An Introduction to the Proximal Galerkin Method[1]

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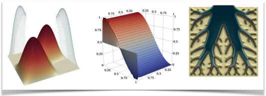
SCAN Meeting, December 7, 2023

[1] Recently mentioned in Popular Science(!): *These 10 scientists are on the cusp of changing the world, It's the Brilliant 10 class of 2023.* `https://www.popsci.com/science/brilliant-10-2023/`

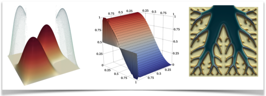
Overview



1. **History and Background**
2. **Algorithms and Numerical Experiments**
3. **Extensions of Proximal Galerkin**
4. **The Latent Variable Proximal Point Method**

B. Keith and T.M. Surowiec.
Proximal galerkin: A structure-preserving finite element method for pointwise bound constraints.
Submitted (2023), https://arxiv.org/pdf/2307.12444.pdf

Dirichlet's Principle[2]



In contemporary language, this energy principle states that for all functions $f \in L^2(\Omega)$ and $g \in H^1(\Omega)$, the (weak) solution of Poisson's equation over a Lipschitz domain $\Omega \subset \mathbb{R}^n$,

$$-\Delta u = f \quad \text{in } \Omega, \qquad u = g \quad \text{on } \partial\Omega, \tag{1}$$

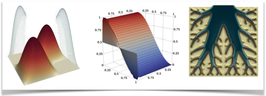
can be obtained as the $H^1(\Omega)$-minimizer of the Dirichlet energy,

$$E(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 \mathrm{d}x - \int_\Omega v f \mathrm{d}x\,, \tag{2}$$

confined to the constraint set $H^1_g(\Omega) = g + H^1_0(\Omega) = \{v \in H^1(\Omega) \mid v = g \text{ on } \partial\Omega\}$.

[2] Actually discovered by William Thomson, 1st Lord Kelvin 1847 and C.F. Gauß. Named after his teacher, P.G.L. Dirichlet, by G.F. Riemann in 1900.

A Variational Inequality



Since $H^1_g(\Omega)$ is nonempty, closed, and convex, the Lions–Stampacchia theorem (1967) states that the energy minimizer $u^* \in K = H^1_g(\Omega)$ is the unique solution to the variational inequality (VI)

$$\int_\Omega \nabla u^* \cdot \nabla (v - u^*) \mathrm{d}x \geq \int_\Omega f(v - u^*) \mathrm{d}x \text{ for all } v \in K.$$

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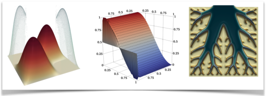

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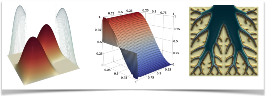
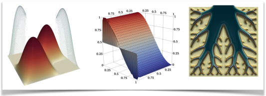
But no one solves Poisson's problem (1) *as a variational inequality. Why not?*

Back to the Dirichlet's Principle



- $K = H^1_g(\Omega)$ is affine and for all $w \in H^1_0(\Omega)$ and $v \in H^1_g(\Omega)$, $v + w \in H^1_g(\Omega)$, as well.

Back to the Dirichlet's Principle



- $K = H_g^1(\Omega)$ is affine and for all $w \in H_0^1(\Omega)$ and $v \in H_g^1(\Omega)$, $v + w \in H_g^1(\Omega)$, as well.
- Taking $v = u^* \pm w$ for any $w \in H_0^1(\Omega)$ here

$$\int_\Omega \nabla u^* \cdot \nabla(v - u^*)\mathrm{d}x \geq \int_\Omega f(v - u^*)\mathrm{d}x \text{ for all } v \in K,$$

brings us back to Dirichlet's principle: Find $u^* \in H_g^1(\Omega)$ such that

$$\int_\Omega \nabla u^* \cdot \nabla w \mathrm{d}x = \int_\Omega f w \mathrm{d}x \text{ for all } w \in H_0^1(\Omega).$$

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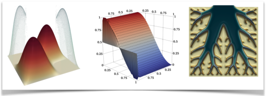

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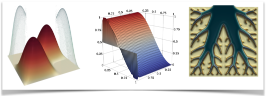
$$\int_\Omega \nabla u^* \cdot \nabla w \mathrm{d}x = \int_\Omega f w \mathrm{d}x \text{ for all } w \in H^1_0(\Omega).$$

We use the explicit *geometry* of the feasible set to derive a simpler problem.

The Obstacle Problem[3]



- Now minimize Dirichlet's energy over the set K defined by

$$K = \{v \in H_0^1(\Omega) \mid v \geq 0 \text{ a.e.}\} = H_0^1(\Omega) \cap H_+^1(\Omega).$$

- K is no longer an affine set, but it is a *closed convex cone*:

[3] Introduced by G. Stampacchia around 1963. Variational inequalities proposed by A. Signorini (1959) and studied by G. Fichera (1963) and onwards.

