

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

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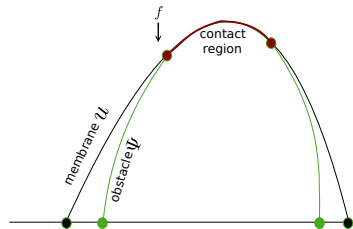
$$\text{Find } \mathbf{u} \in \mathcal{K}_g \quad a(\mathbf{u}, \mathbf{v} - \mathbf{u}) \geq \ell(\mathbf{v} - \mathbf{u}) \quad \forall \mathbf{v} \in \mathcal{K}_g$$

Application to several problems in contact mechanics

Obstacle problem: Find $\mathbf{u} \in \mathcal{K}_g := \{v \in H^1(\Omega) \text{ s.t. } v = g \text{ on } \partial\Omega, \text{ and } v \geq \Psi \text{ in } \Omega\}$ 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
- $f \in L^2(\Omega)$: force acting on the membrane
- $g \in H^{\frac{1}{2}}(\partial\Omega)$: Dirichlet boundary datum for \mathbf{u}



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

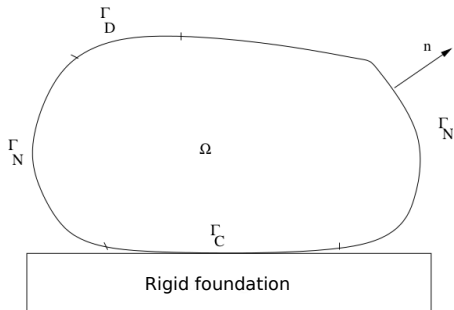
Γ_D : Dirichlet boundary conditions, Γ_N : Neumann boundary conditions

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

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

- $\mathbf{g} \in [H^{\frac{1}{2}}(\Gamma_D)]^2$: 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 elastic solid
- $\sigma(\mathbf{u})$: stress tensor
- ϵ : strain tensor
- $\sigma(\mathbf{u}) = \mathbb{A}\epsilon(\mathbf{u})$ where \mathbb{A} is the fourth-order elasticity tensor

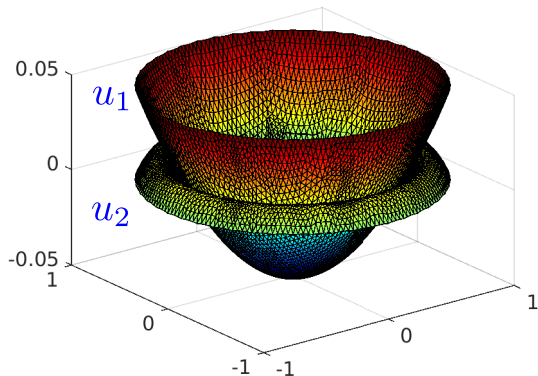


Contact between two membranes:

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

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

- $\mu_1, \mu_2 > 0$: tensions of the membranes
- $g_1 \geq g_2$: boundary data
- $f_1 \in L^2(\Omega), f_2 \in L^2(\Omega)$: external sources



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Propose several numerical schemes

- The finite element method, the discontinuous Galerkin method, the hybrid high-order method (HHO)

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Quantify the error

- A posteriori error estimates : $\| \mathbf{u} - \mathbf{u}_h \|_{\#} \leq \eta(\mathbf{u}_h)$
- Identify each error components : numerical discretization, nonlinear algorithms, linear algorithms,...

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Save computational time

- Adaptivity

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Extension to unsteady problems?

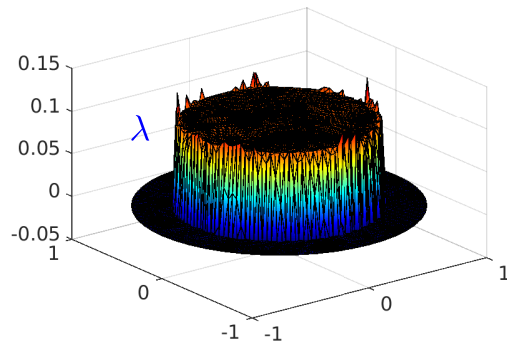
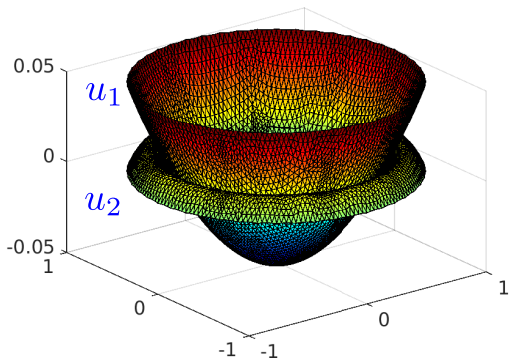
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Model problem and settings: contact between two membranes

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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other interpretation

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other interpretation

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

The finite element method

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For any $p \geq 1$

Spaces for the discretization:

$$X_{g_\alpha h}^p = \{v_h \in C^0(\bar{\Omega}), v_h|_K \in \mathbb{P}_p(K), \forall K \in \mathcal{T}_h, v_h = g_\alpha \text{ on } \partial\Omega\} \quad \mathcal{V}_d^p: \text{ set of nodes}$$

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

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

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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)

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

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

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

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

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

Saddle point formulation

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

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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

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

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

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Matrix representation of (DS2)

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

Matrix representation of (DS2)

$$u_{1h} = \sum_{l=1}^{\mathcal{N}_d^{p,int}} (\mathbf{X}_{1h})_l \underbrace{\psi_{h,\mathbf{x}_l}}_{\text{Lagrange basis}}, \quad u_{2h} = \sum_{l=1}^{\mathcal{N}_d^{p,int}} (\mathbf{X}_{2h})_l \psi_{h,\mathbf{x}_l}, \quad \lambda_h = \sum_{l=1}^{\mathcal{N}_d^{p,int}} (\mathbf{X}_{3h})_l \underbrace{\Theta_{h,\mathbf{x}_l}}_{\text{dual basis}}$$

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

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

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

Remark

The construction of Λ_h^p and the dual basis Θ_{h,\mathbf{x}_l} are essential to obtain equivalence between DS and DR

The Discontinuous Galerkin method

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Discontinuous spaces:

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

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

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The Discontinuous Galerkin method

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

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

The Discontinuous Galerkin method

Discontinuous spaces:

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

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

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$$\mathcal{A}_h(u_{\alpha h}, v_{\alpha h}) = \underbrace{\sum_{K \in \mathcal{T}_h} (\nabla u_{\alpha h}, \nabla v_{\alpha h})_K}_{\text{bilinear form}} + \underbrace{\delta_h(u_{\alpha h}, v_{\alpha h})}_{\text{consistency and stabilization terms [SIPG, NIPG]}}$$

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$$\mathcal{A}_h(u_{\alpha h}, v_{\alpha h}) = \underbrace{\sum_{K \in \mathcal{T}_h} (\nabla u_{\alpha h}, \nabla v_{\alpha h})_K}_{\text{bilinear form}} + \underbrace{\delta_h(u_{\alpha h}, v_{\alpha h})}_{\text{consistency and stabilization terms [SIPG, NIPG]}}$$

[SIPG] $\delta_h(u_{\alpha h}, v_{\alpha h}) = - \sum_{F \in \mathcal{E}_h} (\{\{\nabla v_{\alpha h}\}\}_F, \llbracket u_{\alpha h} \rrbracket_F + \{\{\nabla u_{\alpha h}\}\}_F, \llbracket v_{\alpha h} \rrbracket_F, 1)_F + \sum_{F \in \mathcal{E}_h} \frac{\gamma}{h_F} (\llbracket v_{\alpha h} \rrbracket_F, \llbracket u_{\alpha h} \rrbracket_F)$

Discrete complementarity problem

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

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

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

Discrete complementarity problem

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

Discrete complementarity problem

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

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

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

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

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

The Hybrid High-Order method

The unknowns are polynomial functions attached to the cells and the edges of the mesh.

Discontinuous spaces:

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

$$X_h^p := \prod_{K \in \mathcal{T}_h} \mathbb{P}_p(K) \times \prod_{F \in \mathcal{E}_h} \mathbb{P}_{p-1}(F), \quad X_{h,K}^p := \mathbb{P}_p(K) \times \prod_{F \in \mathcal{E}_K} \mathbb{P}_{p-1}(F)$$

$$X_{g_\alpha h}^p := \{v_h \in X_h^p \text{ s.t. } v_h = g_\alpha \text{ on } \partial\Omega\} : u_1, u_2 \quad \Lambda_h := \prod_{K \in \mathcal{T}_h} \mathbb{P}_p(K) : \lambda$$

$$\mathcal{K}_{gh}^p := \left\{ \mathbf{v}_h := (v_{1h}, v_{2h}) \in X_{g_1 h}^p \times X_{g_2 h}^p \text{ s.t. } (v_{1h} - v_{2h})|_K(\mathbf{x}_l) \geq 0 \quad \forall \mathbf{x}_l \in \mathcal{V}_K \quad \forall K \in \mathcal{T}_h \right\}$$

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

In HHO we employ two operators:

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

$$(\mathbf{G}_K(\hat{v}_K), \mathbf{q})_K := (\nabla \hat{v}_K, \mathbf{q})_K + (v_{\partial K} - \hat{v}_K, \mathbf{q} \cdot \mathbf{n}_K)_{\partial K}, \quad \forall \hat{v}_K \in X_{h,K}^p, \quad \forall \mathbf{q} \in \mathbb{P}_p(K; \mathbb{R}^2),$$

It approximates the gradient at the continuous level

- **Stabilization operator**

$$s_h(\hat{u}_h, \hat{v}_h) := \sum_{K \in \mathcal{T}_h} h_K^{-1} \left(\Pi_{\partial K}^{p-1}(u_{\partial K} - \hat{u}_K), v_{\partial K} - \hat{v}_K \right)_{\partial K}$$

