

High-order numerical discretizations and a posteriori error estimates for variational inequalities

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Seminar of Numerical Analysis and Scientific Computing, January 21st 2021

Outline

- 1 Introduction
- 2 Model problem and discretization
- 3 Semismooth Newton and first numerical results
- 4 A posteriori analysis
- 5 Extension to unsteady problems
- 6 Conclusion

Motivation

$\Omega \subset \mathbb{R}^2$: smooth connected domain, $\mathcal{H}$: Hilbert space, $\mathcal{K}_g$: convex set.
 $a : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$: bilinear continuous coercive form, $\ell : \mathcal{H} \rightarrow \mathbb{R}$: linear continuous form

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

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Application to several problems in contact mechanics

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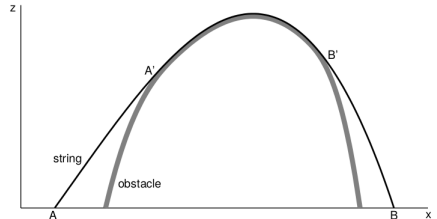
$$\text{Find } \mathbf{u} \in \mathcal{K}_g \quad a(\mathbf{u}, \mathbf{v} - \mathbf{u}) \geq \ell(\mathbf{v} - \mathbf{u}) \quad \forall \mathbf{v} \in \mathcal{K}_g$$

Application to several problems in contact mechanics

Obstacle problem: Find $\mathbf{u} \in \mathcal{K}_g := \{ \mathbf{v} \in H^1(\Omega) \text{ s.t. } \mathbf{v} = g \text{ on } \partial\Omega, \text{ and } \mathbf{v} \geq \psi \text{ in } \Omega \}$ such that

$$(\nabla \mathbf{u}, \nabla(\mathbf{v} - \mathbf{u}))_{\Omega} \geq (f, \mathbf{v} - \mathbf{u})_{\Omega} \quad \forall \mathbf{v} \in \mathcal{K}_g$$

- $\mathbf{u}$: displacement of an elastic membrane
- $\psi \in H^1(\Omega)$: position of the lower obstacle
- $g \in H^{\frac{1}{2}}(\partial\Omega)$: Dirichlet boundary datum for $\mathbf{u}$
- $f \in L^2(\Omega)$: force acting on the membrane



Signorini problem: $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_C$.

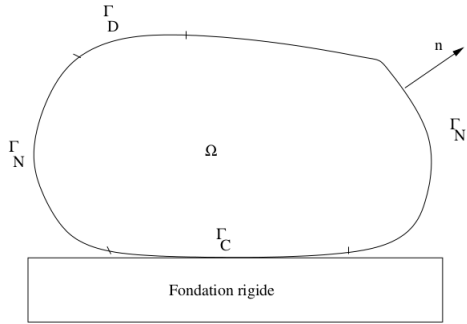
Γ_D : Dirichlet boundary conditions, Γ_N : Neumann boundary conditions

Γ_C : Unilateral contact boundary conditions

Find $\mathbf{u} \in \mathcal{K}_g := \{ \mathbf{v} \in [H^1(\Omega)]^2 \text{ s.t. } \mathbf{v} = \mathbf{g} \text{ on } \Gamma_D, \text{ and } \mathbf{v} \cdot \mathbf{n} \leq 0 \text{ on } \Gamma_C \}$ such that

$$(\sigma(\mathbf{u}), \epsilon(\mathbf{v} - \mathbf{u}))_\Omega \geq (\mathbf{f}, \mathbf{v} - \mathbf{u})_\Omega + (\mathbf{g}_N, \mathbf{v} - \mathbf{u})_{\Gamma_N} \quad \forall \mathbf{v} \in \mathcal{K}_g$$

- $\mathbf{g} \in H^{\frac{1}{2}}(\Gamma_D)$: Dirichlet boundary datum for $\mathbf{u}$
- $\mathbf{g}_N \in [L^2(\Gamma_N)]^2$: Neumann boundary data
- $\mathbf{f} \in [L^2(\Omega)]^2$: force acting on the solid elastic.

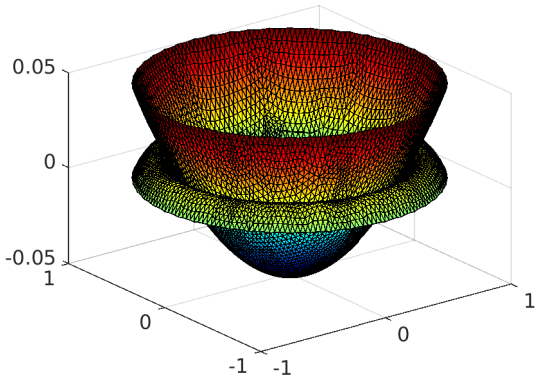


Contact between two membranes:

Find $\mathbf{u} := (u_1, u_2) \in \mathcal{K}_g := \{ \mathbf{v} = (v_1, v_2) \in H^1_{g_1}(\Omega) \times H^1_{g_2}(\Omega) \text{ s.t. } v_1 - v_2 \geq 0 \text{ a.e. in } \Omega \}$ such that

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

- μ_1, μ_2 : tensions of the membranes
- $g_1 \geq g_2$: boundary data



Study the contact problem between two membranes

Propose robust algorithms

- Discretization by the finite element method, the discontinuous Galerkin method, the hybrid high-order method

Nonlinear resolution

- Semismooth Newton methods

Quantify the error

- A posteriori error estimates
- Distinction of each error components

Save computational time

- Adaptivity

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Extension to unsteady problems?

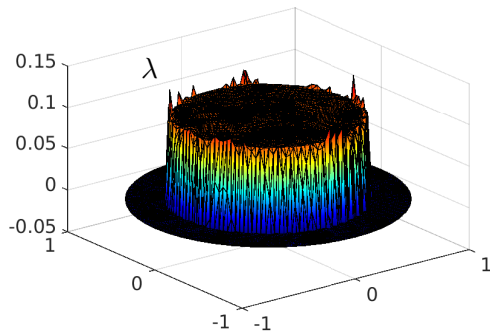
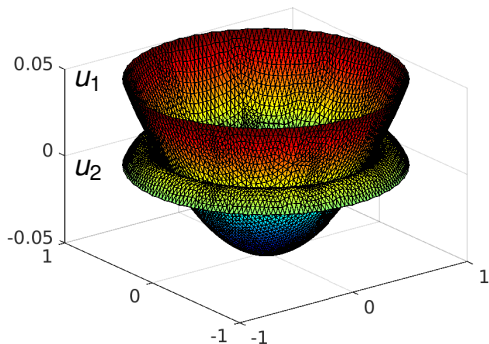
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Model problem and settings: contact between two membranes

Find u_1, u_2, λ such that

$$\begin{cases} -\mu_1 \Delta u_1 - \lambda = f_1 & \text{in } \Omega, \\ -\mu_2 \Delta u_2 + \lambda = f_2 & \text{in } \Omega, \\ u_1 - u_2 \geq 0, \quad \lambda \geq 0, \quad (u_1 - u_2)\lambda = 0 & \text{in } \Omega, \\ u_1 = g_1, \quad u_2 = g_2 & \text{on } \partial\Omega. \end{cases}$$



Continuous problem

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

Saddle point type weak formulation: For $(f_1, f_2) \in [L^2(\Omega)]^2$ and $g > 0$ find $(u_1, u_2, \lambda) \in H_{g_1}^1(\Omega) \times H_{g_2}^1(\Omega) \times \Lambda$ such that

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

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

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

equivalent to

Continuous problem

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

equivalent to

Variational inequality:

- $\mathcal{K}_g := \{(v_1, v_2) \in H_{g_1}^1(\Omega) \times H_{g_2}^1(\Omega), v_1 - v_2 \geq 0 \text{ a.e. in } \Omega\}$ **convex**

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

The finite element method

For any $p \geq 1$

Spaces for the discretization:

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

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

$$\mathcal{K}_{gh}^p = \left\{ (v_{1h}, v_{2h}) \in X_{g_1 h}^p \times X_{g_2 h}^p, v_{1h}(\mathbf{x}_I) - v_{2h}(\mathbf{x}_I) \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^p \right\} \not\subset \mathcal{K}_g \quad \forall p \geq 2$$

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

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

Well-posed problem (Lions–Stampacchia)

The finite element method

For any $p \geq 1$

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

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

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

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

Saddle point formulation

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Continuous weak formulation

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

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Discrete weak formulation Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{g_1h}^p \times X_{g_2h}^p \times \Lambda_h^p$ s.t.

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

$$\langle \chi_h - \lambda_h, u_{1h} - u_{2h} \rangle_h \geq 0 \quad \forall \chi_h \in \Lambda_h^p.$$

Discrete complementarity problem

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

$$(u_{1h} - u_{2h})(\mathbf{x}_I) \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, \psi_{h,\mathbf{x}_I} \rangle_h \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad \langle \lambda_h, u_{1h} - u_{2h} \rangle_h = 0. \quad (\text{DS2})$$

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Matrix representation of (DS2)

Discrete complementarity problem

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

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

Matrix representation of (DS2)

$$p \geq 1: u_{1h} = \sum_{l=1}^{\mathcal{N}_d^{p,\text{int}}} (\mathbf{x}_{1h})_l \psi_{h,\mathbf{x}_l}, \quad u_{2h} = \sum_{l=1}^{\mathcal{N}_d^{p,\text{int}}} (\mathbf{x}_{2h})_l \psi_{h,\mathbf{x}_l}, \quad \lambda_h = \sum_{l=1}^{\mathcal{N}_d^{p,\text{int}}} (\mathbf{x}_{3h})_l \Theta_{h,\mathbf{x}_l}.$$

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

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

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

The Discontinuous Galerkin method

Discontinuous spaces:

$$X_h^p := \left\{ v_h \in L^2(\Omega) \text{ s.t. } v_h|_K \in \mathbb{P}_p(K) \ \forall K \in \mathcal{T}_h \right\}$$

$$X_{g_\alpha h}^p := \left\{ v_h \in L^2(\Omega) \text{ s.t. } v_h|_K \in \mathbb{P}_p(K) \ \forall K \in \mathcal{T}_h \text{ and } v_h = g_\alpha \text{ on } \partial\Omega \right\}$$

$$\mathcal{K}_{gh}^p := \left\{ \mathbf{v}_h := (v_{1h}, v_{2h}) \in X_{g_1h}^p \times X_{g_2h}^p \text{ s.t. } (v_{1h} - v_{2h})|_K(\mathbf{x}_I) \geq 0 \ \forall \mathbf{x}_I \in \mathcal{V}_K^{\text{int}} \ \forall K \in \mathcal{T}_h \right\}$$

