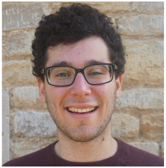
Hierarchical proximal Galerkin: a fast *hp*-FEM solver for variational problems with pointwise inequality constraints

John Papadopoulos[1]

[1]Weierstrass Institute Berlin,

April 11, 2025, Brown University Scientific Computing Seminar



Introduction

Pointwise constraints appear everywhere, e.g. contact mechanics (non-penetration), stress constraints in elasticity, sandpile growth, financial mathematics, pattern formation, engineering design, biological models...

Obstacle problem

Given a forcing term $f \in L^2(\Omega)$ and an obstacle $\varphi \in H^1(\Omega)$, the obstacle problem seeks $u : \Omega \to \mathbb{R}$ minimizing the Dirichlet energy

$$\min_{u \in H_0^1(\Omega)} \int_\Omega \frac{1}{2}|\nabla u|^2 - fu \,\mathrm{d}x \quad \text{subject to } u(x) \leq \varphi(x) \text{ for almost every } x \in \Omega.$$

- primal-dual active set, multigrid, finite-dimensional constrained optimizers (often mesh dependent, confined to low-order[1]).
- penalty methods (infeasible solutions, suboptimal for high-order, ill-conditioning).

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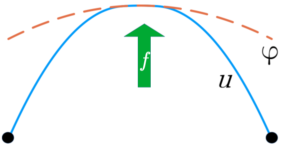

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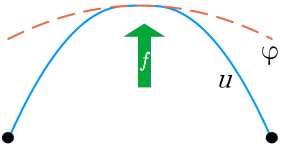

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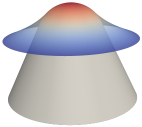

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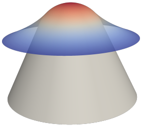

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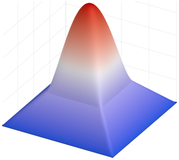

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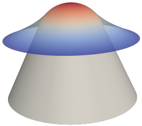

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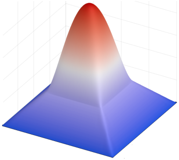

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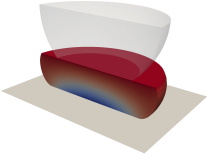

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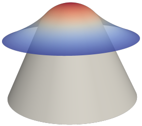

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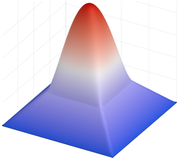

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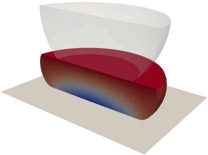

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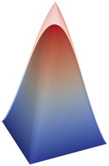

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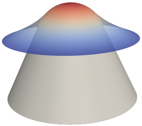

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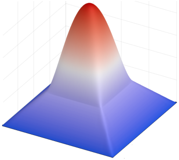

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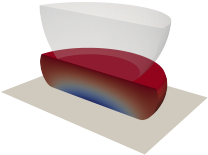

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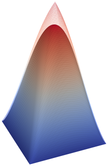

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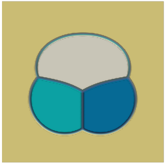

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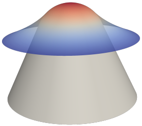

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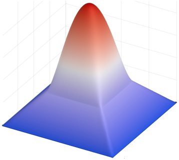

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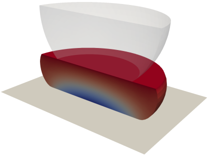

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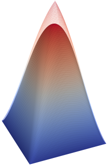

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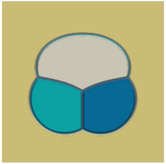

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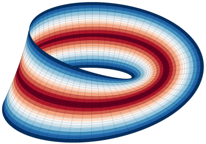

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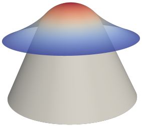

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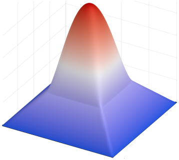

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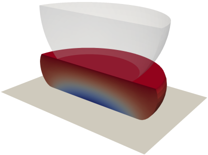

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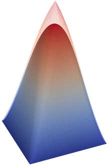

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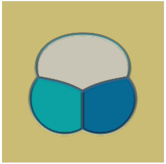

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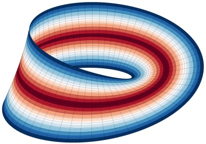

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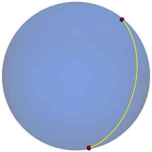

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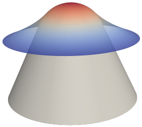

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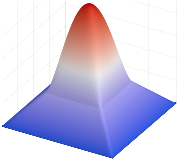

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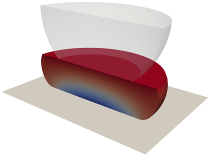

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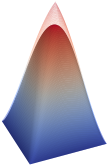

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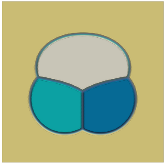

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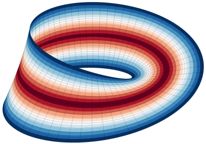

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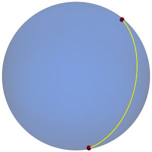

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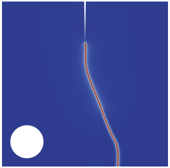
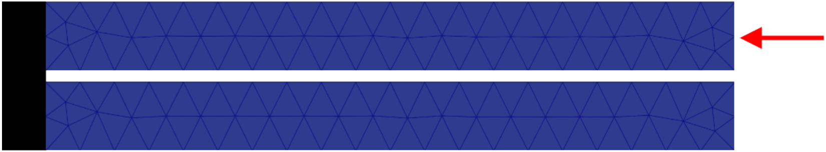


Fracture.