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

$$\mathcal{A}_h(\hat{v}_h, \hat{w}_h) := \sum_{K \in \mathcal{T}_h} (\mathbf{G}_K(\hat{v}_K), \mathbf{G}_K(\hat{w}_K))_K + s_h(\hat{v}_h, \hat{w}_h)$$

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

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

Well-posed problem (Lions–Stampacchia)

Discrete complementarity problem

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

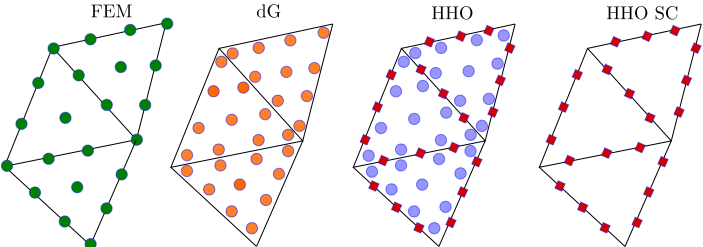
$$\mathbf{X}_{1h}^C - \mathbf{X}_{2h}^C \geq 0, \quad \mathbf{X}_{3h} \geq 0, \quad (\mathbf{X}_{1h}^C - \mathbf{X}_{2h}^C) \cdot \mathbf{X}_{3h} = 0.$$

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

HHO performance

- In dG-SIPG, \mathcal{A}_h is coercive provided that the coefficient $\gamma > 0$ (stabilization term) is large enough. The matrix associated to \mathcal{A}_h is symmetric.
- In dG-NIPG, the stability is unconditional but the matrix associated to \mathcal{A}_h is not symmetric.
- In HHO, \mathcal{A}_h is always coercive and the associated matrix is symmetric. The polynomials attached to the cells can be eliminated through a static condensation procedure.

Static condensation: It occurs within the assembly part. A linear system expressed on the faces is derived. To recover the cell unknowns we solve local problems.



The blue DOFs are eliminated!

Summary

Find u_1, u_2, λ such that

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

We proposed several numerical schemes : FEM, dG, HHO leading to a discrete system of PDEs with complementarity constraints:

$$\begin{aligned} \mathbb{E} \mathbf{X}_h &= \mathbf{F}, \\ \mathbf{X}_{1h} - \mathbf{X}_{2h} &\geq 0, \quad \mathbf{X}_{3h} \geq 0, \quad (\mathbf{X}_{1h} - \mathbf{X}_{2h}) \cdot \mathbf{X}_{3h} = 0. \end{aligned}$$

How can we solve the nonlinear problem ?

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

How to solve the nonlinear problem

$$\begin{aligned}
 \mathbb{E}\mathbf{X}_h &= \mathbf{F}, \\
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 \end{aligned}$$

Definition

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

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

C-functions

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min: $(\min\{\mathbf{x}, \mathbf{y}\})_l := \min\{\mathbf{x}_l, \mathbf{y}_l\}$, **Fischer–Burmeister:** $(f_{\text{FB}}(\mathbf{x}, \mathbf{y}))_l := \sqrt{\mathbf{x}_l^2 + \mathbf{y}_l^2} - \mathbf{x}_l - \mathbf{y}_l$

C-functions

How to solve the nonlinear problem

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

C-functions

How to solve the nonlinear problem

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

The C-function is not Fréchet differentiable. We 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 semismooth Newton method

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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,*

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



J. DABAGHI, G. DELAY, A unified framework for high-order numerical discretizations of variational inequalities. *Computers & Mathematics with Applications* (2021).

Numerical experiments

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

First test case

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

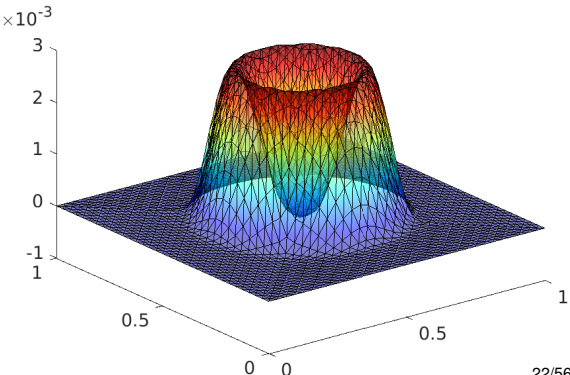
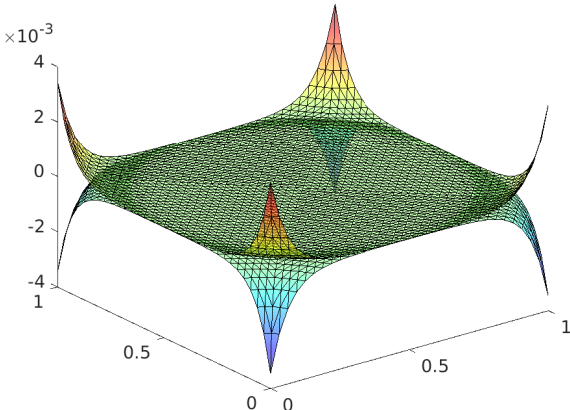
- $r := \sqrt{(x - 0.5)^2 + (y - 0.5)^2}$: distance to the center of the domain,
- $R := 1/3$: radius of the disk where contact occurs,
- $N := 6$

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

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

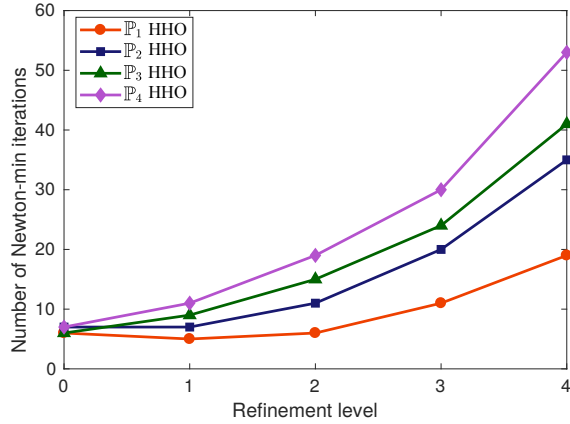
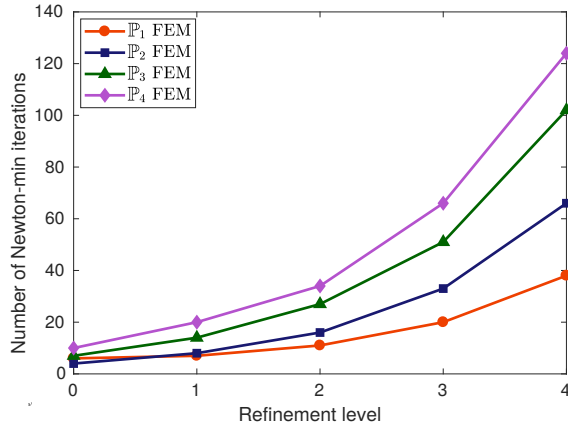


HHO with static condensation

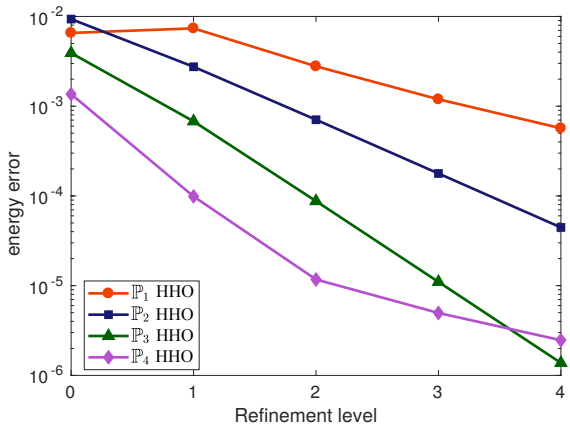
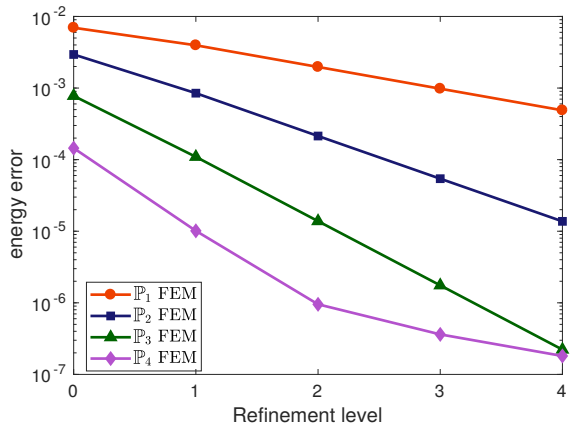
Mesh	\mathbb{P}_1 DOFs		\mathbb{P}_2 DOFs		\mathbb{P}_3 DOFs		\mathbb{P}_4 DOFs	
	no SC	SC	no SC	SC	no SC	SC	no SC	SC
\mathcal{T}_0	752	176	1504	352	2448	528	3584	704
\mathcal{T}_1	3040	736	6080	1472	9888	2208	14464	2944
\mathcal{T}_2	12224	3008	24448	6016	39744	9024	58112	12032
\mathcal{T}_3	49024	12160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

- Important reduction of the system size

Number of Newton-min iterations



Convergence

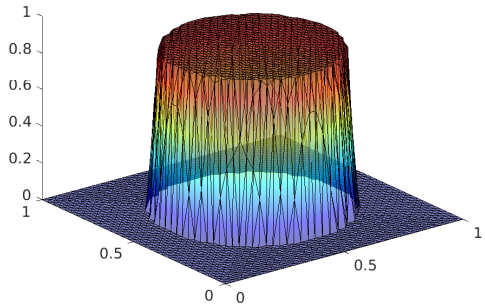
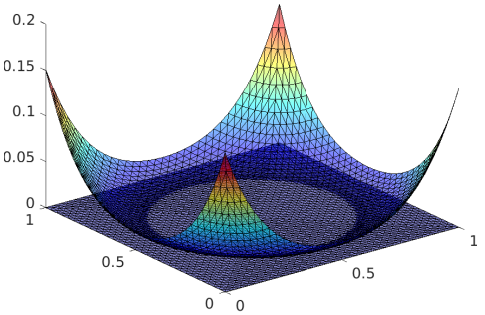


