol{a} \in \mathcal{V}_d^{1,\mathrm{int}} \right\} \subset \boldsymbol{\Lambda}$ Ben Belgacem, Bernardi, Blouza, and Vohralík (2012).

$p \geq 2$ **(new):** $\Lambda_h^p := \left\{ v_h \in X_h^p\ \left(v_h, \psi_{h,\boldsymbol{x}_l}\right)_\Omega \geq 0\ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}\ \left(v_h, \psi_{h,\boldsymbol{x}_l}\right)_\Omega = 0\ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{ext}} \right\} \not\subset \boldsymbol{\Lambda}$

$$\langle w_h, v_h\rangle_h := \sum_{\boldsymbol{a}\in\mathcal{V}_h} w_h(\boldsymbol{a}) v_h(\boldsymbol{a}) \left(\psi_{h,\boldsymbol{a}}, 1\right)_{\omega_h^{\boldsymbol{a}}} \quad \text{if} \quad p = 1 \quad \text{and} \quad \langle w_h, v_h\rangle_h := (w_h, v_h)_\Omega \quad \text{if} \quad p \geq 2$$

Continuous weak formulation

$$\sum_{\alpha=1}^{2} \mu_\alpha \left(\nabla u_\alpha, \nabla v_\alpha\right)_\Omega - (\lambda, v_1 - v_2)_\Omega = \sum_{\alpha=1}^{2} (f_\alpha, v_\alpha)_\Omega \quad \forall (v_1, v_2) \in \left[H_0^1(\Omega)\right]^2 \qquad (\mathrm{S})$$

$$(\chi - \lambda, u_1 - u_2)_\Omega \geq 0 \quad \forall \chi \in \Lambda$$

Saddle point formulation

Recall $\Lambda = \{\chi \in L^2(\Omega),\ \chi \geq 0 \text{ a.e. in } \Omega\}$

$p = 1$: $\Lambda_h^1 := \left\{ v_h \in X_{0h}^1\ v_h(\boldsymbol{a}) \geq 0\ \forall \boldsymbol{a} \in \mathcal{V}_d^{1,\mathrm{int}} \right\} \subset \boldsymbol{\Lambda}$ Ben Belgacem, Bernardi, Blouza, and Vohralík (2012).

$p \geq 2$ **(new)**: $\Lambda_h^p := \left\{ v_h \in X_h^p\ \left(v_h, \psi_{h,\boldsymbol{x}_l}\right)_\Omega \geq 0\ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}\ \left(v_h, \psi_{h,\boldsymbol{x}_l}\right)_\Omega = 0\ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{ext}} \right\} \not\subset \boldsymbol{\Lambda}$

$$\langle w_h, v_h\rangle_h := \sum_{\boldsymbol{a}\in\mathcal{V}_h} w_h(\boldsymbol{a}) v_h(\boldsymbol{a}) \left(\psi_{h,\boldsymbol{a}}, 1\right)_{\omega_h^{\boldsymbol{a}}} \quad \text{if} \quad p = 1 \quad \text{and} \quad \langle w_h, v_h\rangle_h := (w_h, v_h)_\Omega \quad \text{if} \quad p \geq 2$$

Discrete weak formulation Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{gh}^p \times X_{0h}^p \times \Lambda_h^p$ s.t. $\forall (z_{1h}, z_{2h}) \in [X_{0h}^p]^2$

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

Discrete complementarity problems

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

$$(u_{1h} - u_{2h})(\boldsymbol{x}_l) \geq 0 \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}, \ \langle \lambda_h, \psi_{h,\boldsymbol{x}_l} \rangle_h \geq 0 \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}, \ \langle \lambda_h, u_{1h} - u_{2h} \rangle_h = 0. \quad \text{(DS2)}$$

Discrete complementarity problems

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

$$(u_{1h} - u_{2h})(\boldsymbol{x}_l) \geq 0 \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}, \ \left\langle \lambda_h, \psi_{h,\boldsymbol{x}_l} \right\rangle_h \geq 0 \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}, \ \langle \lambda_h, u_{1h} - u_{2h} \rangle_h = 0. \quad \text{(DS2)}$$

Matrix representation of (DS2)

Discrete complementarity problems

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

$$(u_{1h} - u_{2h})(\boldsymbol{x}_l) \geq 0 \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}, \ \langle \lambda_h, \psi_{h,\boldsymbol{x}_l} \rangle_h \geq 0 \ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}, \ \langle \lambda_h, u_{1h} - u_{2h} \rangle_h = 0. \quad \text{(DS2)}$$

Matrix representation of (DS2)

$p \geq 1$: $$u_{1h} = \sum_{l=1}^{\mathcal{N}_{\mathrm{d}}^{p,\mathrm{int}}} (\boldsymbol{X}_{1h})_l \psi_{h,\boldsymbol{x}_l} + g, \quad u_{2h} = \sum_{l=1}^{\mathcal{N}_{\mathrm{d}}^{p,\mathrm{int}}} (\boldsymbol{X}_{2h})_l \psi_{h,\boldsymbol{x}_l} \quad \lambda_h = \sum_{l=1}^{\mathcal{N}_{\mathrm{d}}^{p,\mathrm{int}}} (\boldsymbol{X}_{3h})_l \Theta_{h,\boldsymbol{x}_l}.$$

$$\mathbb{E}\boldsymbol{X}_h = \boldsymbol{F},$$

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

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

Resolution

C-functions

Definition

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

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

C-functions

Definition

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

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

min function: $(\min\{\boldsymbol{x}, \boldsymbol{y}\})_l := \min\{\boldsymbol{x}_l, \boldsymbol{y}_l\} \qquad l = 1, \dots, m$

C-functions

Definition

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

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

min function: $(\min\{\boldsymbol{x}, \boldsymbol{y}\})_l := \min\{\boldsymbol{x}_l, \boldsymbol{y}_l\} \qquad l = 1, \ldots, m$

Fischer–Burmeister function: $(f_{\mathrm{FB}}(\boldsymbol{x}, \boldsymbol{y}))_l := \sqrt{\boldsymbol{x}_l^2 + \boldsymbol{y}_l^2} - (\boldsymbol{x}_l + \boldsymbol{y}_l) \quad l = 1, \ldots, m$

C-functions

Definition

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

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

min function: $(\min\{\boldsymbol{x}, \boldsymbol{y}\})_l := \min\{\boldsymbol{x}_l, \boldsymbol{y}_l\} \qquad l = 1, \ldots, m$

Fischer–Burmeister function: $(f_{\mathrm{FB}}(\boldsymbol{x}, \boldsymbol{y}))_l := \sqrt{\boldsymbol{x}_l^2 + \boldsymbol{y}_l^2} - (\boldsymbol{x}_l + \boldsymbol{y}_l) \quad l = 1, \ldots, m$

$\boldsymbol{x} = \boldsymbol{X}_{1h} + g\mathbf{1} - \boldsymbol{X}_{2h}$, $\boldsymbol{y} = \boldsymbol{X}_{3h}$ ($m = \mathcal{N}_{\mathrm{d}}^{p,\mathrm{int}}$), $\mathbf{C}(\boldsymbol{X}_h) = \tilde{\mathbf{C}}(\boldsymbol{X}_{1h} + g\mathbf{1} - \boldsymbol{X}_{2h}, \boldsymbol{X}_{3h})$.

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

C-functions

Definition

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

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

min function: $(\min\{\boldsymbol{x}, \boldsymbol{y}\})_l := \min\{\boldsymbol{x}_l, \boldsymbol{y}_l\} \qquad l = 1, \ldots, m$

Fischer–Burmeister function: $(f_{\mathrm{FB}}(\boldsymbol{x}, \boldsymbol{y}))_l := \sqrt{\boldsymbol{x}_l^2 + \boldsymbol{y}_l^2} - (\boldsymbol{x}_l + \boldsymbol{y}_l) \quad l = 1, \ldots, m$

$\boldsymbol{x} = \boldsymbol{X}_{1h} + g\boldsymbol{1} - \boldsymbol{X}_{2h}$, $\boldsymbol{y} = \boldsymbol{X}_{3h}$ ($m = \mathcal{N}_{\mathrm{d}}^{p,\mathrm{int}}$), $\mathbf{C}(\boldsymbol{X}_h) = \tilde{\mathbf{C}}(\boldsymbol{X}_{1h} + g\boldsymbol{1} - \boldsymbol{X}_{2h}, \boldsymbol{X}_{3h})$.

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

The C-function is not Fréchet differentiable.

C-functions

Definition

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

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

min function: $(\min\{\boldsymbol{x}, \boldsymbol{y}\})_l := \min\{\boldsymbol{x}_l, \boldsymbol{y}_l\} \qquad l = 1, \dots, m$

Fischer–Burmeister function: $(f_{\mathrm{FB}}(\boldsymbol{x}, \boldsymbol{y}))_l := \sqrt{\boldsymbol{x}_l^2 + \boldsymbol{y}_l^2} - (\boldsymbol{x}_l + \boldsymbol{y}_l) \quad l = 1, \dots, m$

$\boldsymbol{x} = \boldsymbol{X}_{1h} + g\mathbf{1} - \boldsymbol{X}_{2h}$, $\boldsymbol{y} = \boldsymbol{X}_{3h}$ $(m = \mathcal{N}_{\mathrm{d}}^{p,\mathrm{int}})$, $\mathbf{C}(\boldsymbol{X}_h) = \tilde{\mathbf{C}}(\boldsymbol{X}_{1h} + g\mathbf{1} - \boldsymbol{X}_{2h}, \boldsymbol{X}_{3h})$.

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

The C-function is not Fréchet differentiable.

We will use semismooth Newton algorithms.

Facchinei and Pang (2003), Bonnans, Gilbert, Lemaréchal, and Sagastizábal (2006).

Inexact semismooth Newton method

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

$$\mathbb{A}^{k-1}\boldsymbol{X}_h^k = \boldsymbol{B}^{k-1},$$

where

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

Inexact semismooth Newton method

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

$$\mathbb{A}^{k-1}\boldsymbol{X}_h^k = \boldsymbol{B}^{k-1},$$

where

$$\mathbb{A}^{k-1} := \begin{bmatrix} \mathbb{E} \\ \mathbf{J_C}(\boldsymbol{X}_h^{k-1}) \end{bmatrix}, \qquad \boldsymbol{B}^{k-1} := \begin{bmatrix} \boldsymbol{F} \\ \mathbf{J_C}(\boldsymbol{X}_h^{k-1})\boldsymbol{X}_h^{k-1} - \mathbf{C}(\boldsymbol{X}_h^{k-1}) \end{bmatrix}.$$

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

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

where $\boldsymbol{R}_h^{k,i} \in \mathbb{R}^{3\mathcal{N}_{\mathrm{d}}^{p,\mathrm{int}}}$ is the algebraic residual vector.