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

$$\sum_{\alpha=1}^2 \mu_{\alpha} \mathcal{A}_h(u_{\alpha h}, v_{\alpha h} - u_{\alpha h}) \geq \sum_{\alpha=1}^2 \sum_{K \in \mathcal{T}_h} (f_{\alpha}|_K, v_{\alpha h}|_K - u_{\alpha h}|_K)_K \quad \forall \mathbf{v}_h = (v_{1h}, v_{2h}) \in \mathcal{K}_{gh}^p \quad (\text{DR})$$

 $\mathcal{A}_h$: bilinear form a + consistency and stability terms [SIPG, NIPG]

Well-posed problem (Lions–Stampacchia)

Discrete complementarity problem

$$\Lambda_h^p := \left\{ v_h \in X_h^p \text{ s.t. } (v_h|_K, \psi_{h,\mathbf{x}_I}|_K)_K \geq 0 \ \forall K \in \mathcal{T}_h, \ \forall \mathbf{x}_I \in \mathcal{V}_K^{\text{int}}, \text{ and } (v_h|_K, \psi_{h,\mathbf{x}_I}|_K)_K = 0 \right. \\ \left. \forall K \in \mathcal{T}_h \ \forall \mathbf{x}_I \in \mathcal{V}_K^{\text{ext}} \right\} \quad p \geq 2$$

Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{g_1h}^p \times X_{g_2h}^p \times \Lambda_h^p$ such that

$$\sum_{\alpha=1}^2 \mu_\alpha \mathcal{A}_h(u_{\alpha h}, v_{\alpha h}) - \sum_{K \in \mathcal{T}_h} (v_{1h}|_K - v_{2h}|_K, \lambda_h|_K)_K = \sum_{\alpha=1}^2 \sum_{K \in \mathcal{T}_h} (f_\alpha|_K, v_{\alpha h}|_K)_K \quad \forall \mathbf{v}_h \in [X_{0h}^p]^2, \\ (u_{1h}|_K - u_{2h}|_K)(\mathbf{x}_I) \geq 0 \ \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \ (\lambda_h|_K, \psi_{h,\mathbf{x}_I}) \geq 0 \ \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \ (\lambda_h|_K, u_{1h}|_K - u_{2h}|_K) = 0.$$

Discrete complementarity problem

$$\Lambda_h^p := \left\{ \mathbf{v}_h \in X_h^p \text{ s.t. } (\mathbf{v}_h|_K, \psi_{h,\mathbf{x}_I}|_K)_K \geq 0 \quad \forall K \in \mathcal{T}_h, \quad \forall \mathbf{x}_I \in \mathcal{V}_K^{\text{int}}, \text{ and } (\mathbf{v}_h|_K, \psi_{h,\mathbf{x}_I}|_K)_K = 0 \right. \\ \left. \forall K \in \mathcal{T}_h \quad \forall \mathbf{x}_I \in \mathcal{V}_K^{\text{ext}} \right\} \quad p \geq 2$$

Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{g_1h}^p \times X_{g_2h}^p \times \Lambda_h^p$ such that

$$\sum_{\alpha=1}^2 \mu_\alpha \mathcal{A}_h(u_{\alpha h}, \mathbf{v}_{\alpha h}) - \sum_{K \in \mathcal{T}_h} (\mathbf{v}_{1h}|_K - \mathbf{v}_{2h}|_K, \lambda_h|_K)_K = \sum_{\alpha=1}^2 \sum_{K \in \mathcal{T}_h} (f_\alpha|_K, \mathbf{v}_{\alpha h}|_K)_K \quad \forall \mathbf{v}_h \in [X_{0h}^p]^2, \\ (u_{1h}|_K - u_{2h}|_K)(\mathbf{x}_I) \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad (\lambda_h|_K, \psi_{h,\mathbf{x}_I}) \geq 0 \quad \forall \mathbf{x}_I \in \mathcal{V}_d^{p,\text{int}}, \quad (\lambda_h|_K, u_{1h}|_K - u_{2h}|_K) = 0.$$

Matrix representation $\mathbf{X}_h := [\mathbf{X}_{1h}, \mathbf{X}_{2h}, \mathbf{X}_{3h}] \in \mathbb{R}^{3\mathcal{N}_h^{\text{int}}}$

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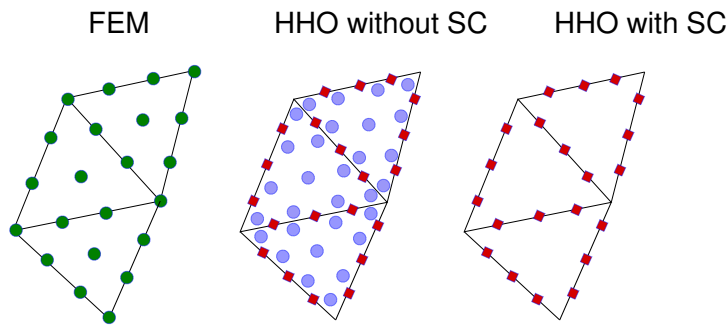
$$\mathbb{E} \mathbf{X}_h = \mathbf{F},$$

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

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

The Hybrid High-Order method

The unknowns are polynomial functions attached to the cells and the edges of the mesh. The polynomials attached to the cells can be eliminated through a static condensation procedure.



The blue DOFs are eliminated!

HHO papers: Di Pietro, Ern (2015), Cockburn, Di Pietro, Ern (2016), Cascavita, Chouly, Ern (2019), Cicuttin, Ern, Gudi (2020), Chouly, Ern, Pignet (2020)

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Discontinuous spaces: $\mathcal{E}_h$: set of edges, $\mathcal{V}_K$: DOFs in a triangle

$$\begin{aligned}
 X_h^p &:= \prod_{K \in \mathcal{T}_h} \mathbb{P}_p(K) \times \prod_{F \in \mathcal{E}_h} \mathbb{P}_{p-1}(F), & X_{h,K}^p &:= \mathbb{P}_p(K) \times \prod_{F \in \mathcal{E}_K} \mathbb{P}_{p-1}(F) \\
 X_{g_\alpha h}^p &:= \{v_h \in X_h^p \text{ s.t. } v_h = g_\alpha \text{ on } \partial\Omega\} : \textcolor{red}{u_1, u_2} & \Lambda_h &:= \prod_{K \in \mathcal{T}_h} \mathbb{P}_p(K) : \textcolor{red}{\lambda} \\
 \mathcal{K}_{gh}^p &:= \left\{ \mathbf{v}_h := (v_{1h}, v_{2h}) \in X_{g_1 h}^p \times X_{g_2 h}^p \text{ s.t. } (v_{1h} - v_{2h})|_K(\mathbf{x}_l) \geq 0 \ \forall \mathbf{x}_l \in \mathcal{V}_K \ \forall K \in \mathcal{T}_h \right\}
 \end{aligned}$$

Gradient reconstruction operator in every cell: $\mathbf{G}_K : X_{h,K}^p \rightarrow \mathbb{P}_p(K; \mathbb{R}^2)$ such that

$$(\mathbf{G}_K(\hat{v}_K), \mathbf{q})_K := (\nabla v_K, \mathbf{q})_K + \sum_{F \in \mathcal{E}_K} (v_F - v_K, \mathbf{q} \cdot \mathbf{n}_K)_F, \quad \forall \hat{v}_K \in X_{h,K}^p, \quad \forall \mathbf{q} \in \mathbb{P}_p(K; \mathbb{R}^2),$$

Bilinear form: $\forall \hat{v}_h \in X_h^p, \forall \hat{w}_h \in X_h^p$

$$\mathcal{A}_h(\hat{v}_h, \hat{w}_h) := \sum_{K \in \mathcal{T}_h} \left((\mathbf{G}_K(\hat{v}_K), \mathbf{G}_K(\hat{w}_K))_K + h_K^{-1} \sum_{F \in \mathcal{E}_K} \left(\Pi_F^{p-1}(v_K - v_F), w_K - w_F \right)_F \right),$$

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

$$\sum_{\alpha=1}^2 \mu_{\alpha} \mathcal{A}_h(u_{\alpha h}, v_{\alpha h} - u_{\alpha h}) \geq \sum_{\alpha=1}^2 \sum_{K \in \mathcal{T}_h} (f_{\alpha}|_K, v_{\alpha h}|_K - u_{\alpha h}|_K)_K \quad \forall \mathbf{v}_h = (v_{1h}, v_{2h}) \in \mathcal{K}_{gh}^p \quad (\text{DR})$$

Well-posed problem (Lions–Stampacchia)

HHO without static condensation:

$$\mathbb{E} := \begin{bmatrix} \mu_1 \mathbb{S}_{CC} & \mu_1 \mathbb{S}_{CF} & \mathbf{0} & \mathbf{0} & -\mathbb{I}_d \\ \mu_1 \mathbb{S}_{FC} & \mu_1 \mathbb{S}_{FF} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mu_2 \mathbb{S}_{CC} & \mu_2 \mathbb{S}_{CF} & \mathbb{I}_d \\ \mathbf{0} & \mathbf{0} & \mu_2 \mathbb{S}_{FC} & \mu_2 \mathbb{S}_{FF} & \mathbf{0} \end{bmatrix}, \quad \mathbf{F} := \begin{bmatrix} \mathbf{F}_1 \\ \mathbf{0} \\ \mathbf{F}_2 \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{x}_h := \begin{bmatrix} \mathbf{x}_{1h}^C \\ \mathbf{x}_{1h}^F \\ \mathbf{x}_{2h}^C \\ \mathbf{x}_{2h}^F \\ \mathbf{x}_{3h} \end{bmatrix}.$$

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Static condensation procedure: Later, need the semismooth resolution!

Outline

- 1 Introduction
- 2 Model problem and discretization
- 3 Semismooth Newton and first numerical results
- 4 A posteriori analysis
- 5 Extension to unsteady problems
- 6 Conclusion

C-functions

Definition

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

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

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The C-function is not Fréchet differentiable.