A second test case

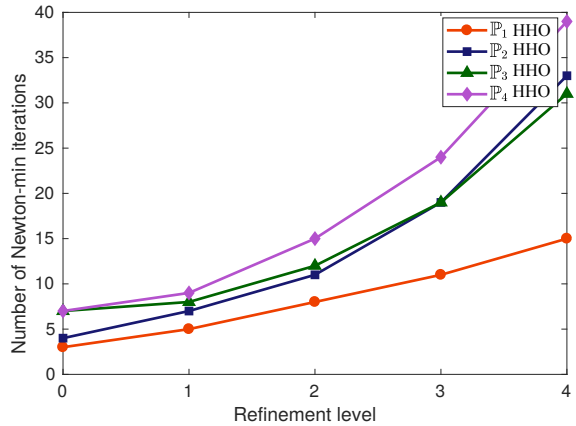
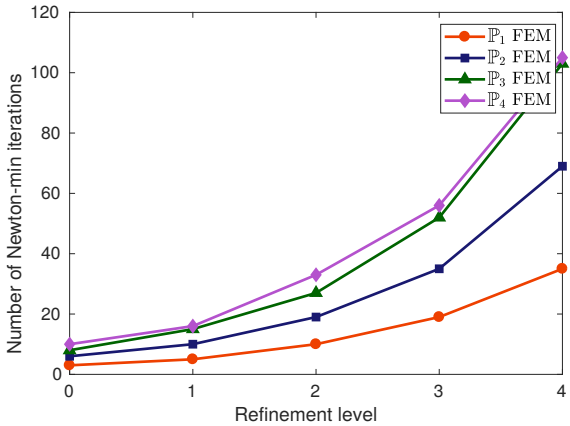
$$u_1(r) := \begin{cases} 0 & \text{if } r \leq R, \\ (r^2 - R^2)^2 & \text{if } r > R, \end{cases} \quad u_2(r) := 0, \quad \lambda(r) := \begin{cases} 1 & \text{if } r \leq R, \\ 0 & \text{if } r > R, \end{cases}$$

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

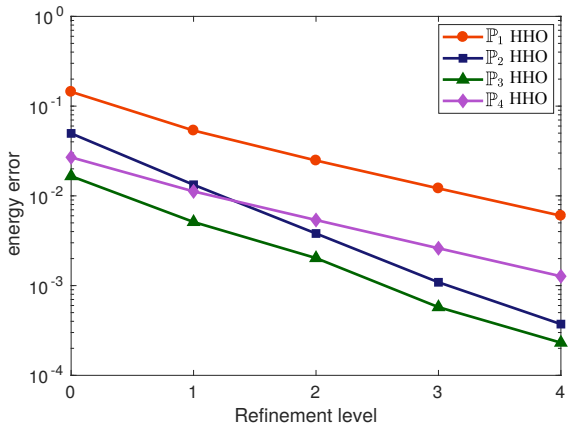
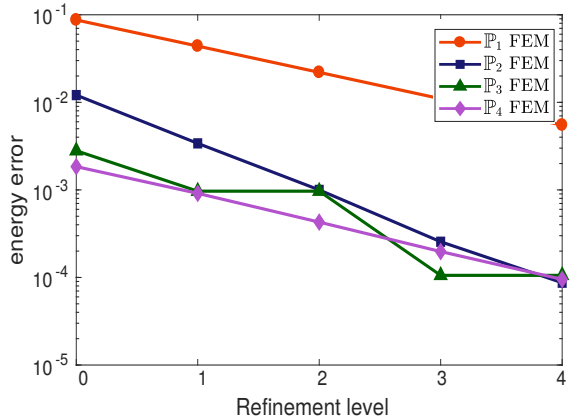
$$f_1(r) := \begin{cases} -8R^2 & \text{if } r \leq R, \\ 8R^2 - 16r^2 & \text{if } r > R, \end{cases} \quad f_2(r) := \begin{cases} 8R^2 & \text{if } r \leq R, \\ 0 & \text{if } r > R. \end{cases}$$



Number of Newton-min iterations



Convergence



J. DABAGHI, G. DELAY, A unified framework for high-order numerical discretizations of variational inequalities. *Computers & Mathematics with Applications* (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

A posteriori analysis for finite elements

Goal: Derive an upper bound on the error which is fully computable

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

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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

Recall

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

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Discretization flux reconstruction solving local mixt problems on patches:

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Estimators

Violations of physical properties of the numerical solution

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Flux estimator:

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

Residual estimator:

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

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Nonconform estimator for the \mathcal{K}_g violation $\eta_{\text{nonc},1}^{k,i} = \left\| \tilde{\mathbf{s}}_h^{k,i} - \mathbf{u}_h^{k,i} \right\|_K$ with $\tilde{\mathbf{s}}_h^{k,i} \in \mathcal{K}_g$

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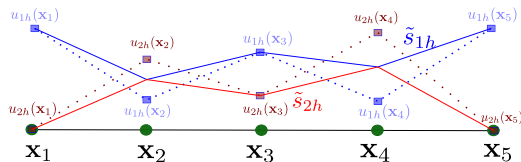
Nonconform estimator for the \mathcal{K}_g violation $\eta_{\text{nonc},1}^{k,i} = \left\| \tilde{\mathbf{s}}_h^{k,i} - \mathbf{u}_h^{k,i} \right\|_K$ with $\tilde{\mathbf{s}}_h^{k,i} \in \mathcal{K}_g$

The procedure to construct $\tilde{\mathbf{s}}_h^{k,i}$ is easy!

$$(\tilde{\mathbf{s}}_{1h}^{k,i}(\mathbf{a}), \tilde{\mathbf{s}}_{2h}^{k,i}(\mathbf{a})) = (u_{1h}^{k,i}(\mathbf{a}), u_{2h}^{k,i}(\mathbf{a})) \text{ if } \mathbf{u}_h^{k,i} \in \mathcal{K}_g$$

$$(\tilde{\mathbf{s}}_{1h}^{k,i}(\mathbf{a}), \tilde{\mathbf{s}}_{2h}^{k,i}(\mathbf{a})) = \left(\frac{u_{1h}^{k,i} + u_{2h}^{k,i}}{2}(\mathbf{a}), \frac{u_{1h}^{k,i} + u_{2h}^{k,i}}{2}(\mathbf{a}) \right)$$

$$\text{if } \mathbf{u}_h^{k,i} \notin \mathcal{K}_g \Rightarrow \tilde{\mathbf{s}}_{1h}^{k,i} - \tilde{\mathbf{s}}_{2h}^{k,i} \geq 0$$



Other nonconform estimators for the Λ violation

$$\eta_{\text{nonc},2}^{k,i} = C_{\Omega,\mu} \left\| \lambda_h^{k,i,\text{neg}} \right\|_K \quad \text{with} \quad \lambda_h^{k,i,\text{neg}} = \min \left\{ 0, \lambda_h^{k,i} \right\}$$

$$\eta_{\text{nonc},3}^{k,i} = 2C_{\Omega,\mu} \left\| \lambda_h^{k,i,\text{pos}} \right\|_K \left\| \tilde{\mathbf{s}}_h^{k,i} - \mathbf{u}_h^{k,i} \right\|_K \quad \text{with} \quad \lambda_h^{k,i,\text{pos}} = \max \left\{ 0, \lambda_h^{k,i} \right\}$$

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Remark

When $k, i \rightarrow +\infty$, $\eta_{\text{nonc},1}^{k,i} \rightarrow 0$, $\eta_{\text{nonc},2}^{k,i} \rightarrow 0$, $\eta_{\text{nonc},3}^{k,i} \rightarrow 0$.

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

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

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The procedure to construct $\tilde{\mathbf{s}}_h$ is more complex!

$p \geq 2$: at convergence and at each inexact semismooth step:

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

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

The procedure to construct $\tilde{\mathbf{s}}_h$ is more complex!

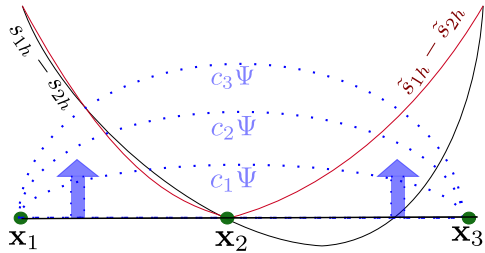
Step 1: Construct \mathbf{s}_h in each nodes as

$$\mathbf{s}_h(\mathbf{x}_l) = \left(\underbrace{\frac{u_{1h} + u_{2h}}{2}(\mathbf{x}_l)}_{s_{1h}(\mathbf{x}_l)}, \underbrace{\frac{u_{1h} + u_{2h}}{2}(\mathbf{x}_l)}_{s_{2h}(\mathbf{x}_l)} \right).$$

We have $s_{1h}(\mathbf{x}_l) - s_{2h}(\mathbf{x}_l) \geq 0$ but $\mathbf{s}_h \notin \mathcal{K}_g$.

