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

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Outline

Motivation

$\Omega \subset \mathbb{R}^2$: smooth connected domain, $\mathcal{H}$: Hilbert space, $\mathcal{K}_g$: convex set.

$a : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$: bilinear continuous coercive form, $\ell : \mathcal{H} \to \mathbb{R}$: linear continuous form

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

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Application to several problems in contact mechanics

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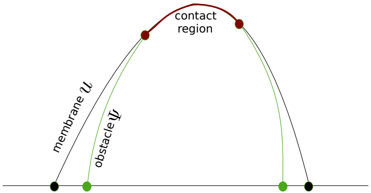
Application to several problems in contact mechanics

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

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

- 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 u
- $f \in L^2(\Omega)$: force acting on the membrane



Signorini problem: $\partial\Omega = \Gamma_{\mathrm{D}} \cup \Gamma_{\mathrm{N}} \cup \Gamma_{\mathrm{C}}$.

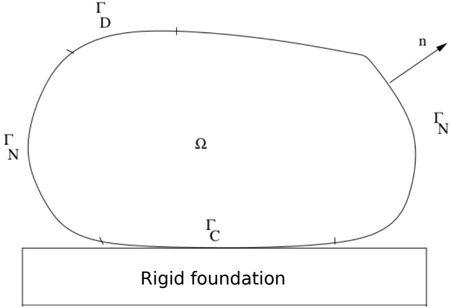
Γ_{D}: Dirichlet boundary conditions, Γ_{N}: Neumann boundary conditions

Γ_{C}: Unilateral contact boundary conditions

Find $\boldsymbol{u} \in \mathcal{K}_g := \left\{ \boldsymbol{v} \in [H^1(\Omega)]^2 \text{ s.t. } \boldsymbol{v} = \boldsymbol{g} \text{ on } \Gamma_{\mathrm{D}}, \text{ and } \boldsymbol{v}\cdot\boldsymbol{n} \leq 0 \text{ on } \Gamma_{\mathrm{C}} \right\}$ such that

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

- $\boldsymbol{g} \in \left[H^{\frac{1}{2}}(\Gamma_{\mathrm{D}})\right]^2$: Dirichlet boudary datum for $\boldsymbol{u}$
- $\boldsymbol{g}_{\mathrm{N}} \in [L^2(\Gamma_{\mathrm{N}})]^2$: Neumann boundary data
- $f \in [L^2(\Omega)]^2$: force acting on the elastic solid.
- $\sigma(\boldsymbol{u})$: stress tensor
- ϵ : strain tensor

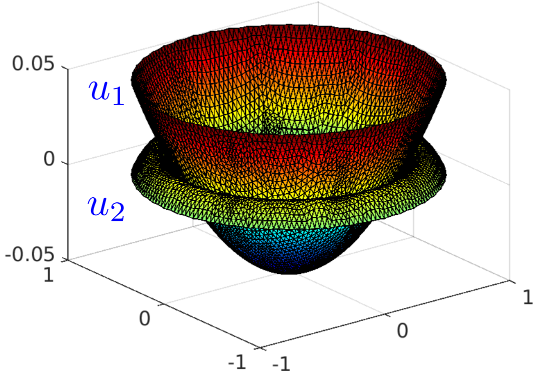


Contact between two membranes:

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

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

- μ_1, μ_2: tensions of the membranes
- $g_1 \geq g_2$: boundary data
- f_1, f_2: external sources



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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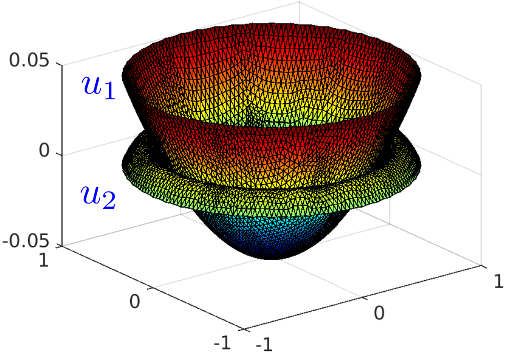
Extension to unsteady problems?

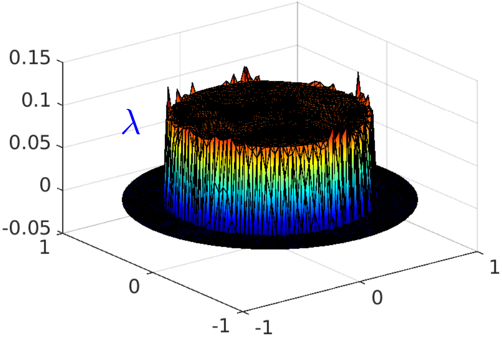
Outline

Model problem and settings: contact between two membranes

Find u_1, u_2, λ such that

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





Continuous problem

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

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

$$\sum_{\alpha=1}^{2} \mu_\alpha (\nabla u_\alpha, \nabla v_\alpha)_\Omega - (\lambda, v_1 - v_2)_\Omega = \sum_{\alpha=1}^{2} (f_\alpha, v_\alpha)_\Omega \quad \forall (v_1, v_2) \in \left[H^1_0(\Omega)\right]^2$$
$$(\chi - \lambda, u_1 - u_2)_\Omega \geq 0 \quad \forall \chi \in \Lambda \qquad (\mathbb{S})$$

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other interpretation

Continuous problem

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

other interpretation

Variational inequality:

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

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

The finite element method

For any $p \geq 1$

Spaces for the discretization:

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

$\mathcal{V}^p_{\mathrm{d}}$: set of nodes

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

$$\mathcal{K}^p_{gh} = \left\{(v_{1h}, v_{2h}) \in X^p_{g_1 h} \times X^p_{g_2 h},\ v_{1h}(\boldsymbol{x}_l) - v_{2h}(\boldsymbol{x}_l) \geq 0\ \ \forall \boldsymbol{x}_l \in \mathcal{V}^p_{\mathrm{d}}\right\} \not\subset \mathcal{K}_g \quad \forall p \geq 2$$

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

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

Well-posed problem (Lions–Stampacchia)

The finite element method

For any $p \geq 1$

Spaces for the discretization:

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

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

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

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

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Discrete weak formulation Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{g_1 h}^p \times X_{g_2 h}^p \times \Lambda_h^p$ s.t.

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

Discrete complementarity problem

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

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

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Matrix representation of (DS2)

Discrete complementarity problem

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Matrix representation of (DS2)

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

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

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

Remark

The construction of $\mathcal{N}_h^p$ and the dual basis $\Theta_{h,\boldsymbol{x}_l}$ are essential to obtain equivalence between DS *and* DR

The Discontinuous Galerkin method

Discontinuous spaces:

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

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

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

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

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

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

Well-posed problem (Lions–Stampacchia)

Discrete complementarity problem

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

Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{g_1 h}^p \times X_{g_2 h}^p \times \Lambda_h^p$ such that

$$\sum_{\alpha=1}^{2} \mu_\alpha \mathcal{A}_h(u_{\alpha h}, v_{\alpha h}) - \sum_{K\in\mathcal{T}_h} (v_{1h}|_K - v_{2h}|_K, \lambda_h|_K)_K = \sum_{\alpha=1}^{2} \sum_{K\in\mathcal{T}_h} (f_\alpha|_K, v_{\alpha h}|_K)_K \quad \forall \boldsymbol{v}_h \in \left[X_{0h}^p\right]^2,$$

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

Discrete complementarity problem

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

Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{g_1 h}^p \times X_{g_2 h}^p \times \Lambda_h^p$ such that

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

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

Discrete complementarity problem

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

Find $(u_{1h}, u_{2h}, \lambda_h) \in X_{g_1 h}^p \times X_{g_2 h}^p \times \Lambda_h^p$ such that

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

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

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

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

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

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

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

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

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**: $\mathbf{G}_K : X^p_{h,K} \to \mathbb{P}_p(K;\mathbb{R}^2)$ such that

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

  It approximates the gradient at the continuous level

- **Stabilization operator**

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

Bilinear form: $\forall \hat{v}_h \in X^p_h, \forall \hat{w}_h \in X^p_h$

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

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

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

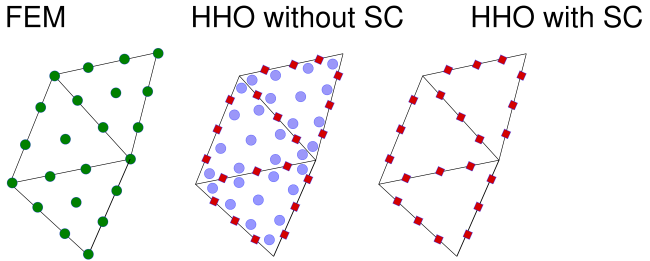
Well-posed problem (Lions–Stampacchia)

Discrete complementarity problem

$$\mathbb{E}\boldsymbol{X}_h = \boldsymbol{F},$$
$$\boldsymbol{X}^{\mathrm{C}}_{1h} - \boldsymbol{X}^{\mathrm{C}}_{2h} \geq 0, \quad \boldsymbol{X}_{3h} \geq 0, \quad (\boldsymbol{X}^{\mathrm{C}}_{1h} - \boldsymbol{X}^{\mathrm{C}}_{2h}) \cdot \boldsymbol{X}_{3h} = 0.$$

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

- In dG-SIPG, $\mathcal{A}_h$ is coercive provided that the coefficient $\gamma > 0$ (stablization 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!

