A semismooth Newton method for obstacle-type quasivariational inequalities

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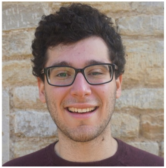   

What are obstacle-type QVIs?

An example of an obstacle-type QVI

Consider the feasible set: $K(u) \coloneqq \{v \in H_0^1(\Omega) : v \leq \Phi(u) \text{ a.e.}\}$.
Find $u \in H_0^1(\Omega)$ that satisfies $u \leq \Phi(u)$ and

$$(\nabla u, \nabla(v - u))_{L^2(\Omega)} \geq (f, v - u)_{L^2(\Omega)} \quad \text{for all } v \in K(u).$$

Examples of $\Phi(u)$?

- $\Phi(u) = C + \epsilon \min(0, u)$,
- $-\Delta(\Phi(u)) + k^2\Phi(u) = u^2$.

Applications include contact mechanics, thermoforming, elastic bilayers, image processing, option pricing, fluid flow with pressure constraints...
Why doesn't everyone model with QVIs? ...because they are very hard to solve!

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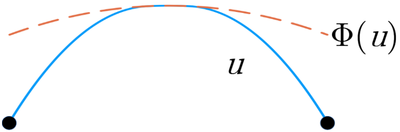

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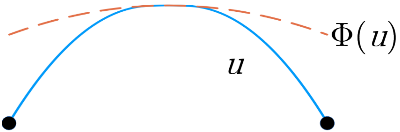

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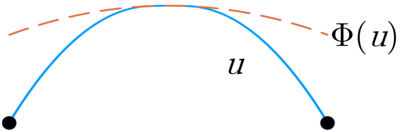

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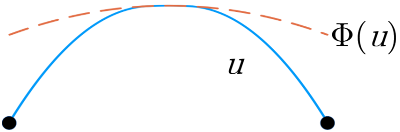

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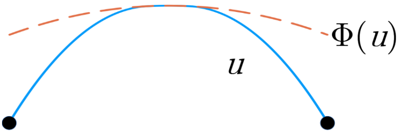

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Semismooth Newton method

Rewrite the QVI as the fixed point problem

$$u = S(\Phi(u)).$$

Obstacle map $S : H_0^1(\Omega) \to H_0^1(\Omega)$, $S : \phi \mapsto u_\phi$

$u_\phi = S(\phi)$ maps from the obstacle $\to$ solution of the obstacle VI, i.e.

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⚠Evaluating $\Phi(u)$ might require a nonlinear PDE solve.

⚠Evaluating $S(\phi)$ requires a VI solve.

SSN step for the QVI

Let $R(u) = u - S(\Phi(u))$. We want $u_* : R(u_*) = 0$. The $i+1$-th SSN iteration is

(i) Solve $G_R(u_i)\delta = -R(u_i)$ for δ. (ii) $u_{i+1} = u_i + \delta$.

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Evaluating the right-hand side $R(u_i)$

Recall $R(u) = u - S(\Phi(u))$.

Obstacle problem

The difficulty lies in evaluating $S(\phi)$ i.e. find $u_\phi \in H_0^1(\Omega)$ that satisfies:

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Solver

- Delivers a feasible solution $\tilde{u}_\phi \leq \phi$ a.e.;
- Enjoys mesh independence (the number of iterations does not grow in an unbounded manner as the mesh is refined).

💡 Use a path-following smoothed Moreau–Yosida regularization [mesh independence] followed by a few iterations of the primal-dual active set strategy [feasibility].

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Semismooth/Newton differentiable

Definition

A mapping $F : D \subset X \to Z$ (X, Z Banach) is *semismooth* or *Newton differentiable* in an open set $U \subset D$ if $\exists$ a family of mappings $G_F : U \to \mathcal{L}(X, Z)$ such that, for every $u \in U$,

$$\lim_{\delta \to 0} \frac{1}{\|\delta\|} \|F(u + \delta) - F(u) - G_F(u + \delta)\delta\| = 0$$

Application

$$\text{Find } u_* \in X : F(u_*) = 0.$$

(i) Solve $G_F(u_i)\delta_i = -F(u_i)$ for δ_i and (ii) $u_{i+1} = u_i + \delta_i$.

The semismooth property implies that, if $\|u_* - u_0\|$ is sufficiently small, the Newton method converges at a local superlinear rate.