Step 2: solve the minimization problem : find $c_K > 0$ such that $c_K = \min_{c>0} (s_{1h} - s_{2h})_K + c\Psi_K$

Step 3: We set $\tilde{s}_{1h}|_K = s_{1h}|_K + \frac{1}{2}c_K\Psi_K$ and $\tilde{s}_{2h}|_K = s_{2h}|_K - \frac{1}{2}c_K\Psi_K$



Theorem (A posteriori error estimate)

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

Theorem (A posteriori error estimate)

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

Corollary (Distinction of the error components)

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

Theorem (A posteriori error estimate)

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Corollary (Distinction of the error components)

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

Adaptive algorithm

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

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)

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

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Adaptive algorithm

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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)

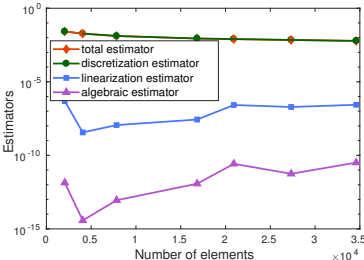
$$\eta_{\text{disc},K}^{k,i} \lesssim \sum_{\mathbf{a} \in \mathcal{V}_h} \left(\left\| \nabla \left(u_\alpha - u_{\alpha h}^{k,i} \right) \right\|_{\omega_h^{\mathbf{a}}} + \left\| \lambda - \lambda_h^{k,i}(\mathbf{a}) \right\|_{H_*^{-1}(\omega_h^{\mathbf{a}})} \right) + \text{contact term}$$

Numerical experiments

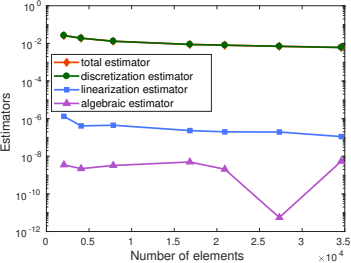
Numerical experiments \mathbb{P}_2

- semismooth solver: **Newton-min**. Linear solver: **GMRES** with ILU preconditionner.
- We compare three strategies: exact Newton, inexact Newton, adaptive inexact Newton.

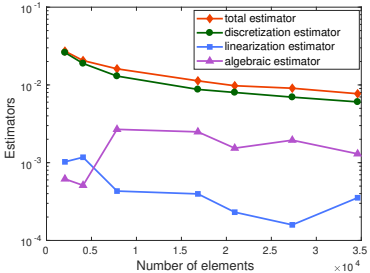
Exact Newton



Inexact Newton



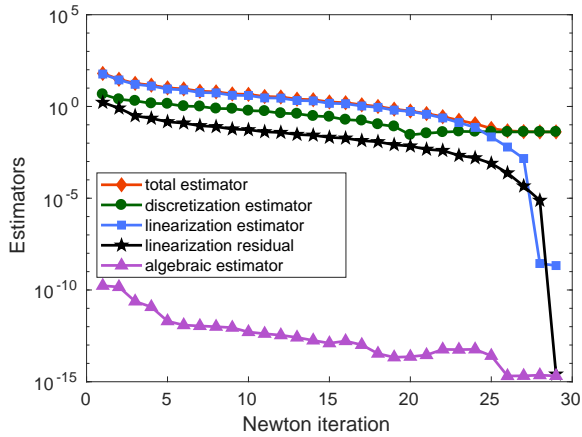
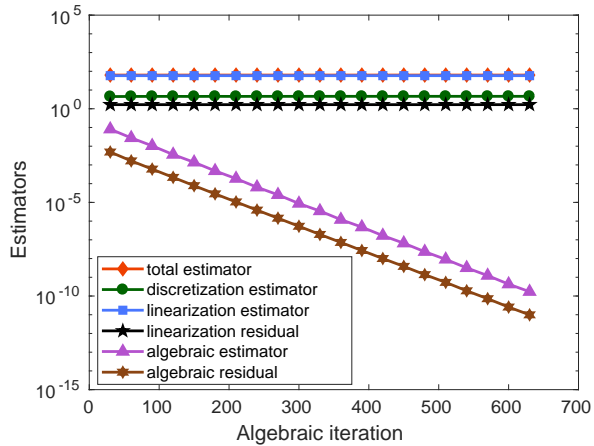
Adaptive inexact Newton



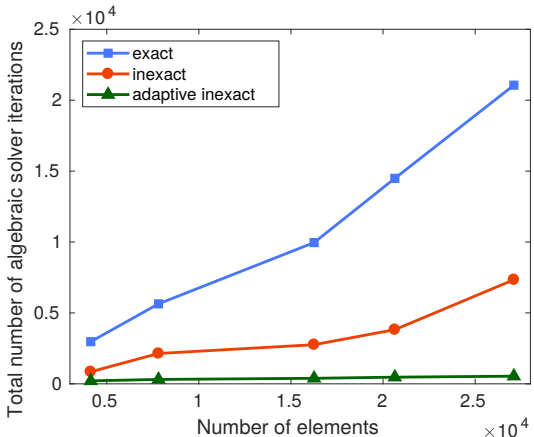
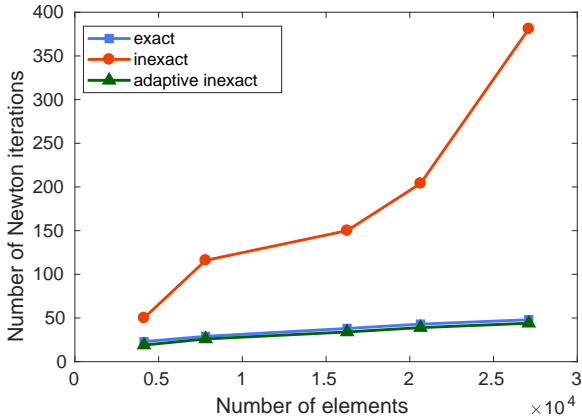
Precision is preserved for adaptive inexact semismooth Newton method.

Adaptivity

Exact Newton/Adaptive inexact Newton

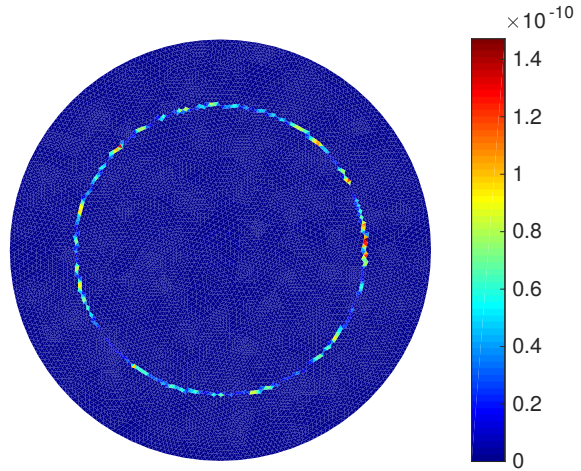
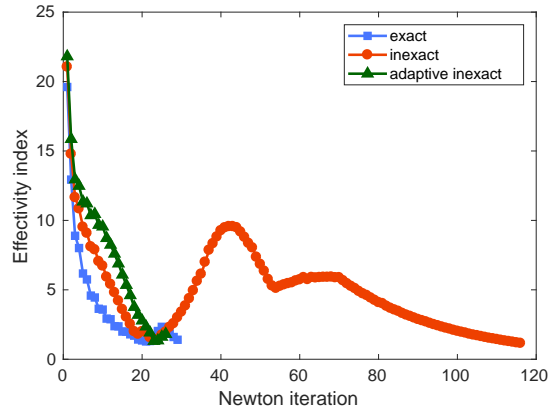


Overall performance



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

contact estimator



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

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

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

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

Discrete complementarity problems for finite elements

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

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

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

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

Discrete complementarity problems for finite elements

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Employing a C-function our problem reads

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

Discrete complementarity problems for finite elements

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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 analysis

We employ the methodology of equilibrated flux reconstructions

Theorem (Guaranteed upper bound)

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

Corollary (Distinction of the error components)

$$\left\| \left\| \mathbf{u} - \mathbf{u}_{h\tau}^{k,i} \right\| \right\|_{L^2(0,T;H_0^1(\Omega))} \leq \eta_{\text{disc}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i} + \eta_{\text{init}}$$

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

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

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

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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)

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

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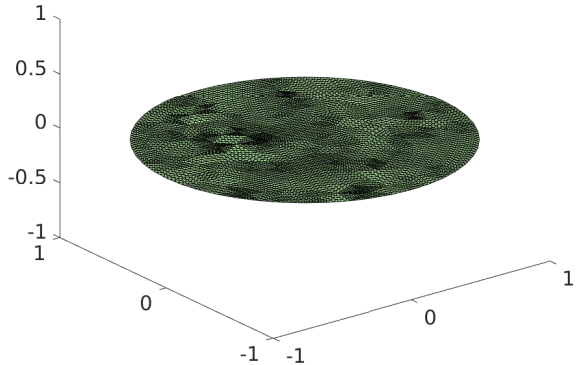
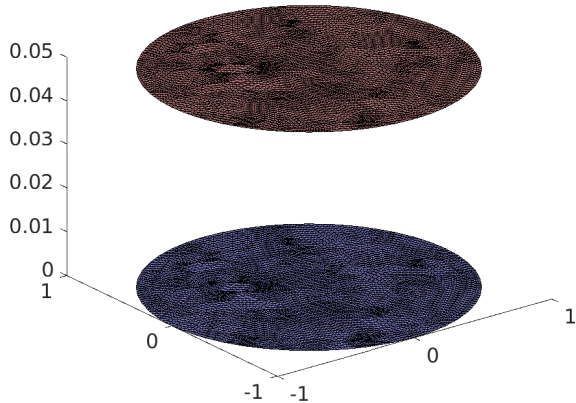
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Lemma

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

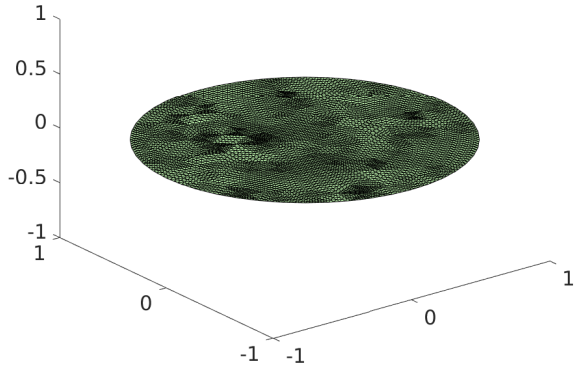
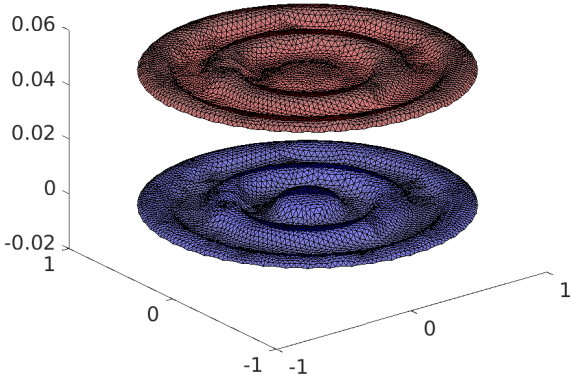
Numerical experiments $p = 1$