Outline

C-functions

How to solve the nonlinear problem

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

Definition

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

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

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

C-functions

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

C-functions

How to solve the nonlinear problem

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

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

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

Inexact semismooth Newton method

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

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

where

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

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

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

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

Newton-min convergence

Theorem

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

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

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

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

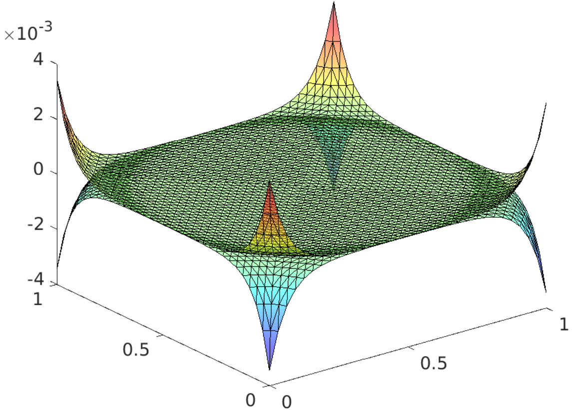
- $r := \sqrt{(x-0.5)^2 + (y-0.5)^2}$: distance to the center of the domain,
- $R := 1/3$: radius of the disk where contact occurs,
- $N := 6$

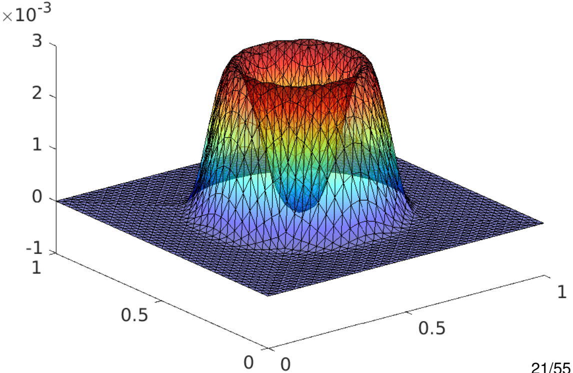
This solution is associated to the right-hand sides f_1 and f_2 defined by

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

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

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



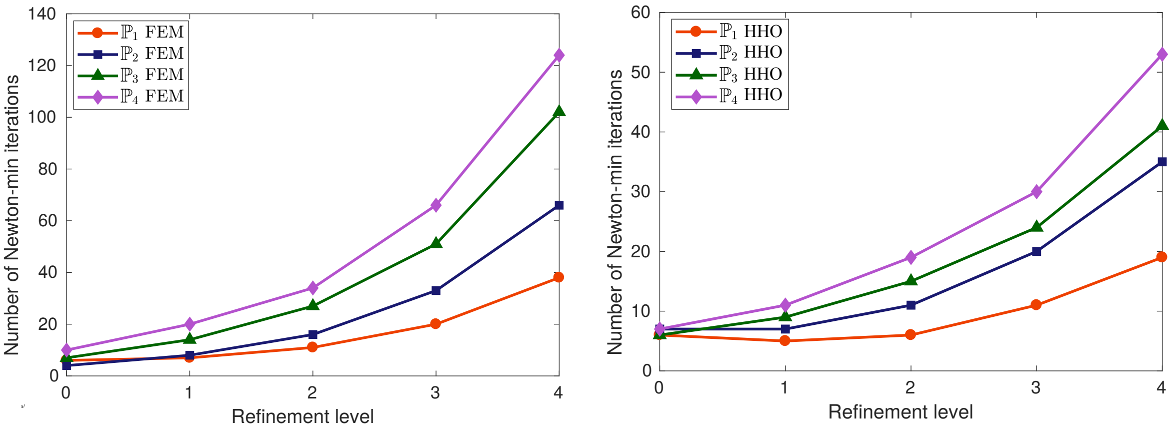


HHO with static condensation

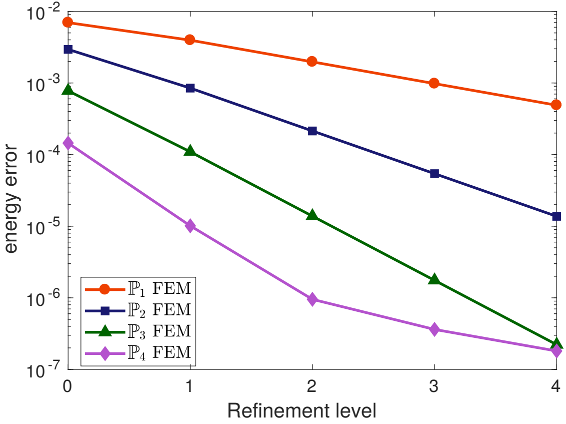
	$\mathbb{P}_1$ DOFs		$\mathbb{P}_2$ DOFs		$\mathbb{P}_3$ DOFs		$\mathbb{P}_4$ DOFs	
Mesh	no SC	SC	no SC	SC	no SC	SC	no SC	SC
$\mathcal{T}_0$	752	176	1504	352	2448	528	3584	704
$\mathcal{T}_1$	3040	736	6080	1472	9888	2208	14464	2944
$\mathcal{T}_2$	12224	3008	24448	6016	39744	9024	58112	12032
$\mathcal{T}_3$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

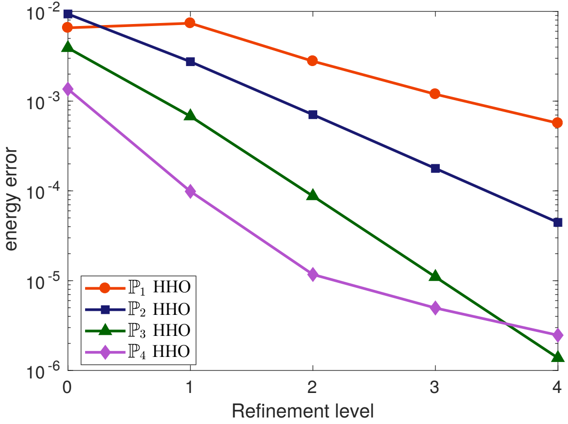
- Important reduction of the system size

Number of Newton-min iterations



Convergence



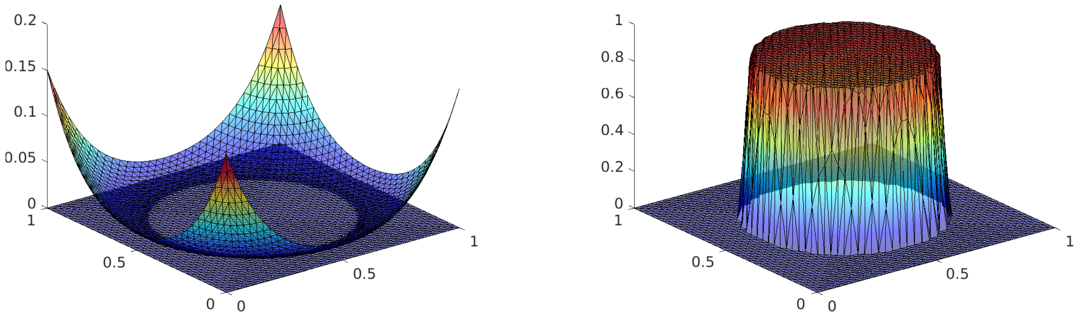


A second test case

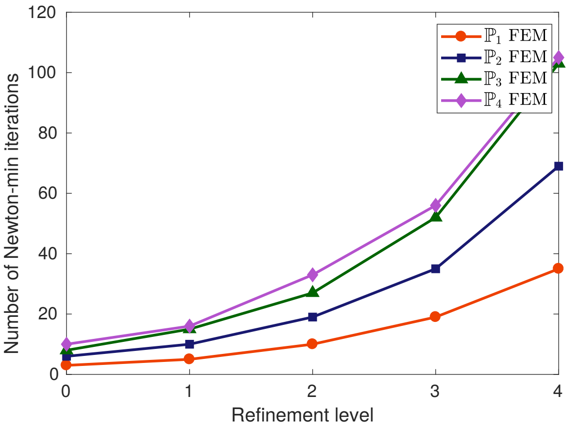
$$u_1(r) := \begin{cases} 0 & \text{if } r \le R, \\ (r^2 - R^2)^2 & \text{if } r > R, \end{cases} \quad u_2(r) := 0, \quad \lambda(r) := \begin{cases} 1 & \text{if } r \le R, \\ 0 & \text{if } r > R, \end{cases}$$