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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: $\mathbf{x}_h^0 := (\mathbf{x}_{1h}^0, \mathbf{x}_{2h}^0, \mathbf{x}_{3h}^0)^T \in \mathbb{R}^{3m}$, on step $k \geq 1$, one looks for $\mathbf{x}_h^k \in \mathbb{R}^{3m}$ such that

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

where

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

Inexact solver initial vector: $\mathbf{x}_h^{k,0} \in \mathbb{R}^{3m}$, often taken as $\mathbf{x}_h^{k,0} = \mathbf{x}_h^{k-1}$, this yields on step $i \geq 1$ an approximation $\mathbf{x}_h^{k,i}$ to $\mathbf{x}_h^k$ satisfying

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

where $\mathbf{R}_h^{k,i} \in \mathbb{R}^{3m}$ is the algebraic residual vector.

Newton-min convergence

Theorem

The Newton-min Algorithm is well defined. Moreover, if the first guess $\mathbf{X}_h^0$ is close enough to the solution $\mathbf{X}_h^$ to the nonlinear system, then the sequence $(\mathbf{X}_h^k)_{k \geq 1}$ converges to $\mathbf{X}_h^*$ with a finite number of semismooth iterations and the local convergence is quadratic. In other words,*

$$\left\| \mathbf{X}_h^k - \mathbf{X}_h^* \right\|_2 \leq K \left\| \mathbf{X}_h^{k-1} - \mathbf{X}_h^* \right\|_2^2,$$

HHO with static condensation

- Express the cell components from the face components by local problems
- By substitution derive from the global system the edge unknowns problem
- Recover the solution attached to the cells
- Important computational speed-up

	$\mathbb{P}_1$ DOFs		$\mathbb{P}_2$ DOFs		$\mathbb{P}_3$ DOFs		$\mathbb{P}_4$ DOFs	
Mesh	no SC	SC	no SC	SC	no SC	SC	no SC	SC
$\mathcal{T}_0$	752	176	1504	352	2448	528	3584	704
$\mathcal{T}_1$	3040	736	6080	1472	9888	2208	14464	2944
$\mathcal{T}_2$	12224	3008	24448	6016	39744	9024	58112	12032
$\mathcal{T}_3$	49024	12160	98048	24320	159360	36480	232960	48640
$\mathcal{T}_4$	196352	48896	392704	97792	638208	146688	932864	195584

Numerical experiments

- unit square domain $\Omega := (0, 1) \times (0, 1)$
- We compare the performance of FEM and HHO

First test case

$$u_1(r) := -u_2(r) := \begin{cases} (r^2 - R^2)^N & \text{if } r \geq R, \\ 0 & \text{otherwise,} \end{cases} \quad \lambda(r) := \begin{cases} 0 & \text{if } r \geq R, \\ 1000r^3(R^2 - r^2)^3 & \text{otherwise,} \end{cases}$$

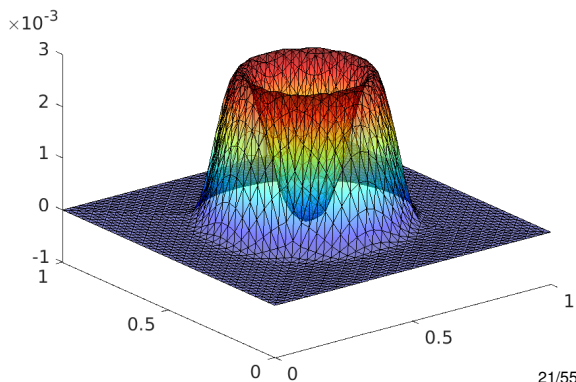
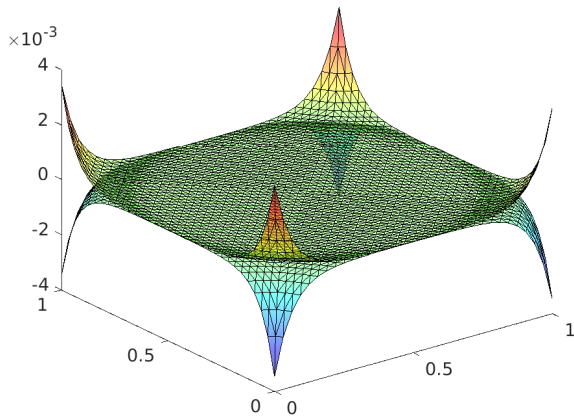
- $r := \sqrt{(x - 0.5)^2 + (y - 0.5)^2}$: distance to the center of the domain,
- $R := 1/3$: radius of the disk where contact occurs,
- $N := 6$

This solution is associated to the right-hand sides f_1 and f_2 defined by

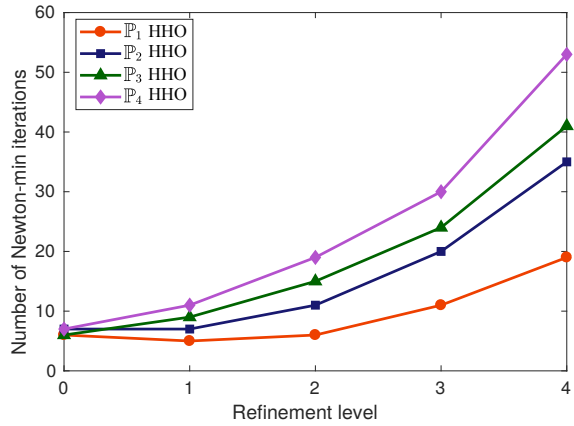
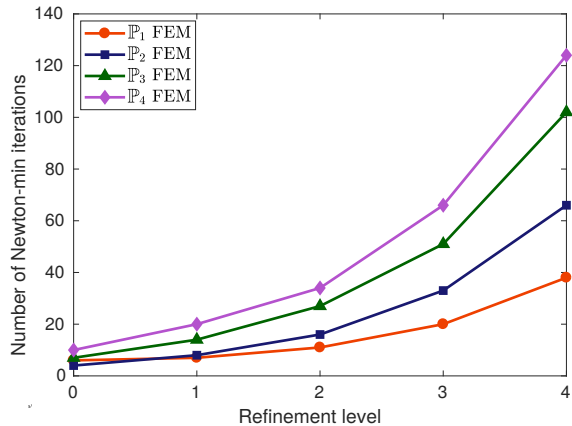
$$f_1(r) := -f_2(r) := \begin{cases} -4N(r^2 - R^2)^{N-2}(Nr^2 - R^2) & \text{if } r \geq R, \\ -1000r^3(R^2 - r^2)^3 & \text{otherwise.} \end{cases}$$

For both schemes, the errors are reported in the energy norm

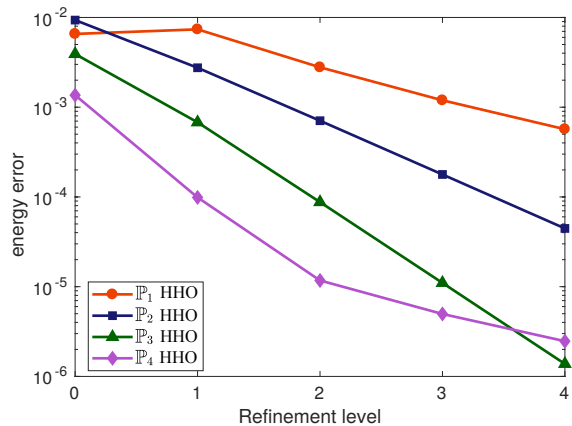
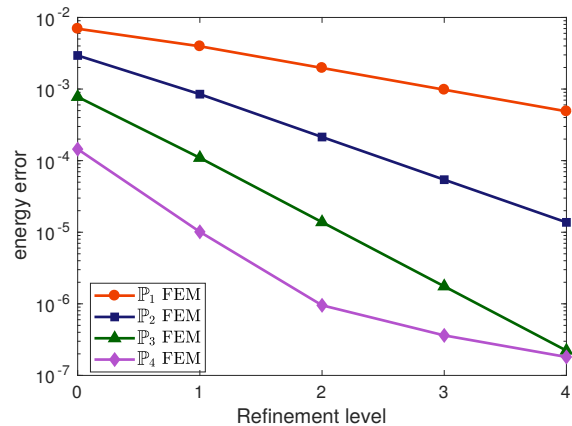
$$\| \mathbf{u} - \mathbf{u}_h \|_{\Omega} := \left(\sum_{K \in \mathcal{T}_h} \mu_1 \| \nabla(u_1 - u_{1K}) \|_{L^2(K)}^2 + \mu_2 \| \nabla(u_2 - u_{2K}) \|_{L^2(K)}^2 \right)^{\frac{1}{2}},$$



Number of Newton-min iterations



Convergence

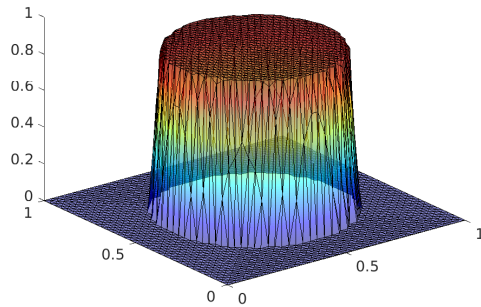
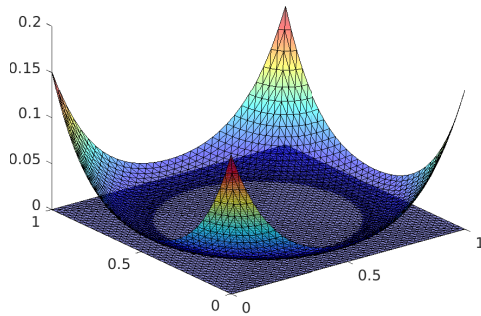