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



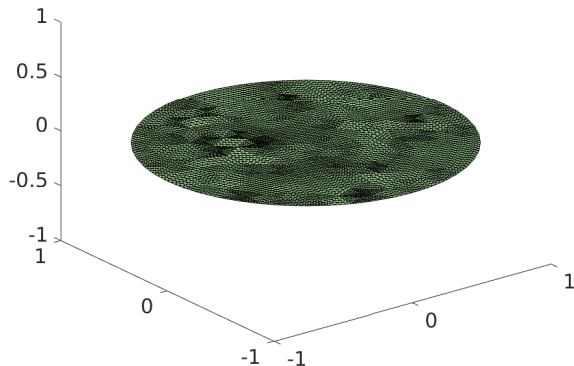
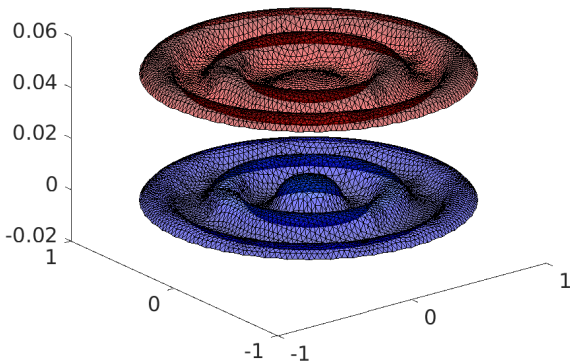
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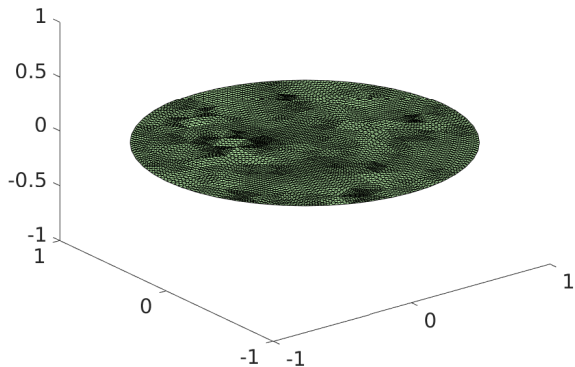
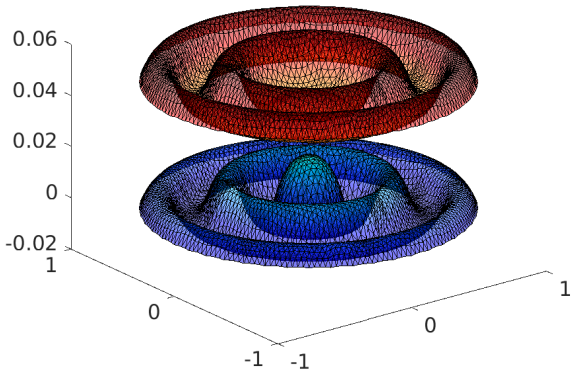
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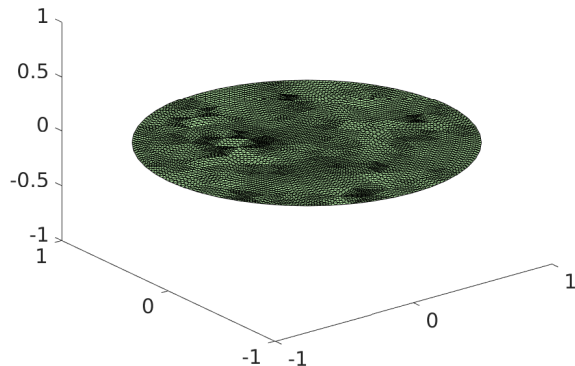
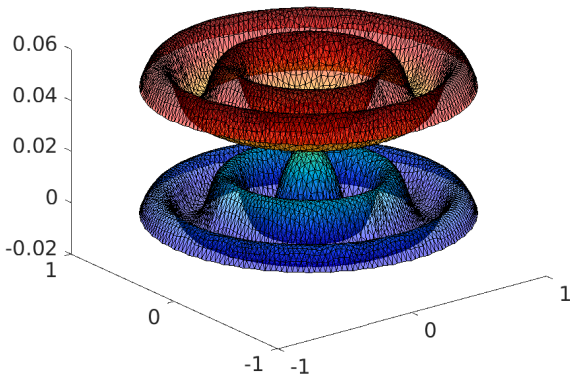
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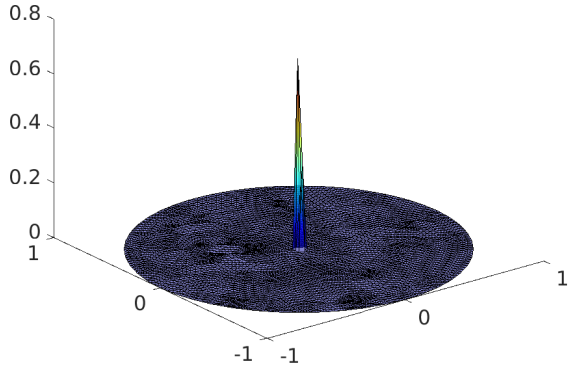
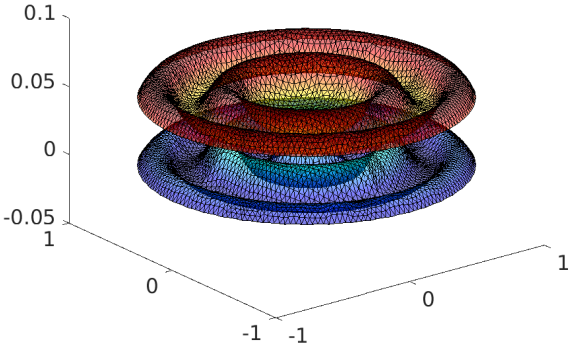
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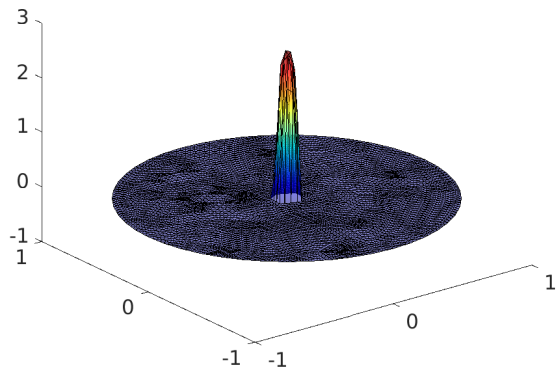
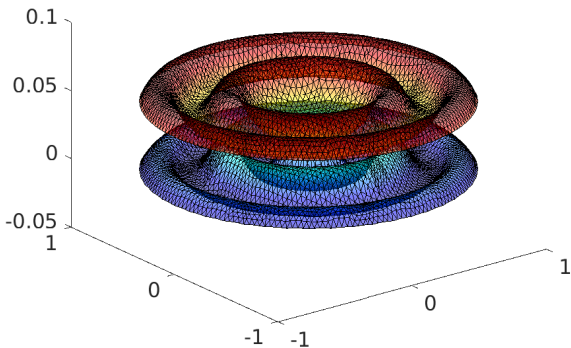
Numerical experiments $p = 1$