Contact problems



Contact problems

Problems of interest

Consider the constrained optimization problem:

$$\min_{u \in U} J(u) \quad \text{subject to} \quad Bu(x) \in C(x) \text{ for a.e. } x \in \Omega.$$

Examples

- (Obstacle problem.) Find $u : \Omega \to \mathbb{R}$

$$\min_{u \in H_0^1(\Omega)} \int_\Omega \frac{1}{2}|\nabla u|^2 - fu \,\mathrm{d}x \quad \text{subject to } u(x) \leq \varphi(x).$$

- (Elastic-plastic torsion.) Find $u : \Omega \to \mathbb{R}$,

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The LVPP algorithm

$$\min_{u \in U} J(u) \text{ subject to } Bu(x) \in C(x) \text{ for a.e. } x \in \Omega.$$

LVPP is an iterative algorithm where at each iteration we solve a *smooth* nonlinear system of PDEs:

The LVPP subproblem

Given ψ^{k-1}, for $k = 1, 2, \ldots$, we seek (u^k, ψ^k) satisfying

$$\alpha_k J'(u^k) + B^* \psi^k = B^* \psi^{k-1} \text{ in } U^*$$
$$Bu^k - G(\psi^k) = 0 \text{ a.e.,}$$

- Pick proximal parameters α_k such that $\sum_{j=1}^{\infty} \alpha_j \to \infty$.
- Pick pointwise operator G such that $G^{-1}(Bu)(x) \to \infty$ as $Bu(x) \to \partial C(x)$.

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LVPP for the obstacle problem

Obstacle problem

$U = H_0^1(\Omega)$, $B = B^* = \mathrm{id}$, $J' = -\Delta - f$, and $G(\psi) = \varphi - \mathrm{e}^{-\psi}$.

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Theorem (B. Keith, T. Surowiec, FoCM, 2024)

Suppose that Ω is an open, bounded and Lipschitz domain, $f \in L^\infty(\Omega)$ and $\varphi \in \{\phi \in H^1(\Omega) \cap C(\bar{\Omega}) : \Delta\phi \in L^\infty(\Omega)\}$, then

$$\|u^* - u^k\|_{H^1(\Omega)} \lesssim \left(\sum_{j=1}^{k} \alpha_j\right)^{-1/2}.$$

Note that $u^k \to u^*$ in $H^1(\Omega)$ even if $\alpha_k = 1$ for all $k \in \mathbb{N}$.

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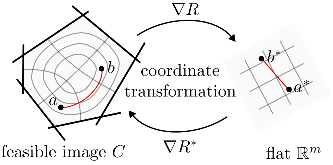
Advantages of the LVPP algorithm

1. It has an infinite-dimensional formulation.
2. Observed discretization-independent number of linear system solves.
3. A simple mechanism for enforcing pointwise constraints on the discrete level (without the need for a projection).
4. Ease of implementation — the algorithm reduces to the repeated solve of a smooth nonlinear system of PDEs *without requiring specialized discretizations*.
5. Robust numerical performance since convergence occurs as α_k can be kept small.



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1. It has an infinite-dimensional formulation.
2. Observed discretization-independent number of linear system solves.
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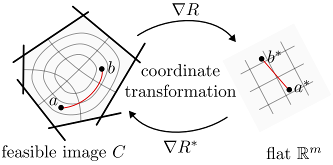

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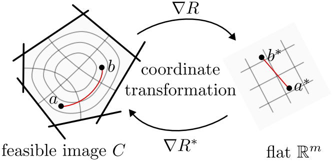

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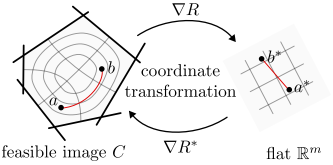

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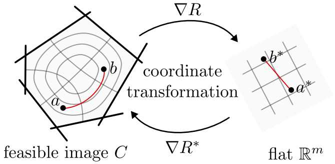
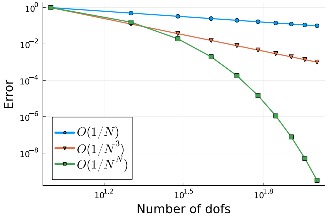


High-order finite element methods

A “high-order” discretization is one where we are approximating the solution with piecewise polynomials of high degree, e.g. $p \geq 4$.



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Naive implementations lead to slow quadrature, dense linear systems, capped convergence and, therefore, slow solve times.

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Utilize a sparsity-promoting high-order basis that admits fast quadrature via the DCT.

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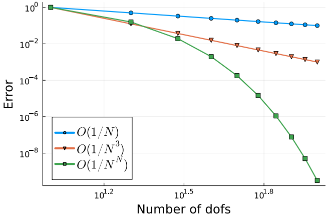

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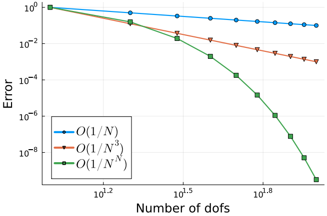

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Weak form and a finite element discretization

Weak form of LVPP for the obstacle problem

The k^{th} LVPP subproblem seeks $(u^k, \psi^k) \in H_0^1(\Omega) \times L^\infty(\Omega)$ satisfying for all $(v, q) \in H_0^1(\Omega) \times L^\infty(\Omega)$:

$$\alpha_k(\nabla u^k, \nabla v) + (\psi^k, v) = \alpha_k(f, v) + (\psi^{k-1}, v)$$
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FEM discretization

Pick finite-dimensional spaces $V_{hp} \subset H_0^1(\Omega)$, $Q_{hp} \subset L^\infty(\Omega)$ and seek $(u_{hp}^k, \psi_{hp}^k) \in V_{hp} \times Q_{hp}$ satisfying for all $(v_{hp}, q_{hp}) \in V_{hp} \times Q_{hp}$:

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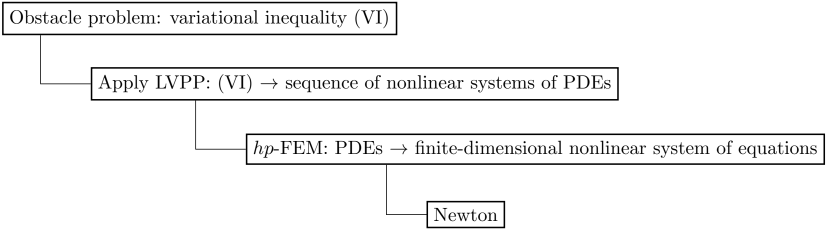

LVPP solver pipeline.