A second test case

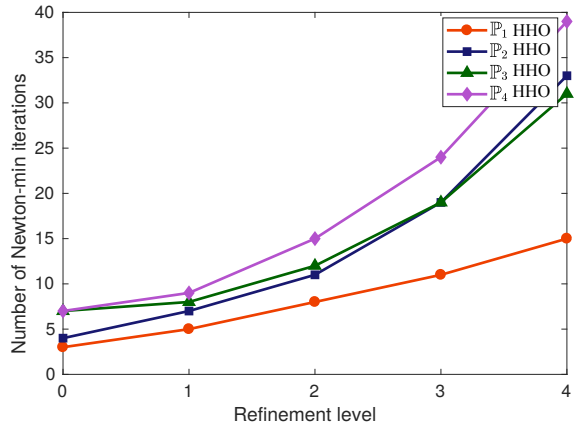
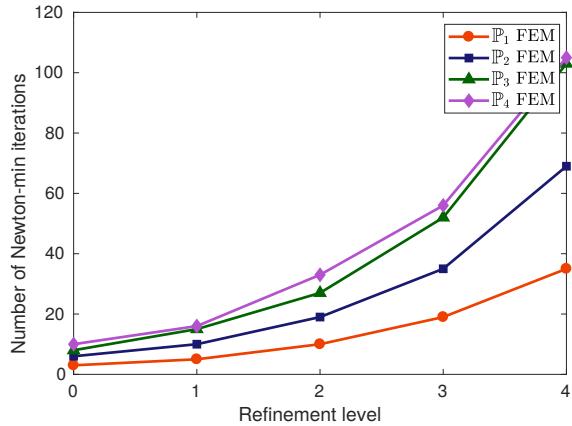
$$u_1(r) := \begin{cases} 0 & \text{if } r \leq R, \\ (r^2 - R^2)^2 & \text{if } r > R, \end{cases} \quad u_2(r) := 0, \quad \lambda(r) := \begin{cases} 1 & \text{if } r \leq R, \\ 0 & \text{if } r > R, \end{cases}$$

This solution is associated to the right-hand sides f_1 and f_2 given by

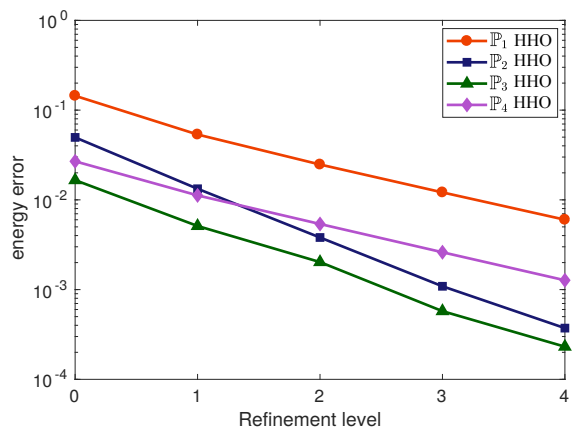
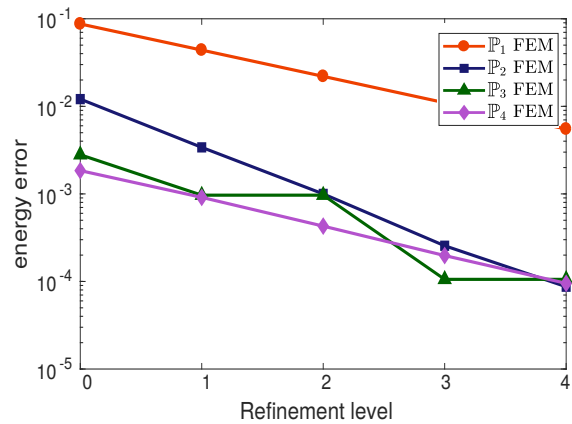
$$f_1(r) := \begin{cases} -8R^2 & \text{if } r \leq R, \\ 8R^2 - 16r^2 & \text{if } r > R, \end{cases} \quad f_2(r) := \begin{cases} 8R^2 & \text{if } r \leq R, \\ 0 & \text{if } r > R. \end{cases}$$



Number of Newton-min iterations



Convergence



Outline

- 1 Introduction
- 2 Model problem and discretization
- 3 Semismooth Newton and first numerical results
- 4 A posteriori analysis**
- 5 Extension to unsteady problems
- 6 Conclusion

A posteriori analysis for finite elements

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

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

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- $\eta_K(\mathbf{u}_h^{k,i}) \leq \text{local error} + \underbrace{\text{local contact term}}_{\text{typically very small}}$: 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:

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

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Flux reconstruction:

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

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Decomposition of the flux:

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

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Algebraic error flux reconstruction:

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

Papež, Růde, Vohralík and Wohlmuth (2020).

Component flux reconstruction

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

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Discretization flux reconstruction:

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

Estimators

Violations of physical properties of the numerical solution

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

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

Flux estimator:

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

Residual estimator:

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

Violations of the complementarity constraints

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p = 1: at convergence:

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

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

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Contact estimator:

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

Violations of the complementarity constraints

p = 1: at convergence:

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

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

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

Theorem (A posteriori error estimate)

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

Theorem (A posteriori error estimate)

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

Corollary (Distinction of the error components)

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

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Adaptive algorithm

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

Stop linear solver

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

Stop nonlinear solver

Theorem (A posteriori error estimate)

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

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Adaptive algorithm

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

Stop linear solver

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

Stop nonlinear solver

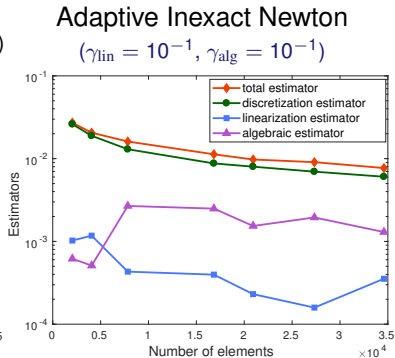
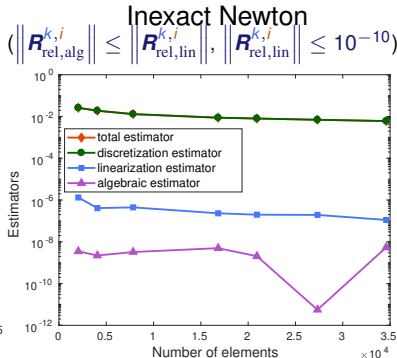
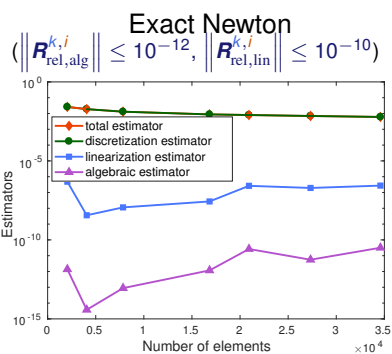
Theorem (Local efficiency under adaptive stopping criteria : $p=1$)

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

Numerical experiments

Numerical experiments $\mathbb{P}_2$

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



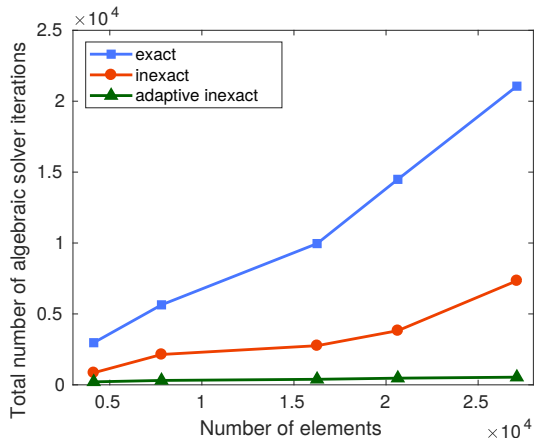
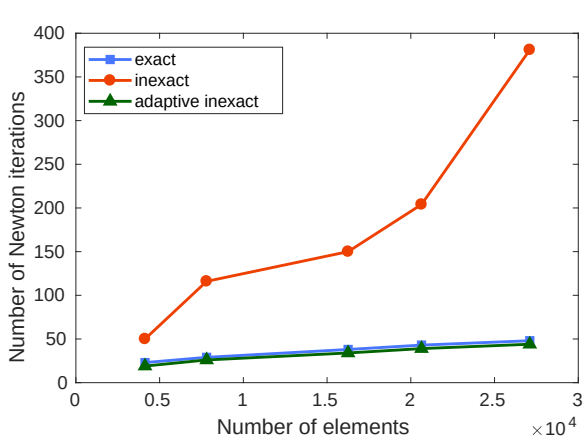
Precision is preserved for adaptive inexact semismooth Newton method.

Figure 10 is a log-linear plot showing the convergence of various estimators and residuals over algebraic iterations. The y-axis is logarithmic, ranging from 10^{-15} to 10^5 . The x-axis is linear, ranging from 0 to 700. The plot includes six data series:

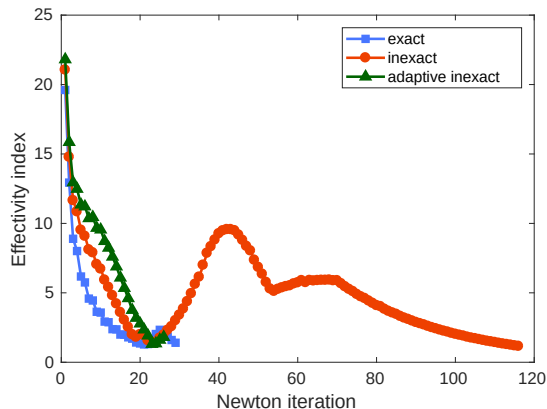
- total estimator** (red diamonds): Constant at approximately 10^2 .
- discretization estimator** (green circles): Constant at approximately 10^1 .
- linearization estimator** (blue squares): Constant at 10^0 .
- linearization residual** (black stars): Constant at 10^0 .
- algebraic estimator** (magenta triangles): Decreases linearly on the log scale, reaching approximately 10^{-10} at 650 iterations.
- algebraic residual** (brown stars): Decreases linearly on the log scale, reaching approximately 10^{-11} at 650 iterations.