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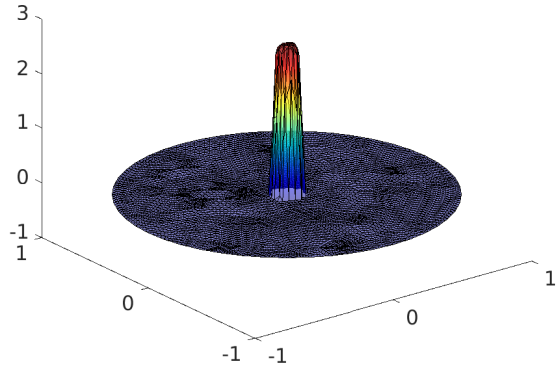
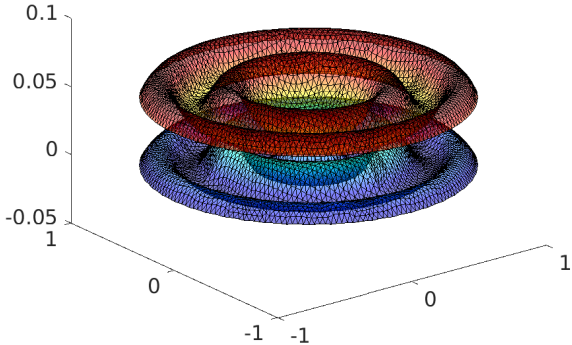
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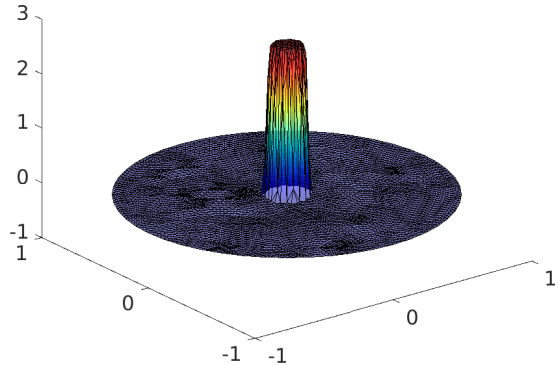
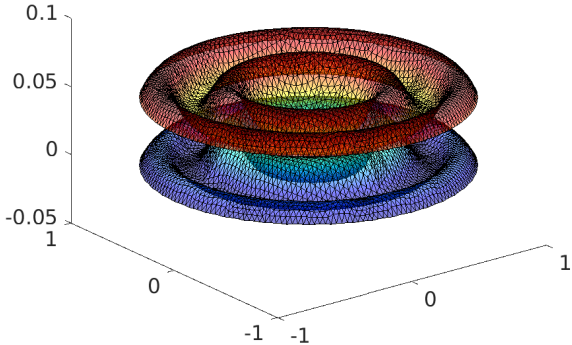
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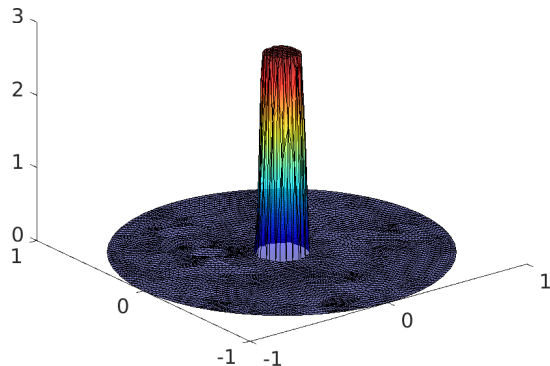
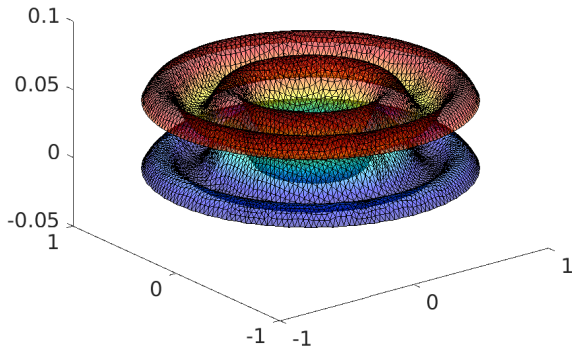
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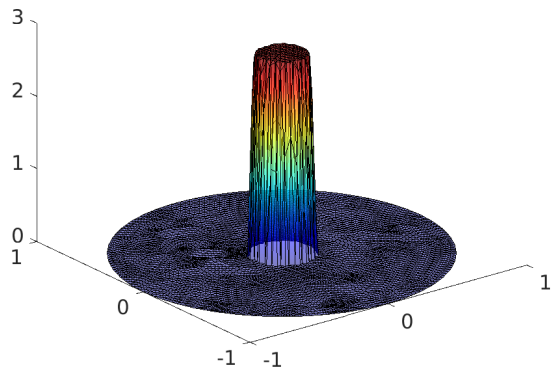
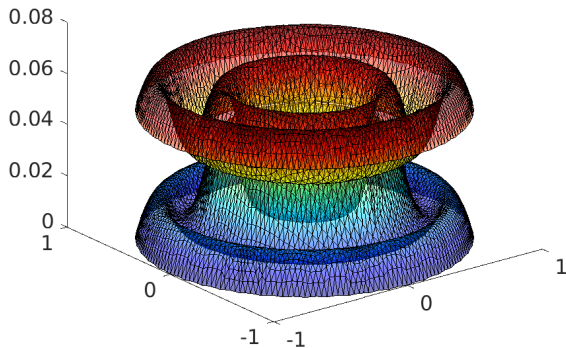
Numerical experiments $p = 1$

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



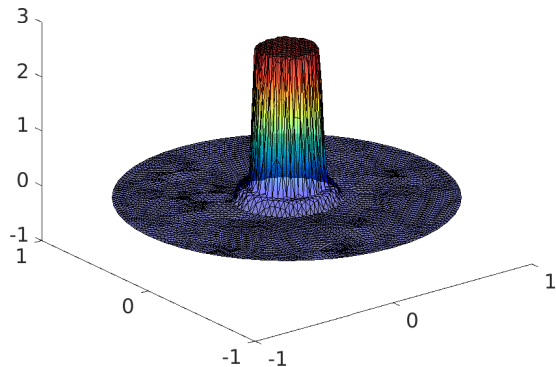
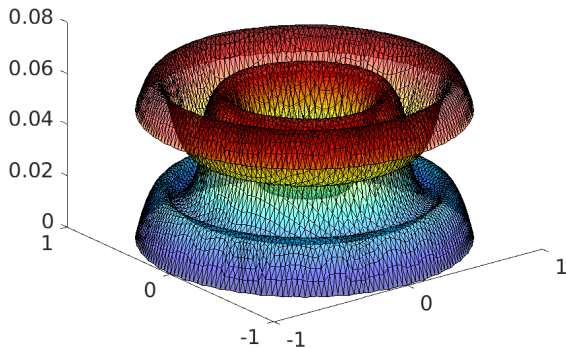
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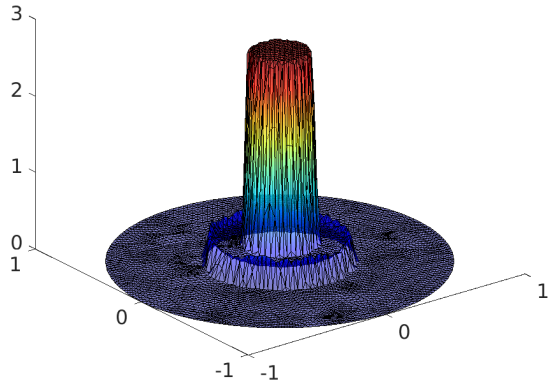
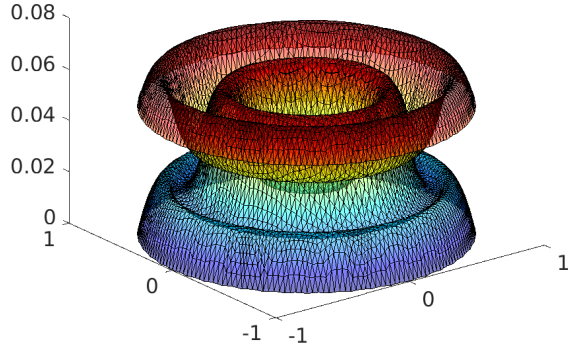
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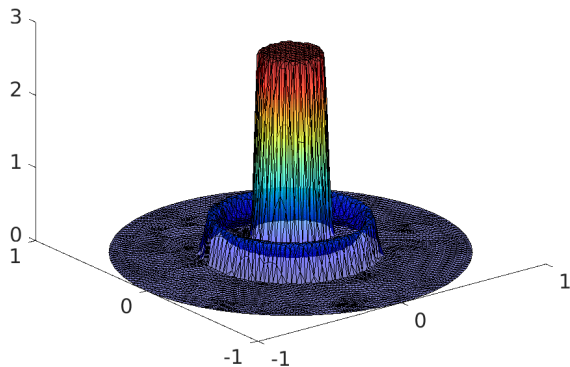
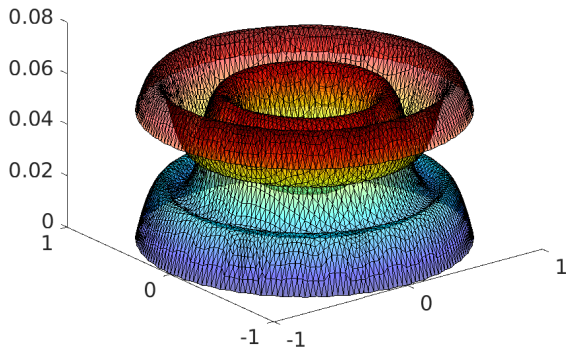
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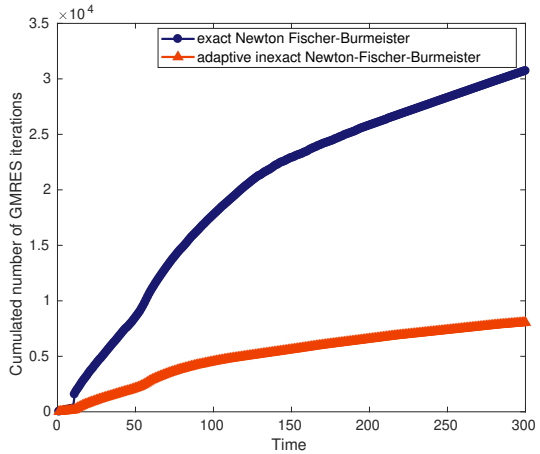
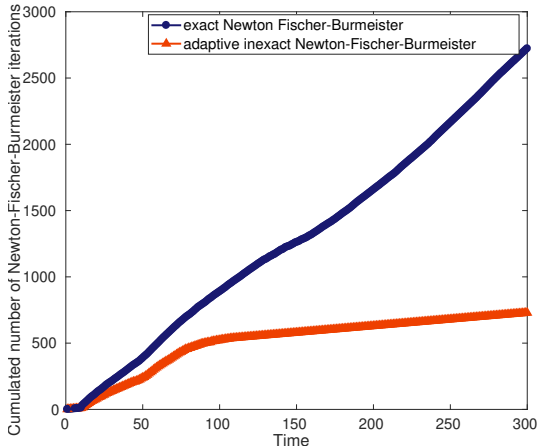


Numerical experiments $p = 1$

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



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

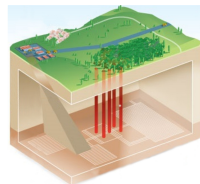
Two-phase flow with phase appearance and disappearance

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$$\partial_t l_w(S^l) + \nabla \cdot [\gamma_1 \mathbf{q}^l(S^l, P^l) - \mathbf{J}_h^l(S^l, \chi_h^l)] = Q_w,$$

$$\partial_t h(S^l, P^l, \chi_h^l) + \nabla \cdot [\gamma_2 \chi_h^l \mathbf{q}^l(S^l, P^l) + \gamma_3 P^g \mathbf{q}^g(S^l, P^l) + \mathbf{J}_h^l(S^l, \chi_h^l)] = Q_h,$$

$$1 - S^l \geq 0, \quad HP^g - \beta_1 \chi_h^l \geq 0, \quad [1 - S^l] \cdot [HP^g - \beta_1 \chi_h^l] = 0$$