Newton linear systems

In matrix-vector form we are solving

$$\begin{pmatrix} \alpha_k A & B \\ B^\top & -D_{\psi^k} \end{pmatrix} \begin{pmatrix} \boldsymbol{\delta}_u \\ \boldsymbol{\delta}_\psi \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_u \\ \boldsymbol{b}_\psi \end{pmatrix},$$

where for basis function $\phi_i \in V_{hp}$ and $\zeta_i \in Q_{hp}$,

$$A_{ij} = (\nabla\phi_i, \nabla\phi_j), \quad B_{ij} = (\phi_i, \zeta_j), \quad \text{and} \quad [D_\psi]_{ij} = (\zeta_i, \mathrm{e}^{-\psi_{hp}}\zeta_j).$$

Goal

Pick FEM bases $\{\phi_i\} \subset V_{hp}$ and $\{\zeta_j\} \subset Q_{hp}$ that contain high-degree polynomials but also

- Keep A, B and D_ψ sparse.
- Allow for fast assembly or action of D_ψ.

💡 use a discontinuous piecewise Legendre polynomial basis for ψ_{hp} and the (Babuška–Szabó) hierarchical continuous p-FEM basis for u_{hp}.

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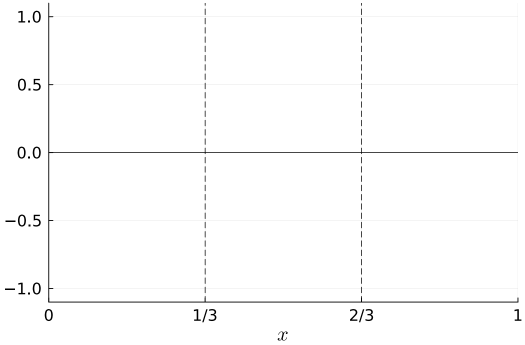
The Legendre polynomials $P_n(x)$, $n \in \mathbb{N}_0$ satisfy $\int_{-1}^{1} P_n P_m \, \mathrm{d}x \simeq \delta_{nm}$.
We can shift-and-scale the polynomials to construct a 1D basis such that $(\zeta_i, \zeta_j) \simeq \delta_{ij}$ for all basis functions $\zeta_i \in Q_{hp}$. This basis has *fast* transforms.



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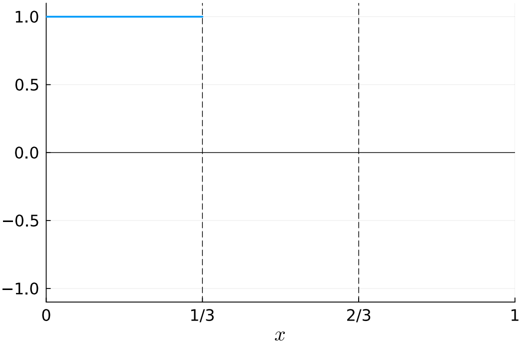

Shift-and-scale constant $P_0(x)$ on each cell.

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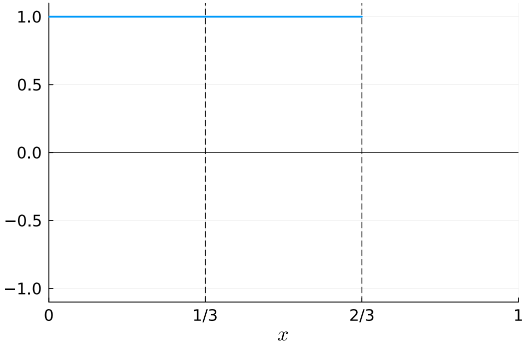

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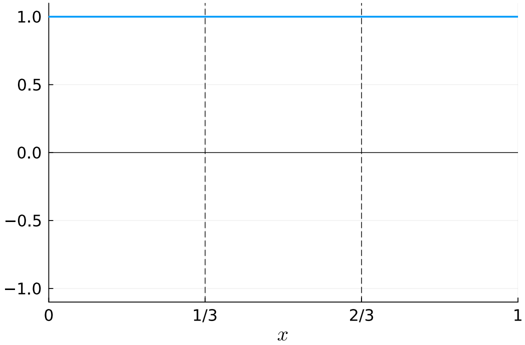

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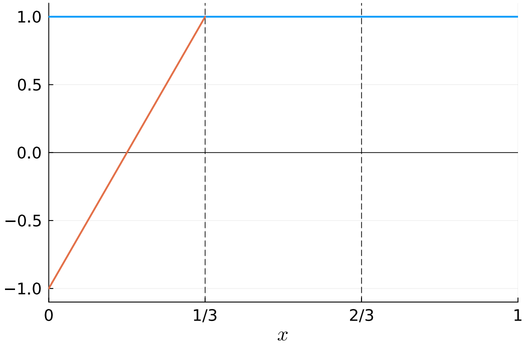

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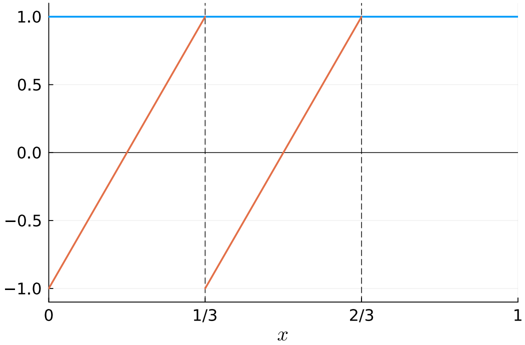

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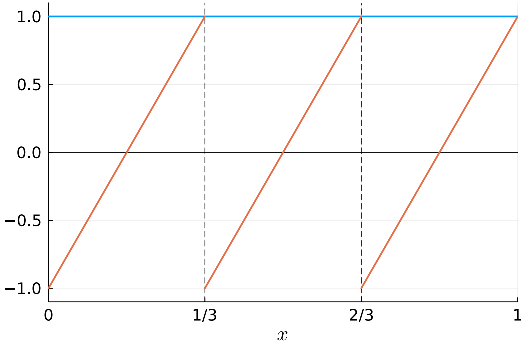

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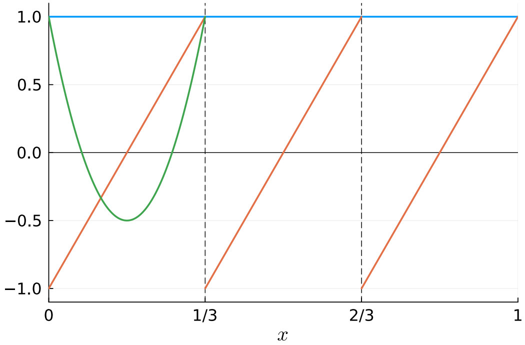