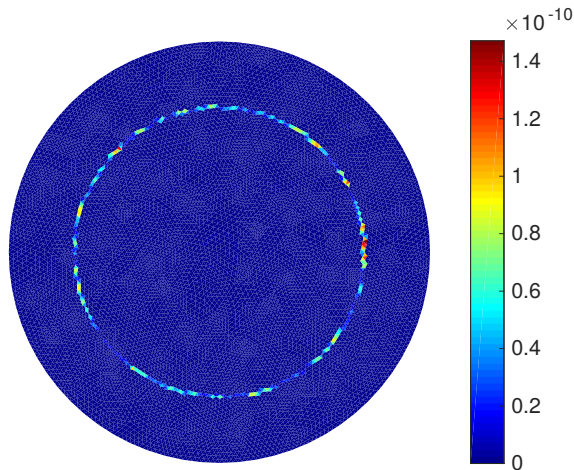
Overall performance



Effectivity indices: $I_{\text{eff}} := \frac{\eta^{k,i}}{\|u - u_h^{k,i}\|_{\Omega}}$



contact estimator



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Parabolic model problem with linear complementarity constraints

$$\begin{cases} \partial_t u_1 - \mu_1 \Delta u_1 - \lambda = f_1 & \text{in } \Omega \times]0, T[, \\ \partial_t u_2 - \mu_2 \Delta u_2 + \lambda = f_2 & \text{in } \Omega \times]0, T[, \\ u_1 - u_2 \geq 0, \quad \lambda \geq 0, \quad \lambda(u_1 - u_2) = 0 & \text{in } \Omega \times]0, T[, \\ u_1 = g_1 & \text{on } \partial\Omega \times]0, T[, \\ u_2 = g_2 & \text{on } \partial\Omega \times]0, T[, \\ u_1(\mathbf{x}, 0) = u_1^0(\mathbf{x}), \quad u_2(\mathbf{x}, 0) = u_2^0(\mathbf{x}), \quad u_1^0(\mathbf{x}) - u_2^0(\mathbf{x}) \geq 0 & \text{in } \Omega. \end{cases}$$

Parabolic model problem with linear complementarity constraints

$$\left\{ \begin{array}{ll} \partial_t u_1 - \mu_1 \Delta u_1 - \lambda = f_1 & \text{in } \Omega \times]0, T[, \\ \partial_t u_2 - \mu_2 \Delta u_2 + \lambda = f_2 & \text{in } \Omega \times]0, T[, \\ u_1 - u_2 \geq 0, \quad \lambda \geq 0, \quad \lambda(u_1 - u_2) = 0 & \text{in } \Omega \times]0, T[, \\ u_1 = g_1 & \text{on } \partial\Omega \times]0, T[, \\ u_2 = g_2 & \text{on } \partial\Omega \times]0, T[, \\ u_1(\mathbf{x}, 0) = u_1^0(\mathbf{x}), \quad u_2(\mathbf{x}, 0) = u_2^0(\mathbf{x}), \quad u_1^0(\mathbf{x}) - u_2^0(\mathbf{x}) \geq 0 & \text{in } \Omega. \end{array} \right.$$

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 $(u_1, u_2, \lambda) \in L^2(0, T; H_{g_1}^1(\Omega)) \times L^2(0, T; H_{g_2}^1(\Omega)) \times L^2(0, T; \Lambda)$
- Parabolic variational inequality: $\mathbf{u} \in \mathcal{K}_g^t$

$$\mathcal{K}_g^t := \left\{ \mathbf{v} \in L^2(0, T; H_{g_1}^1(\Omega)) \times L^2(0, T; H_{g_2}^1(\Omega)), \mathbf{v}(t) \in \mathcal{K}_g \quad \text{a.e. in }]0, T[\right\}$$

Discrete complementarity problems for finite elements

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

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$$\begin{aligned}
 \mathbb{E}^n \mathbf{X}_h^n &= \mathbf{F}^n, \\
 \mathbf{X}_{1h}^n - \mathbf{X}_{2h}^n &\geq \mathbf{0} \quad \mathbf{X}_{3h}^n \geq \mathbf{0} \quad (\mathbf{X}_{1h}^n - \mathbf{X}_{2h}^n) \cdot \mathbf{X}_{3h}^n = 0.
 \end{aligned}
 \quad
 \mathbb{E}^n := \begin{bmatrix}
 \mu_1 \mathbb{S} + \frac{1}{\Delta t_n} \mathbb{M} & \mathbf{0} & -\mathbb{D} \\
 \mathbf{0} & \mu_2 \mathbb{S} + \frac{1}{\Delta t_n} \mathbb{M} & +\mathbb{D}
 \end{bmatrix}$$

Discrete complementarity problems for finite elements

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Employing a C-function our problem reads

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

Inexact semismooth Newton method:

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

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

$$\| \mathbf{u} - \mathbf{u}_{h\tau} \|_{L^2(0,T;H_0^1(\Omega))}^2 + \| \mathbf{u} - \mathbf{z} \|_{L^2(0,T;H_0^1(\Omega))}^2 + \| (\mathbf{u} - \mathbf{u}_{h\tau})(\cdot, T) \|_{\Omega}^2 \leq 5\eta^2$$

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

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

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

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

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 & \| \mathbf{u} - \mathbf{u}_{h\tau} \|_{L^2(0,T;H_0^1(\Omega))}^2 + \| \mathbf{u} - \mathbf{z} \|_{L^2(0,T;H_0^1(\Omega))}^2 + \| (\mathbf{u} - \mathbf{u}_{h\tau})(\cdot, T) \|_{\Omega}^2 \leq 5\eta^2 \\
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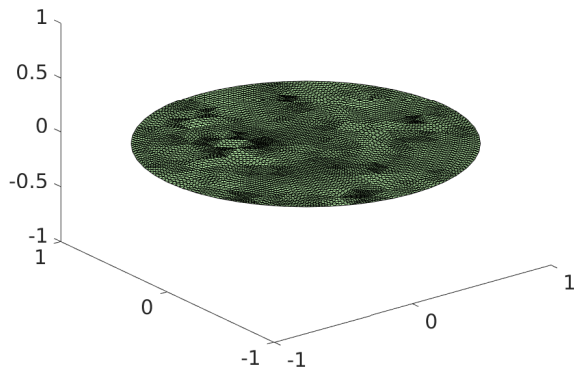
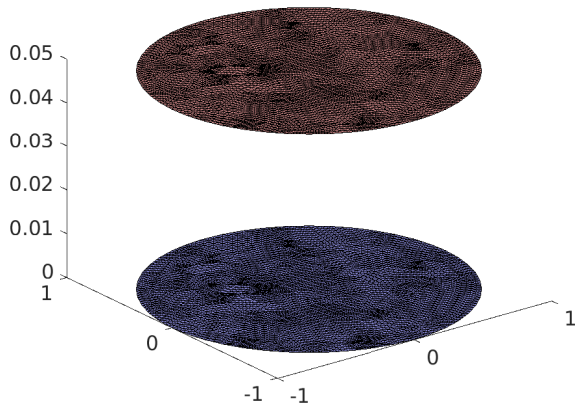
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Lemma

$$\| \mathbf{u} - \mathbf{z} \|_{L^2(0,T;H_0^1(\Omega))} \lesssim \left(\int_0^T \sum_{\alpha=1}^2 \| \partial_t(u_{\alpha} - u_{\alpha h\tau}) \|_{H^{-1}(\Omega)}^2 (t) dt \right)^{\frac{1}{2}} + \left(\int_0^T \| \lambda_{h\tau} - \lambda \|_{H^{-1}(\Omega)}^2 (t) dt \right)^{\frac{1}{2}}$$

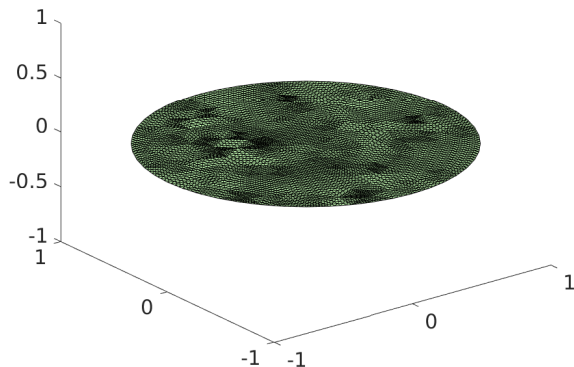
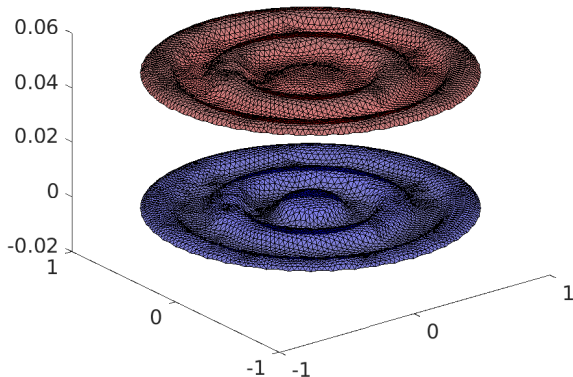
Numerical experiments $p = 1$