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Chain rule: $R(u) = u - S(\Phi(u))$

$$G_R(u_i) = \mathrm{Id} - G_S(\Phi(u_i))G_\Phi(u_i).$$

Theorem

Let $Y_p := \{\psi \in H_0^1(\Omega) : \Delta\psi \in L^p(\Omega)\}$, $\max(1, 2d/(d+2)) < p \leq \infty$. Then the obstacle map $S : \phi \mapsto u_\phi$, $S : Y_p \to H_0^1(\Omega)$ is *semismooth* with a Newton derivative G_S where $\|G_S\| \leq 1$. Moreover,

$$G_S(\phi)\zeta = \zeta + z_\zeta$$

where $z_\zeta \in H_0^1(\mathcal{I}(\phi))$ satisfies

$$(\nabla z_\zeta - \nabla\zeta, \nabla v) = 0 \;\text{ for all } v \in H_0^1(\mathcal{I}(\phi))$$

and $\mathcal{I}(\phi) = \{x \in \Omega : S(\phi)(x) < \phi(x) \text{ a.e.}\} \subseteq \Omega$.

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$$G_R(u_i) = \mathrm{Id} - G_S(\Phi(u_i))G_\Phi(u_i).$$

Theorem

Let $Y_p := \{\psi \in H_0^1(\Omega) : \Delta\psi \in L^p(\Omega)\}$, $\max(1, 2d/(d+2)) < p \leq \infty$. Then the obstacle map $S : \phi \mapsto u_\phi$, $S : Y_p \to H_0^1(\Omega)$ is *semismooth* with a Newton derivative G_S where $\|G_S\| \leq 1$. Moreover,

$$G_S(\phi)\zeta = \zeta + z_\zeta$$

where $z_\zeta \in H_0^1(\mathcal{I}(\phi))$ satisfies

$$(\nabla z_\zeta - \nabla\zeta, \nabla v) = 0 \;\text{ for all } v \in H_0^1(\mathcal{I}(\phi))$$

and $\mathcal{I}(\phi) = \{x \in \Omega : S(\phi)(x) < \phi(x) \text{ a.e.}\} \subseteq \Omega$.

Deriving the SSN System

SSN System

SSN update δ satisfies

$$[\mathrm{Id} - G_S(\Phi(u_i))G_\Phi(u_i)]\delta = -R(u_i).$$

Introduce auxiliary variables $\eta = G_\Phi(u_i)\delta$ and $\mu = G_S(\Phi(u_i))\eta - \eta$. Reformulate SSN system as

$$\begin{pmatrix} \mathrm{Id} & -\mathrm{Id} & -\mathrm{Id}|_{\mathcal{I}(u_i)} \\ G_\Phi(u_i) & -\mathrm{Id} & 0 \\ 0 & (G_S(\Phi(u_i)) - \mathrm{Id})|_{\mathcal{I}(u_i)} & -\mathrm{Id}|_{\mathcal{I}(u_i)} \end{pmatrix} \begin{pmatrix} \delta \\ \eta \\ \mu \end{pmatrix} = -\begin{pmatrix} R(u_i) \\ 0 \\ 0 \end{pmatrix}.$$

where $\mathcal{I}(u_i) := \{x \in \Omega : S(\Phi(u_i))(x) < \Phi(u_i)(x) \text{ a.e.}\}$.

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Implementing the active-set

After a continuous piecewise (bi)linear FEM discretization, the active set can be directly implemented by deleting the corresponding discrete active set rows and columns.

Active-set SSN system

$$\begin{pmatrix} M & -M & -M_{:,\mathfrak{I}} \\ A & -M & 0 \\ 0 & B_{\mathfrak{I},:} & -M_{\mathfrak{I},\mathfrak{I}} \end{pmatrix} \begin{pmatrix} \boldsymbol{\delta} \\ \boldsymbol{\eta} \\ \boldsymbol{\mu}_{\mathfrak{I}} \end{pmatrix} = \begin{pmatrix} -\boldsymbol{r} \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{\mu}_{\mathrm{dofs}\setminus\mathfrak{I}} = 0,$$

$\mathfrak{I} = \{j \in \mathrm{dofs} : [S(\Phi(u_i))]_j < [\Phi(u_i)]_j\}$, $A \approx G_\Phi(u_i)$ and $B \approx G_S(\Phi(u_i)) - \mathrm{Id}$.