Two-phase flow with phase appearance and disappearance

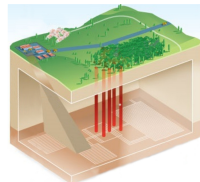
Storage of radioactive wastes in deep geological layers

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Unknowns: liquid saturation S^l , liquid pressure P^l , mole fraction of liquid hydrogen χ_h^l



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Storage of radioactive wastes in deep geological layers

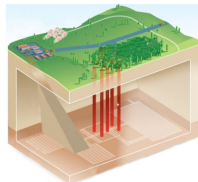
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Unknowns: liquid saturation S^l , liquid pressure P^l , mole fraction of liquid hydrogen χ_h^l

Linear functions: amount of water l_w , amount of hydrogen l_h



Two-phase flow with phase appearance and disappearance

Storage of radioactive wastes in deep geological layers

$$\partial_t l_w(S^l) + \nabla \cdot [\gamma_1 \mathbf{q}^l(S^l, P^l) - \mathbf{J}_h^l(S^l, \chi_h^l)] = Q_w,$$

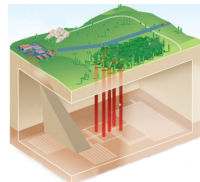
$$\partial_t l_h(S^l, P^l, \chi_h^l) + \nabla \cdot [\gamma_2 \chi_h^l \mathbf{q}^l(S^l, P^l) + \gamma_3 P^g \mathbf{q}^g(S^l, P^l) + \mathbf{J}_h^l(S^l, \chi_h^l)] = Q_h,$$

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Nonlinear fluxes: Darcy fluxes \mathbf{q}^l and \mathbf{q}^g + Fick flux \mathbf{J}_h^l



Two-phase flow with phase appearance and disappearance

Storage of radioactive wastes in deep geological layers

$$\partial_t l_w(S^l) + \nabla \cdot [\gamma_1 \mathbf{q}^l(S^l, P^l) - \mathbf{J}_h^l(S^l, \chi_h^l)] = Q_w,$$

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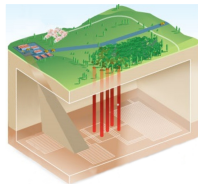
Linear functions: amount of water l_w , amount of hydrogen l_h

Nonlinear fluxes: Darcy fluxes \mathbf{q}^l and \mathbf{q}^g + Fick flux \mathbf{J}_h^l

Nonlinear complementarity constraints: $1 - S^l = 0$ and $HP^g - \beta_1 \chi_h^l > 0 \Rightarrow$ no gas.

If $1 - S^l > 0$ and $HP^g - \beta_1 \chi_h^l = 0 \Rightarrow$ gas appearance.

Ben Gharbia and Jaffré (2014)



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 by the finite volume method

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

Discretization of each component equation and the nonlinear complementarity constraints

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

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

Discretization by the finite volume method

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Discretization of each component equation and the nonlinear complementarity constraints

$$\begin{aligned}
 S_{c,K}^n(\mathbf{U}^n) &= 0 \quad \forall K \in \mathcal{T}_h \quad \forall c \in \{w, h\} \\
 \mathcal{K}(\mathbf{U}_K^n) &\geq 0, \quad \mathcal{G}(\mathbf{U}_K^n) \geq 0, \quad \mathcal{K}(\mathbf{U}_K^n) \cdot \mathcal{G}(\mathbf{U}_K^n) = 0 \quad \forall K \in \mathcal{T}_h
 \end{aligned}$$

- We reformulate the complementarity constraints with C-functions
- We employ inexact semismooth linearization

A posteriori error estimates

Recall:

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

A posteriori error estimates

Recall:

$$\begin{cases} \partial_t l_w(\mathbf{S}^l) + \nabla \cdot \Phi_w(\mathbf{S}^l, \mathbf{P}^l, \chi_h^1) = Q_w, \\ \partial_t l_h(\mathbf{S}^l, \mathbf{P}^l, \chi_h^1) + \nabla \cdot \Phi_h(\mathbf{S}^l, \mathbf{P}^l, \chi_h^1) = Q_h, \\ \mathbf{1} - \mathbf{S}^l \geq 0, \quad H\mathbf{P}^g - \beta_1 \chi_h^1 \geq 0, \quad [\mathbf{1} - \mathbf{S}^l] \cdot [H\mathbf{P}^g - \beta_1 \chi_h^1] = 0 \end{cases}$$

Very complicated to define a weak solution and an upper bound on the error as:

$$\| \| P^l - P_{1,h\tau} \| \| + \| \| S^l - S_{1,h\tau} \| \| + \| \| \chi_h^1 - \chi_{h,h\tau}^1 \| \| \leq \eta(P_{1,h\tau}, S_{1,h\tau}, \chi_{h,h\tau}^1) \quad (*)$$

A posteriori error estimates

Recall:
$$\begin{cases} \partial_t l_w(\mathbf{S}^l) + \nabla \cdot \Phi_w(\mathbf{S}^l, P^l, \chi_h^1) = Q_w, \\ \partial_t l_h(\mathbf{S}^l, P^l, \chi_h^1) + \nabla \cdot \Phi_h(\mathbf{S}^l, P^l, \chi_h^1) = Q_h, \\ \mathbf{1} - \mathbf{S}^l \geq 0, HP^g - \beta_1 \chi_h^1 \geq 0, [\mathbf{1} - \mathbf{S}^l] \cdot [HP^g - \beta_1 \chi_h^1] = 0 \end{cases}$$

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Assumption: There exists a unique weak solution satisfying

$$l_c \in H^1((0, t_F); L^2(\Omega)), \mathbf{1} - \mathbf{S}^l \in L^2_+((0, t_F); L^\infty(\Omega)), \Phi_c \in L^2((0, t_F); \mathbf{H}(\text{div}, \Omega))$$

$$\int_0^{t_F} (\partial_t l_c, \varphi)_\Omega(t) dt - \int_0^{t_F} (\Phi_c, \nabla \varphi)_\Omega(t) dt = \int_0^{t_F} (Q_c, \varphi)_\Omega(t) dt \quad \forall \varphi \in L^2((0, t_F); H^1(\Omega))$$

$$\int_0^{t_F} (\lambda - (\mathbf{1} - \mathbf{S}^l), H[P^l + P_{cp}(\mathbf{S}^l)] - \beta^1 \chi_h^1)_\Omega(t) dt \geq 0 \quad \forall \lambda \in L^2_+((0, t_F); L^\infty(\Omega))$$

A posteriori error estimates

Recall:
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Very complicated to define a weak solution and an upper bound on the error as:

$$\| \| P^l - P_{1,h\tau} \| \| + \| \| \mathbf{S}^l - \mathbf{S}_{1,h\tau} \| \| + \| \| \chi_h^l - \chi_{h,h\tau}^l \| \| \leq \eta(P_{1,h\tau}, \mathbf{S}_{1,h\tau}, \chi_{h,h\tau}^l) \quad (*)$$

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Dual norm of the residual for the components

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

Post-processing of the pressure and the molar fraction

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

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

The darcy velocity involves a pressure gradient and the Fick flux involves a molar fraction gradient!

Step 1: Piecewise polynomial reconstruction

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

Step 2: Conforming reconstruction with Oswald interpolation operator

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

Error measure

1 Dual norm of the residual for the components

2 Residual for the constraints

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

3 Error measure for the nonconformity of the unknowns $\mathcal{N}_p(P_{hr}^{n,k,i})$ and $\mathcal{N}_\chi(\chi_{hr}^{n,k,i})$

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

Theorem

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

Error measure

1 Dual norm of the residual for the components

2 Residual for the constraints

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

3 Error measure for the nonconformity of the unknowns $\mathcal{N}_\rho(\mathbf{P}_{h\tau}^{n,k,i})$ and $\mathcal{N}_\chi(\chi_{h\tau}^{n,k,i})$

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

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

Error measure

- 1 Dual norm of the residual for the components
- 2 Residual for the constraints

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

- 3 **Error measure for the nonconformity of the unknowns** $\mathcal{N}_p(P_{h\tau}^{n,k,i})$ and $\mathcal{N}_\chi(\chi_{h\tau}^{n,k,i})$

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

Theorem

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

Numerical experiments

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

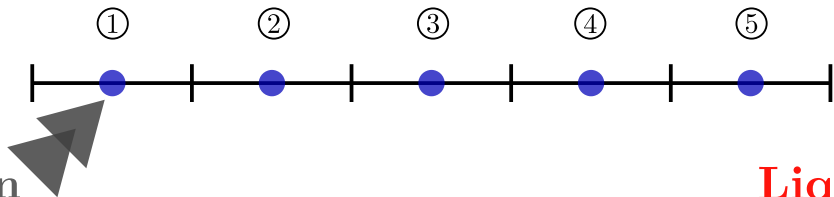
Semismooth solver: Newton-min

Iterative algebraic solver: GMRES.