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



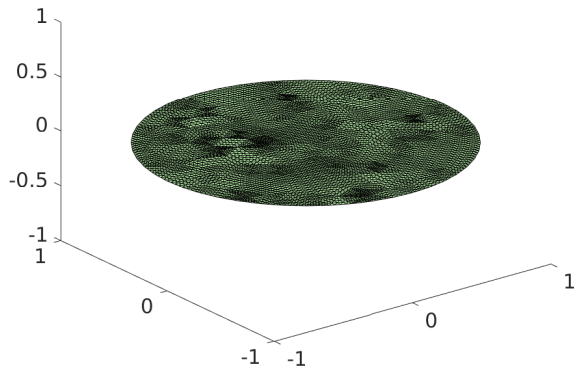
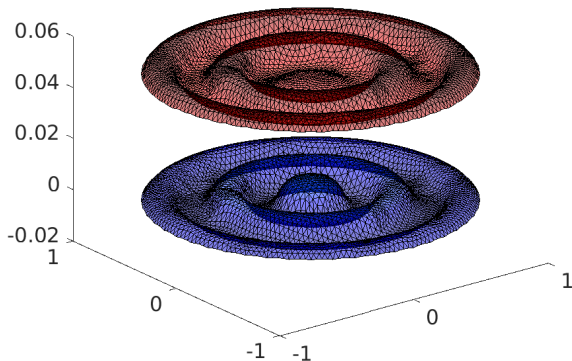
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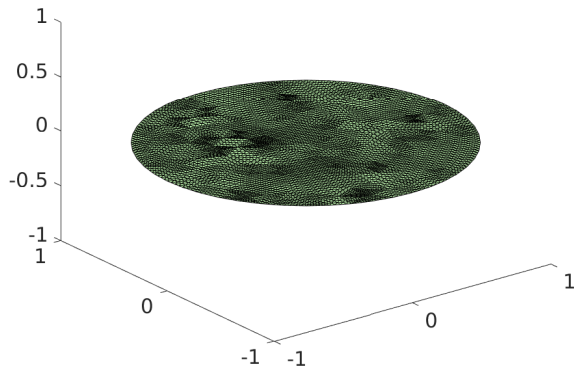
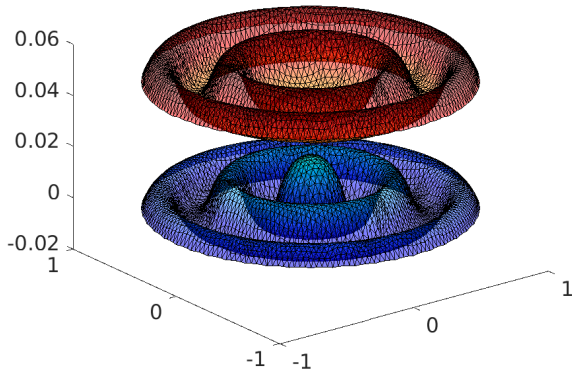
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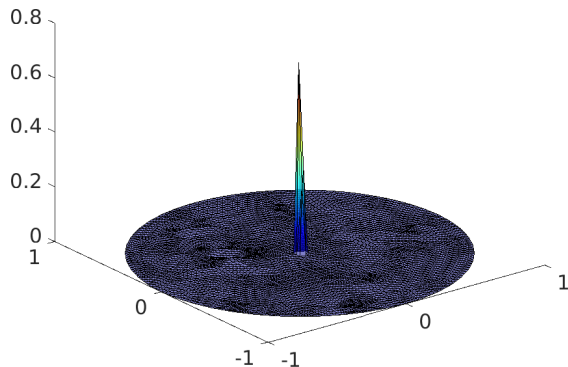
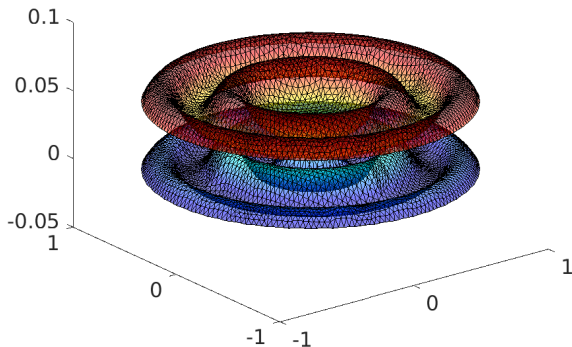
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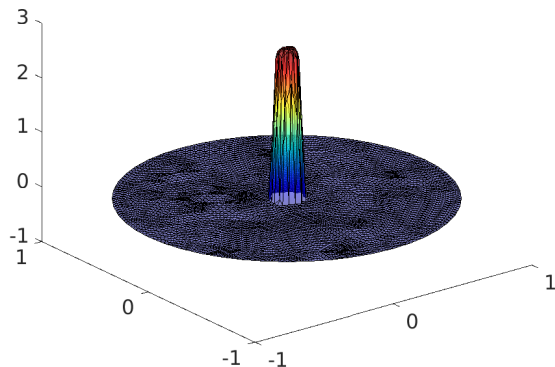
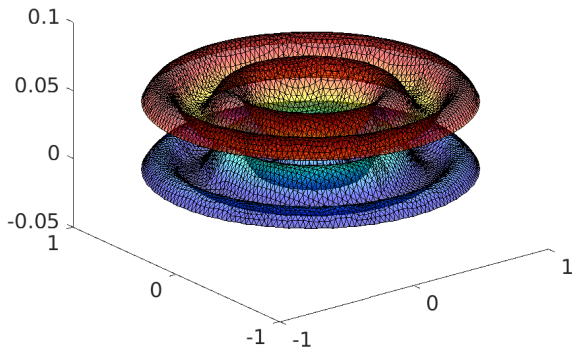
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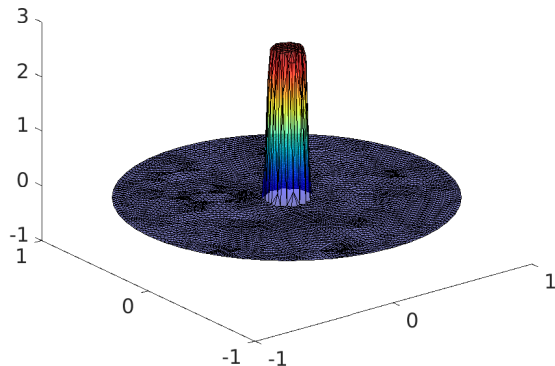
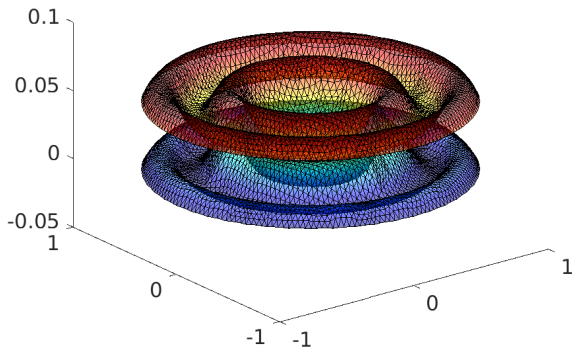
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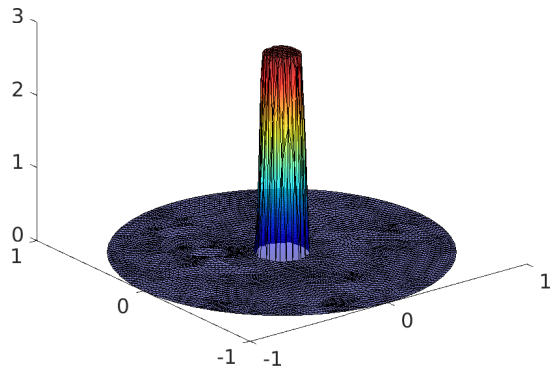
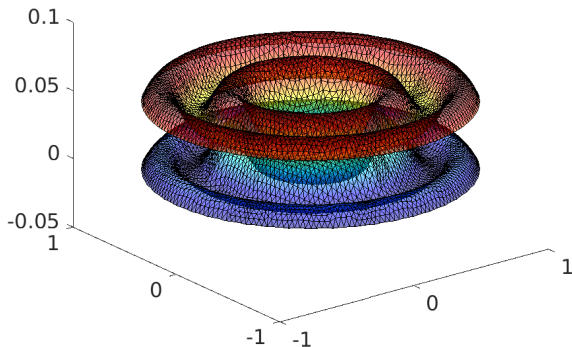
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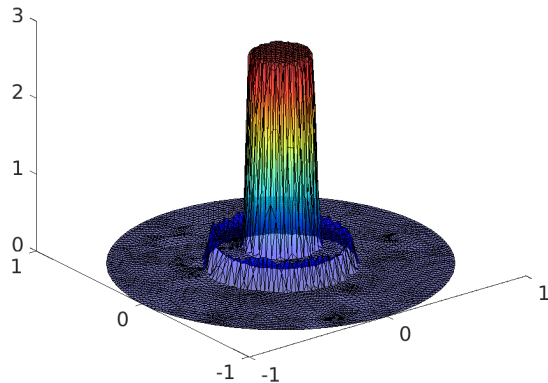
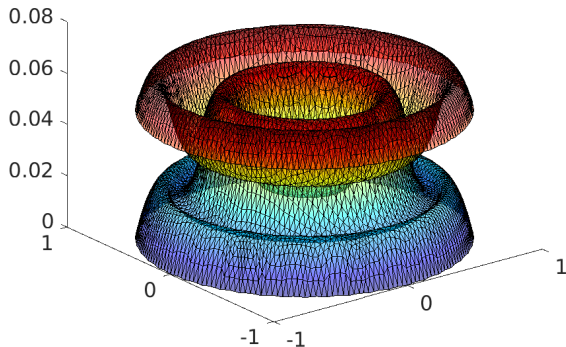
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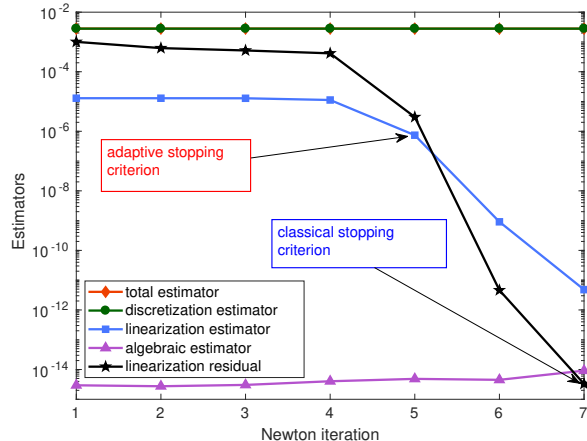
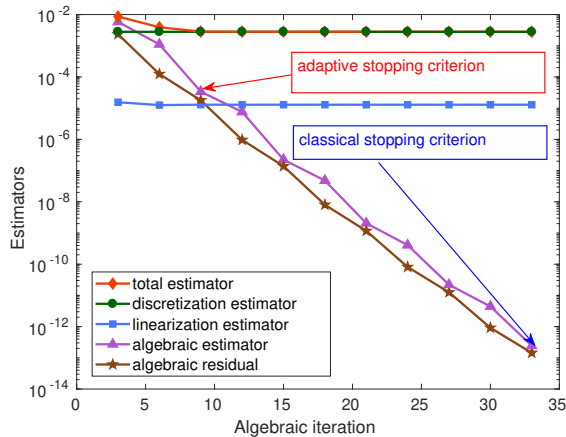
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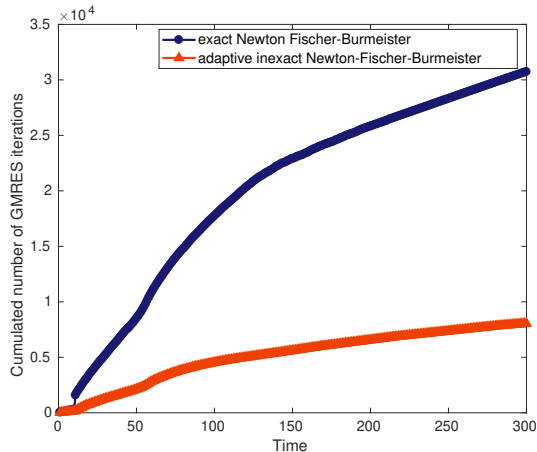
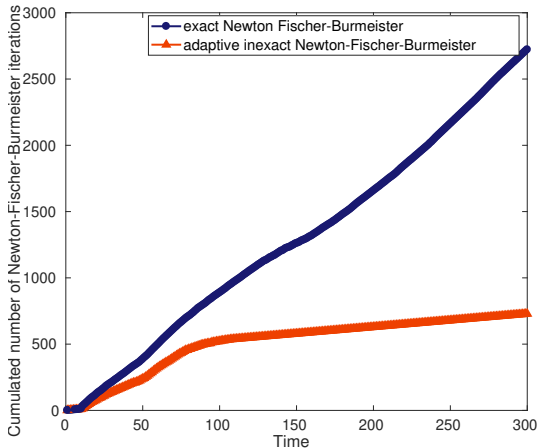


Newton–Fischer–Burmeister adaptivity

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



Newton–Fischer–Burmeister performance



J. DABAGHI, V. MARTIN, M. VOHRALÍK, A posteriori estimates distinguishing the error components and adaptive stopping criteria for numerical approximations of parabolic variational inequalities. *Computer methods in applied mechanics and engineering* (2020).