Inexact semismooth Newton method

A posteriori error estimates

A posteriori analysis

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

- $\eta_K(\boldsymbol{u}_h^{k,i})$ local estimator depending on the approximate solution
- $\eta^{k,i} \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i}$: identification of the error components
- $\eta_K(\boldsymbol{u}_h^{k,i}) \leq$ local error + $\underbrace{\text{local contact term}}_{\text{typically very small}}$: local efficiency
- adaptive inexact stopping criteria based on the error components

A posteriori analysis

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

- $\eta_K(\boldsymbol{u}_h^{k,i})$ local estimator depending on the approximate solution
- $\eta^{k,i} \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i}$: identification of the error components
- $\eta_K(\boldsymbol{u}_h^{k,i}) \leq$ local error + $\underbrace{\text{local contact term}}_{\text{typically very small}}$: local efficiency
- 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:

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

Component flux reconstruction

Motivation:

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

Flux reconstruction:

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

Component flux reconstruction

Motivation:

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

Flux reconstruction:

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

Decomposition of the flux:

$$\boldsymbol{\sigma}_{\alpha h}^{k,i} = \boldsymbol{\sigma}_{\alpha h,\mathrm{alg}}^{k,i} + \boldsymbol{\sigma}_{\alpha h,\mathrm{disc}}^{k,i}$$

Component flux reconstruction

Motivation:

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

Flux reconstruction:

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

Decomposition of the flux:

$$\boldsymbol{\sigma}_{\alpha h}^{k,i} = \boldsymbol{\sigma}_{\alpha h,\mathrm{alg}}^{k,i} + \boldsymbol{\sigma}_{\alpha h,\mathrm{disc}}^{k,i}$$

Algebraic error flux reconstruction:

$\boldsymbol{\sigma}_{\alpha h,\mathrm{alg}}^{k,i} \in \mathbf{H}(\mathrm{div},\Omega) \quad \nabla\cdot\boldsymbol{\sigma}_{\alpha h,\mathrm{alg}}^{k,i} = r_{\alpha h}^{k,i}$ where $r_{\alpha h}^{k,i}$ is the functional representation of $\boldsymbol{R}_{\alpha h}^{k,i}$

Papež, Rüde, Vohralík and Wohlmuth (2017).

Component flux reconstruction

Motivation:

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

Flux reconstruction:

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

Decomposition of the flux:

$$\boldsymbol{\sigma}_{\alpha h}^{k,i} = \boldsymbol{\sigma}_{\alpha h,\mathrm{alg}}^{k,i} + \boldsymbol{\sigma}_{\alpha h,\mathrm{disc}}^{k,i}$$

Algebraic error flux reconstruction:

$\boldsymbol{\sigma}_{\alpha h,\mathrm{alg}}^{k,i} \in \mathbf{H}(\mathrm{div},\Omega)$ $\quad \nabla\cdot\boldsymbol{\sigma}_{\alpha h,\mathrm{alg}}^{k,i} = r_{\alpha h}^{k,i}$ where $r_{\alpha h}^{k,i}$ is the functional representation of $\boldsymbol{R}_{\alpha h}^{k,i}$

Papež, Rüde, Vohralík and Wohlmuth (2017).

Discretization flux reconstruction:

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

Estimators

Violations of physical properties of the numerical solution

$$\boldsymbol{\sigma}_{\alpha h}^{k,i} \neq -\nabla u_{\alpha h}^{k,i}, \qquad \nabla\cdot\boldsymbol{\sigma}_{\alpha h}^{k,i} \neq f_\alpha - (-1)^\alpha \lambda_h^{k,i}$$

Estimators

Violations of physical properties of the numerical solution

$$\boldsymbol{\sigma}_{\alpha h}^{k,i} \neq -\nabla u_{\alpha h}^{k,i}, \qquad \nabla\cdot\boldsymbol{\sigma}_{\alpha h}^{k,i} \neq f_\alpha - (-1)^\alpha \lambda_h^{k,i}$$

Flux estimator:

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

Residual estimator:

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

Violations of the complementarity constraints

Violations of the complementarity constraints

p = 1: at convergence:

$$(u_{1h}-u_{2h})(\boldsymbol{a}) \geq 0 \Rightarrow \boldsymbol{u}_h \in \mathcal{K}_g,\ \lambda_h(\boldsymbol{a}) \geq 0 \Rightarrow \lambda_h \in \Lambda,\ \lambda_h(\boldsymbol{a})\cdot(u_{1h}-u_{2h})(\boldsymbol{a}) = 0 \not\Rightarrow \lambda_h\cdot(u_{1h}-u_{2h}) = 0$$

Violations of the complementarity constraints

p = 1: at convergence:

$$(u_{1h}-u_{2h})(\boldsymbol{a})\geq 0 \Rightarrow \boldsymbol{u}_h\in\mathcal{K}_g,\ \lambda_h(\boldsymbol{a})\geq 0\Rightarrow\lambda_h\in\Lambda,\ \lambda_h(\boldsymbol{a})\cdot(u_{1h}-u_{2h})(\boldsymbol{a})=0\not\Rightarrow\lambda_h\cdot(u_{1h}-u_{2h})=0$$

p = 1: at each inexact semismooth step:

$$(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\not\geq 0 \quad \lambda_h^{k,i}(\boldsymbol{a})\not\geq 0 \quad \lambda_h^{k,i}(\boldsymbol{a})\cdot(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\neq 0 \quad \forall\boldsymbol{a}\in\mathcal{V}_h^{\mathrm{int}}$$

Violations of the complementarity constraints

p = 1: **at convergence:**

$$(u_{1h}-u_{2h})(\boldsymbol{a})\geq 0\Rightarrow \boldsymbol{u}_h\in\mathcal{K}_g,\ \lambda_h(\boldsymbol{a})\geq 0\Rightarrow\lambda_h\in\Lambda,\ \lambda_h(\boldsymbol{a})\cdot(u_{1h}-u_{2h})(\boldsymbol{a})=0\not\Rightarrow\lambda_h\cdot(u_{1h}-u_{2h})=0$$

p = 1: **at each inexact semismooth step:**

$$(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\not\geq 0\quad \lambda_h^{k,i}(\boldsymbol{a})\not\geq 0\quad \lambda_h^{k,i}(\boldsymbol{a})\cdot(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\neq 0\quad \forall \boldsymbol{a}\in\mathcal{V}_h^{\text{int}}$$

$p\geq 2$: **at convergence:**

$$(u_{1h}-u_{2h})(\boldsymbol{x}_l)\geq 0\not\Rightarrow \boldsymbol{u}_h\in\mathcal{K}_g\ ,\ \left(\lambda_h,\psi_{h,\boldsymbol{x}_l}\right)_\Omega\geq 0\not\Rightarrow\lambda_h\in\Lambda$$

$$(\lambda_h, u_{1h}-u_{2h})_\Omega=0\not\Rightarrow\lambda_h\cdot(u_{1h}-u_{2h})=0$$

Violations of the complementarity constraints

p = 1: **at convergence:**

$$(u_{1h}-u_{2h})(\boldsymbol{a})\geq 0 \Rightarrow \boldsymbol{u}_h\in\mathcal{K}_g,\ \lambda_h(\boldsymbol{a})\geq 0\Rightarrow\lambda_h\in\Lambda,\ \lambda_h(\boldsymbol{a})\cdot(u_{1h}-u_{2h})(\boldsymbol{a})=0 \not\Rightarrow \lambda_h\cdot(u_{1h}-u_{2h})=0$$

p = 1: **at each inexact semismooth step:**

$$(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\ngeq 0 \quad \lambda_h^{k,i}(\boldsymbol{a})\ngeq 0 \quad \lambda_h^{k,i}(\boldsymbol{a})\cdot(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\neq 0 \quad \forall \boldsymbol{a}\in\mathcal{V}_h^{\mathrm{int}}$$

$p \geq 2$: **at convergence:**

$$(u_{1h}-u_{2h})(\boldsymbol{x}_l)\geq 0 \not\Rightarrow \boldsymbol{u}_h\in\mathcal{K}_g\ ,\ \left(\lambda_h,\psi_{h,\boldsymbol{x}_l}\right)_\Omega\geq 0 \not\Rightarrow \lambda_h\in\Lambda$$

$$(\lambda_h,u_{1h}-u_{2h})_\Omega=0 \not\Rightarrow \lambda_h\cdot(u_{1h}-u_{2h})=0$$

$p \geq 2$: **at each inexact semismooth step:**

$$(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{x}_l)\ngeq 0\ ,\ \left(\lambda_h^{k,i},\psi_{h,\boldsymbol{x}_l}\right)_\Omega\ngeq 0\ \forall\boldsymbol{x}_l\in\mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}\ \left(\lambda_h^{k,i},u_{1h}^{k,i}-u_{2h}^{k,i}\right)_\Omega\neq 0$$

Violations of the complementarity constraints

p = 1: **at convergence:**

$$(u_{1h}-u_{2h})(\boldsymbol{a})\geq 0\Rightarrow \boldsymbol{u}_h\in\mathcal{K}_g,\ \lambda_h(\boldsymbol{a})\geq 0\Rightarrow\lambda_h\in\Lambda,\ \lambda_h(\boldsymbol{a})\cdot(u_{1h}-u_{2h})(\boldsymbol{a})=0\not\Rightarrow\lambda_h\cdot(u_{1h}-u_{2h})=0$$

p = 1: **at each inexact semismooth step:**

$$(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\ngeq 0 \quad \lambda_h^{k,i}(\boldsymbol{a})\ngeq 0 \quad \lambda_h^{k,i}(\boldsymbol{a})\cdot(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{a})\neq 0 \quad \forall \boldsymbol{a}\in\mathcal{V}_h^{\mathrm{int}}$$

$p\geq 2$: **at convergence:**

$$(u_{1h}-u_{2h})(\boldsymbol{x}_l)\geq 0\not\Rightarrow \boldsymbol{u}_h\in\mathcal{K}_g\ ,\ \left(\lambda_h,\psi_{h,\boldsymbol{x}_l}\right)_\Omega\geq 0\not\Rightarrow\lambda_h\in\Lambda$$

$$(\lambda_h,u_{1h}-u_{2h})_\Omega=0\not\Rightarrow\lambda_h\cdot(u_{1h}-u_{2h})=0$$

$p\geq 2$: **at each inexact semismooth step:**

$$(u_{1h}^{k,i}-u_{2h}^{k,i})(\boldsymbol{x}_l)\ngeq 0\ ,\ \left(\lambda_h^{k,i},\psi_{h,\boldsymbol{x}_l}\right)_\Omega\ngeq 0\ \forall\boldsymbol{x}_l\in\mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}}\ \left(\lambda_h^{k,i},u_{1h}^{k,i}-u_{2h}^{k,i}\right)_\Omega\neq 0$$

Contact estimator:

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

Violations of the complementarity constraints

p = 1: **at convergence:**

$$(u_{1h}-u_{2h})(\boldsymbol{a}) \geq 0 \Rightarrow \boldsymbol{u}_h \in \mathcal{K}_g,\ \lambda_h(\boldsymbol{a}) \geq 0 \Rightarrow \lambda_h \in \Lambda,\ \lambda_h(\boldsymbol{a})\cdot(u_{1h}-u_{2h})(\boldsymbol{a}) = 0 \not\Rightarrow \lambda_h\cdot(u_{1h}-u_{2h}) = 0$$

p = 1: **at each inexact semismooth step:**

$$(u_{1h}^{k,i} - u_{2h}^{k,i})(\boldsymbol{a}) \ngeq 0 \quad \lambda_h^{k,i}(\boldsymbol{a}) \ngeq 0 \quad \lambda_h^{k,i}(\boldsymbol{a}) \cdot (u_{1h}^{k,i} - u_{2h}^{k,i})(\boldsymbol{a}) \neq 0 \quad \forall \boldsymbol{a} \in \mathcal{V}_h^{\mathrm{int}}$$

$p \geq 2$: **at convergence:**

$$(u_{1h} - u_{2h})(\boldsymbol{x}_l) \geq 0 \not\Rightarrow \boldsymbol{u}_h \in \mathcal{K}_g\ ,\ (\lambda_h, \psi_{h,\boldsymbol{x}_l})_\Omega \geq 0 \not\Rightarrow \lambda_h \in \Lambda$$

$$(\lambda_h, u_{1h} - u_{2h})_\Omega = 0 \not\Rightarrow \lambda_h \cdot (u_{1h} - u_{2h}) = 0$$

$p \geq 2$: **at each inexact semismooth step:**

$$(u_{1h}^{k,i} - u_{2h}^{k,i})(\boldsymbol{x}_l) \ngeq 0\ ,\ \left(\lambda_h^{k,i}, \psi_{h,\boldsymbol{x}_l}\right)_\Omega \ngeq 0\ \forall \boldsymbol{x}_l \in \mathcal{V}_{\mathrm{d}}^{p,\mathrm{int}} \quad \left(\lambda_h^{k,i}, u_{1h}^{k,i} - u_{2h}^{k,i}\right)_\Omega \neq 0$$

Contact estimator:

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

Nonconformity estimators: We construct $\widetilde{\mathcal{K}}_{gh}^{p} \subset \mathcal{K}_g$, $\lambda_h^{k,i} = \lambda_h^{k,i,\mathrm{pos}} + \lambda_h^{k,i,\mathrm{neg}} \Rightarrow$ 3 estimators.