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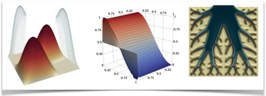

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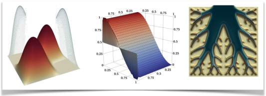

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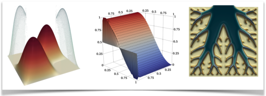

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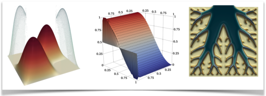

- Now minimize Dirichlet's energy over the set K defined by

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We can no longer reduce the variational inequality to a system of equations, but maybe we can use the geometry to define an iterative method in which we **solve** *a sequence of (nonlinear) equations?*

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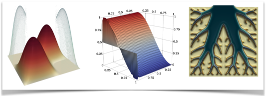
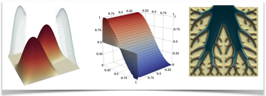
Solving Variational Inequalities



- There are many possibilities: penalty methods, interior point/barrier functions, augmented Lagrangian.

Solving Variational Inequalities



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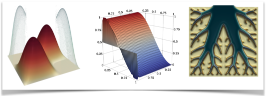
Solving Variational Inequalities

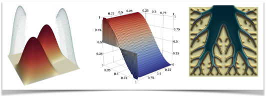


- There are many possibilities: penalty methods, interior point/barrier functions, augmented Lagrangian.
- We take an idea from convex optimization: the proximal point method and use an adaptive form of *entropy regularization*.
- Keep in mind...The obstacle problem can be viewed as a *mixed complementarity problem*: Find $(u, \lambda) \in H_0^1(\Omega) \times H^{-1}(\Omega)$ s.t.

$$\underbrace{-\Delta u - \lambda = f,}_{\text{PDE}} \quad \underbrace{u \geq 0 \quad \text{``}\lambda \geq 0\text{''}, \quad \langle \lambda, u \rangle = 0}_{\text{Complementarity}}.$$

The Lagrange multiplier λ has low regularity, this is the source of *mesh dependence* (non scalability) for many methods.

A Meta-Algorithm



Algorithm 1: Entropic proximal point algorithm for an obstacle problem.

input: Step size parameter $\alpha > 0$ and initial solution guess $w \in H^1_g(\Omega) \cap L^\infty(\Omega)$ s.t. $\operatorname{ess\,inf} w > 0$. $f \in L^\infty(\Omega)$ and $g_{|\partial\Omega} \in C(\partial\Omega)$ s.t. $\operatorname{ess\,inf}_{\partial\Omega} g > 0$.

repeat

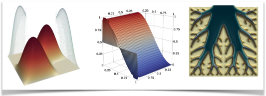
Solve the *entropic Poisson equation*,

$$\begin{cases} -\Delta u + \alpha^{-1} \ln u = f + \alpha^{-1} \ln w & \text{in } \Omega\,, \\ u = g & \text{on } \partial\Omega\,. \end{cases} \tag{3}$$

Assign $w \leftarrow u$.

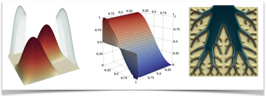
until *a convergence test is satisfied*

Entropic Poisson $\to$ Saddle Point



- Formally, we can introduce **latent variables** $\psi, \widetilde{\psi}$ such that $u = \exp(\psi)$ and $\widetilde{\psi} = \ln w$.

Entropic Poisson $\rightarrow$ Saddle Point



- Formally, we can introduce **latent variables** $\psi, \widetilde{\psi}$ such that $u = \exp(\psi)$ and $\widetilde{\psi} = \ln w$.
- This transforms into a nonlinear saddle point problem in (u, ψ):

$$\begin{cases} \text{Find } u \in H^1_g(\Omega) \text{ and } \psi \in W \text{ such that} \\ \displaystyle\int_\Omega \alpha \nabla u \cdot \nabla v \mathrm{d}x + \int_\Omega \psi v \mathrm{d}x = \int_\Omega (\alpha f + \widetilde{\psi})\, v \mathrm{d}x & \text{for all } v \in H^1_0(\Omega)\,, \\ \displaystyle\int_\Omega u \varphi \mathrm{d}x - \int_\Omega \exp(\psi) \varphi \mathrm{d}x = 0 & \text{for all } \varphi \in U\,. \end{cases}$$

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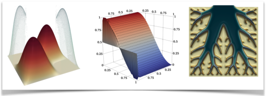

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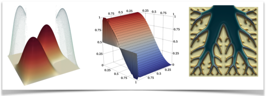
Regardless *of the choice or order of approximating spaces for* $H^1_g(\Omega)$*,* W*, and* U*, the discrete solution* ψ_h *yields a* **latent solution** $\widetilde{u}_h := \exp(\psi_h)$ *that is globally feasible on the discrete level.*

Proximal Galerkin



Algorithm 2:

Input : Step size parameter $\alpha > 0$, linear subspaces $V_h \subset H_0^1(\Omega)$ and $W_h \subset L^\infty(\Omega)$, and initial solution guess $\psi_h \in W_h$.
Output: Approximate solutions u_h and $\widetilde{u}_h = \exp \psi_h$, and approximate Lagrange multiplier, $\lambda_h = (\omega_h - \psi_h)/\alpha$.