Two-phase flow with phase appearance and disappearance

Storage of radioactive wastes in deep geological layers

$$\left\{ \begin{array}{l} \partial_t l_w(\mathbf{S}^l) + \nabla \cdot \Phi_w(\mathbf{S}^l, \mathbf{P}^l, \chi_h^l) = Q_w, \\ \partial_t l_h(\mathbf{S}^l, \mathbf{P}^l, \chi_h^l) + \nabla \cdot \Phi_h(\mathbf{S}^l, \mathbf{P}^l, \chi_h^l) = Q_h, \\ 1 - \mathbf{S}^l \geq 0, H[\mathbf{P}^l + P_{cp}(\mathbf{S}^l)] - \beta_1 \chi_h^l \geq 0, [1 - \mathbf{S}^l] \cdot [H[\mathbf{P}^l + P_{cp}(\mathbf{S}^l)] - \beta_1 \chi_h^l] = 0 \end{array} \right.$$

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Unknowns: liquid saturation $\mathbf{S}^l$, liquid pressure $\mathbf{P}^l$, mole fraction of liquid hydrogen χ_h^l

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Nonlinear complementarity constraints: $\Rightarrow$ Phase change

Discretization by the finite volume method

Numerical solution:

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

Discretization of the water equation

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

Discretization by the finite volume method

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

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

Discrete complementarity problem and semismoothness

Discretization of the nonlinear complementarity constraints

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

The discretization reads

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

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

- 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

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The discretization reads

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

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

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

Weak solution

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

Assumption: There exists a unique weak solution satisfying

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

Error measure

1 Dual norm of the residual for the components

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

2 Residual for the constraints

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

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

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

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

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Post-processing

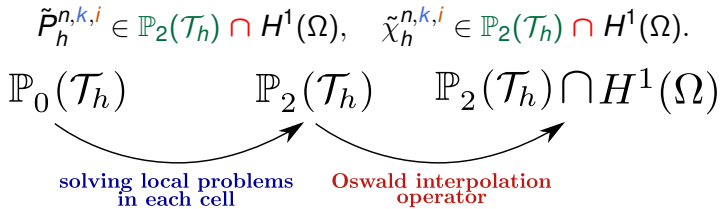
The discrete liquid pressure and discrete molar fraction **are piecewise constant**

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

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:



A posteriori error estimate distinguishing the error components

Theorem

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

Construction of the estimators:

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

Numerical experiments

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

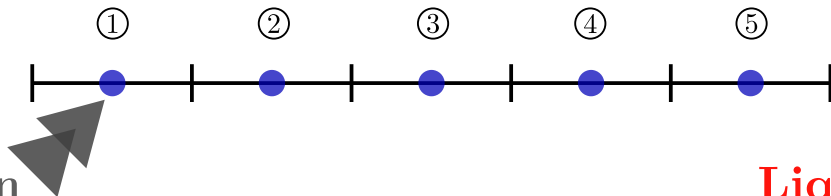
Semismooth solver: Newton-min

Iterative algebraic solver: GMRES.

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

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

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

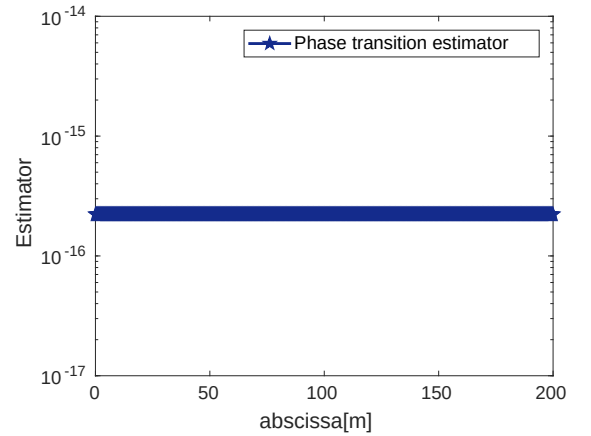
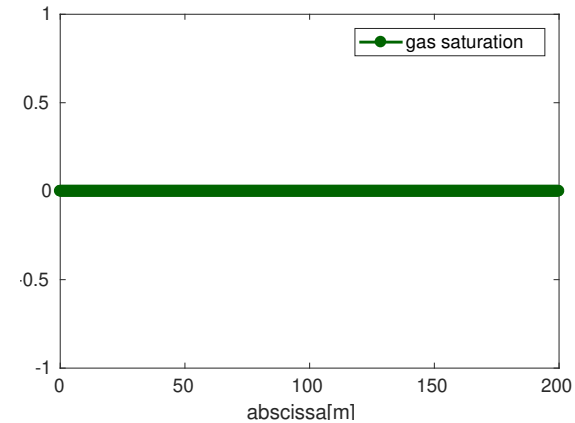


Gas injection

Liquid

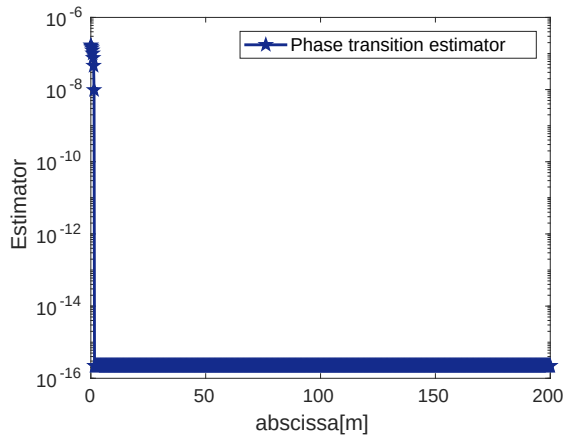
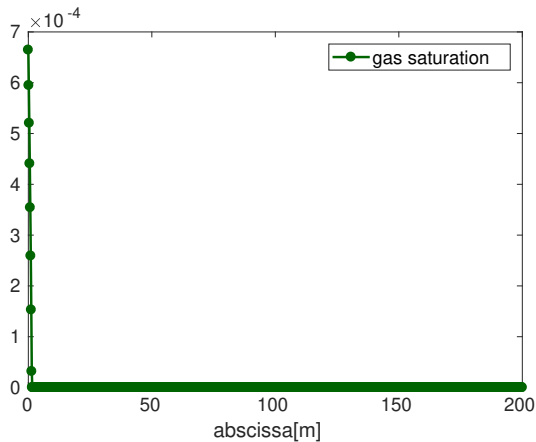
Phase transition estimator

$t = 2500$ years



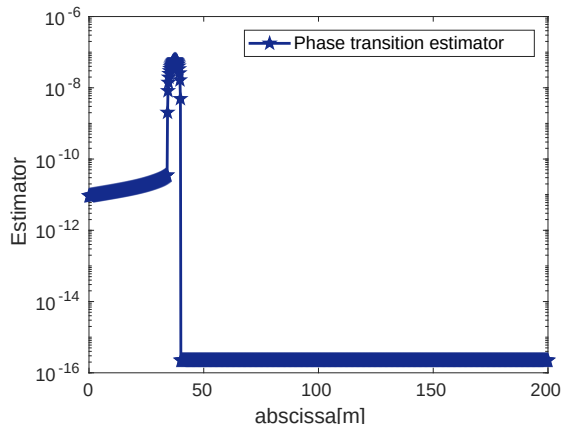
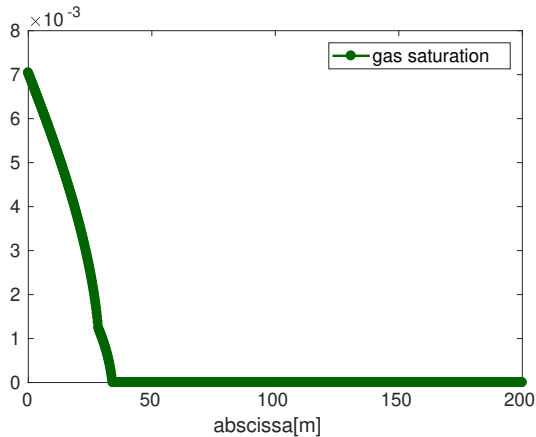
Phase transition estimator

$t = 1.25 \times 10^4$ years

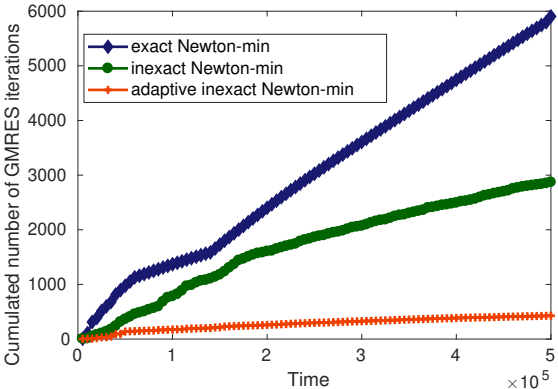
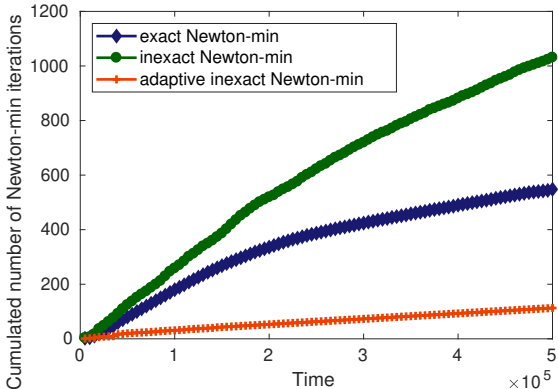