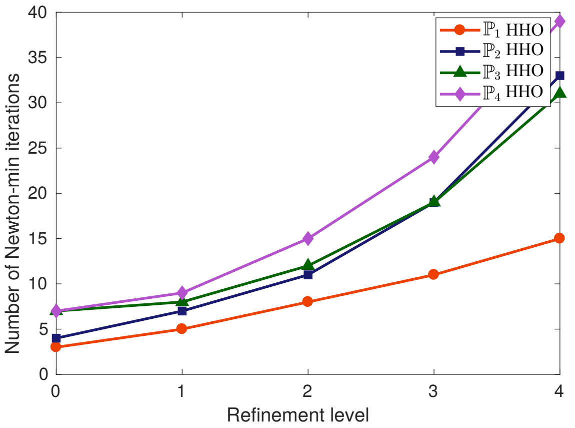
This solution is associated to the right-hand sides f_1 and f_2 given by

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

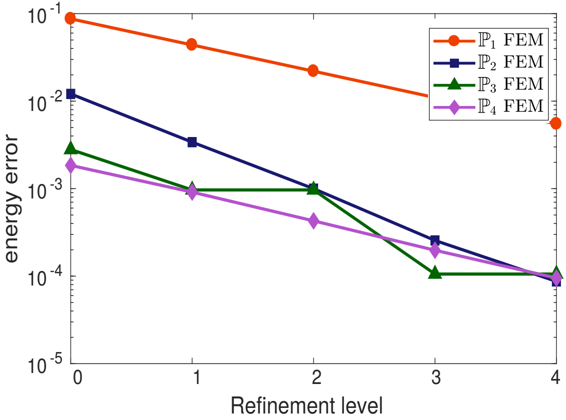


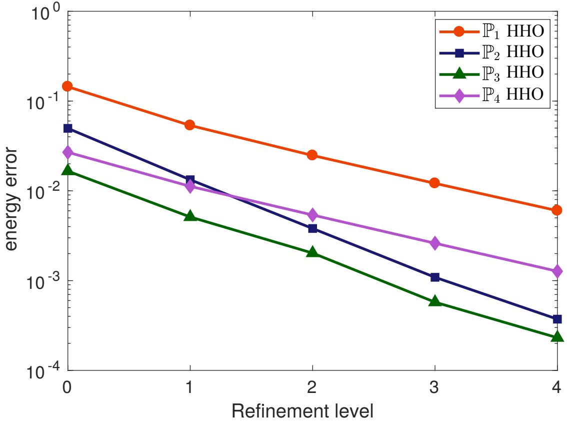
Number of Newton-min iterations





Convergence





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

Outline

A posteriori analysis for finite elements

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

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

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- $\eta_K(\boldsymbol{u}_h^{k,i})$ local estimator depending on the approximate solution

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- $\eta_K(\boldsymbol{u}_h^{k,i})$ local estimator depending on the approximate solution
- $\eta^{k,i} \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i}$: identification of the error components

A posteriori analysis for finite elements

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

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

- $\eta_K(\boldsymbol{u}_h^{k,i})$ local estimator depending on the approximate solution
- $\eta^{k,i} \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i}$: identification of the error components
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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

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

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Estimators

Violations of physical properties of the numerical solution

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

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Flux estimator:

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

Residual estimator:

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

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p = 1: **at convergence:**

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

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

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

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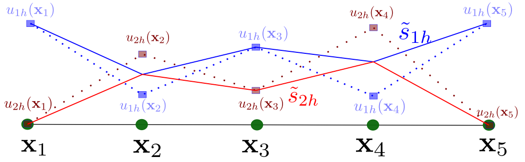
The procedure to construct $\tilde{\boldsymbol{s}}_h^{k,i}$ is easy!

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

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

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



Other nonconform estimators for the Λ violation

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

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

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Remark

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

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

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

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

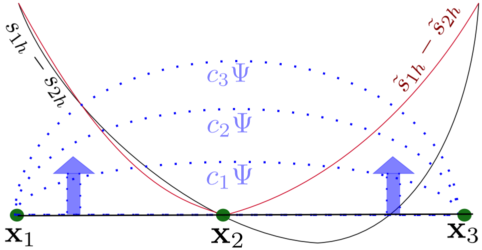
Step 1: Construct $\boldsymbol{s}_h$ in each nodes as

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

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

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)

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

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Corollary (Distinction of the error components)

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

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Adaptive algorithm

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

Stop linear solver

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

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

Stop linear solver

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

Stop nonlinear solver

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

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

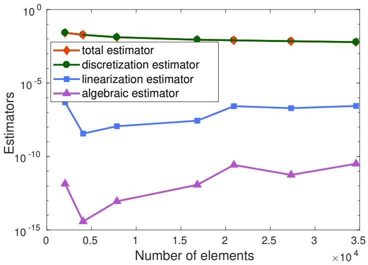
$$+ \text{ contact term}$$

Numerical experiments

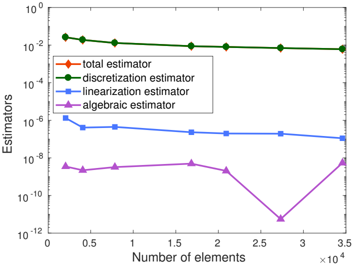
Numerical experiments $\mathbb{P}_2$

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

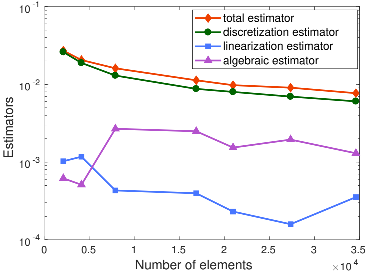
Exact Newton



Inexact Newton



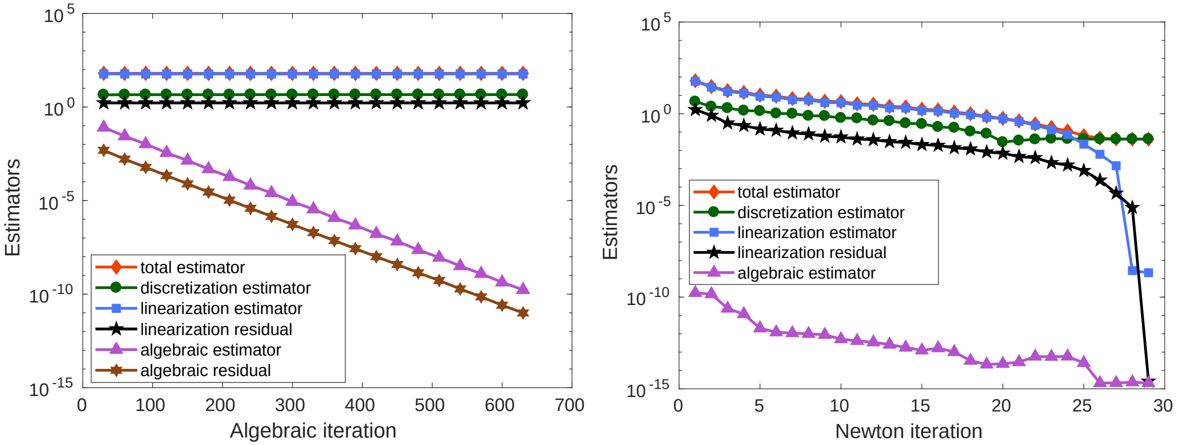
Adaptive inexact Newton



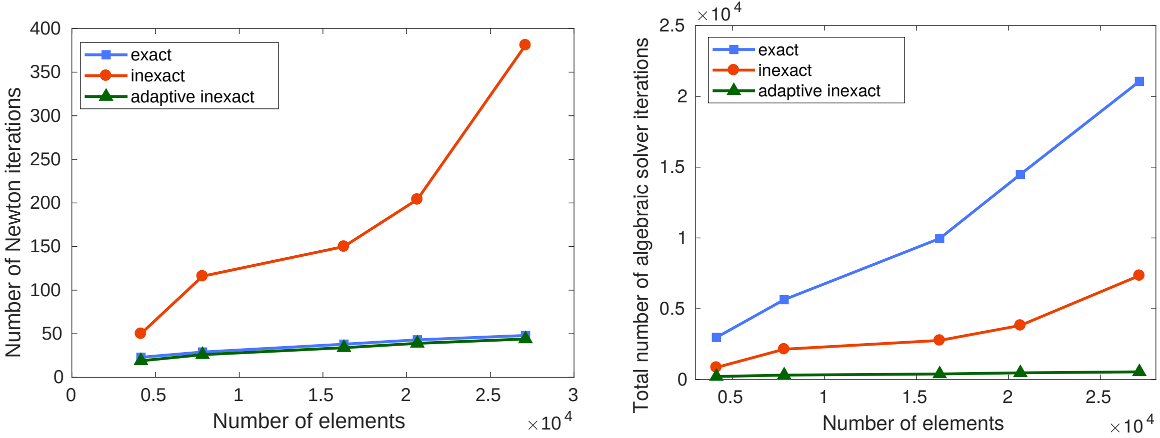
Precision is preserved for adaptive inexact semismooth Newton method.