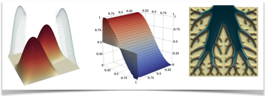
repeat

Assign $\omega_h \leftarrow \psi_h$.
Solve the following (nonlinear) discrete saddle-point problem:

$$\begin{cases} \text{Find } u_h \in g_h + V_h \text{ and } \psi_h \in W_h \text{ such that} \\ \displaystyle\int_\Omega \alpha \nabla u_h \cdot \nabla v \mathrm{d}x + \int_\Omega \psi_h v \mathrm{d}x = \int_\Omega (f + \omega_h)\, v \mathrm{d}x \quad \text{for all } v \in V_h\,, \\ \displaystyle\int_\Omega u_h \varphi \mathrm{d}x - \int_\Omega \exp(\psi_h) \varphi \mathrm{d}x = 0 \qquad \text{for all } \varphi \in U_h\,. \end{cases}$$

until *a convergence test is satisfied*

Proximal Galerkin



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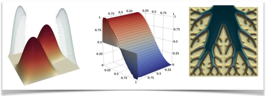
until *a convergence test is satisfied*

- The *full algorithm* involves updating α, ω and repeating Algorithm 2.
- $\alpha > 0$ can remain fixed or updated successively provided $\sum \alpha = \infty$.
- Convergence of this *outer loop* is provided (on an ∞-dimensional level) by the classical proximal point method with a rate $O((\sum \alpha)^{-1/2})$.

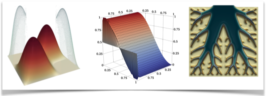
Finite Element Spaces I



- $\mathcal{T}_h$ shape-regular partition of $\Omega \subset \mathbb{R}^2$.
- $T \in \mathcal{T}_h$ open connected triangular mesh cells with Lipschitz boundaries ∂T.
- $\Omega := \bigcup_{T \in \mathcal{T}_h} \overline{T}$.
- $h = \max_{T \in \mathcal{T}_h} \operatorname{diam}(T)$ is the mesh size.
- $\mathbb{P}_p(T)$ space of polynomials of total order up to and including p on a triangle T.
- $\mathbb{X}(T)$ of polynomials over an element $T \in \mathcal{T}_h$.
- We define "broken" polynomials

$$\mathbb{X}(\mathcal{T}_h) = \{\varphi \in L^\infty(\Omega) \mid \varphi_{|T} \in \mathbb{X}(T) \text{ for every } T \in \mathcal{T}_h\}.$$

Finite Element Spaces II



- We require spaces of degree-q polynomials on whose traces on the cell boundary ∂T have lower polynomial degree $p < q$.
- Define the sets of bubble functions in $\mathbb{P}_q(T)$ and $\mathbb{Q}_q(T)$ to be

$$\mathring{\mathbb{P}}^q(T) = \{\varphi \in \mathbb{P}_q(T) \mid \varphi_{|\partial T} = 0\}$$

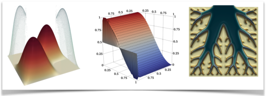
- Then define

$$\hat{\mathbb{P}}_p(T) = \mathbb{P}_p(T) \setminus \mathring{\mathbb{P}}^p(T)$$

- Finally let

$$\mathbb{P}_p^q(T) = \hat{\mathbb{P}}_p(T) \oplus \mathring{\mathbb{P}}^q(T). \tag{4}$$

Finite Element Spaces III

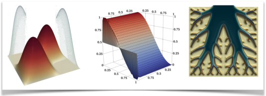


For any integer $p \geq 1$, we define the following pairs of spaces: We refer to the following as the $(\mathbb{P}_p\text{-bubble}, \mathbb{P}_{p-1}\text{-broken})$ pairing:

$$V_h = \mathbb{P}_p^{p+2}(\mathcal{T}_h) \cap H_0^1(\Omega)\,, \qquad W_h = \mathbb{P}_{p-1}(\mathcal{T}_h)\,.$$

- Example, $p = 1$: V_h is composed of the direct sum of piecewise linear functions and 3rd order bubble functions and W_h is piecewise constants.

Finite Element Spaces III



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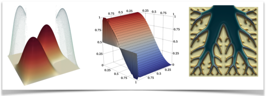
- Example, $p = 1$: V_h is composed of the direct sum of piecewise linear functions and 3rd order bubble functions and W_h is piecewise constants.
- For shape regular $\mathcal{T}_h$, these pairs of spaces are **stable** for the linearized, singularly perturbed saddle point problems.
- The paper contains similar spaces for quadrilateral mesh cells and alternative pairs without bubble functions that are also stable.

Discrete Domains



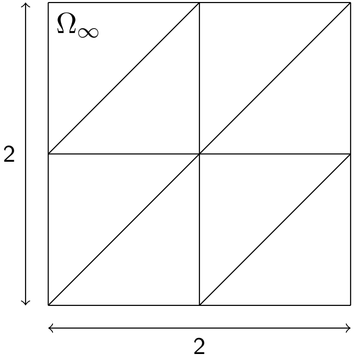
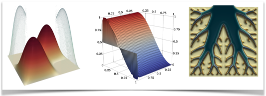


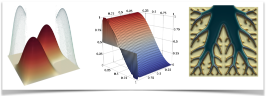
Figure: Initial FE meshes for domain Ω_∞ mesh sizes $h = h_\infty$, respectively. (I): Initial triangular mesh for $(\mathbb{P}_p\text{-bubble}, \mathbb{P}_{p-1}\text{-broken})$ pair on Ω_∞. We consider various polynomial orders $p \geq 1$ and mesh sizes.

Experiment 1



How does PG behave over various meshes and polynomials orders?