Globalization & inexactness

Globalization

For $u, v \in X$ and a $\gamma \in [0,1)$ suppose that

$$\|S(\Phi(u)) - S(\Phi(v))\|_X \leq \gamma \|u - v\|_X,$$

$$\sup_{u \in X} \|G_S(\Phi(u)) G_\Phi(u)\| \leq \gamma.$$

A simple safeguarding technique that ensures globalization is take the next iterate as

$$u_{i+1} = \begin{cases} u_i + \delta & \text{if } \|R(u_i + \delta)\|_X \leq \|R(S(\Phi(u_i)))\|_X, \\ S(\Phi(u_i)) & \text{if } \|R(S(\Phi(u_i)))\|_X < \|R(u_i + \delta)\|_X. \end{cases}$$

⚠Globalization techniques require efficient evaluations of $R(u)$. Here each evaluation requires an obstacle problem solve.

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Inexactness

The SSN update δ does not need to be computed exactly. An inexact strategy considers the updates

$$\|R(u_i) + G_R(u_i)\delta\|_X \leq \rho_i \|R(u_i)\|_X.$$

If $\rho_i \to 0$ as $i \to \infty$ then the SSN strategy converges with a local superlinear rate to the solution.

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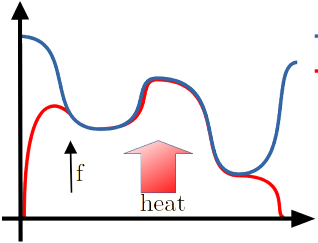
Thermoforming: an obstacle-type QVI



Model

Find $u \in H_0^1(\Omega)$ satisfying $u \leq \Phi(u) := \Phi_0 + \psi T$ and

$$(\nabla u, \nabla(v-u))_{L^2(\Omega)} - (f, v-u)_{L^2(\Omega)} \geq 0 \quad \text{for all } v \in H_0^1(\Omega), v \leq \Phi(u),$$

with T as the solution of

$$kT - \Delta T = g(\Phi_0 + \psi T - u) \text{ in } \Omega, \qquad \partial_\nu T = 0 \text{ on } \partial\Omega,$$

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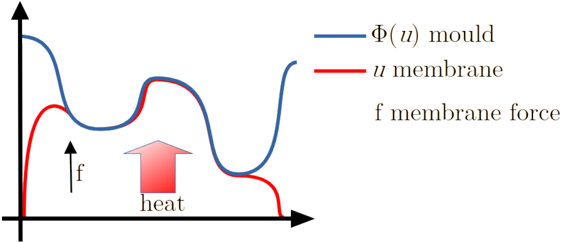

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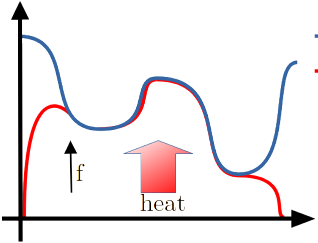

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Some properties of the thermoforming problem

Assumptions

- $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, is a Lipschitz domain;
- $\Phi_0 \in L^{2+\epsilon}(\Omega)$ for some $\epsilon > 0$ and $\psi \in C^2(\bar{\Omega})$ and $\psi = 0$ on $\partial\Omega$;
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Results

- There exists a solution (u, T) to the thermoforming problem;
- Φ is Newton differentiable from $H_0^1(\Omega)$ to Y_2;
- Φ is locally Lipschitz from $H_0^1(\Omega)$ to Y_2,

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FEM discretization & algorithm

Continuous piecewise (bi)linear FEM discretization for u and T.

Algorithm for SSN step

`Step 1.` Compute $R(u_i) = u_i - S(\Phi(u_i))$.

`Step 1.1.` $\Phi(u_i)$ requires a nonlinear solve [Newton].

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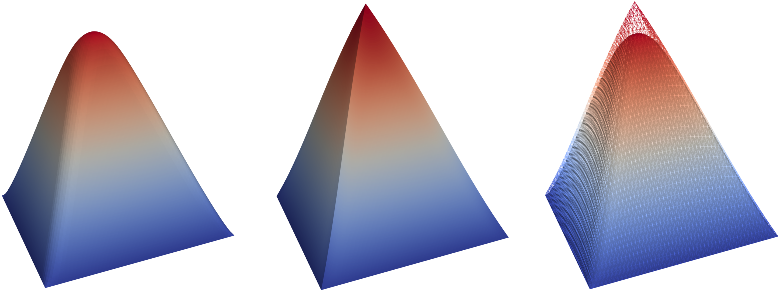
Leibniz Association

Example 1: setup

$$\Omega = (0,1)^2, \qquad \Phi_0(x_1,x_2) = 1 - 2\max(|x_1 - 0.5|, |x_2 - 0.5|),$$

$$f(x_1,x_2) = 25, \qquad \psi(x_1,x_2) = \sin(\pi x_1)\sin(\pi x_2), \qquad k = 1,$$