Adaptivity

Exact Newton/Adaptive inexact Newton

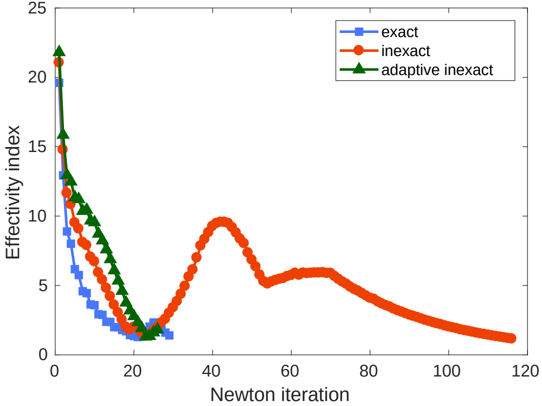


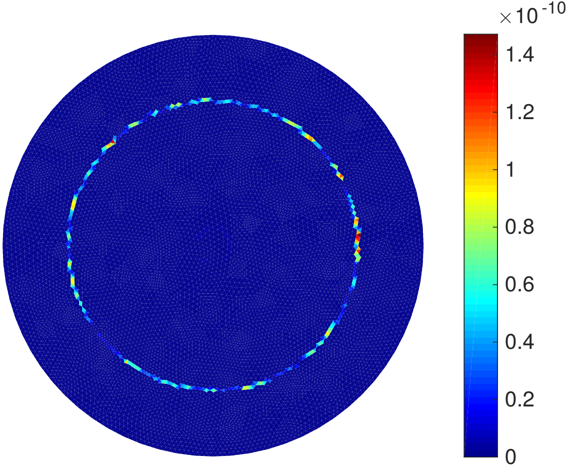
Overall performance



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

contact estimator





J. Dabaghi, V. Martin, M. Vohralík, Adaptive Inexact Semismooth Newton Methods for the Contact Problem Between Two Membranes. *Journal of Scientific Computing (2020).*

Outline

Parabolic model problem with linear complementarity constraints

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

Parabolic model problem with linear complementarity constraints

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

Two possibilities to characterize the weak solution

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

- Saddle point formulation $(u_1, u_2, \lambda) \in L^2(0,T; H^1_{g_1}(\Omega)) \times L^2(0,T; H^1_{g_2}(\Omega)) \times L^2(0,T;\Lambda)$
- Parabolic variational inequality: $\boldsymbol{u} \in \mathcal{K}_g^{\mathrm{t}}$

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

Discrete complementarity problems for finite elements

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

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

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Employing a C-function our problem reads

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

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Inexact semismooth Newton method:

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

A posteriori analysis

We employ the methodology of equilibrated flux reconstructions

Theorem (Guaranteed upper bound)

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

Corollary (Distinction of the error components)

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

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

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

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

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

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

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

A posteriori error at convergence for $p = 1$

Theorem (Guaranteed upper bound)

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

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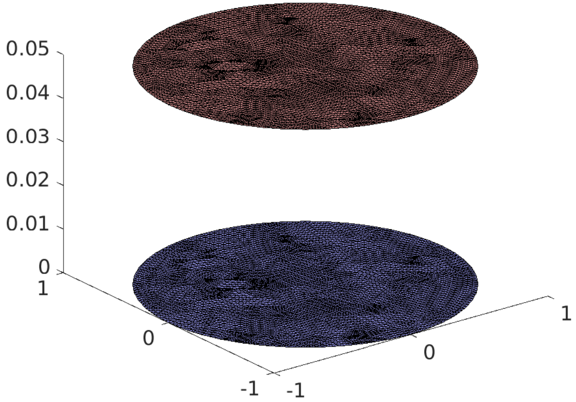
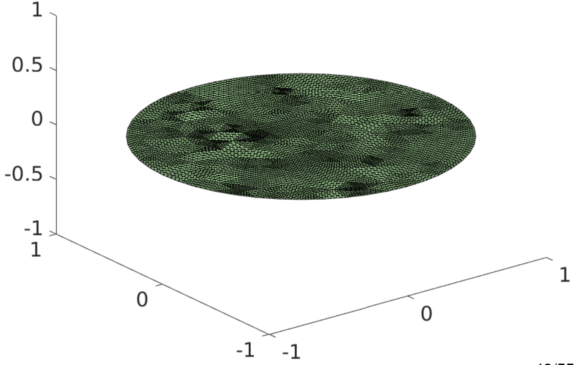
Lemma

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

Numerical experiments $p = 1$

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





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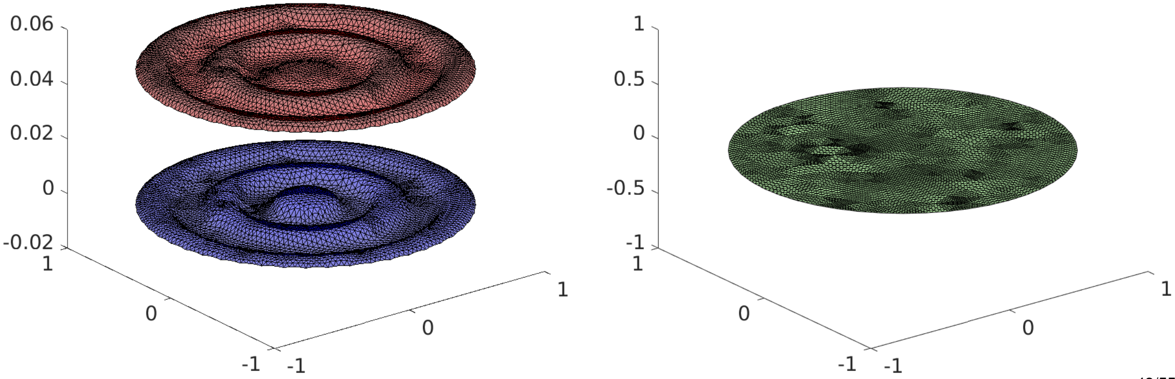

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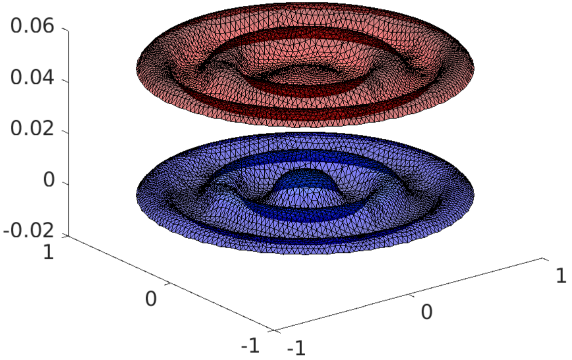

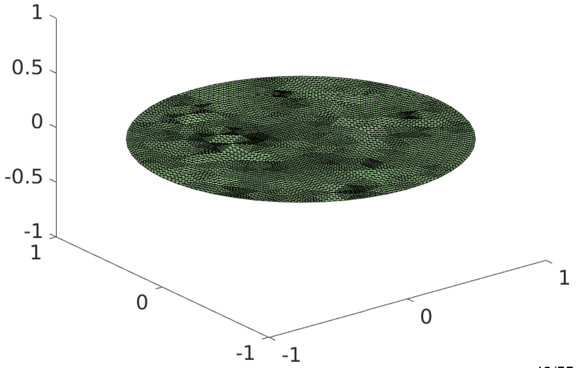

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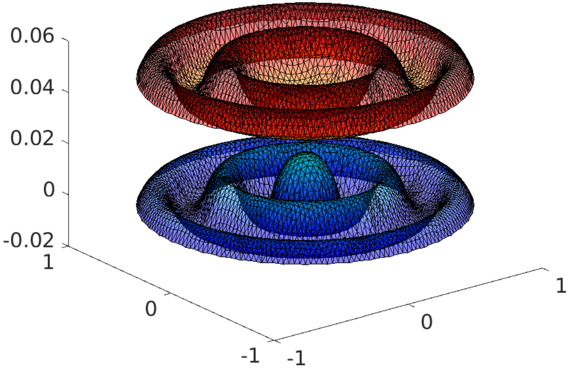