Experiment 1



- Set $g = u$, where $u(x, y)$ is the smooth manufactured solution

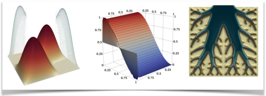
$$u(x,y) = \begin{cases} 0 & \text{if } x < 0\,, \\ x^4 & \text{otherwise,} \end{cases} \quad \text{implied by} \quad f(x,y) = \begin{cases} 0 & \text{if } x < 0\,, \\ -12x^2 & \text{otherwise.} \end{cases} \tag{5}$$

- $\lambda \equiv 0$: this is a **biactive** solution, meaning problem is nonsmooth at the solution.
- Proximal point is a (slow) fixed point method if α is left fixed. We choose:

$$\alpha_1 = 1\,, \quad \alpha_k = \min\{\max\{\alpha_1, r^{q^{k-1}} - \alpha_{k-1}\}, 10^{10}\}\,, \quad k = 2, 3, \dots, \tag{6}$$

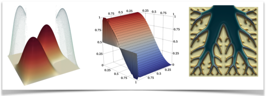
  where $r = q = 1.5$.
- Once $\alpha_k = 10^{10}$, we can check successive iterates as a stopping criterion.

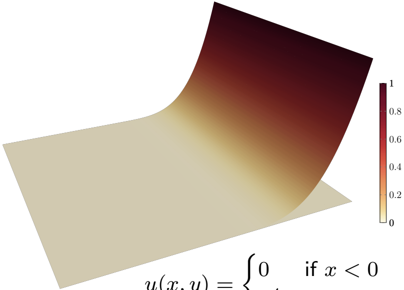
Experiment 1: Results



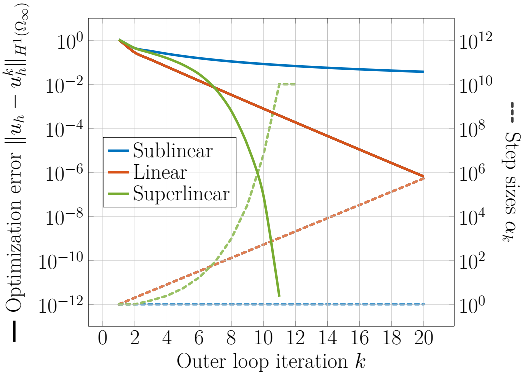
		Progress of the iterates $\|u_h^k - u_h^{k-1}\|_{H^1(\Omega_\infty)}$ for various h and p				
		Polynomial order $p = 1$			Polynomial order $p = 2$	
k	α_k	$h_\infty/16$	$h_\infty/32$	$h_\infty/64$	$h_\infty/16$	$h_\infty/32$
1	1.0	$2.10 \cdot 10^{0}$	$2.10 \cdot 10^{0}$	$2.10 \cdot 10^{0}$	$2.10 \cdot 10^{0}$	$2.10 \cdot 10^{0}$
2	1.0	$6.45 \cdot 10^{-1}$	$6.45 \cdot 10^{-1}$	$6.45 \cdot 10^{-1}$	$6.45 \cdot 10^{-1}$	$6.45 \cdot 10^{-1}$
3	1.49	$1.73 \cdot 10^{-1}$	$1.73 \cdot 10^{-1}$	$1.73 \cdot 10^{-1}$	$1.73 \cdot 10^{-1}$	$1.73 \cdot 10^{-1}$
4	2.43	$1.10 \cdot 10^{-1}$	$1.10 \cdot 10^{-1}$	$1.10 \cdot 10^{-1}$	$1.10 \cdot 10^{-1}$	$1.10 \cdot 10^{-1}$
5	5.35	$7.76 \cdot 10^{-2}$	$7.77 \cdot 10^{-2}$	$7.77 \cdot 10^{-2}$	$7.77 \cdot 10^{-2}$	$7.77 \cdot 10^{-2}$
6	$1.64 \cdot 10^{1}$	$4.76 \cdot 10^{-2}$	$4.77 \cdot 10^{-2}$	$4.77 \cdot 10^{-2}$	$4.77 \cdot 10^{-2}$	$4.77 \cdot 10^{-2}$
7	$8.50 \cdot 10^{1}$	$2.24 \cdot 10^{-2}$	$2.25 \cdot 10^{-2}$	$2.25 \cdot 10^{-2}$	$2.25 \cdot 10^{-2}$	$2.25 \cdot 10^{-2}$
8	$9.35 \cdot 10^{2}$	$5.82 \cdot 10^{-3}$	$5.84 \cdot 10^{-3}$	$5.85 \cdot 10^{-3}$	$5.85 \cdot 10^{-3}$	$5.85 \cdot 10^{-3}$
9	$3.17 \cdot 10^{4}$	$6.04 \cdot 10^{-4}$	$6.07 \cdot 10^{-4}$	$6.07 \cdot 10^{-4}$	$6.07 \cdot 10^{-4}$	$6.07 \cdot 10^{-4}$
10	$5.85 \cdot 10^{6}$	$1.80 \cdot 10^{-5}$	$1.81 \cdot 10^{-5}$	$1.81 \cdot 10^{-5}$	$1.81 \cdot 10^{-5}$	$1.81 \cdot 10^{-5}$
11	$1 \cdot 10^{10}$	$9.41 \cdot 10^{-8}$	$9.47 \cdot 10^{-8}$	$9.49 \cdot 10^{-8}$	$9.50 \cdot 10^{-8}$	$9.50 \cdot 10^{-8}$
12	$1 \cdot 10^{10}$	$2.10 \cdot 10^{-12}$	$2.00 \cdot 10^{-12}$	$1.96 \cdot 10^{-12}$	$1.92 \cdot 10^{-12}$	$1.95 \cdot 10^{-10}$
Tot. linear solves		21	20	19	19	19

Experiment 1: Results

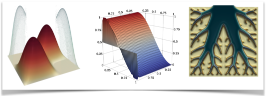




$$u(x,y) = \begin{cases} 0 & \text{if } x < 0 \\ x^4 & \text{otherwise} \end{cases}$$

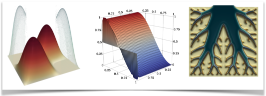


Experiment 2



How does PG fare with optimality conditions and strict complementarity?