Theorem (A posteriori error estimate)

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

Theorem (A posteriori error estimate)

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

Corollary (Distinction of the error components)

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

Theorem (A posteriori error estimate)

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

Corollary (Distinction of the error components)

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

Adaptive algorithm

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

Stop linear solver

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

Stop nonlinear solver

Theorem (A posteriori error estimate)

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

Corollary (Distinction of the error components)

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

Adaptive algorithm

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

Stop linear solver

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

Stop nonlinear solver

Theorem (Local efficiency under adaptive stopping criteria : p=1)

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

$$+ \text{contact term}$$

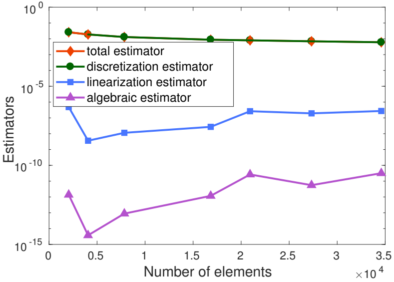
Numerical experiments

Numerical experiments

- semismooth solver: Newton-min. Linear solver: GMRES with ILU preconditionner.

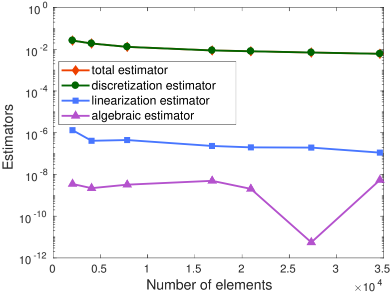
Exact Newton

$\left(\left\|\boldsymbol{R}^{k,i}_{\mathrm{rel,alg}}\right\| \leq 10^{-12}, \left\|\boldsymbol{R}^{k,i}_{\mathrm{rel,lin}}\right\| \leq 10^{-10}\right)$



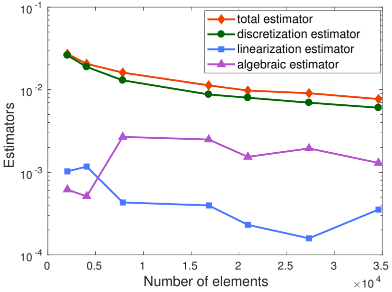
Inexact Newton

$\left(\left\|\boldsymbol{R}^{k,i}_{\mathrm{rel,alg}}\right\| \leq \left\|\boldsymbol{R}^{k,i}_{\mathrm{rel,lin}}\right\|, \left\|\boldsymbol{R}^{k,i}_{\mathrm{rel,lin}}\right\| \leq 10^{-10}\right)$



Adaptive Inexact Newton

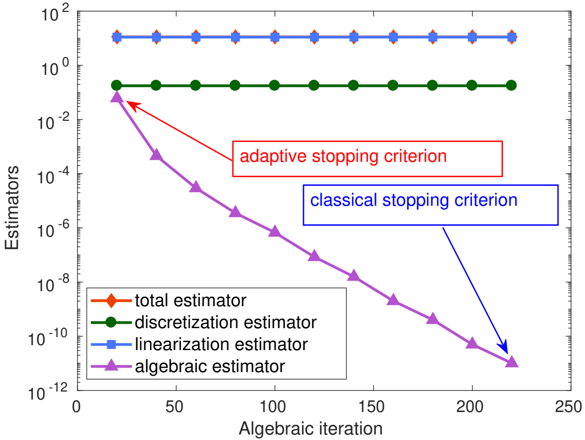
$(\gamma_{\mathrm{lin}} = 10^{-1}, \gamma_{\mathrm{alg}} = 10^{-1})$

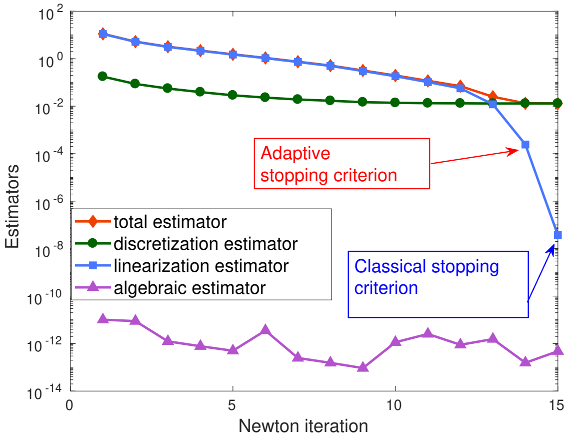


Precision is preserved for adaptive inexact semismooth Newton method.

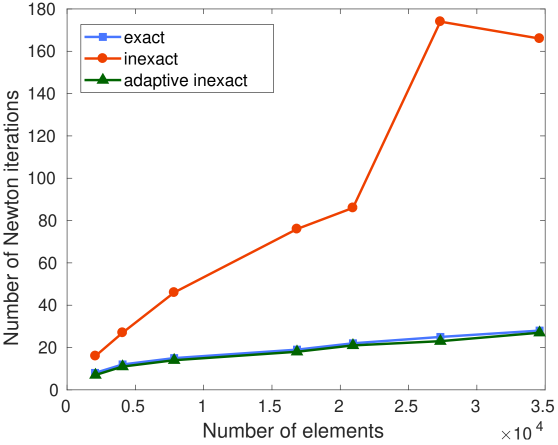
Adaptivity

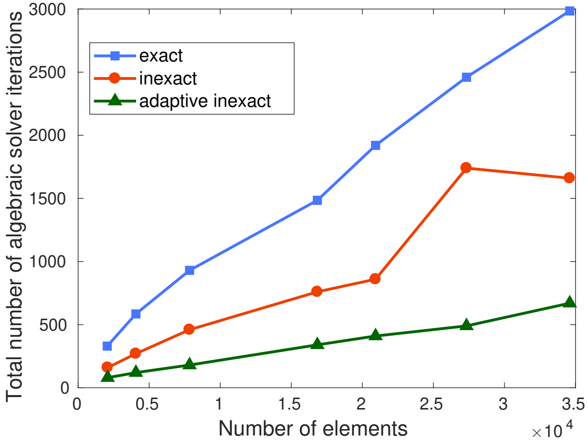
Exact Newton/Adaptive inexact Newton



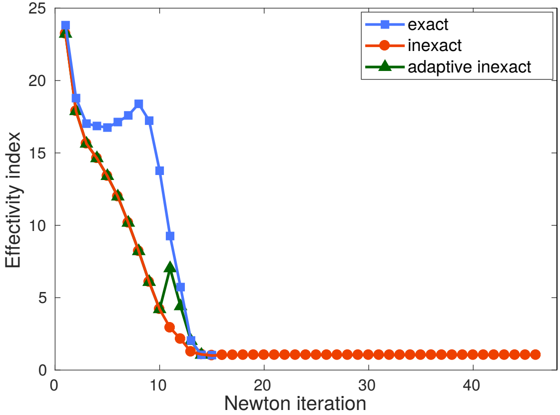


Overall performance

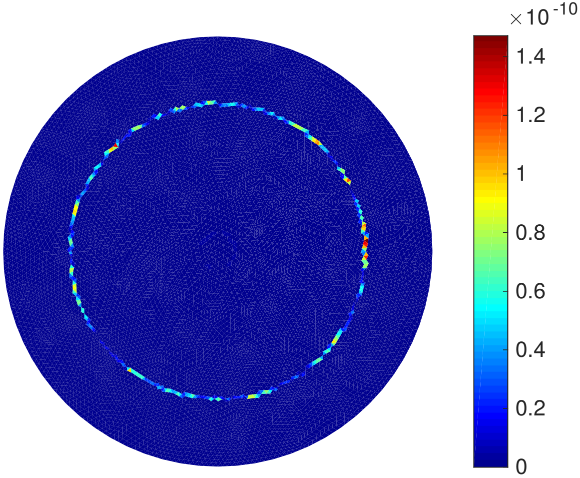




Effectivity indices: $\mathrm{I}_{\mathrm{eff}} := \dfrac{\eta^{k,i}}{\left|\!\left|\!\left| \boldsymbol{u} - \boldsymbol{u}_h^{k,i} \right|\!\right|\!\right|_{\Omega}}$



contact estimator



Outline

Parabolic model problem with linear complementarity constraints

$$\begin{cases} \partial_t u_1 - \mu_1 \Delta u_1 - \lambda = f_1 & \text{in} \quad \Omega \times]0,T[\,, \\ \partial_t u_2 - \mu_2 \Delta u_2 + \lambda = f_2 & \text{in} \quad \Omega \times]0,T[\,, \\ u_1 - u_2 \geq 0, \quad \lambda \geq 0, \quad \lambda(u_1 - u_2) = 0 & \text{in} \quad \Omega \times]0,T[\,, \\ u_1 = g & \text{on} \quad \partial\Omega \times]0,T[\,, \\ u_2 = 0 & \text{on} \quad \partial\Omega \times]0,T[\,, \\ u_1(\boldsymbol{x},0) = u_1^0(\boldsymbol{x}),\ u_2(\boldsymbol{x},0) = u_2^0(\boldsymbol{x}),\ u_1^0(\boldsymbol{x}) - u_2^0(\boldsymbol{x}) \geq 0 & \text{in} \quad \Omega. \end{cases}$$

Parabolic model problem with linear complementarity constraints

$$\begin{cases} \partial_t u_1 - \mu_1 \Delta u_1 - \lambda = f_1 & \text{in} \quad \Omega \times]0,T[\,, \\ \partial_t u_2 - \mu_2 \Delta u_2 + \lambda = f_2 & \text{in} \quad \Omega \times]0,T[\,, \\ u_1 - u_2 \geq 0, \quad \lambda \geq 0, \quad \lambda(u_1 - u_2) = 0 & \text{in} \quad \Omega \times]0,T[\,, \\ u_1 = g & \text{on} \quad \partial\Omega \times]0,T[\,, \\ u_2 = 0 & \text{on} \quad \partial\Omega \times]0,T[\,, \\ u_1(\boldsymbol{x},0) = u_1^0(\boldsymbol{x}),\ u_2(\boldsymbol{x},0) = u_2^0(\boldsymbol{x}),\ u_1^0(\boldsymbol{x}) - u_2^0(\boldsymbol{x}) \geq 0 & \text{in} \quad \Omega. \end{cases}$$

Two possibilities to characterize the weak solution

Recall $\Lambda = \{\chi \in L^2(\Omega),\ \chi \geq 0 \text{ a.e. in } \Omega\}$

- Saddle point formulation $(u_1, u_2, \lambda) \in L^2(0,T; H_g^1(\Omega)) \times L^2(0,T; H_0^1(\Omega)) \times L^2(0,T;\Lambda)$
- Parabolic variational inequality: $\boldsymbol{u} \in \mathcal{K}_g^{\mathrm{t}}$

$$\mathcal{K}_g^{\mathrm{t}} := \left\{ \boldsymbol{v} \in L^2(0,T; H_g^1(\Omega)) \times L^2(0,T; H_0^1(\Omega)),\ \boldsymbol{v}(t) \in \mathcal{K}_g \quad \text{a.e in }]0,T[\right\}$$

Discrete complementarity problems

$n \geq 1$, $p \geq 1$:

Discrete complementarity problems

$n \geq 1, \ p \geq 1$:

$$\mathbb{E}^n \boldsymbol{X}_h^n = \boldsymbol{F}^n,$$

$$\boldsymbol{X}_{1h}^n + g\mathbf{1} - \boldsymbol{X}_{2h}^n \geq 0 \ \boldsymbol{X}_{3h}^n \geq 0 \ (\boldsymbol{X}_{1h}^n + g\mathbf{1} - \boldsymbol{X}_{2h}^n) \cdot \boldsymbol{X}_{3h}^n = 0.$$

$$\mathbb{E}^n := \begin{bmatrix} \mu_1 \mathbb{S} + \frac{1}{\Delta t_n} \mathbb{M} & \mathbf{0} & -\mathbb{D} \\ \mathbf{0} & \mu_2 \mathbb{S} + \frac{1}{\Delta t_n} \mathbb{M} & +\mathbb{D} \end{bmatrix}$$

Discrete complementarity problems

$n \geq 1, \ p \geq 1$:

$$\mathbb{E}^n \boldsymbol{X}_h^n = \boldsymbol{F}^n,$$
$$\boldsymbol{X}_{1h}^n + g\mathbf{1} - \boldsymbol{X}_{2h}^n \geq 0 \ \boldsymbol{X}_{3h}^n \geq 0 \ (\boldsymbol{X}_{1h}^n + g\mathbf{1} - \boldsymbol{X}_{2h}^n) \cdot \boldsymbol{X}_{3h}^n = 0.$$

$$\mathbb{E}^n := \begin{bmatrix} \mu_1 \mathbb{S} + \frac{1}{\Delta t_n}\mathbb{M} & \mathbf{0} & -\mathbb{D} \\ \mathbf{0} & \mu_2 \mathbb{S} + \frac{1}{\Delta t_n}\mathbb{M} & +\mathbb{D} \end{bmatrix}$$

Employing a C-function our problem reads

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

Discrete complementarity problems

$n \geq 1, \;\; p \geq 1$:

$$\mathbb{E}^n \boldsymbol{X}_h^n = \boldsymbol{F}^n, \qquad \mathbb{E}^n := \begin{bmatrix} \mu_1 \mathbb{S} + \frac{1}{\Delta t_n}\mathbb{M} & \mathbf{0} & -\mathbb{D} \\ \mathbf{0} & \mu_2 \mathbb{S} + \frac{1}{\Delta t_n}\mathbb{M} & +\mathbb{D} \end{bmatrix}$$

$$\boldsymbol{X}_{1h}^n + g\mathbf{1} - \boldsymbol{X}_{2h}^n \geq 0 \;\; \boldsymbol{X}_{3h}^n \geq 0 \;\; (\boldsymbol{X}_{1h}^n + g\mathbf{1} - \boldsymbol{X}_{2h}^n) \cdot \boldsymbol{X}_{3h}^n = 0.$$

Employing a C-function our problem reads

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

Inexact semismooth Newton method:

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

A posteriori error estimates

A posteriori analysis

We employ the methodology of equilibrated flux reconstructions

Theorem (Guaranteed upper bound)

$$\forall p \geq 1,\ \forall k \geq 0,\ \forall i \geq 0, \quad \left\lvert\!\left\lvert\!\left\lvert \boldsymbol{u} - \boldsymbol{u}_{h\tau}^{k,i} \right\rvert\!\right\rvert\!\right\rvert_{L^2(0,T;H_0^1(\Omega))} \leq \eta^{k,i}$$

Corollary (Distinction of the error components)

$$\left\lvert\!\left\lvert\!\left\lvert \boldsymbol{u} - \boldsymbol{u}_{h\tau}^{k,i} \right\rvert\!\right\rvert\!\right\rvert_{L^2(0,T;H_0^1(\Omega))} \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{init}}$$

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

$$|||\boldsymbol{u} - \boldsymbol{u}_{h\tau}|||^2_{L^2(0,T;H^1_0(\Omega))} + |||\boldsymbol{u} - \boldsymbol{z}|||^2_{L^2(0,T;H^1_0(\Omega))} + \|(\boldsymbol{u} - \boldsymbol{u}_{h\tau})(\cdot, T)\|^2_{\Omega} \leq 5\eta^2$$

$$\eta^2 := \sum_{n=1}^{N_{\mathrm{t}}} \int_{I_n} \sum_{K \in \mathcal{T}_h} \left(\sum_{\alpha=1}^{2} \left(\eta^n_{\mathrm{R},K,\alpha} + \eta^n_{\mathrm{F},K,\alpha}\right)^2 + \eta^n_{\mathrm{C},K} \right)(t)\,\mathrm{d}t + \|(\boldsymbol{u} - \boldsymbol{u}_{h\tau})(\cdot, 0)\|^2_{\Omega}.$$

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

$$|||\boldsymbol{u} - \boldsymbol{u}_{h\tau}|||^2_{L^2(0,T;H^1_0(\Omega))} + |||\boldsymbol{u} - \boldsymbol{z}|||^2_{L^2(0,T;H^1_0(\Omega))} + \|(\boldsymbol{u} - \boldsymbol{u}_{h\tau})(\cdot, T)\|^2_\Omega \leq 5\eta^2$$

$$\eta^2 := \sum_{n=1}^{N_t} \int_{I_n} \sum_{K\in\mathcal{T}_h} \left(\sum_{\alpha=1}^{2} \left(\eta^n_{\mathrm{R},K,\alpha} + \eta^n_{\mathrm{F},K,\alpha}\right)^2 + \eta^n_{\mathrm{C},K} \right)(t)\,\mathrm{d}t + \|(\boldsymbol{u} - \boldsymbol{u}_{h\tau})(\cdot, 0)\|^2_\Omega .$$

Auxiliary problem: Given $\boldsymbol{u} \in \mathcal{K}^{\mathrm{t}}_g$ and $\boldsymbol{u}_{h\tau} \in \mathcal{K}^{\mathrm{t}}_g$, let $\boldsymbol{z} \in \mathcal{K}^{\mathrm{t}}_g$ be such that $\forall \boldsymbol{v} \in \mathcal{K}^{\mathrm{t}}_g$

$$\int_0^T a(\boldsymbol{z} - \boldsymbol{u}, \boldsymbol{v} - \boldsymbol{z})(t)\,\mathrm{d}t \geq -\int_0^T \sum_{\alpha=1}^{2} \langle \partial_t(u_\alpha - u_{\alpha h\tau}) - (-1)^\alpha \lambda_{h\tau}, v_\alpha - z_\alpha\rangle (t)\,\mathrm{d}t$$

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

$$|||\boldsymbol{u} - \boldsymbol{u}_{h\tau}|||^2_{L^2(0,T;H^1_0(\Omega))} + |||\boldsymbol{u} - \boldsymbol{z}|||^2_{L^2(0,T;H^1_0(\Omega))} + \|(\boldsymbol{u} - \boldsymbol{u}_{h\tau})(\cdot, T)\|^2_\Omega \leq 5\eta^2$$

$$\eta^2 := \sum_{n=1}^{N_\mathrm{t}} \int_{I_n} \sum_{K\in\mathcal{T}_h} \left(\sum_{\alpha=1}^{2} \left(\eta^n_{\mathrm{R},K,\alpha} + \eta^n_{\mathrm{F},K,\alpha}\right)^2 + \eta^n_{\mathrm{C},K} \right)(t)\,\mathrm{d}t + \|(\boldsymbol{u} - \boldsymbol{u}_{h\tau})(\cdot, 0)\|^2_\Omega .$$

Auxiliary problem: Given $\boldsymbol{u} \in \mathcal{K}^{\mathrm{t}}_g$ and $\boldsymbol{u}_{h\tau} \in \mathcal{K}^{\mathrm{t}}_g$, let $\boldsymbol{z} \in \mathcal{K}^{\mathrm{t}}_g$ be such that $\forall \boldsymbol{v} \in \mathcal{K}^{\mathrm{t}}_g$

$$\int_0^T a(\boldsymbol{z} - \boldsymbol{u}, \boldsymbol{v} - \boldsymbol{z})(t)\,\mathrm{d}t \geq -\int_0^T \sum_{\alpha=1}^{2} \langle \partial_t(u_\alpha - u_{\alpha h\tau}) - (-1)^\alpha \lambda_{h\tau}, v_\alpha - z_\alpha\rangle(t)\,\mathrm{d}t$$

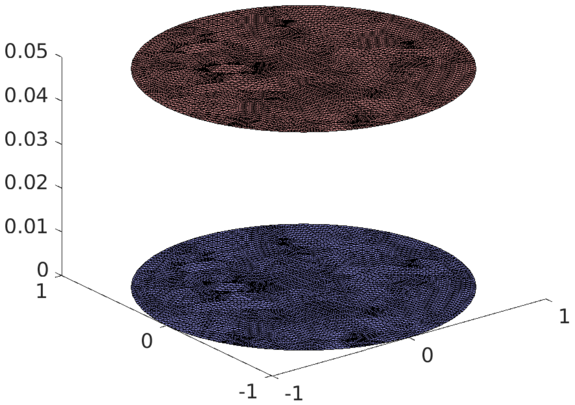
Lemma

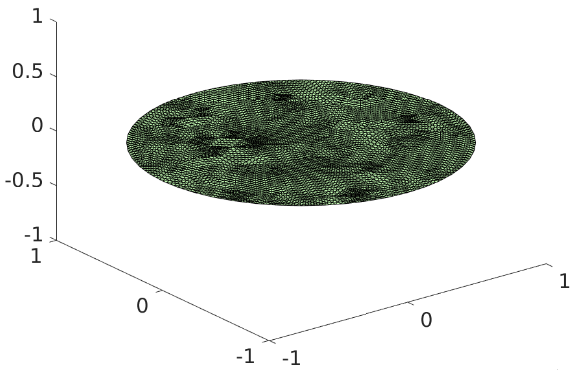
$$|||\boldsymbol{u} - \boldsymbol{z}|||_{L^2(0,T;H^1_0(\Omega))} \lesssim \left(\int_0^T \sum_{\alpha=1}^{2} \|\partial_t (u_\alpha - u_{\alpha h\tau})\|^2_{H^{-1}(\Omega)}(t)\,\mathrm{d}t \right)^{\frac{1}{2}} + \left(\int_0^T \|\lambda_{h\tau} - \lambda\|^2_{H^{-1}(\Omega)}(t)\,\mathrm{d}t \right)^{\frac{1}{2}}$$

Numerical experiments

Numerical experiments $p = 1$

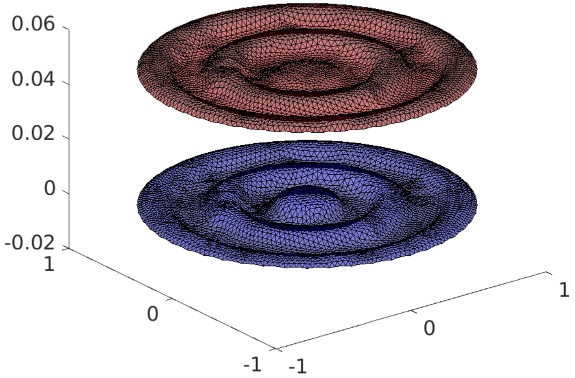
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