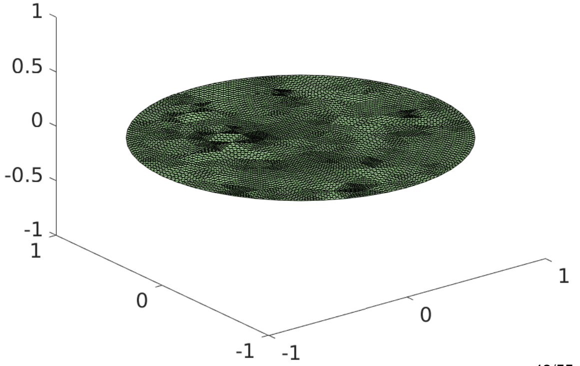

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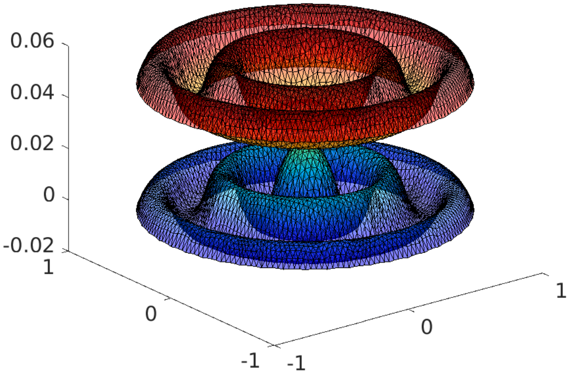

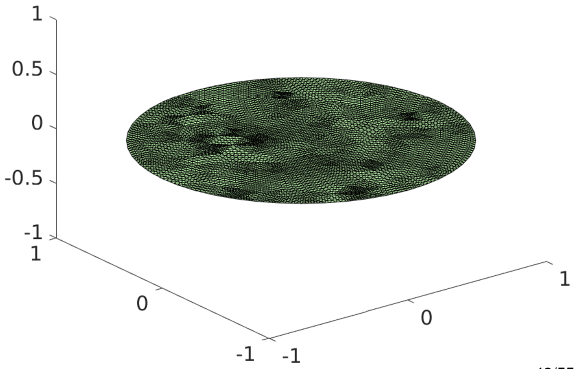

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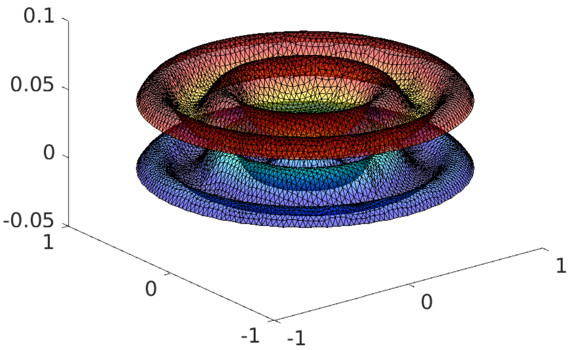

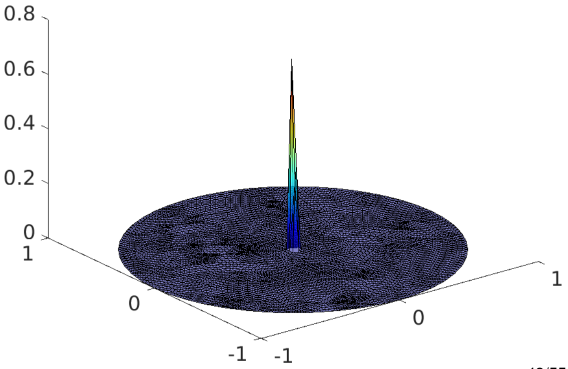

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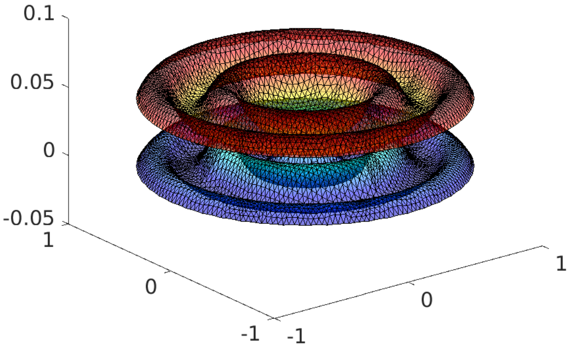

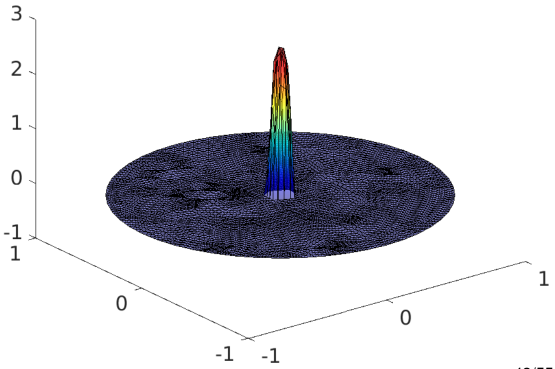

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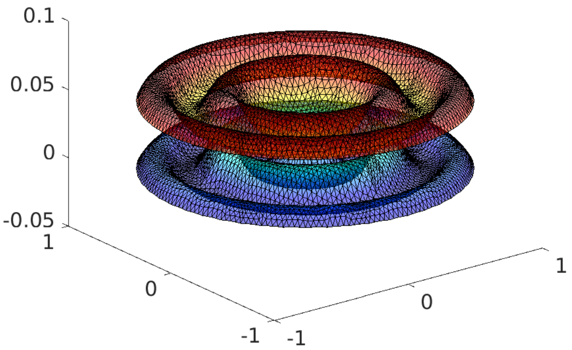

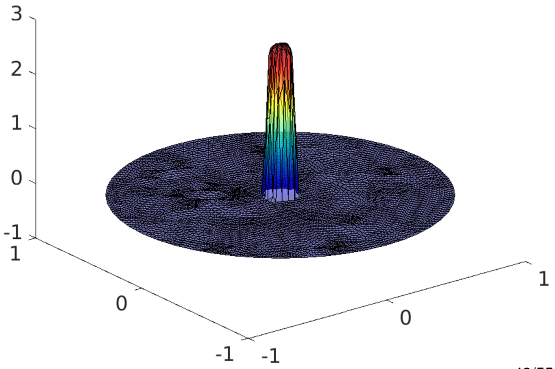

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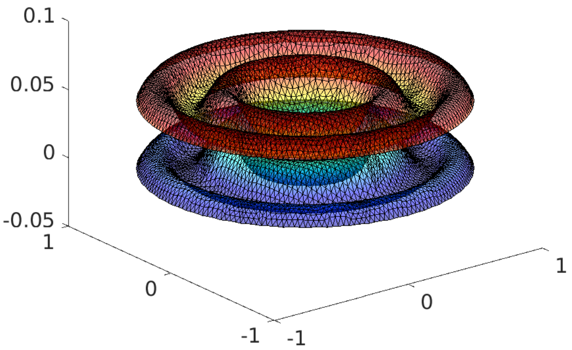

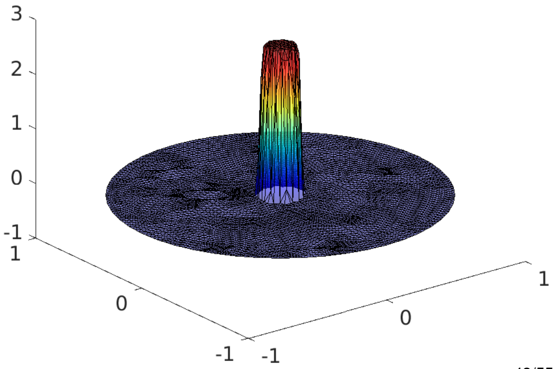

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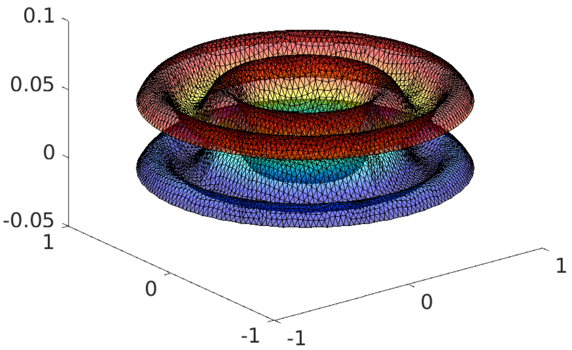