Experiment 2



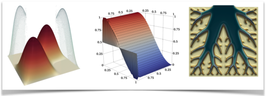
- In this experiment, we set $g = 0$ and define

$$f(x, y) = 2\pi^2 \sin(\pi x) \sin(\pi y)\,. \tag{7}$$

- We aim to check convergence of the discrete solution via the KKT conditions:

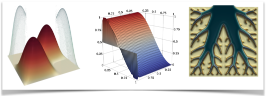
$$\begin{aligned}
\left| \int_\Omega \lambda u \mathrm{d}x \right| &= 0, \text{ complementary slackness,} \\
\int_\Omega \max\{-u, 0\} \mathrm{d}x &= 0, \text{ primal feasibility,} \\
\int_\Omega \max\{-\lambda, 0\} \mathrm{d}x &= 0, \text{ dual feasibility.}
\end{aligned}$$

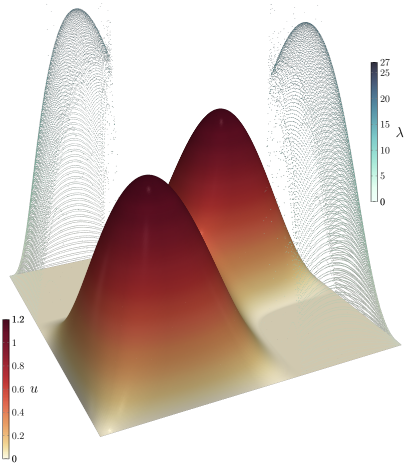
Experiment 2: Results

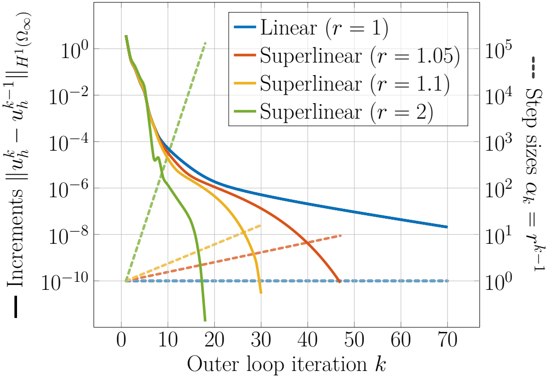


h	Complementarity $\left\lvert \int_{\Omega_\infty} \lambda_h u_h \mathrm{d}x \right\rvert$	Primal feasibility $\int_{\Omega_\infty} \max\{-u_h, 0\}\mathrm{d}x$	Dual feasibility $\int_{\Omega_\infty} \max\{-\lambda_h, 0\}\mathrm{d}x$
h_∞	(all less than 10^{-14})	$6.97 \cdot 10^{-3}$	(all less than 10^{-12})
$h_\infty/2$		$9.09 \cdot 10^{-3}$	
$h_\infty/4$		$1.16 \cdot 10^{-3}$	
$h_\infty/8$		$1.69 \cdot 10^{-4}$	
$h_\infty/16$		$4.08 \cdot 10^{-5}$	
$h_\infty/32$		$4.53 \cdot 10^{-6}$	

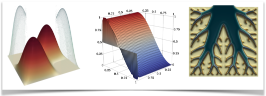
Experiment 2: Results





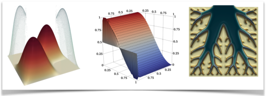


Experiment 3



How does PG do with nontrivial obstacles and higher order spaces?

Experiment 3



- Set $f = 0$, $g = 0$ and define the obstacle to be the upper surface of a sphere of radius $1/2$, namely
$$\phi(x, y) = \sqrt{1/4 - x^2 - y^2}\,, \tag{8}$$
if $\sqrt{x^2 + y^2} \leq 1/2$, and assume that ϕ is sufficiently negative when $\sqrt{x^2 + y^2} > 1/2$ so that no contact happens on that subdomain.
- The exact solution on the circular domain $\Omega = \Omega_2$ is found to be
$$u(x, y) = \begin{cases} A \ln \sqrt{x^2 + y^2} & \text{if } \sqrt{x^2 + y^2} > a, \\ \phi(x, y) & \text{otherwise}, \end{cases} \tag{9}$$
where $a = \exp\left(W_{-1}\left(\frac{-1}{2e^2}\right)/2 + 1\right) \approx 0.34898$, $A = \sqrt{1/4 - a^2}/\ln a \approx -0.34012$, and $W_j(\cdot)$ is the j-th branch of the Lambert W-function.