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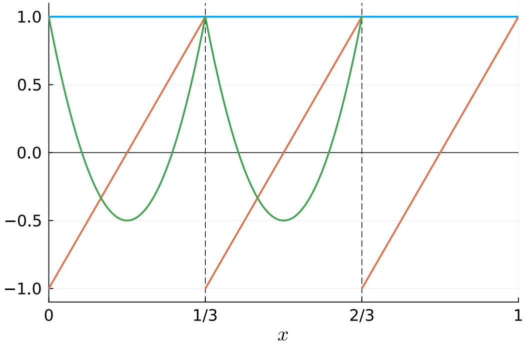

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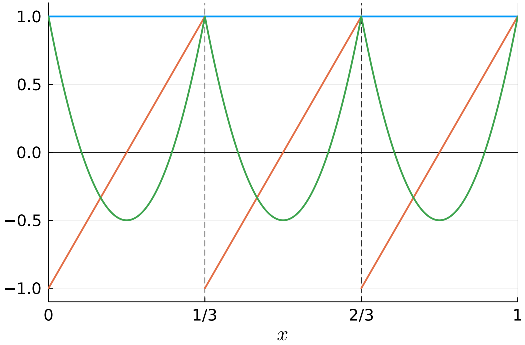

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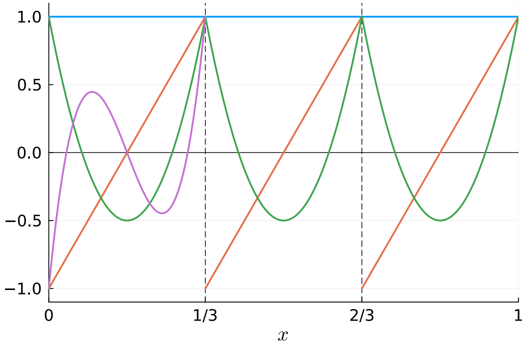

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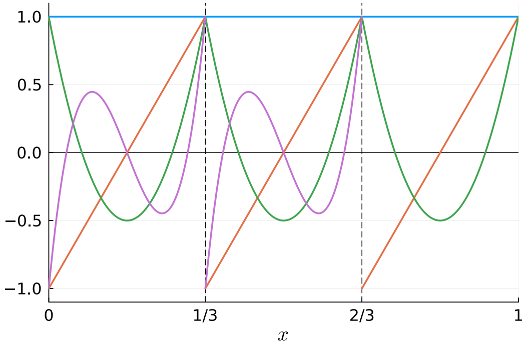

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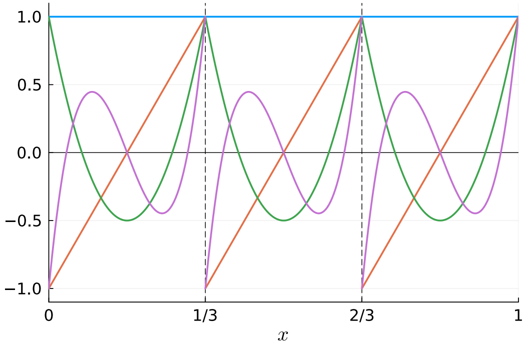

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The continuous hierarchical *p*-FEM basis in 1D

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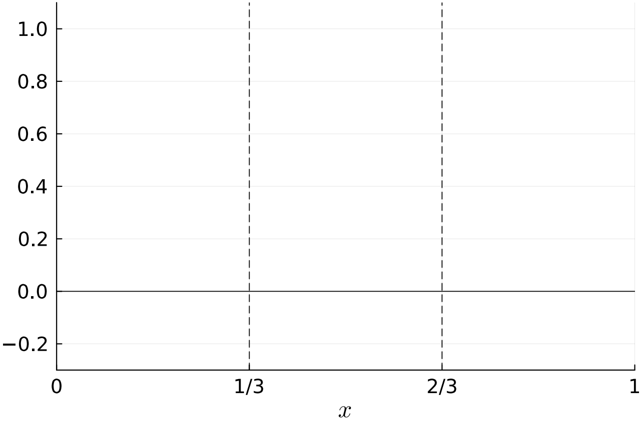

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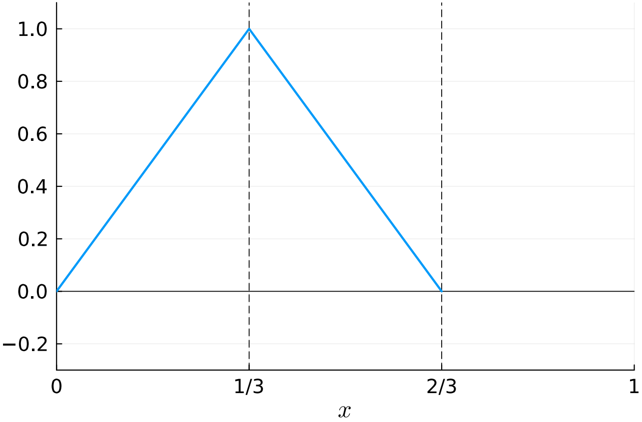

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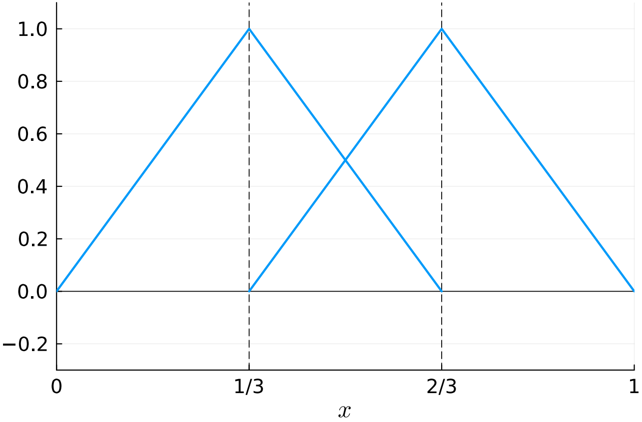

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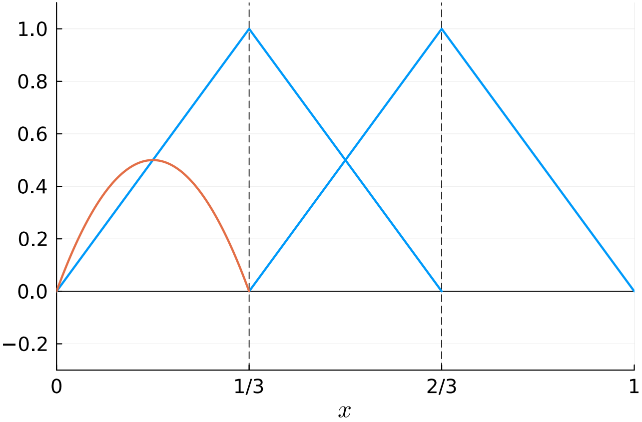

Next add quadratic "bubble" polynomials only supported on one element each.