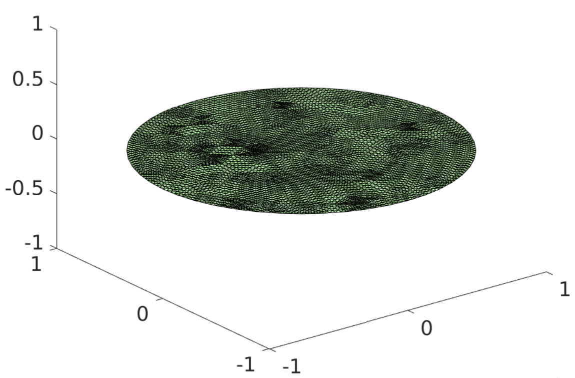




Numerical experiments $p = 1$

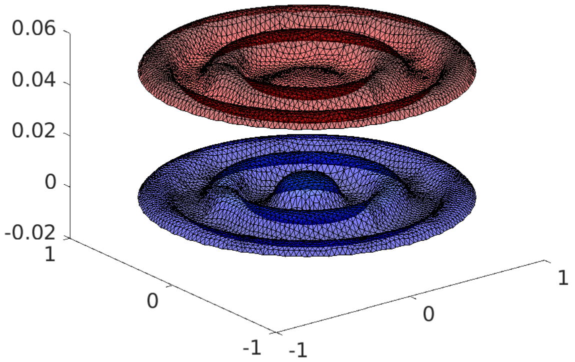
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

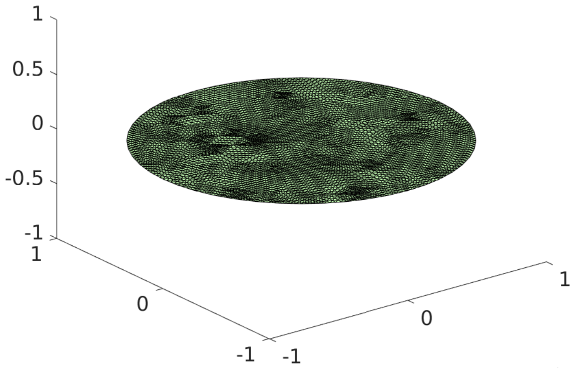




Numerical experiments $p = 1$

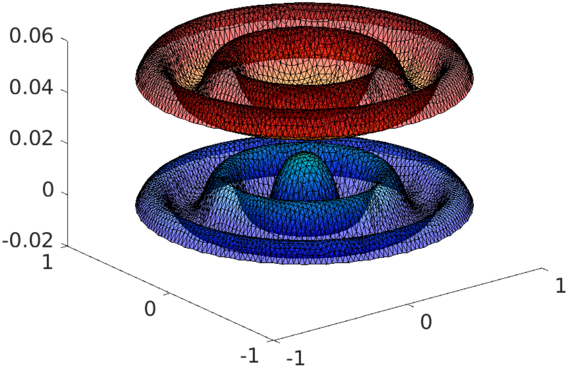
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

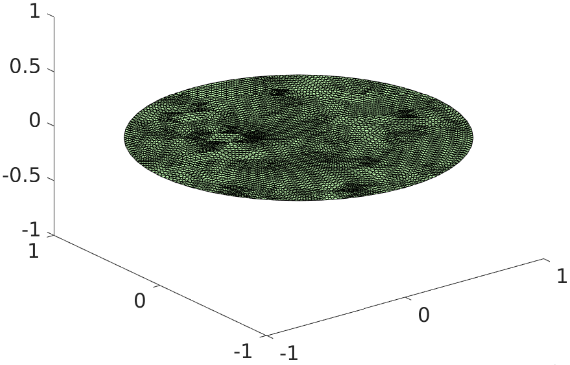




Numerical experiments $p = 1$

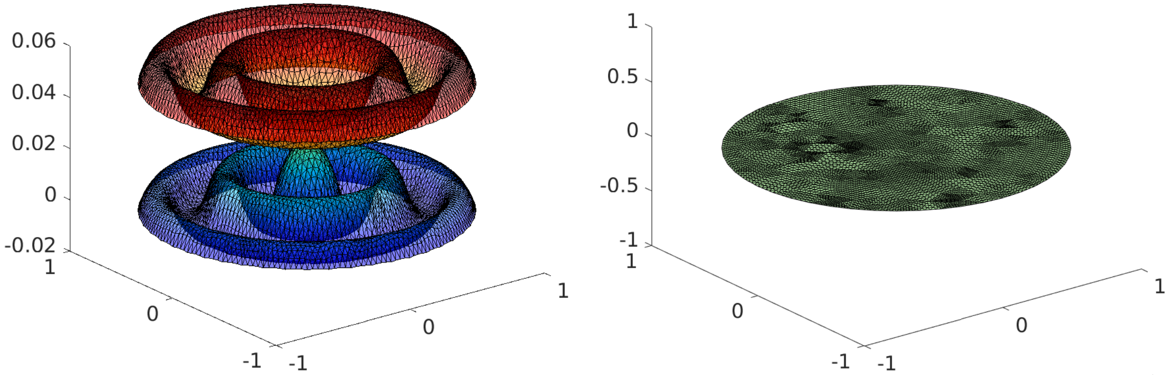
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner





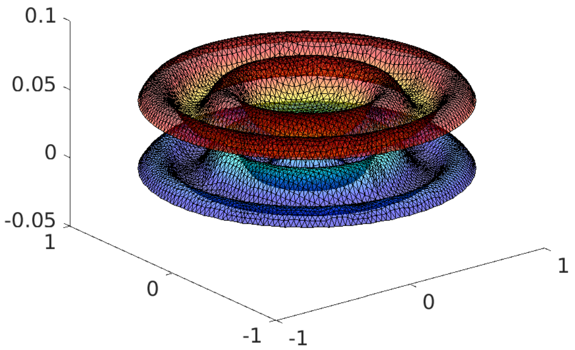
Numerical experiments $p = 1$

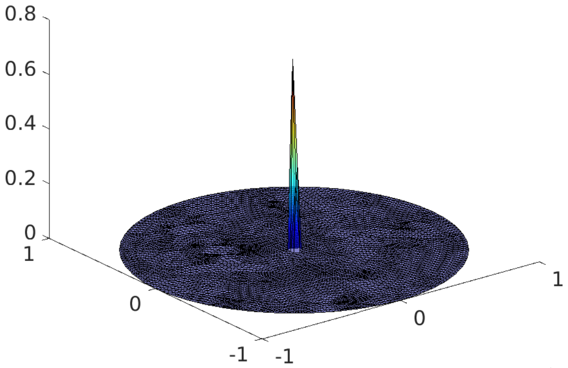
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner



Numerical experiments $p = 1$

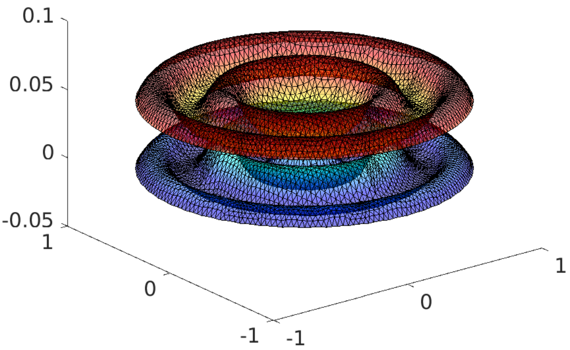
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

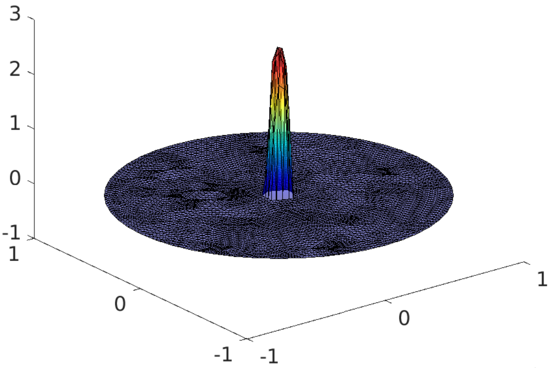




Numerical experiments $p = 1$

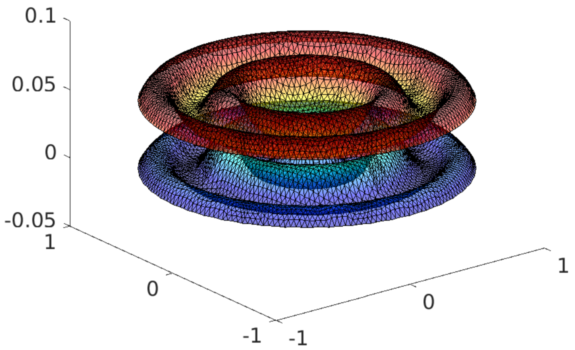
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

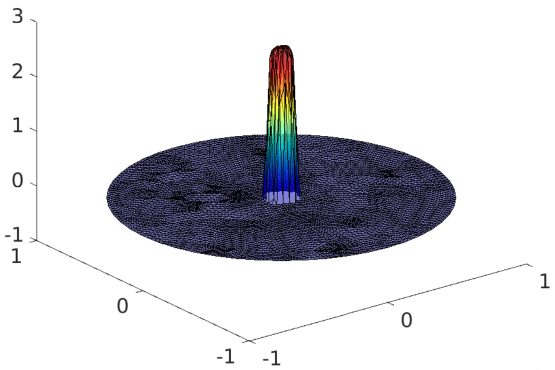




Numerical experiments $p = 1$

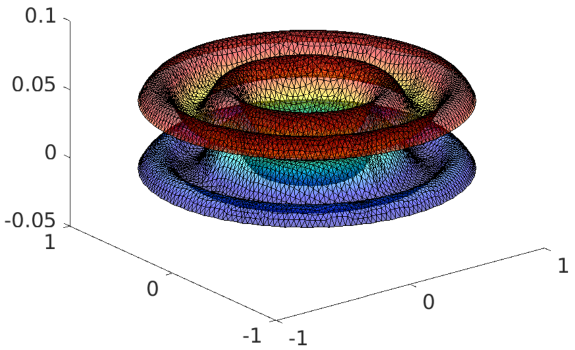
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

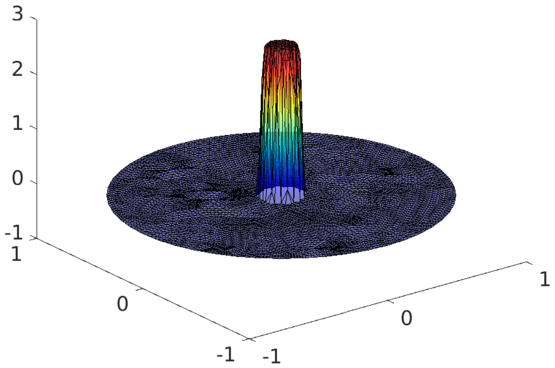




Numerical experiments $p = 1$

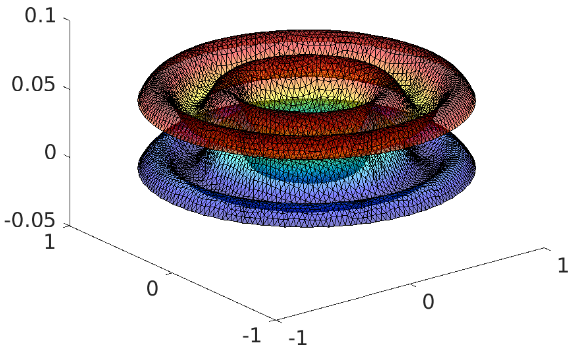
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

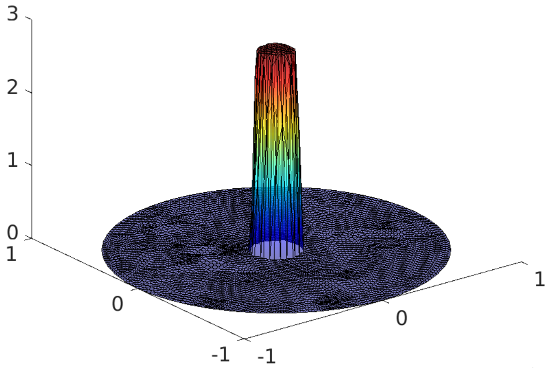




Numerical experiments $p = 1$

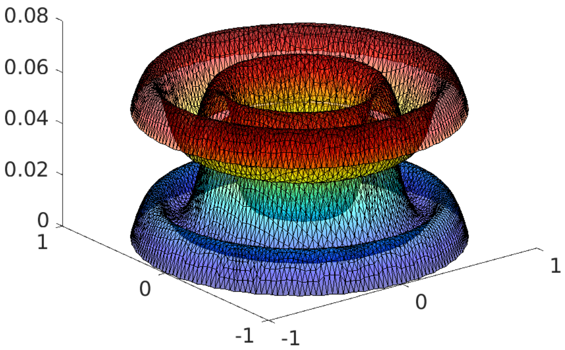
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