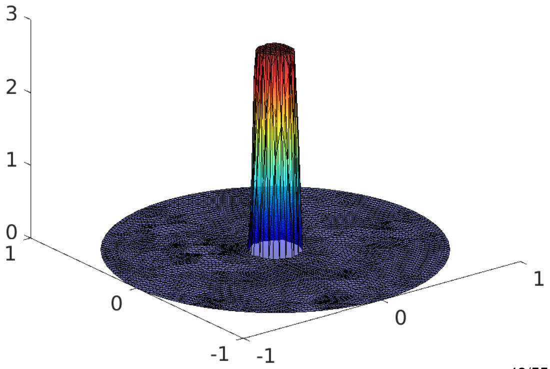

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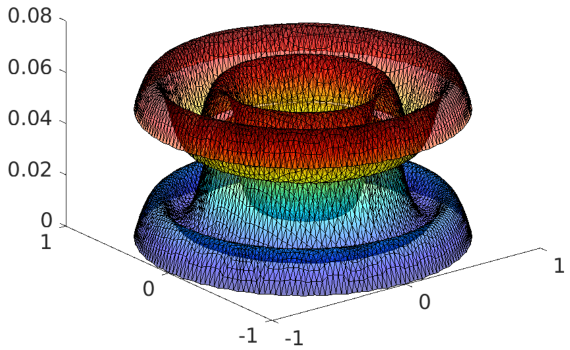

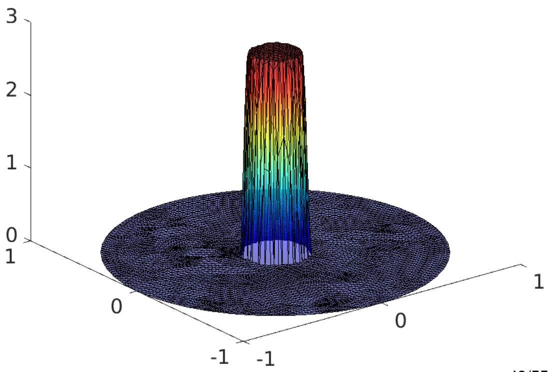

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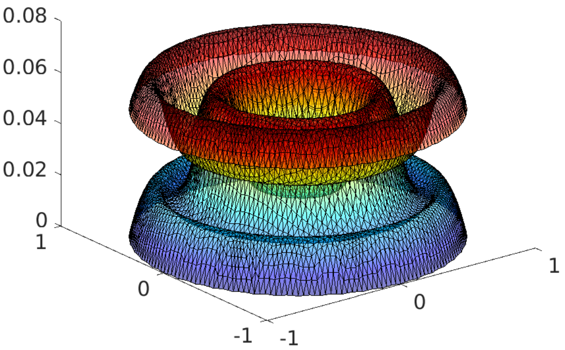

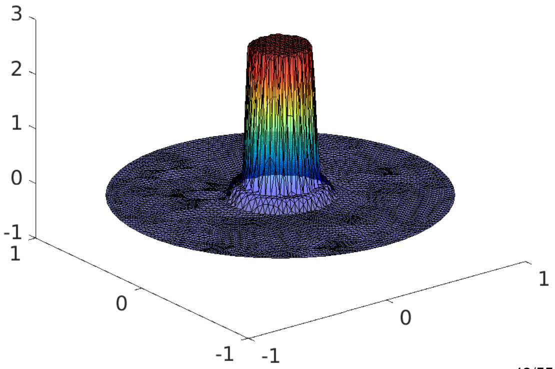

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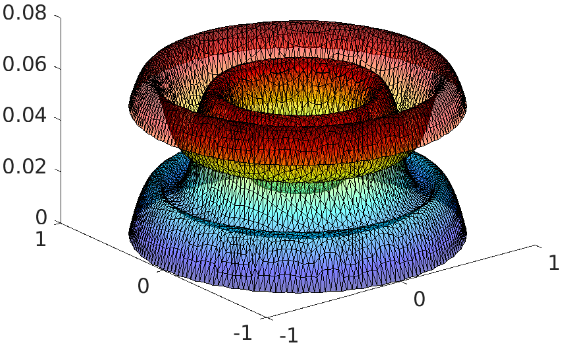

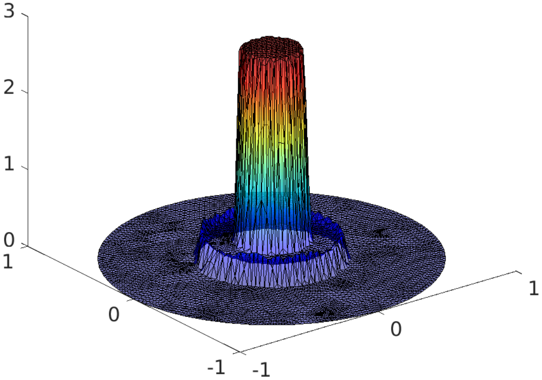

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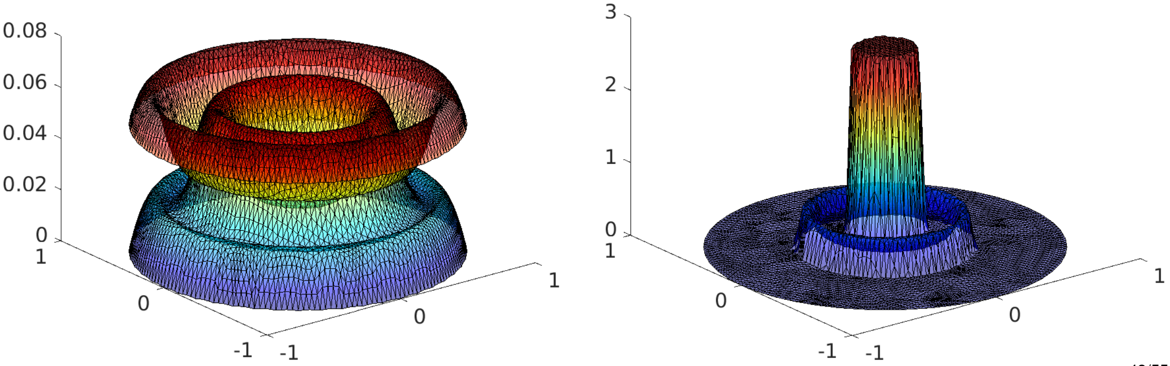
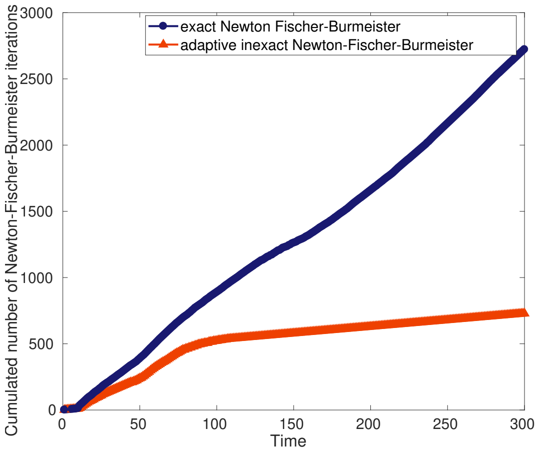
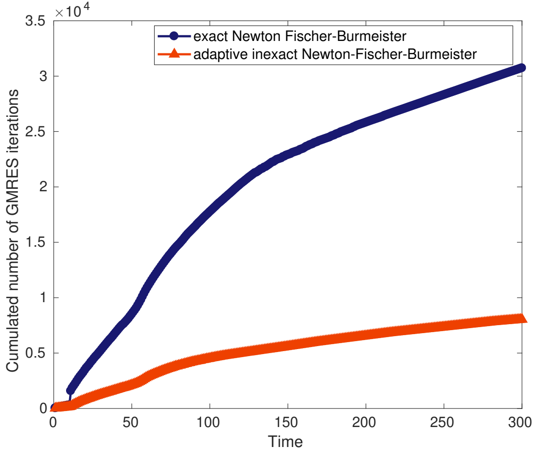


Newton–Fischer–Burmeister performance





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 engeneering (2020).*

Two-phase flow with phase appearance and disappearance

Storage of radioactive wastes in deep geological layers

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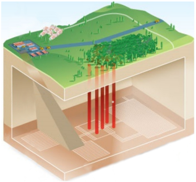
Storage of radioactive wastes in deep geological layers