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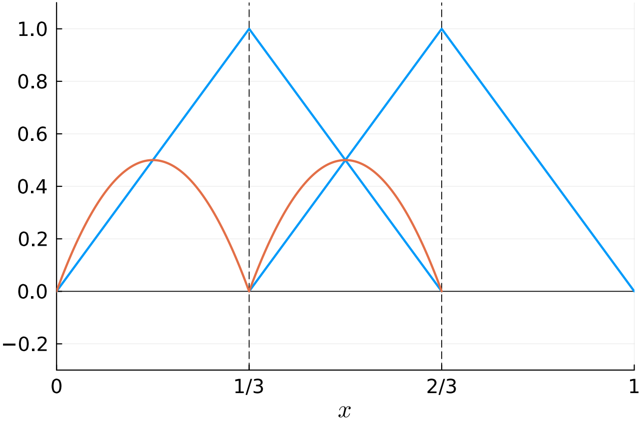

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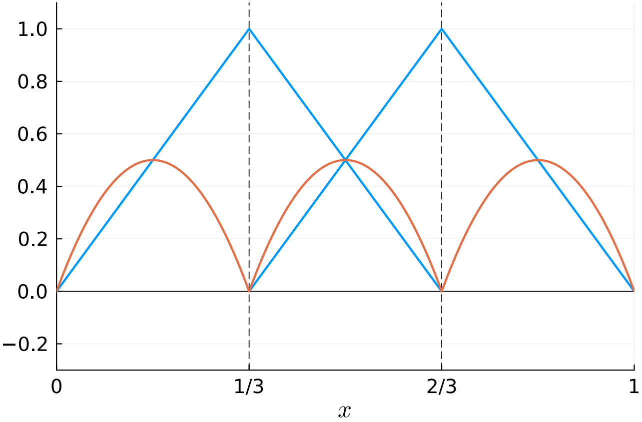

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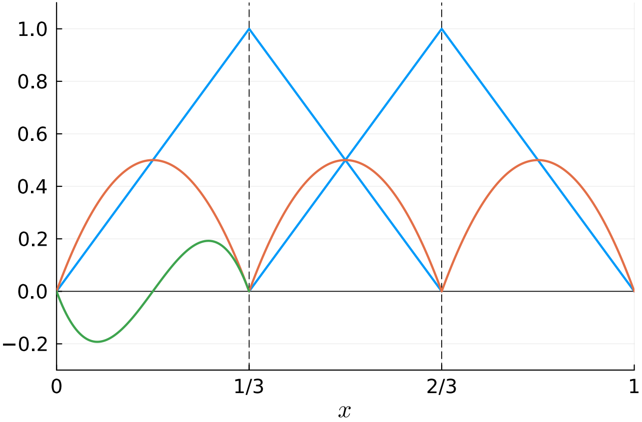

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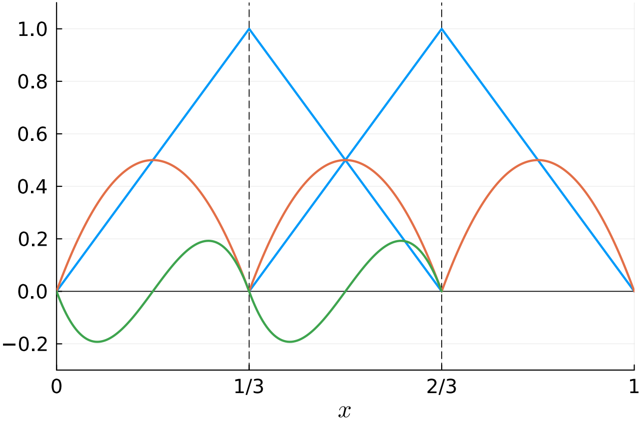

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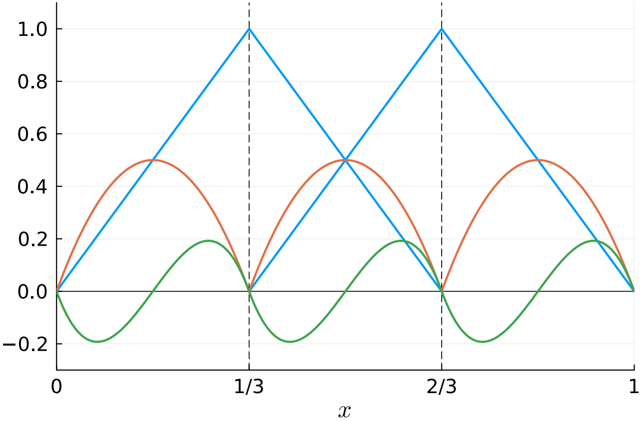

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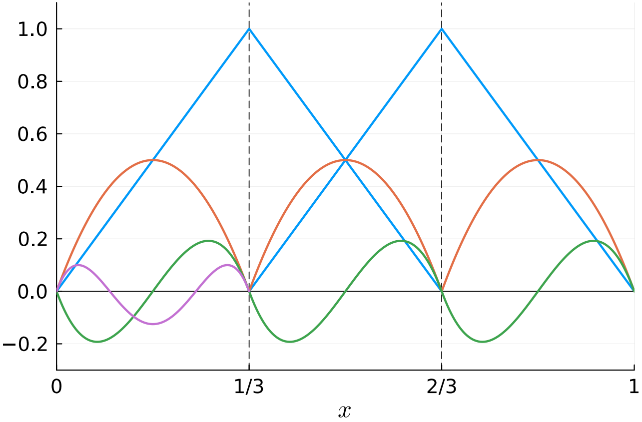