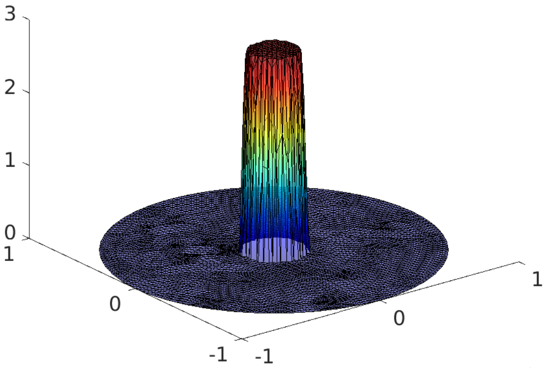




Numerical experiments $p = 1$

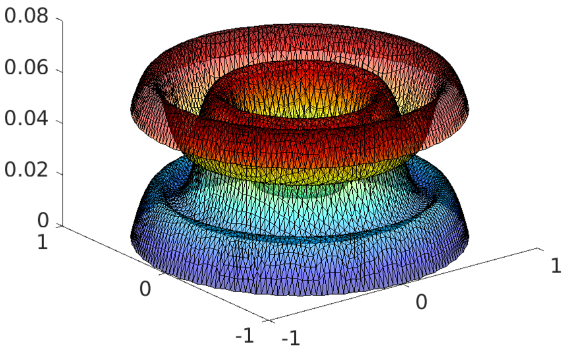
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

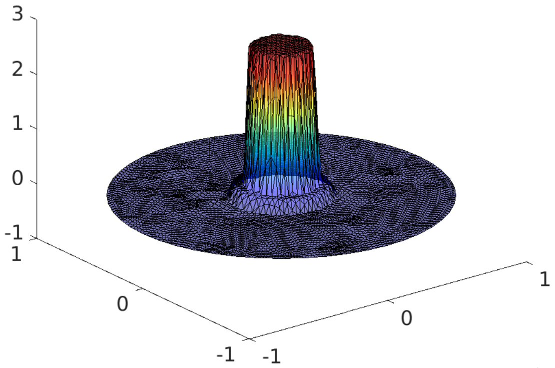




Numerical experiments $p = 1$

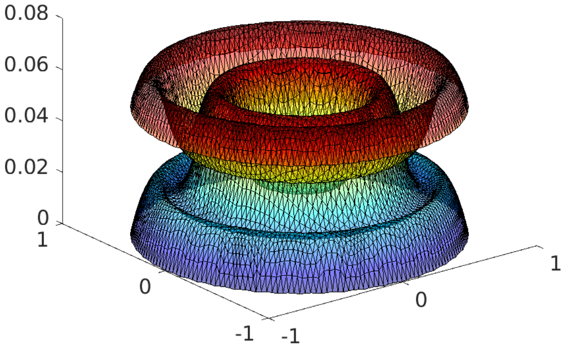
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner

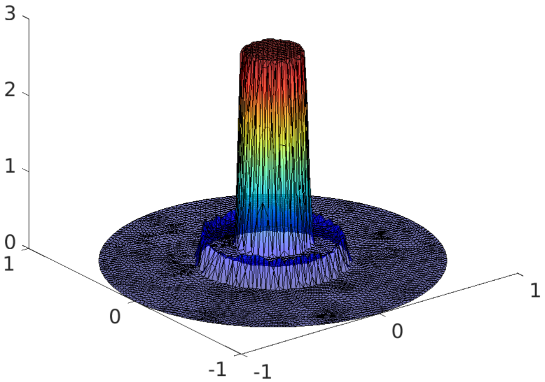




Numerical experiments $p = 1$

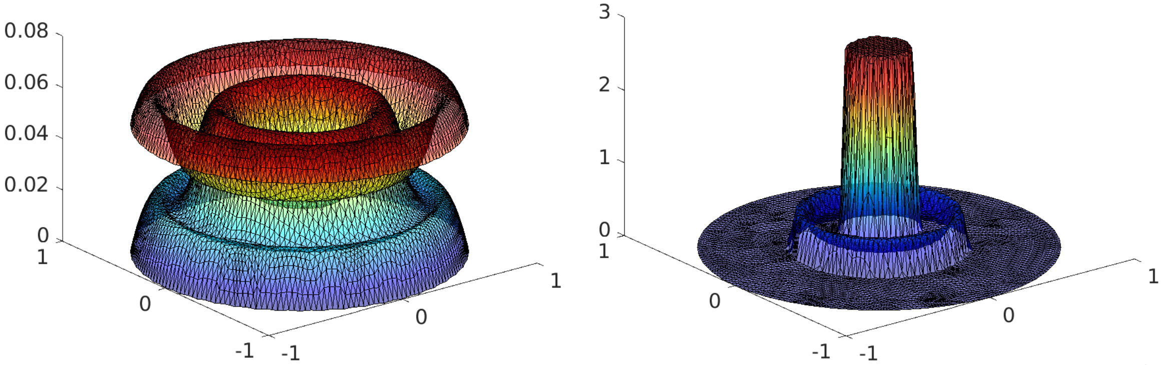
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner





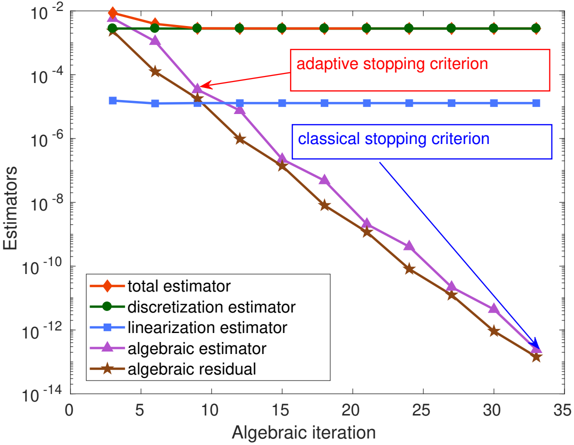
Numerical experiments $p = 1$

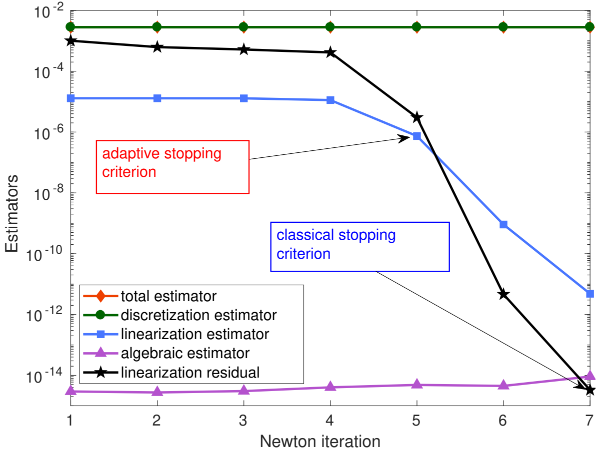
- semismooth solver: Newton–Fischer–Burmeister
- iterative algebraic solver : GMRES with ILU preconditionner



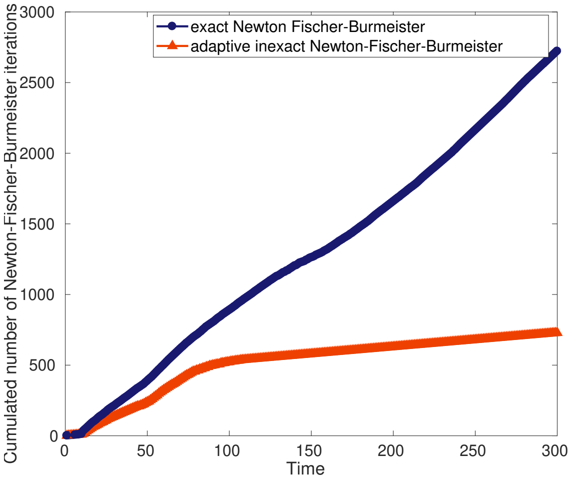
Newton–Fischer–Burmeister adaptivity

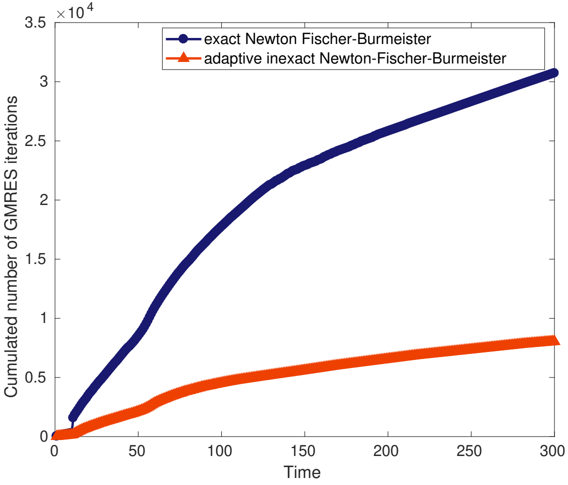
$\gamma_{\mathrm{lin}} = \gamma_{\mathrm{alg}} = 10^{-3}$





Newton–Fischer–Burmeister performance





Outline

Two-phase flow with phase appearance and disappearance

$$\left\{\begin{array}{l} \partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \boldsymbol{\nabla}\cdot\boldsymbol{\Phi}_{\mathrm{w}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) + \boldsymbol{\nabla}\cdot\boldsymbol{\Phi}_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0,\ H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0,\ \left[1 - S^{\mathrm{l}}\right]\cdot\left[H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right] = 0 \end{array}\right.$$

Two-phase flow with phase appearance and disappearance

$$\begin{cases} \partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \nabla \cdot \mathbf{\Phi}_{\mathrm{w}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) + \nabla \cdot \mathbf{\Phi}_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0, \; H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0, \; \left[1 - S^{\mathrm{l}}\right] \cdot \left[H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right] = 0 \end{cases}$$

Unknowns: liquid saturation S^{l}, liquid pressure P^{l}, mole fraction of liquid hydrogen $\chi_{\mathrm{h}}^{\mathrm{l}}$

Two-phase flow with phase appearance and disappearance

$$\begin{cases} \partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \nabla \cdot \mathbf{\Phi}_{\mathrm{w}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) + \nabla \cdot \mathbf{\Phi}_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0, \; H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0, \; \left[1 - S^{\mathrm{l}}\right] \cdot \left[H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right] = 0 \end{cases}$$

Unknowns: liquid saturation S^{l}, liquid pressure P^{l}, mole fraction of liquid hydrogen $\chi_{\mathrm{h}}^{\mathrm{l}}$

Linear functions: amount of water l_{w}, amount of hydrogen l_{h}

Two-phase flow with phase appearance and disappearance

$$\begin{cases} \partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \boldsymbol{\nabla}\cdot\boldsymbol{\Phi}_{\mathrm{w}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) + \boldsymbol{\nabla}\cdot\boldsymbol{\Phi}_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0,\ H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0,\ \left[1 - S^{\mathrm{l}}\right]\cdot\left[H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right] = 0 \end{cases}$$

Unknowns: liquid saturation S^{l}, liquid pressure P^{l}, mole fraction of liquid hydrogen $\chi_{\mathrm{h}}^{\mathrm{l}}$