Experiment 3: Results

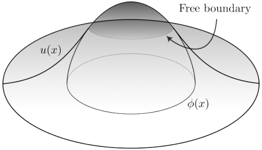
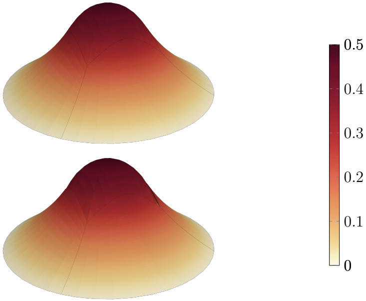


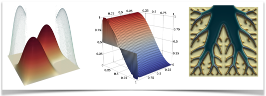
Diagram of problem



Very high order ($p = 12$) proximal Galerkin solutions u_h (top) and $\tilde{u}_h$ (bottom)

Figure: Spherical obstacle. Benchmark obstacle problem. Left: Diagram of the problem set-up. Right: Five-element proximal Galerkin solutions u_h and $\tilde{u}_h$.

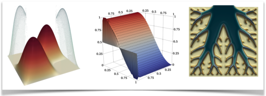
Experiment 3: Results



		Primal errors $\|u - u_h^k\|_{H^1(\Omega_2)}$ for $p = 1$				
k	Linear solves	$h_2/8$	$h_2/16$	$h_2/32$	$h_2/64$	$h_2/128$
1	3	$2.72 \cdot 10^{-1}$	$2.70 \cdot 10^{-1}$	$2.70 \cdot 10^{-1}$	$2.70 \cdot 10^{-1}$	$2.70 \cdot 10^{-1}$
2	1	$1.37 \cdot 10^{-1}$	$1.38 \cdot 10^{-1}$	$1.38 \cdot 10^{-1}$	$1.38 \cdot 10^{-1}$	$1.38 \cdot 10^{-1}$
3	1	$3.62 \cdot 10^{-2}$	$3.33 \cdot 10^{-2}$	$3.31 \cdot 10^{-2}$	$3.31 \cdot 10^{-2}$	$3.31 \cdot 10^{-2}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
Total iterations		11	11	11	11	11
Total linear solves		13	13	13	13	13
Final error		$1.98 \cdot 10^{-2}$	$8.73 \cdot 10^{-3}$	$3.49 \cdot 10^{-3}$	$1.18 \cdot 10^{-3}$	$3.85 \cdot 10^{-4}$

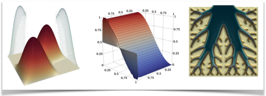
Table: Subproblem error, $\|u - u_h^k\|_{H^1(\Omega_2)}$, for various mesh sizes using $(\mathbb{Q}_2, \mathbb{Q}_0\text{-broken})$ discretization. We used $\alpha_k = 1$ for all $k = 1, \ldots$ and stopped the algorithm when $\|u_h^k - u_h^{k-1}\|_{L^2(\Omega_2)} < 10^{-6}$.

Nonsymmetric VI



What about variational inequalities that do not arise as energy minimization principles?

Ext. 1: Discrete Maximum Principle

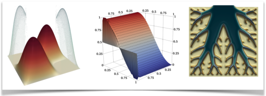


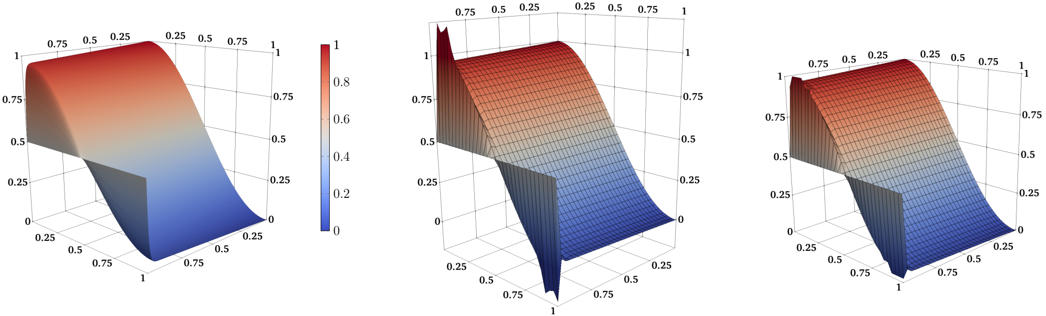
- Let $\epsilon > 0$, $\beta \in \mathbb{R}^d$ be fixed, $f \in L^\infty(\Omega)$, and $g \in H^1(\Omega) \cap C(\overline{\Omega})$.
- The solution u to the advection diffusion equation should satisfy a maximum principle on the continuous and **discrete** level:

$$-\epsilon\Delta u + \beta \cdot \nabla u = f \quad \text{in } \Omega, \qquad u = g \quad \text{on } \partial\Omega\,, \tag{10}$$

- By rewriting (10) as a variational inequality, we can develop a Proximal Galerkin scheme.
- There are (many) details in the paper including a "binary entropic Poisson equation", an implementable algorithm, further pairs of tailored FE spaces for the new saddle point problems.

Ext. 1: Discrete Maximum Principle

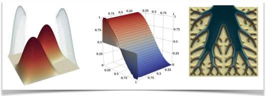




Exact solution u FEM solution Proximal Galerkin solution $\tilde{u}_h$

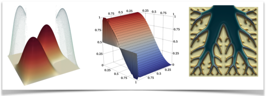
Figure: Erikkson–Johnson problem with $\epsilon = 10^{-2}$. (l): Exact solution. (c): A first-order Bubnov–Galerkin numerical solution that clearly violates the strong maximum principle $0 \le u(x) \le 1$. (r): $(\mathbb{Q}_1, \mathbb{Q}_1)$-proximal Galerkin solution $\tilde{u}_h = \mathrm{expit}(\psi_h)$ satisfies the strong maximum principle, by construction.