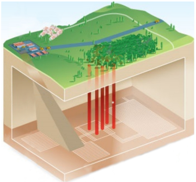
$$\partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \nabla \cdot \left[\gamma_1 \mathbf{q}^{\mathrm{l}}(S^{\mathrm{l}}, P^{\mathrm{l}}) - \mathbf{J}^{\mathrm{l}}_{\mathrm{h}}(S^{\mathrm{l}}, \chi^{\mathrm{l}}_{\mathrm{h}})\right] = Q_{\mathrm{w}},$$

$$\partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi^{\mathrm{l}}_{\mathrm{h}}) + \nabla \cdot \left[\gamma_2 \chi^{\mathrm{l}}_{\mathrm{h}} \mathbf{q}^{\mathrm{l}}(S^{\mathrm{l}}, P^{\mathrm{l}}) + \gamma_3 P^{\mathrm{g}} \mathbf{q}^{\mathrm{g}}(S^{\mathrm{l}}, P^{\mathrm{l}}) + \mathbf{J}^{\mathrm{l}}_{\mathrm{h}}(S^{\mathrm{l}}, \chi^{\mathrm{l}}_{\mathrm{h}})\right] = Q_{\mathrm{h}},$$

$$1 - S^{\mathrm{l}} \geq 0, \; HP^{\mathrm{g}} - \beta_{\mathrm{l}} \chi^{\mathrm{l}}_{\mathrm{h}} \geq 0, \; \left[1 - S^{\mathrm{l}}\right] \cdot \left[HP^{\mathrm{g}} - \beta_{\mathrm{l}} \chi^{\mathrm{l}}_{\mathrm{h}}\right] = 0$$

Two-phase flow with phase appearance and disappearance

Storage of radioactive wastes in deep geological layers



$$\partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \nabla\cdot\left[\gamma_1 \mathbf{q}^{\mathrm{l}}(S^{\mathrm{l}}, P^{\mathrm{l}}) - \mathbf{J}_{\mathrm{h}}^{\mathrm{l}}(S^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}})\right] = Q_{\mathrm{w}},$$

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

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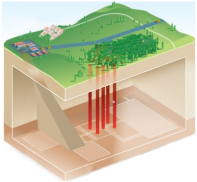

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Unknowns: liquid saturation S^{l}, liquid pressure P^{l}, mole fraction of liquid hydrogen $\chi_{\mathrm{h}}^{\mathrm{l}}$

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

Two-phase flow with phase appearance and disappearance

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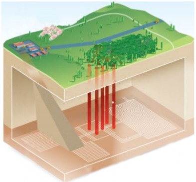

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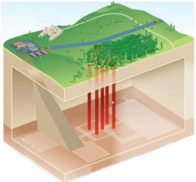

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Unknowns: liquid saturation S^{l}, liquid pressure P^{l}, mole fraction of liquid hydrogen $\chi^{\mathrm{l}}_{\mathrm{h}}$

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

Nonlinear fluxes: Darcy fluxes $\mathbf{q}^{\mathrm{l}}$ and $\mathbf{q}^{\mathrm{g}}$ + Fick flux $\mathbf{J}^{\mathrm{l}}_{\mathrm{h}}$

Nonlinear complementarity constraints: $1 - S^{\mathrm{l}} = 0$ and $HP^{\mathrm{g}} - \beta_{\mathrm{l}} \chi^{\mathrm{l}}_{\mathrm{h}} > 0 \Rightarrow$ no gas.
If $1 - S^{\mathrm{l}} > 0$ and $HP^{\mathrm{g}} - \beta_{\mathrm{l}} \chi^{\mathrm{l}}_{\mathrm{h}} = 0 \Rightarrow$ gas appearance.

Ben Gharbia and Jaffré (2014)

Discretization by the finite volume method

Numerical solution:

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

Discretization by the finite volume method

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

Discretization of each component equation and the nonlinear complementarity constraints

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

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

A posteriori error estimates

Recall:

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

A posteriori error estimates

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

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

A posteriori error estimates

Recall:

$$\begin{cases} \partial_t l_{\mathrm{w}}(S^{\mathrm{l}}) + \nabla\cdot\Phi_{\mathrm{w}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{w}}, \\ \partial_t l_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) + \nabla\cdot\Phi_{\mathrm{h}}(S^{\mathrm{l}}, P^{\mathrm{l}}, \chi_{\mathrm{h}}^{\mathrm{l}}) = Q_{\mathrm{h}}, \\ 1 - S^{\mathrm{l}} \geq 0, \ HP^{\mathrm{g}} - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}} \geq 0, \ \left[1 - S^{\mathrm{l}}\right]\cdot\left[HP^{\mathrm{g}} - \beta_{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right] = 0 \end{cases}$$

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Assumption: There exists a unique weak solution satisfying

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

$$l_c \in Y, \ 1 - S^{\mathrm{l}} \in Z, \ \Phi_c \in L^2((0,t_{\mathrm{F}}); \mathbf{H}(\mathrm{div},\Omega))$$

$$\int_0^{t_{\mathrm{F}}} (\partial_t l_c, \varphi)_\Omega (t)\,\mathrm{dt} - \int_0^{t_{\mathrm{F}}} (\Phi_c, \nabla\varphi)_\Omega (t)\,\mathrm{dt} = \int_0^{t_{\mathrm{F}}} (Q_c, \varphi)_\Omega (t)\,\mathrm{dt} \quad \forall \varphi \in X$$

$$\int_0^{t_{\mathrm{F}}} \left(\lambda - (1 - S^{\mathrm{l}}), H[P^{\mathrm{l}} + P_{\mathrm{cp}}(S^{\mathrm{l}})] - \beta^{\mathrm{l}}\chi_{\mathrm{h}}^{\mathrm{l}}\right)_\Omega (t)\,\mathrm{dt} \geq 0 \quad \forall \lambda \in Z$$

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**

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

2. **Residual for the constraints**

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

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

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

Theorem

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

Error measure

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

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

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

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Theorem

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Error measure

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Theorem

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

Numerical experiments

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

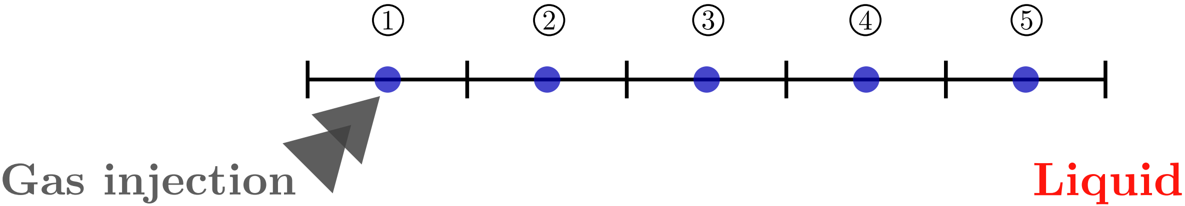
Semismooth solver: Newton-min

Iterative algebraic solver: GMRES.

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

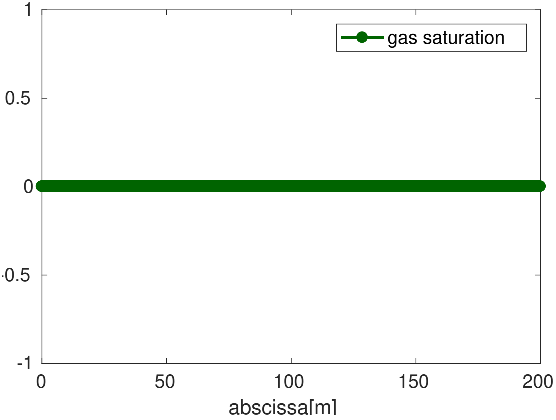
Number of cells: $N_{\mathrm{sp}} = 1000$,

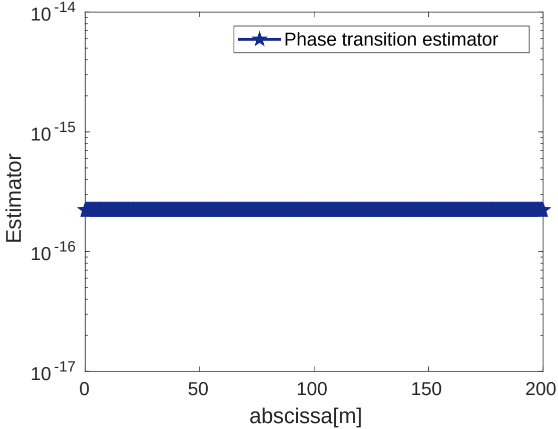
Final simulation time: $t_{\mathrm{F}} = 5 \times 10^5$ years.