Linear functions: amount of water l_{w}, amount of hydrogen l_{h}

Nonlinear function: capillary pressure P_{cp}

Two-phase flow with phase appearance and disappearance

$$\begin{cases} \partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \nabla \cdot \boldsymbol{\Phi}_{\mathrm{w}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) + \nabla \cdot \boldsymbol{\Phi}_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0, \; H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0, \; \left[1 - S^{\mathrm{l}}\right] \cdot \left[H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right] = 0 \end{cases}$$

Unknowns: liquid saturation S^{l}, liquid pressure P^{l}, mole fraction of liquid hydrogen $\chi_{\mathrm{h}}^{\mathrm{l}}$

Linear functions: amount of water l_{w}, amount of hydrogen l_{h}

Nonlinear function: capillary pressure P_{cp}

Nonlinear fluxes: water flux $\underbrace{\boldsymbol{\Phi}_{\mathrm{w}}}_{\text{Darcy+Fick}}$, hydrogen flux $\underbrace{\boldsymbol{\Phi}_{\mathrm{h}}}_{\text{Darcy+Fick}}$

Two-phase flow with phase appearance and disappearance

$$\begin{cases} \partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \nabla \cdot \boldsymbol{\Phi}_{\mathrm{w}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) + \nabla \cdot \boldsymbol{\Phi}_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0, \; H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0, \; \left[1 - S^{\mathrm{l}}\right] \cdot \left[H\left[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})\right] - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right] = 0 \end{cases}$$

Unknowns: liquid saturation S^{l}, liquid pressure P^{l}, mole fraction of liquid hydrogen $\chi_{\mathrm{h}}^{\mathrm{l}}$

Linear functions: amount of water l_{w}, amount of hydrogen l_{h}

Nonlinear function: capillary pressure P_{cp}

Nonlinear fluxes: water flux $\underbrace{\boldsymbol{\Phi}_{\mathrm{w}}}_{\text{Darcy+Fick}}$, hydrogen flux $\underbrace{\boldsymbol{\Phi}_{\mathrm{h}}}_{\text{Darcy+Fick}}$

Nonlinear complementarity constraints: $\Rightarrow$ **Phase change**

Ben Gharbia and Jaffré (2014)

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**

Discretization of the water equation

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

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**

Discretization of the water equation

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

Discretization of the hydrogen equation

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

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**

Discretization of the water equation

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

Discretization of the hydrogen equation

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

At each time step t^n, we obtain the nonlinear system of algebraic equations

$$S_{c,K}^n(\boldsymbol{U}^n) = 0 \quad \forall K \in \mathcal{T}_h \ \forall c \in \{\mathrm{w}, \mathrm{h}\}$$

Discrete complementarity problem and semismoothness

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

$$S_{c,K}^n(\boldsymbol{U}^n) = 0 \quad \forall K \in \mathcal{T}_h \quad \forall c \in \{\mathrm{w}, \mathrm{h}\}$$

$$\mathcal{K}(\boldsymbol{U}_K^n) \geq 0, \quad \mathcal{G}(\boldsymbol{U}_K^n) \geq 0, \quad \mathcal{K}(\boldsymbol{U}_K^n) \cdot \mathcal{G}(\boldsymbol{U}_K^n) = 0 \quad \forall K \in \mathcal{T}_h$$

- **We reformulate the complementarity constraints with C-functions**
- **We employ inexact semismooth linearization**
- **Can we estimate the error?**
- **Can we distinguish the error components?**

Discrete complementarity problem and semismoothness

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

$$S_{c,K}^n(\boldsymbol{U}^n) = 0 \quad \forall K \in \mathcal{T}_h \quad \forall c \in \{\mathrm{w}, \mathrm{h}\}$$
$$\mathcal{K}(\boldsymbol{U}_K^n) \geq 0, \quad \mathcal{G}(\boldsymbol{U}_K^n) \geq 0, \quad \mathcal{K}(\boldsymbol{U}_K^n) \cdot \mathcal{G}(\boldsymbol{U}_K^n) = 0 \quad \forall K \in \mathcal{T}_h$$

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

Discrete complementarity problem and semismoothness

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

$$S_{c,K}^n(\boldsymbol{U}^n) = 0 \quad \forall K \in \mathcal{T}_h \quad \forall c \in \{\mathrm{w}, \mathrm{h}\}$$
$$\mathcal{K}(\boldsymbol{U}_K^n) \geq 0, \quad \mathcal{G}(\boldsymbol{U}_K^n) \geq 0, \quad \mathcal{K}(\boldsymbol{U}_K^n) \cdot \mathcal{G}(\boldsymbol{U}_K^n) = 0 \quad \forall K \in \mathcal{T}_h$$

- **We reformulate the complementarity constraints with C-functions**
- **We employ inexact semismooth linearization**
- **Can we estimate the error?**
- **Can we distinguish the error components?**

A posteriori error estimates

Weak solution

$$X := L^2((0,t_{\mathrm{F}}); H^1(\Omega)),\ \ Y := H^1((0,t_{\mathrm{F}}); L^2(\Omega)),\ \ Z := L^2_+((0,t_{\mathrm{F}}); L^\infty(\Omega))$$

Assumption: There exists a unique weak solution satisfying

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

Error measure

1. **Dual norm of the residual for the components**

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

2. **Residual for the constraints**

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

3. **Error measure for the nonconformity of the pressure $\mathcal{N}_p(P_{h\tau}^{n,k,i})$**
4. **Error measure for nonconformity of the molar fraction $\mathcal{N}_\chi(\chi_{h\tau}^{n,k,i})$**

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

Error measure

1. **Dual norm of the residual for the components**

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

2. **Residual for the constraints**

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

3. **Error measure for the nonconformity of the pressure $\mathcal{N}_p(P_{h\tau}^{n,k,i})$**
4. **Error measure for nonconformity of the molar fraction $\mathcal{N}_\chi(\chi_{h\tau}^{n,k,i})$**

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

Error measure

1. **Dual norm of the residual for the components**

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

2. **Residual for the constraints**

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

3. **Error measure for the nonconformity of the pressure $\mathcal{N}_p(P_{h\tau}^{n,k,i})$**

4. **Error measure for nonconformity of the molar fraction $\mathcal{N}_\chi(\chi_{h\tau}^{n,k,i})$**

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

Error measure

1. **Dual norm of the residual for the components**

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

2. **Residual for the constraints**

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

3. **Error measure for the nonconformity of the pressure $\mathcal{N}_p(P_{h\tau}^{n,k,i})$**
4. **Error measure for nonconformity of the molar fraction $\mathcal{N}_\chi(\chi_{h\tau}^{n,k,i})$**

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

A posteriori error estimate distinguishing the error components

Theorem

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

Construction of the estimators:

- Equilibrated component flux reconstruction in $\mathbf{H}(\mathrm{div}, \Omega)$
- Potential reconstruction in $H^1(\Omega)$

Numerical experiments

Numerical experiments

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

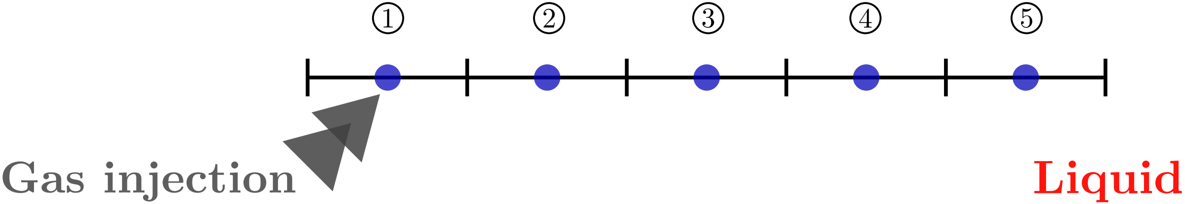
Semismooth solver: Newton-min

Iterative algebraic solver: GMRES.

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

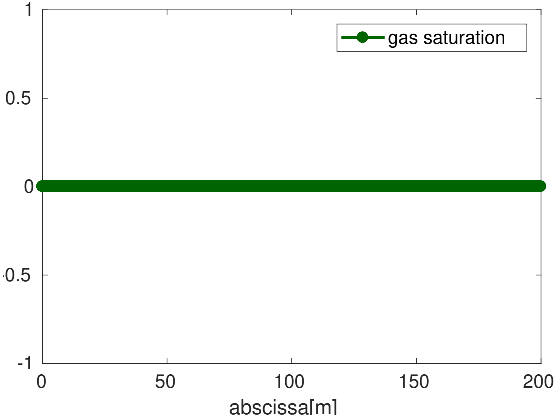
Number of cells: $N_{\mathrm{sp}} = 1000$,

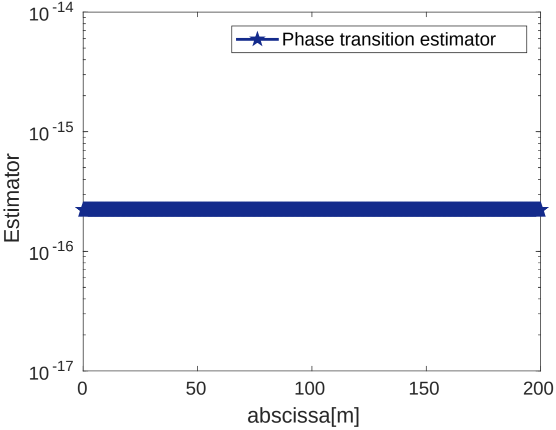
Final simulation time: $t_{\mathrm{F}} = 5 \times 10^5$ years.