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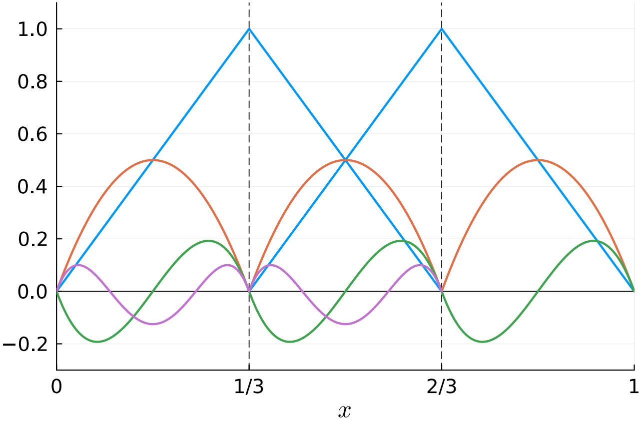

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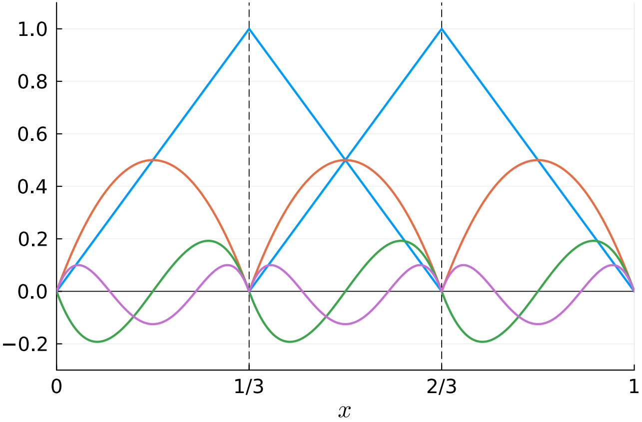

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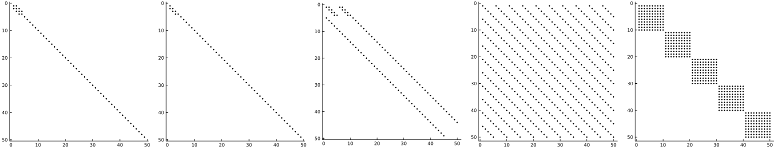
Sparsity of A, B and D_ψ

1D, 5 cells, $p = 10$.



(a) A (b) L^{rchol} (c) B (d) D_ψ (e) Permuted D_ψ

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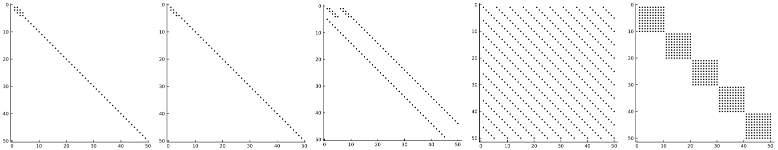

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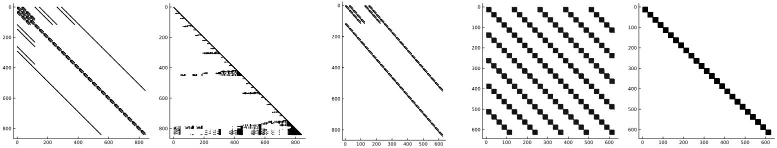
2D, 25 cells, $p = 5$.



(f) A (g) L^{chol} (h) B (i) D_ψ (j) Permuted D_ψ

Solver

- Obstacle problem: variational inequality (VI)
  - Apply LVPP: (VI) → sequence of nonlinear systems of PDEs
    - *hp*-FEM: PDEs → finite-dimensional nonlinear system of equations
      - Newton: nonlinear → sequence of linear saddle point systems
        - LU factorization

LVPP solver pipeline.

Example: oscillatory data in 1D

$$\Omega = (0,1), \quad f(x) = 200\pi^2 \sin(10\pi x), \quad \varphi \equiv 1.$$

$$\min_{u \in H_0^1(\Omega)} \int_\Omega \frac{1}{2}|\nabla u|^2 - fu \,\mathrm{d}x \ \text{ subject to } u(x) \leq \varphi(x).$$

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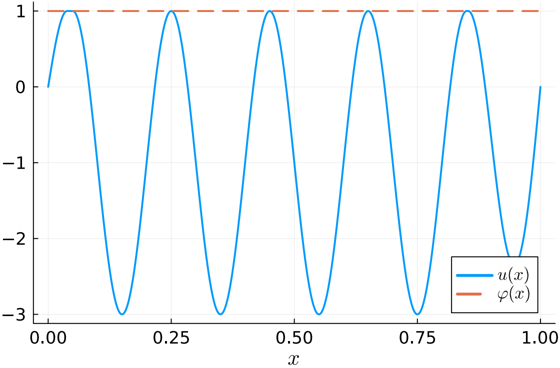

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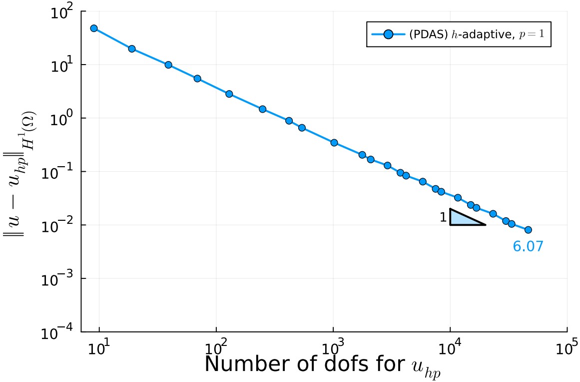

Cholesky factorization for the reduced PDAS stiffness matrix.
LU factorization for LVPP Newton systems with $\alpha_1 = 2^{-7}$, $\alpha_{k+1} = \min(\sqrt{2}\alpha_k, 2^{-3})$ and terminate once $\alpha_k = \alpha_{k-1} = 2^{-3}$. LVPP solver exhibits *hp*-independence (20-30 Newton linear system solves).