Nonconvex Problems



What about nonconvex variational problems?

Ext. 2.: Topology Optimization



Find a material distribution with maximum flexibility and a fixed volume:

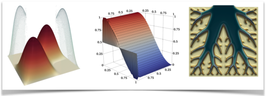
$$\min_{\rho \in L^\infty(\Omega)} \left\{ \widehat{F}(\mathbf{u}, \rho) = \int_\Omega \mathbf{u} \cdot \mathbf{f} \, \mathrm{d}\boldsymbol{x} \right\} , \tag{11}$$

subject to the constraints

$$\begin{cases} -\mathrm{Div}\,(r(\tilde{\rho})\,\boldsymbol{\sigma}) = \mathbf{f} \ \text{ in } \Omega \quad \text{with} \quad \mathbf{u} = 0 \ \text{ on } \Gamma_0 \,, \quad \boldsymbol{\sigma}\mathbf{n} = 0 \ \text{ on } \partial\Omega \setminus \Gamma_0 \,, \\ -\epsilon^2 \Delta\tilde{\rho} + \tilde{\rho} = \rho \ \text{ in } \Omega \quad \text{with} \quad \nabla\tilde{\rho} \cdot \mathbf{n} = 0 \ \text{ on } \partial\Omega \,, \\ \int_\Omega \rho(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \theta|\Omega| \,, \quad 0 \le \rho \le 1 \,, \quad r(\tilde{\rho}) = \underline{\rho} + \tilde{\rho}^3(1 - \underline{\rho}) \,, \end{cases} \tag{12}$$

where $\epsilon > 0$ is a *length scale* and $0 < \theta < 1$ is the desired volume fraction, which constrains the amount of the domain Ω occupied by the design.

Ext. 2: Topology Optimization



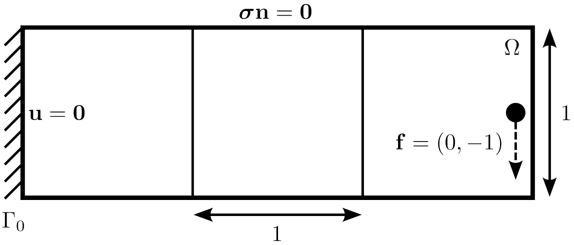
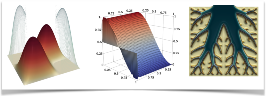


Figure: The design domain Ω for the cantilever beam problem with corresponding boundary conditions and three-element initial mesh with length $h_0 = 1$.

Mirror Descent



- Like proximal point, but replace the objective with its linearization.

Algorithm 4: Entropic mirror descent for topology optimization.

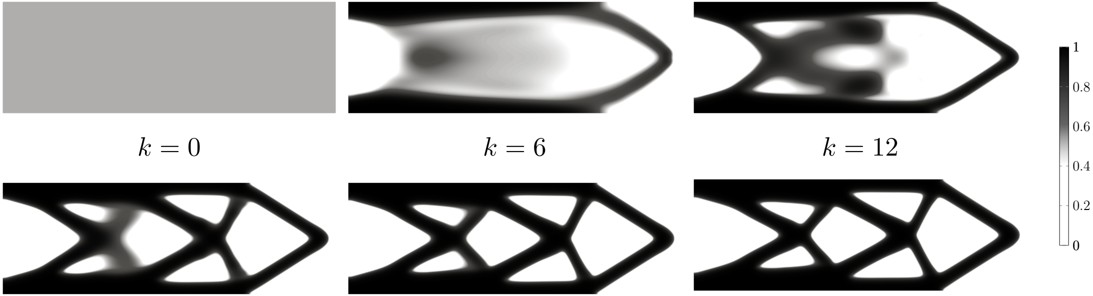
Input : Initial latent variable $\rho^0 \in L^\infty(\Omega)$, sequence of step sizes $\alpha_k > 0$, increment tolerance $\texttt{itol.} > 0$, and normalized tolerance $\texttt{ntol.} > 0$.
Output: Optimized material density $\overline{\rho} = \operatorname{expit}(\psi^k)$.

Initialize $k = 0$.

while $\| \operatorname{expit}(\psi^k) - \operatorname{expit}(\psi^{k-1}) \|_{L^1(\Omega)} > \min\{\alpha_k \, \texttt{ntol.}, \texttt{itol.}\}$ **do**

```
// Latent space gradient descent
```
Assign $\psi^{k+1/2} \leftarrow \psi^k - \alpha_{k+1} \nabla F(\operatorname{expit}(\psi^k))$.
```
// Compute Lagrange multiplier
```
Solve for $c \in \mathbb{R}$ such that $\int_\Omega \operatorname{expit}(\psi^{k+1/2} + c) \mathrm{d}x = \theta |\Omega|$.
```
// Latent space feasibility correction
```
Assign $\psi^{k+1} \leftarrow \psi^{k+1/2} + c$.
Assign $k \leftarrow k + 1$.