Phase transition estimator

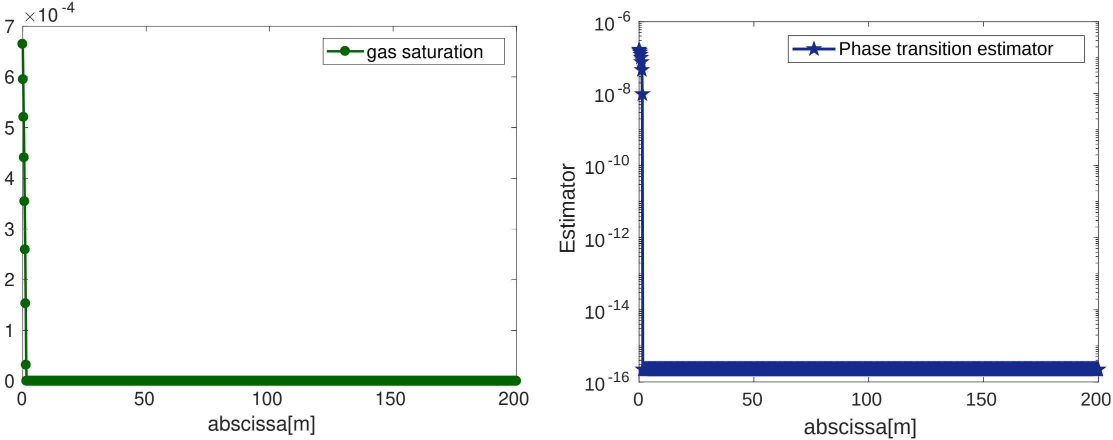
$t = 2500$ **years**





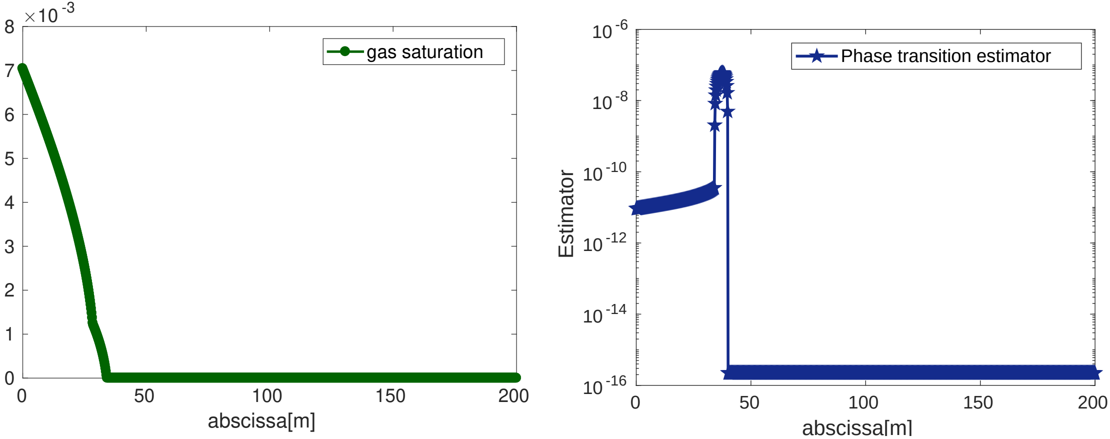
Phase transition estimator

$t = 1.25 \times 10^4$ years

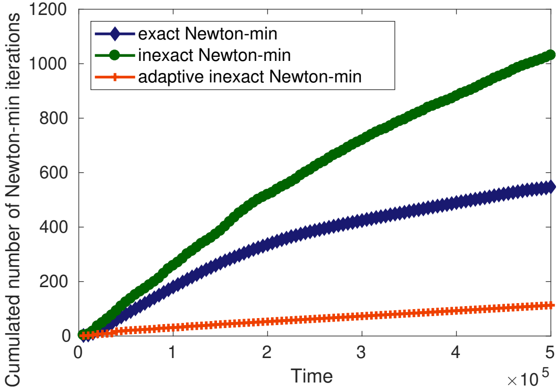


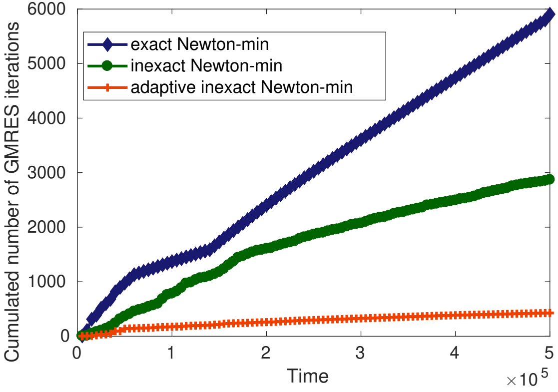
Phase transition estimator

$t = 4.25 \times 10^4$ **years**



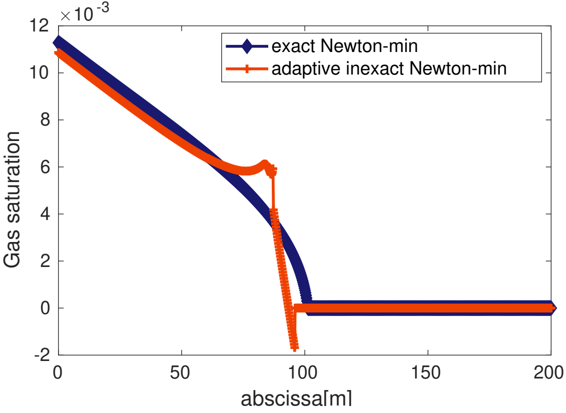
Overall performance $\gamma_{\mathrm{lin}} = \gamma_{\mathrm{alg}} = 10^{-3}$



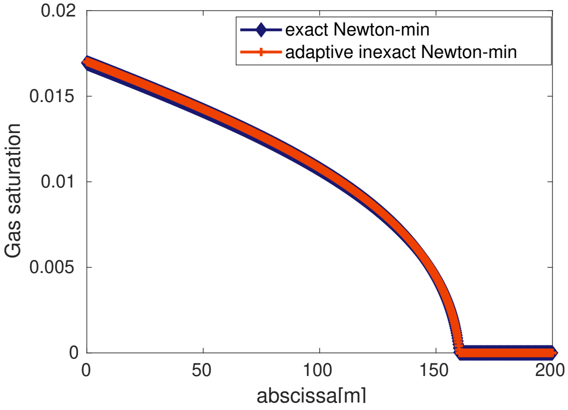


Accuracy $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years



Outline

Conclusion and perspectives

Conclusion

Conclusion and perspectives

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.

Conclusion and perspectives

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.

Perspectives

- Extension of the stationary contact problem to a hyperbolic contact problem between two vibrating membranes
- Devise a proof for the convergence of the semismooth Newton scheme
- Chapter 2: Improve the time derivative a posteriori error
- Construct a posteriori error estimates for a multiphase multi compositional flow with several phase transitions.

Acknowledgements

Ibtihel Ben Gharbia (IFPEN) Simulation in Chapter 3 on the basis of her MATLAB code.
Soleiman Yousef (IFPEN)
Jean-Charles Gilbert (INRIA Paris)
Michel Kern (INRIA Paris)
Jan Papež (INRIA Paris) Simulation in Chapter 1 on the basis of his MATLAB code.
Adel Blouza (Université Rouen)

Thank you for your attention

Discretization flux reconstruction:

$$
\begin{aligned}
\left(\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\alpha h,\mathrm{disc}}, \boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} - \left(\gamma^{k,i,\boldsymbol{a}}_{\alpha h}, \boldsymbol{\nabla}\cdot\boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} &= -\left(\mu_\alpha \psi_{h,\boldsymbol{a}} \boldsymbol{\nabla} u^{k,i,\boldsymbol{a}}_{\alpha h}, \boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} \quad \forall \boldsymbol{\tau}_h \in \mathbf{V}_h^{\boldsymbol{a}},\\
\left(\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\alpha h,\mathrm{disc}}, q_h\right)_{\omega_h^{\boldsymbol{a}}} &= \left(\tilde{g}^{k,i,\boldsymbol{a}}_{\alpha h}, q_h\right)_{\omega_h^{\boldsymbol{a}}} \quad \forall q_h \in Q_h^{\boldsymbol{a}},
\end{aligned}
$$

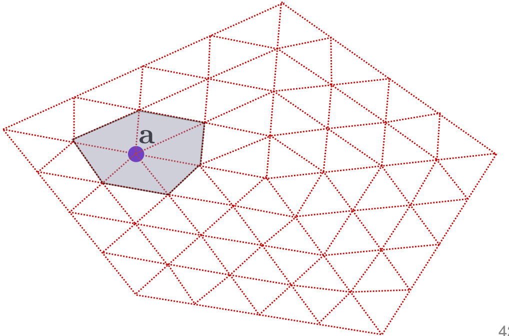
$$\tilde{g}^{k,i,\boldsymbol{a}}_{\alpha h} := \left(f_\alpha - (-1)^\alpha \tilde{\lambda}^{k,i}_{h,\boldsymbol{a}} - r^{k,i}_{\alpha h}\right)\psi_{h,\boldsymbol{a}} - \mu_\alpha \boldsymbol{\nabla} u^{k,i}_{\alpha h}\cdot\boldsymbol{\nabla}\psi_{h,\boldsymbol{a}}$$: depends on the residual

For each internal vertex $\boldsymbol{a} \in \mathcal{V}_h^{\mathrm{int}}$

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

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

$$\boldsymbol{\sigma}^{k,i}_{\alpha h,\mathrm{disc}} := \sum_{\boldsymbol{a}\in\mathcal{V}_h} \boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\alpha h,\mathrm{disc}}$$



Strategy for constructing the estimators

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

Nonconformity estimator 1:

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

Nonconformity estimator 2:

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

Nonconformity estimator 3:

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

Parabolic weak formulation

Weak formulation: For $(f_1, f_2) \in [L^2(0,T;L^2(\Omega))]^2$, $\boldsymbol{u}^0 \in H^1_g(\Omega) \times H^1_0(\Omega)$, find $(u_1, u_2, \lambda) \in L^2(0,T;H^1_g(\Omega)) \times L^2(0,T;H^1_0(\Omega)) \times L^2(0,T;\Lambda)$ s.t. $\partial_t u_\alpha \in L^2(0,T;H^{-1}(\Omega))$, and satisfying $\forall t \in]0,T[$

$$\sum_{\alpha=1}^{2} \langle \partial_t u_\alpha(t), v_\alpha \rangle + \sum_{\alpha=1}^{2} \mu_\alpha \left(\nabla u_\alpha(t), \nabla v_\alpha \right)_\Omega - (\lambda(t), v_1 - v_2)_\Omega = \sum_{\alpha=1}^{2} (f_\alpha, v_\alpha)_\Omega, \ \forall \boldsymbol{v} \in \left[H^1_0(\Omega)\right]^2$$

$$(\chi - \lambda(t), u_1(t) - u_2(t))_\Omega \geq 0 \quad \forall \chi \in \Lambda.$$

Discrete formulation: Given $(u^0_{1h}, u^0_{2h}) \in \mathcal{K}^p_{gh}$, search $(u^n_{1h}, u^n_{2h}, \lambda^n_h) \in X^p_{gh} \times X^p_{0h} \times \Lambda^p_h$ such that for all $(z_{1h}, z_{2h}, \chi_h) \in X^p_{0h} \times X^p_{0h} \times \Lambda^p_h$

$$\frac{1}{\Delta t_n} \sum_{\alpha=1}^{2} \left(u^n_{\alpha h} - u^{n-1}_{\alpha h}, z_{\alpha h} \right)_\Omega + \sum_{\alpha=1}^{2} \mu_\alpha \left(\nabla u^n_{\alpha h}, \nabla z_{\alpha h} \right)_\Omega - \langle \lambda^n_h, z_{1h} - z_{2h} \rangle_h = \sum_{\alpha=1}^{2} (f_\alpha, z_{\alpha h})_\Omega,$$

$$\langle \chi_h - \lambda^n_h, u^n_{1h} - u^n_{2h} \rangle_h \geq 0$$

Post-processing

The discrete liquid pressure and discrete molar fraction **are piecewise constant**

$$\left(P_K^{n,k,i}\right)_{K\in\mathcal{T}_h} \in \mathbb{P}_0(\mathcal{T}_h) \quad \left(\chi_K^{n,k,i}\right)_{K\in\mathcal{T}_h} \in \mathbb{P}_0(\mathcal{T}_h)$$

Piecewise polynomial reconstruction:

$$P_h^{n,k,i} \in \mathbb{P}_2(\mathcal{T}_h), \quad \chi_h^{n,k,i} \in \mathbb{P}_2(\mathcal{T}_h)$$

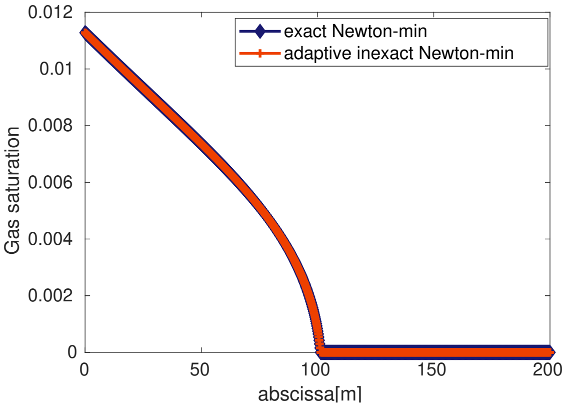
Conforming reconstruction:

$$\tilde{P}_h^{n,k,i} \in \mathbb{P}_2(\mathcal{T}_h) \cap H^1(\Omega), \quad \tilde{\chi}_h^{n,k,i} \in \mathbb{P}_2(\mathcal{T}_h) \cap H^1(\Omega).$$

$$\mathbb{P}_0(\mathcal{T}_h) \xrightarrow[\text{solving local problems in each cell}]{} \mathbb{P}_2(\mathcal{T}_h) \xrightarrow[\text{Oswald interpolation operator}]{} \mathbb{P}_2(\mathcal{T}_h) \bigcap H^1(\Omega)$$

$\gamma_{\mathbf{lin}} = \gamma_{\mathbf{alg}} = \mathbf{10^{-6}}$

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years