Phase transition estimator

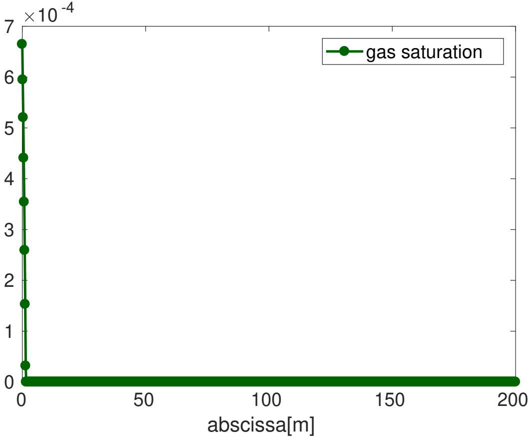
$t = $ 2500 years

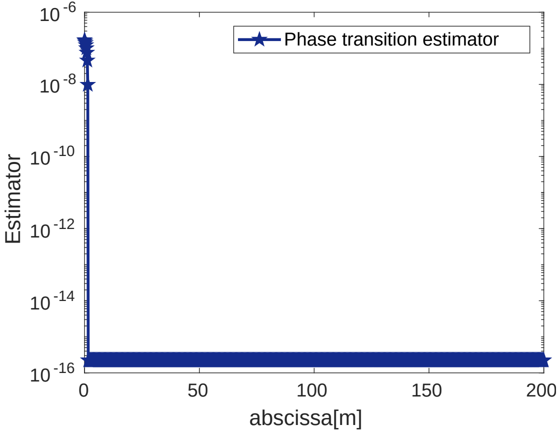




Phase transition estimator

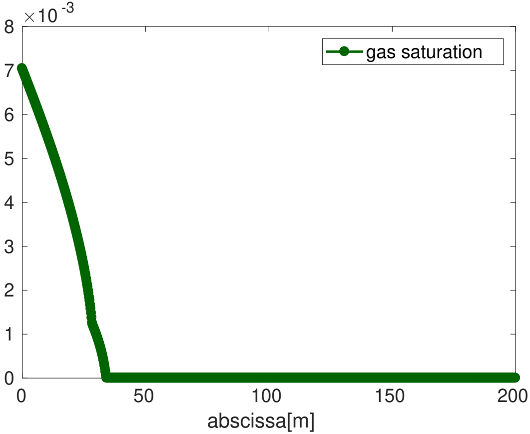
$t = 1.25 \times 10^4$ **years**

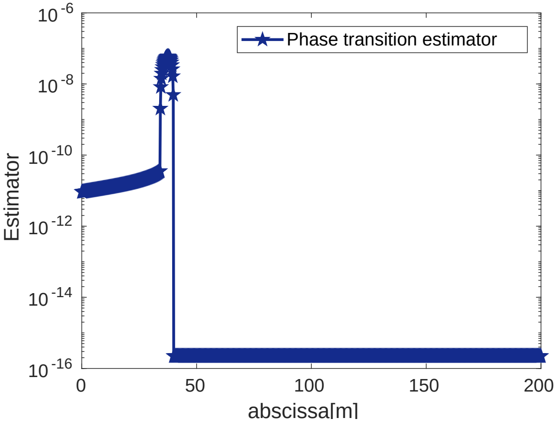




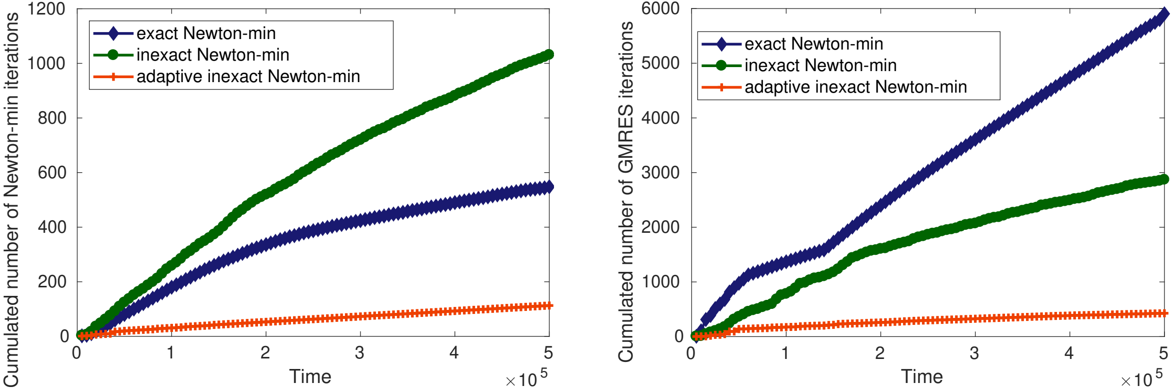
Phase transition estimator

$t = 4.25 \times 10^4$ years



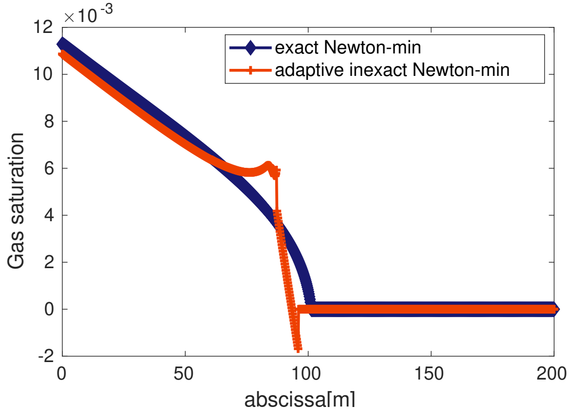


Overall performance $\gamma_{\mathrm{lin}} = \gamma_{\mathrm{alg}} = 10^{-3}$

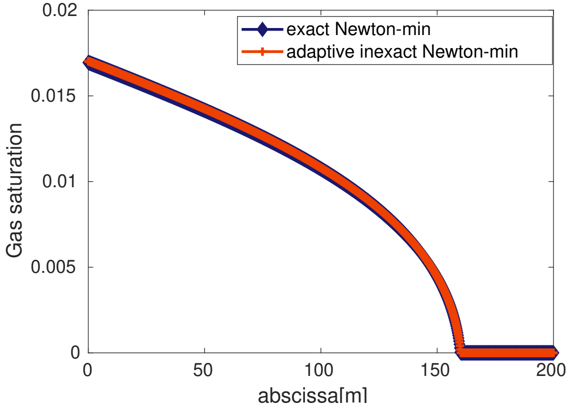


Accuracy $\gamma_{\mathrm{lin}} = \gamma_{\mathrm{alg}} = 10^{-3}$

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years



I. Ben Gharbia J. Dabaghi, V. Martin, M. Vohralík, A posteriori error estimates for a compositional two-phase flow with nonlinear complementarity constraints. *Computational Geosciences (2020).*

Outline

Conclusion and perspectives

Conclusion

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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

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).

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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Discretization flux reconstruction:

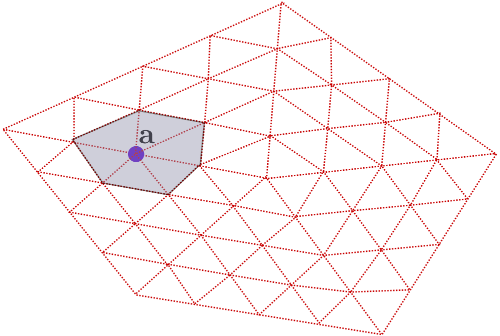
$$
\begin{aligned}
\left(\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\alpha h,\mathrm{disc}}, \boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} - \left(\gamma^{k,i,\boldsymbol{a}}_{\alpha h}, \nabla\cdot\boldsymbol{\tau}_h\right)_{\omega_h^{\boldsymbol{a}}} &= -\left(\mu_\alpha \psi_{h,\boldsymbol{a}}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

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

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

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

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



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

Strategy for constructing the estimators

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

Nonconformity estimator 1:

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

Nonconformity estimator 2:

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

Nonconformity estimator 3:

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

Distinguishing the error components

$p = 1$

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

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

$p \geq 2$

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

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

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

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

Parabolic weak formulation

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

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

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

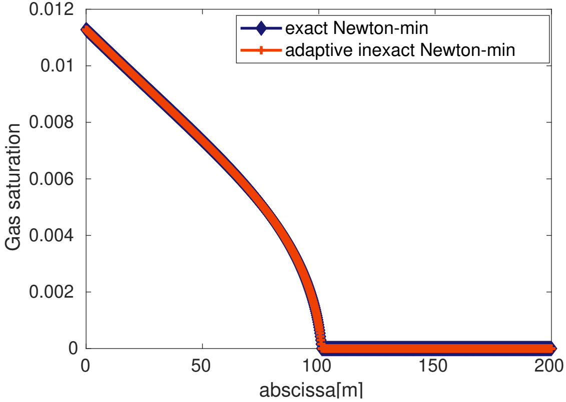
Discrete formulation: Given $(u^0_{1h}, u^0_{2h}) \in \mathcal{K}^p_{gh}$, search $(u^n_{1h}, u^n_{2h}, \lambda^n_h) \in X^p_{gh} \times X^p_{0h} \times \Lambda^p_h$ such that for all $(z_{1h}, z_{2h}, \chi_h) \in X^p_{0h} \times X^p_{0h} \times \Lambda^p_h$

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

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

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

$t = 1.05 \times 10^5$ years



$t = 3.5 \times 10^5$ years