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

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

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

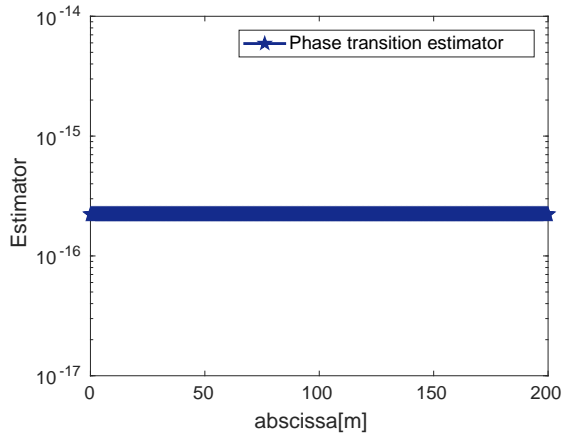
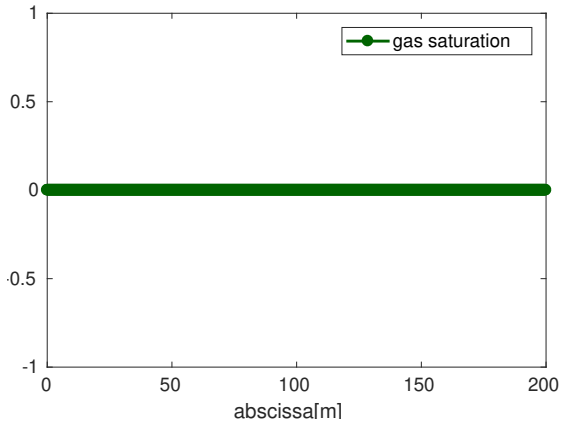


Gas injection

Liquid

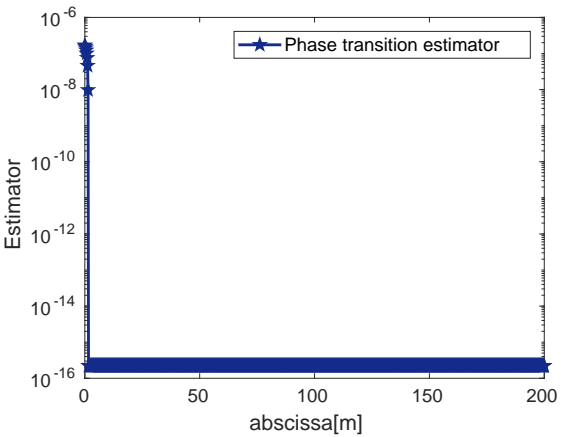
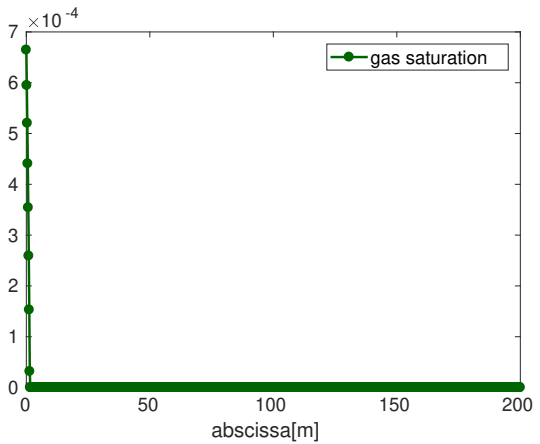
Phase transition estimator

$t = 2500$ years



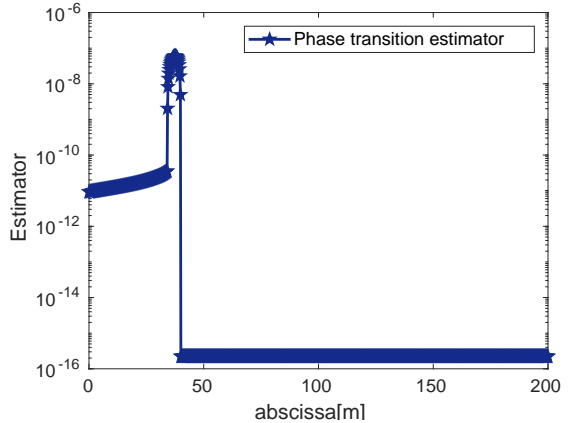
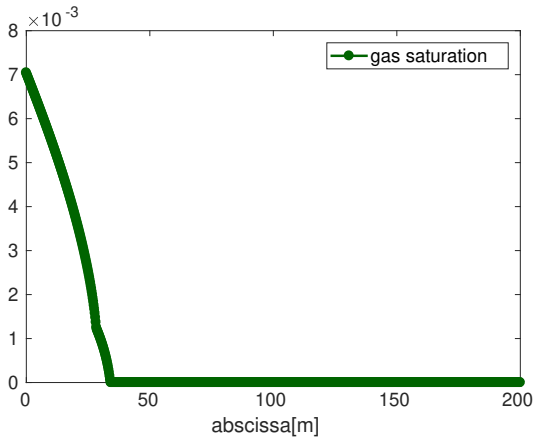
Phase transition estimator

$t = 1.25 \times 10^4$ years

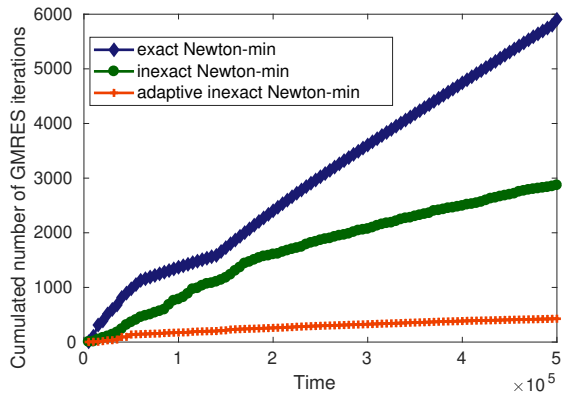
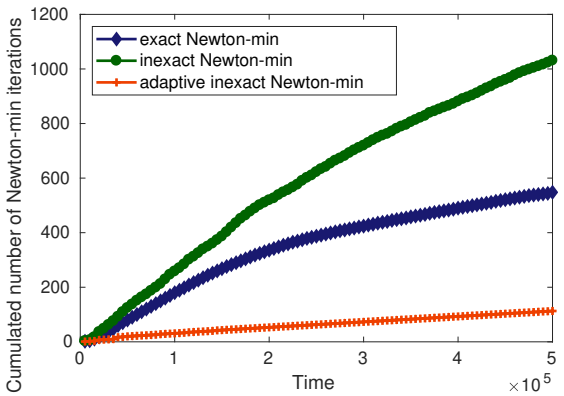


Phase transition estimator

$t = 4.25 \times 10^4$ years

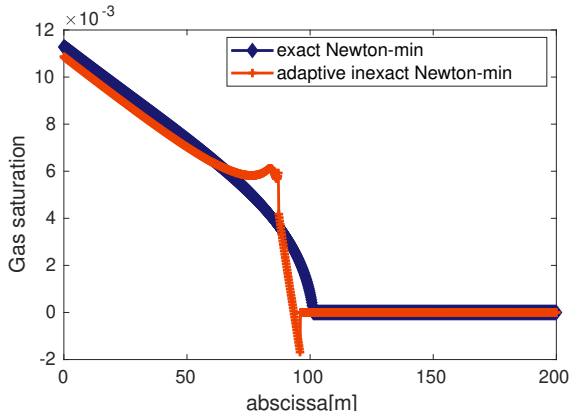


Overall performance $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

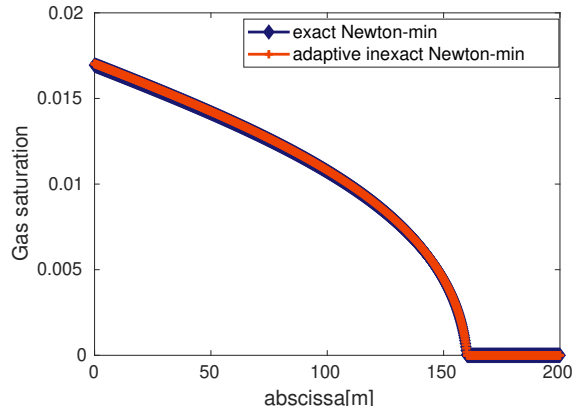


Accuracy $\gamma_{\text{lin}} = \gamma_{\text{alg}} = 10^{-3}$

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years



I. BEN GHARBA 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

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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).

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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.

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Thank you for your attention

Discretization flux reconstruction:

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

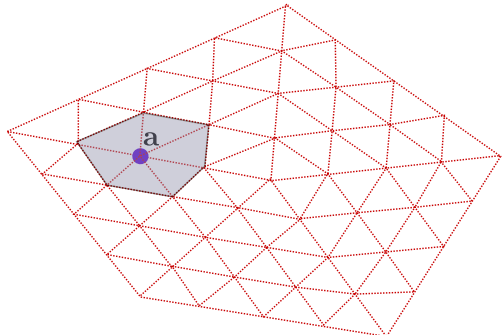
$$\tilde{g}_{\alpha h}^{k,i,a} := \left(f_\alpha - (-1)^\alpha \tilde{\lambda}_{h,a}^{k,i} - r_{\alpha h}^{k,i} \right) \psi_{h,a} - \mu_\alpha \nabla U_{\alpha h}^{k,i} \cdot \nabla \psi_{h,a} : \text{depends on the residual}$$

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

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

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

$p = 1$

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

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

$p \geq 2$

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

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

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

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

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 $\forall t \in]0, T[$

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

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

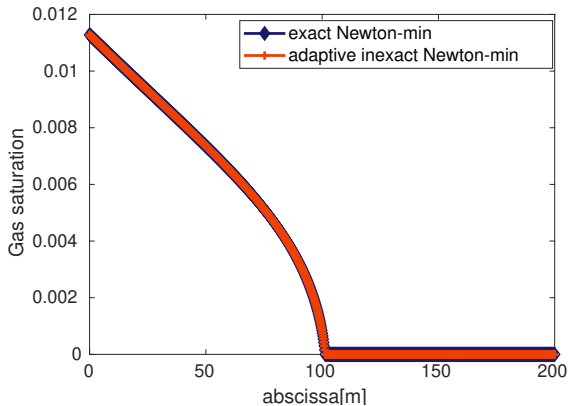
Discrete formulation: Given $(u_{1h}^0, u_{2h}^0) \in \mathcal{K}_{gh}^p$, search $(u_{1h}^n, u_{2h}^n, \lambda_h^n) \in X_{gh}^p \times X_{0h}^p \times \Lambda_h^p$ such that for all $(z_{1h}, z_{2h}, \chi_h) \in X_{0h}^p \times X_{0h}^p \times \Lambda_h^p$

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

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

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

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years