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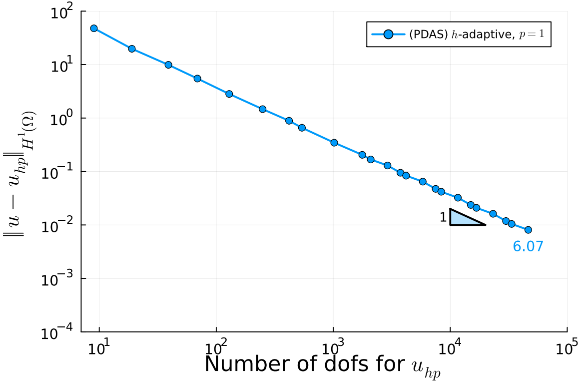

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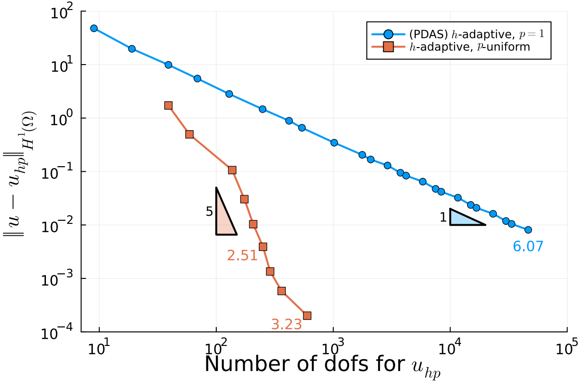

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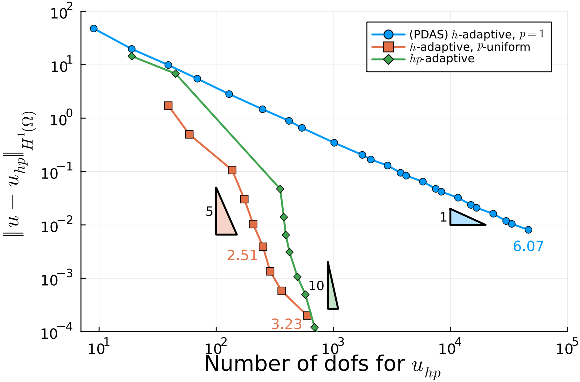

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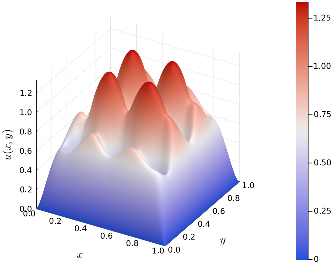
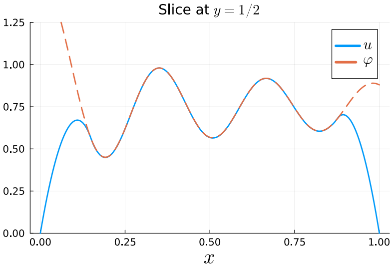
Example: oscillatory obstacle

$$\Omega = (0,1)^2, \quad f(x,y) = 100, \quad \text{and} \quad \varphi(x,y) = (1 + J_0(20x))(1 + J_0(20y)),$$

where J_0 denotes the zeroth order Bessel function of the first kind.





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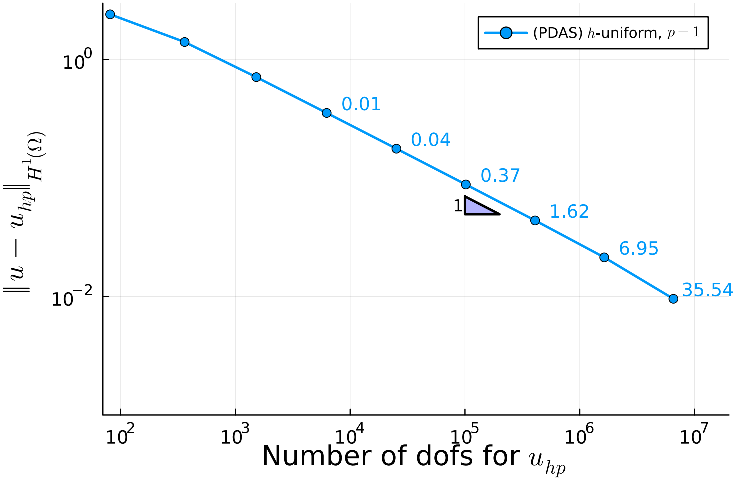

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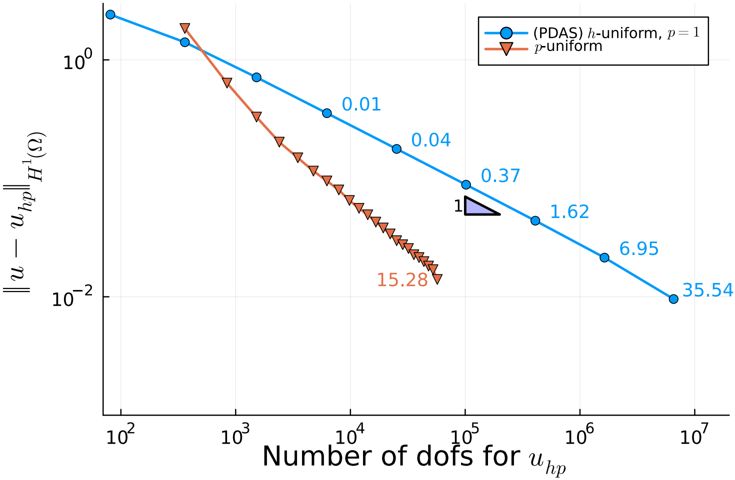

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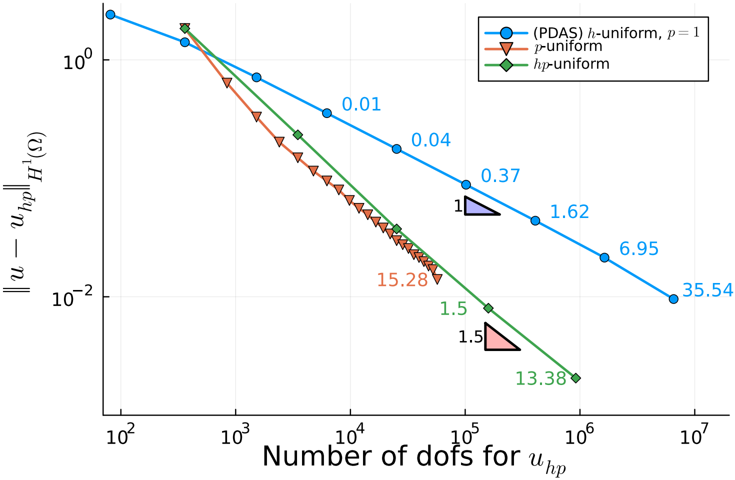

Block preconditioning

Recall we are repeatedly solving (where $A_\alpha := \alpha A$)

$$\begin{pmatrix} A_\alpha & B \\ B^\top & -D_\psi \end{pmatrix} \begin{pmatrix} \boldsymbol{\delta}_u \\ \boldsymbol{\delta}_\psi \end{pmatrix} = \begin{pmatrix} \boldsymbol{b}_u \\ \boldsymbol{b}_\psi \end{pmatrix}.$$

Schur complement factorization

A Schur complement factorization reveals that

$$\delta_u = A_\alpha^{-1}(\boldsymbol{b}_u - B\delta_\psi) \text{ and } \delta_\psi = S^{-1}(\boldsymbol{b}_\psi - B^\top A_\alpha^{-1}\boldsymbol{b}_u),$$

where $S := -(D_\psi + B^\top A_\alpha^{-1} B)$.