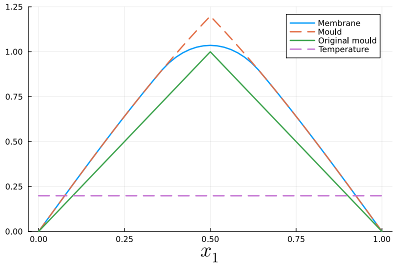
$$g(s) = \begin{cases} 1/5 & \text{if } s \leq 0, \\ (1-s)/5 & \text{if } 0 < s < 1, \\ 0 & \text{otherwise.} \end{cases}$$



(a) Membrane u (b) Mould $\Phi_0 + \psi T$ (c) Membrane & Mould

Example 1: convergence

- MY-Newton: Regularize the QVI with a smoothed Moreau–Yosida penalty in the obstacle problem [Solution is not feasible].
- Fixed point method: $u_{i+1} = S(\Phi(u_i))$ [Converges linearly].



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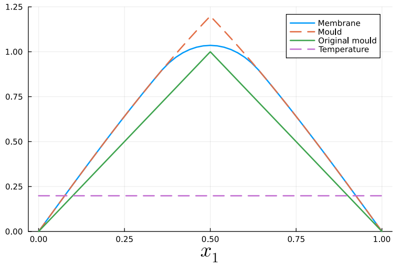

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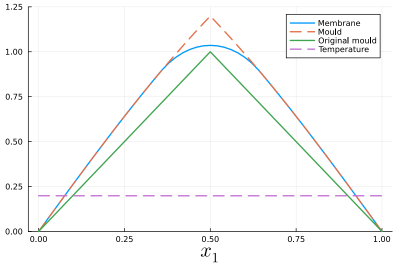
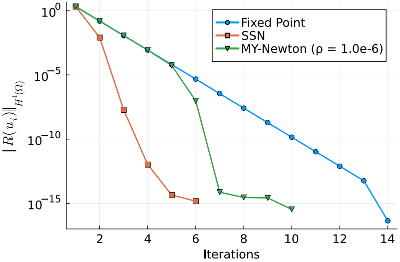




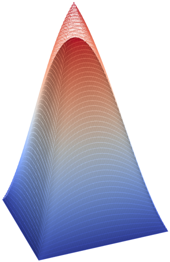
Example 1: mesh independence

	Outer loop	Evaluate Φ	Evaluate S	
h	SSN	Newton	PFMY	+PDAS
0.04	4	9	159	10
0.02	4	9	185	17
0.01	3	8	150	11
0.00667	3	8	158	11
0.005	3	8	158	17
0.004	4	8	199	21
0.00333	4	7	184	21

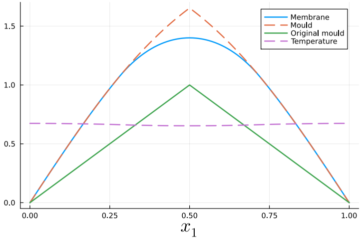
Table: Mesh independence of the SSN.

Example 2: setup

Only change: $$g(s) = \begin{cases} 1 & \text{if } s \leq 0, \\ (1 - 100s) & \text{if } 0 < s < 1/100, \\ 0 & \text{otherwise.} \end{cases}$$

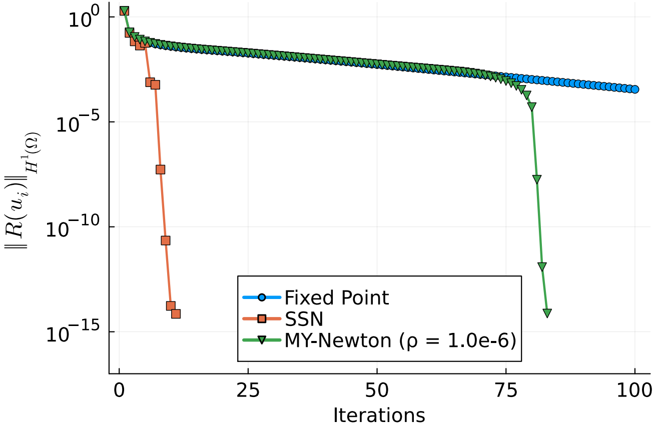


(a) Membrane & Mould



(b) Slice at $x_2 = 1/2$

Example 2: convergence



Conclusions

- A semismooth Newton method for solving obstacle-type QVIs;
- An active-set strategy implemented in Gridap & Firedrake;
- Theory relies on recent semismooth results for the obstacle map S.

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Software packages

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Conclusions

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Thank you for listening!

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