Phase transition estimator

$t = 4.25 \times 10^4$ years

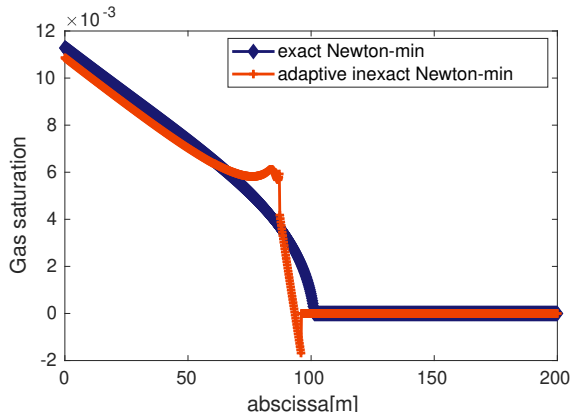


Overall performance $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

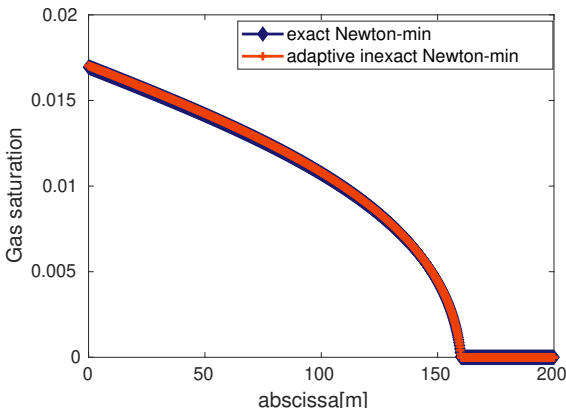


Accuracy $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years



I. BEN GHARBI, J. DABAGHI, V. MARTIN, M. VOHRALÍK, A posteriori error estimates for a compositional two-phase flow with nonlinear complementarity constraints. *Computational Geosciences* (2020).

Outline

- 1 Introduction
- 2 Model problem and discretization
- 3 Semismooth Newton and first numerical results
- 4 A posteriori analysis
- 5 Extension to unsteady problems
- 6 Conclusion**

Conclusion and perspectives

Conclusion

Conclusion and perspectives

Conclusion

- We proposed several numerical schemes for variational inequalities.
- We devised a posteriori error estimates with $\mathbb{P}_p$ finite elements distinguishing the error components.
- Adaptive stopping criteria $\Rightarrow$ reduction of the number of iterations.
- Our a posteriori analysis works for unsteady problems (Two-phase flow with phase transition).

Conclusion and perspectives

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- We proposed several numerical schemes for variational inequalities.
- We devised a posteriori error estimates with $\mathbb{P}_p$ finite elements distinguishing the error components.
- Adaptive stopping criteria $\Rightarrow$ reduction of the number of iterations.
- Our a posteriori analysis works for unsteady problems (Two-phase flow with phase transition).

Perspectives

- Extension of the stationary contact problem to a hyperbolic contact problem between two vibrating membranes.
- Devise a posteriori error estimators for HHO
- Construct a posteriori error estimates for a multiphase multi compositional flow with several phase transitions.

Acknowledgements

- Martin Vohralík (INRIA Paris)
- Vincent Martin (UTC Compiègne)
- Ibtihel Ben Gharbia (IFPEN)
- Guillaume Delay (LJLL)
- Soleiman Yousef (IFPEN)
- Jean-Charles Gilbert (INRIA Paris)

Thank you for your attention

Discretization flux reconstruction:

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

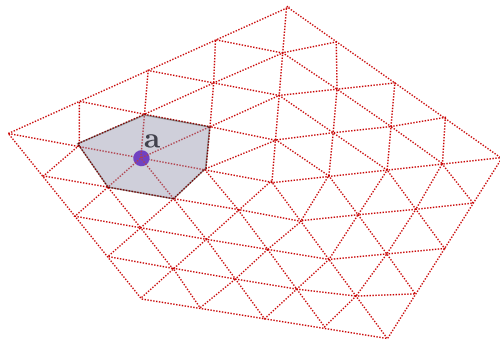
$$\tilde{g}_{\alpha h}^{k,i,a} := \left(f_\alpha - (-1)^\alpha \tilde{\lambda}_{h,a}^{k,i} - r_{\alpha h}^{k,i} \right) \psi_{h,a} - \mu_\alpha \nabla u_{\alpha h}^{k,i} \cdot \nabla \psi_{h,a} : \text{depends on the residual}$$

For each internal vertex $\mathbf{a} \in \mathcal{V}_h^{\text{int}}$

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

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

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



Strategy for constructing the estimators

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

Nonconformity estimator 1:

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

Nonconformity estimator 2:

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

Nonconformity estimator 3:

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

Distinguishing the error components

$p = 1$

$$\eta_{\text{disc}}^{k,i} := \left\{ \sum_{\alpha=1}^2 \sum_{K \in \mathcal{T}_h} \left(\eta_{\text{disc},K,\alpha}^{k,i} + \eta_{\text{osc},K,\alpha} \right)^2 \right\}^{\frac{1}{2}} + \left\{ \left| \sum_{K \in \mathcal{T}_h} \eta_{C,K}^{k,i,\text{pos}} \right| \right\}^{\frac{1}{2}}$$

$$\eta_{\text{lin}}^{k,i} := \eta_{\text{nonc},1}^{k,i} + \eta_{\text{nonc},2}^{k,i} + \left(\eta_{\text{nonc},3}^{k,i} \right)^{\frac{1}{2}}, \quad \eta_{\text{alg}}^{k,i} := \left\{ \sum_{\alpha=1}^2 \sum_{K \in \mathcal{T}_h} \left\| \mu_{\alpha}^{-\frac{1}{2}} \boldsymbol{\sigma}_{\alpha h,\text{alg}}^{k,i} \right\|_K^2 \right\}^{\frac{1}{2}}$$

$p \geq 2$

$$\eta_{\text{disc}}^{k,i} := \left\{ \sum_{\alpha=1}^2 \sum_{K \in \mathcal{T}_h} \left(\eta_{\text{disc},K,\alpha}^{k,i} + \eta_{\text{osc},K,\alpha} \right)^2 \right\}^{\frac{1}{2}} + \left\{ 2 \left| \left(\lambda_h^{k,i,\text{pos}} - \lambda_h^{k,i}, u_{1h}^{k,i} - u_{2h}^{k,i} \right)_{\Omega} \right| \right\}^{\frac{1}{2}}$$

$$+ \left\| \tilde{\mathbf{s}}_h^{k,i} - \mathbf{s}_h^{k,i} \right\| + C_{\Omega,\mu} \left\| \lambda_h^{k,i,\text{neg}} - \tilde{\lambda}_h^{k,i,\text{neg}} \right\|_{\Omega} + \left(2 C_{\Omega,\mu} \left\| \lambda_h^{k,i,\text{pos}} \right\| \right)^{\frac{1}{2}} \left\| \tilde{\mathbf{s}}_h^{k,i} - \mathbf{s}_h^{k,i} \right\|^{\frac{1}{2}}$$

$$\eta_{\text{lin}}^{k,i} := \left\| \mathbf{s}_h^{k,i} - \mathbf{u}_h^{k,i} \right\| + C_{\Omega,\mu} \left\| \tilde{\lambda}_h^{k,i,\text{neg}} \right\|_{\Omega} + \left(2 C_{\Omega,\mu} \left\| \lambda_h^{k,i,\text{pos}} \right\| \right)^{\frac{1}{2}} \left\| \mathbf{s}_h^{k,i} - \mathbf{u}_h^{k,i} \right\|^{\frac{1}{2}}$$

$$+ \left\{ 2 \left| \left(\lambda_h^{k,i}, u_{1h}^{k,i} - u_{2h}^{k,i} \right)_{\Omega} \right| \right\}^{\frac{1}{2}}$$

Parabolic weak formulation

Weak formulation: For $(f_1, f_2) \in [L^2(0, T; L^2(\Omega))]^2$, $\mathbf{u}^0 \in H_g^1(\Omega) \times H_0^1(\Omega)$, find $(u_1, u_2, \lambda) \in L^2(0, T; H_g^1(\Omega)) \times L^2(0, T; H_0^1(\Omega)) \times L^2(0, T; \Lambda)$ s.t. $\partial_t u_\alpha \in L^2(0, T; H^{-1}(\Omega))$, and satisfying $\forall t \in]0, T[$

$$\sum_{\alpha=1}^2 \langle \partial_t u_\alpha(t), v_\alpha \rangle + \sum_{\alpha=1}^2 \mu_\alpha (\nabla u_\alpha(t), \nabla v_\alpha)_\Omega - (\lambda(t), v_1 - v_2)_\Omega = \sum_{\alpha=1}^2 (f_\alpha, v_\alpha)_\Omega, \quad \forall \mathbf{v} \in [H_0^1(\Omega)]^2$$

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

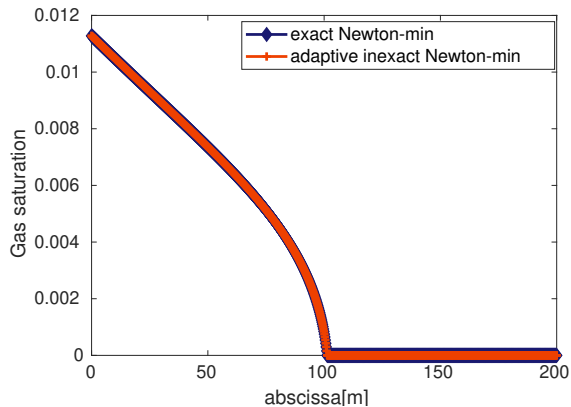
Discrete formulation: Given $(u_{1h}^0, u_{2h}^0) \in \mathcal{K}_{gh}^p$, search $(u_{1h}^n, u_{2h}^n, \lambda_h^n) \in X_{gh}^p \times X_{0h}^p \times \Lambda_h^p$ such that for all $(z_{1h}, z_{2h}, \chi_h) \in X_{0h}^p \times X_{0h}^p \times \Lambda_h^p$

$$\frac{1}{\Delta t_n} \sum_{\alpha=1}^2 (u_{\alpha h}^n - u_{\alpha h}^{n-1}, z_{\alpha h})_\Omega + \sum_{\alpha=1}^2 \mu_\alpha (\nabla u_{\alpha h}^n, \nabla z_{\alpha h})_\Omega - \langle \lambda_h^n, z_{1h} - z_{2h} \rangle_h = \sum_{\alpha=1}^2 (f_\alpha, z_{\alpha h})_\Omega,$$

$$\langle \chi_h - \lambda_h^n, u_{1h}^n - u_{2h}^n \rangle_h \geq 0$$

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

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years