Advantages

A_α and B are sparse and A_α admits a cheap Cholesky factorization that we only compute once.

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Iterative solver & Schur complement approximation

Complication

$S = -(D_\psi + B^\top A_\alpha^{-1} B)$ is dense — it cannot be assembled and factorized quickly.

However, given a vector $\boldsymbol{y}$ we may compute $S\boldsymbol{y}$ efficiently.

Iterative solver

Solve $S\delta_\psi = (\boldsymbol{b}_\psi - B^\top A_\alpha^{-1} \boldsymbol{b}_u)$ with GMRES preconditioned with a block-diagonal Schur complement approximation $\tilde{S}$.

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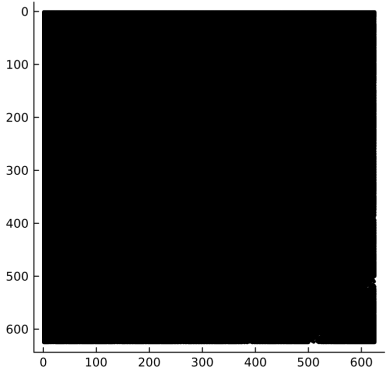
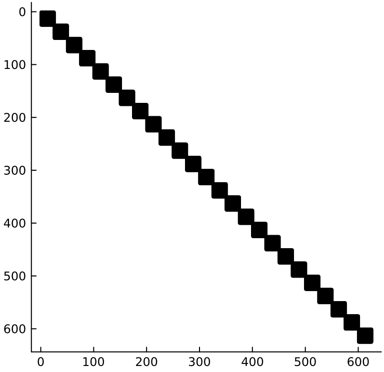


(a) Schur complement S



(b) Block-diagonal approximation $\tilde{S}$

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        - ~~LU factorization~~
        - Schur complement factorization
          - Cholesky for A_α
          - preconditioned GMRES for S

LVPP solver pipeline.

Example: thermoforming

The thermoforming quasi-variational inequality seeks u minimizing

$$\min_{u \in H_0^1(\Omega)} \int_\Omega \frac{1}{2}|\nabla u|^2 - fu \,\mathrm{d}x \text{ subject to } u \leq \varphi(T) := \Phi_0 + \xi T, \qquad (1)$$

where Φ_0 and ξ are given and T satisfies

$$-\Delta T + \gamma T = g(\Phi_0 + \xi T - u), \quad \partial_\nu T = 0 \text{ on } \partial\Omega. \qquad (2)$$

Solver strategy

We will solve the thermoforming problem via a fixed point approach, i.e. repeatedly solve

1. Freeze T and solve the obstacle subproblem (1) for u,
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Leibniz Association

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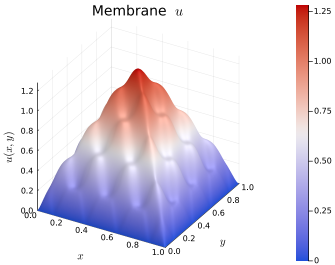

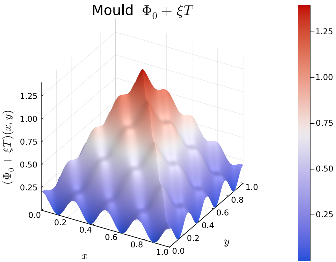

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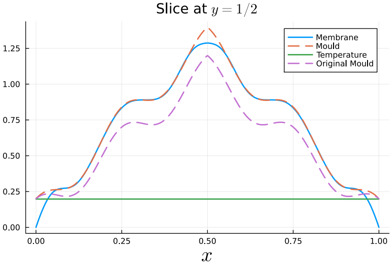

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6	4	15.00	11.00	1.50	2.83
12	4	15.25	15.85	2.00	3.13
22	4	16.00	19.36	2.00	3.00
32	4	16.00	21.09	2.00	3.00
42	4	15.75	21.75	2.25	3.11
52	4	15.00	22.40	2.00	3.00
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p-independent Newton and preconditioned GMRES iteration counts to solve the thermoforming problem. Unbelievable!

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Outer loop

Average Newton steps to solve an obstacle subproblem

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Average preconditioned GMRES iterations per Newton step

Average Newton steps to solve a temperature PDE subproblem

Average preconditioned GMRES iterations per Newton step

p-independent Newton and preconditioned GMRES iteration counts to solve the thermoforming problem. Unbelievable!

Conclusions

- Pointwise constraints can be effectively handled by the latent variable proximal point algorithm resulting in a nonlinear system of smooth PDEs.
- The PDE system is linearized with Newton.
- For the obstacle problem, the nonlinearity is confined to the latent variable ψ which can be discretized with a high-order DG Legendre polynomial basis that admits fast quadrature via the DCT.
- We discretize the membrane u with the hierarchical continuous p-FEM basis.
- This leads to sparse linear systems which admit simple preconditioners.
- **This leads to fast convergence with competitive wall clock solve times.**

Latent variable proximal point

Jørgen S. Dokken, Patrick E. Farrell, Brendan Keith, I. P., Thomas M. Surowiec, *The latent variable proximal point algorithm for variational problems with inequality constraints* (2025), https://arxiv.org/abs/2503.05672.

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Conclusions

- Pointwise constraints can be effectively handled by the latent variable proximal point algorithm resulting in a nonlinear system of smooth PDEs.
- The PDE system is linearized with Newton.
- For the obstacle problem, the nonlinearity is confined to the latent variable ψ which can be discretized with a high-order DG Legendre polynomial basis that admits fast quadrature via the DCT.
- We discretize the membrane u with the hierarchical continuous p-FEM basis.
- This leads to sparse linear systems which admit simple preconditioners.
- **This leads to fast convergence with competitive wall clock solve times.**

Latent variable proximal point

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Thank you for listening!

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