Ext. 2: Results

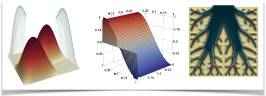


$k = 0$ $k = 6$ $k = 12$

$k = 18$ $k = 24$ $k = 29$ (final)

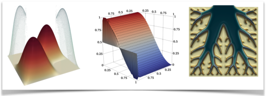
Figure: Subsequence of material densities $\tilde{\rho}_h^k$ from Algorithm 4 for selected iterations k. Results obtained with problem parameters $\epsilon = 2 \cdot 10^{-2}$ and $\theta = 0.5$; algorithm parameters $\texttt{itol.} = 10^{-2}$, $\texttt{ntol.} = 10^{-5}$, and $\alpha_k = 25k$; and discretization parameters $h = h_0/128$ and $p = 1$.

Latent Variable Proximal Point



What is really going on here? (beware: unpublished work follows)

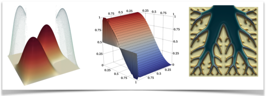
The LVPP Method



- We seek a minimizer $\overline{u}$ of a smooth coercive functional J over a closed convex subset K of a Sobolev space V.

[4] introduced by B. Martinet (1970).

The LVPP Method



- We seek a minimizer $\overline{u}$ of a smooth coercive functional J over a closed convex subset K of a Sobolev space V.
- We assume

$$K = \{ v \in V \,|\, \Lambda v \in C \text{ a.e. } \Omega \} \,,$$

Ω is an open bounded set, Λ is a bounded linear operator into $L^2(\Omega)^n$ or $L^2(\Omega)^{n\times n}$, and C is a nonempty closed convex subset of $\mathbb{R}^n$ or $\mathbb{R}^{n\times n}$.

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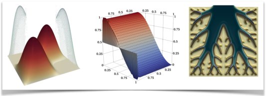
The LVPP Method



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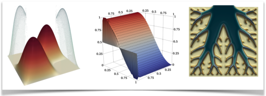
- LVPP contains two essential components: the **P**roximal **P**oint method[4] and the introduction of a **L**atent **V**ariable ψ.

[4] introduced by B. Martinet (1970).

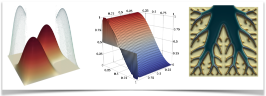
The LVPP Method



- The generalized proximal point method for computing $\overline{u}$ is an iterative procedure that takes a penalty parameter $\alpha > 0$ and a previous iterate v and returns a new approximation u of $\overline{u}$ as the solution of the optimization problem:

$$\min\{J(u) + \alpha^{-1} D(\Lambda u, \Lambda v) : u \in K\}.$$

The LVPP Method



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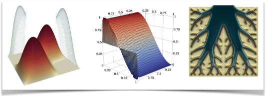
- $D(u, v) = B(u) - B(v) - B'(v)(u - v)$ is a Bregman distance, B captures the geometry of C such that the subproblems can be considered *unconstrained*.

The LVPP Method



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- Consequently, u should solve the optimality system:

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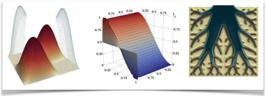
The LVPP Method



- The generalized proximal point method for computing $\overline{u}$ is an iterative procedure that takes a penalty parameter $\alpha > 0$ and a previous iterate v and returns a new approximation u of $\overline{u}$ as the solution of the optimization problem:

$$\min\{J(u) + \alpha^{-1} D(\Lambda u, \Lambda v) : u \in K\}.$$

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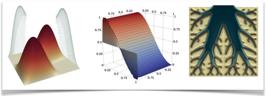
- This still contains a potential difficulty in the term $B'(\Lambda u)$ and it is here that we first introduce the *latent variable* ψ, which we set to be $\psi := B'(\Lambda u)$.

Legendre-Nemitskii Operators



- B should also be an integral functional so that B' is a structured superposition (Nemitskii) operator, i.e. $[B'(y)](x) = \nabla f(y(x))$ for some real-valued mapping f.

[5] Rockafellar (1970)

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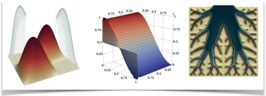

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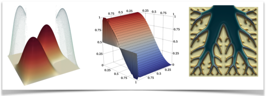

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- Key property: ∇f forms a bijection from $\operatorname{int}\operatorname{dom} f$ to $\operatorname{int}\operatorname{dom} f^*$, where f^* is the Fenchel conjugate of f, i.e. $(\nabla f)^{-1} = \nabla f^*$, where it is defined.

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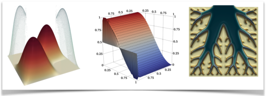

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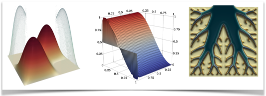

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K	f	Λ	$\Lambda^*\psi$	$\Lambda u = \nabla f^*(\psi)$
$\{\gamma u \geq 0\}$	$x \ln x - x$	γ (trace)	$\gamma^*\psi$	$\gamma u = \exp(\psi)$
$\{\lVert\nabla u\rVert_2 \leq \phi(\cdot)\}$	$-\sqrt{\phi^2(\cdot) - \lVert\vec{x}\rVert_2^2}$	∇ (gradient)	$-\operatorname{div}\vec{\psi}$	$\nabla u = \phi(\cdot)(1 + \lVert\vec{\psi}\rVert_2^2)^{-1/2}\vec{\psi}$
$\{\vec{u} \geq 0,\ \sum_i u_i = 1\}$	$\sum_i x_i \ln(x_i)$	$-$	$\vec{\psi}$	$u_i = \exp(\psi_i)/(\sum_j \exp(\psi_j))$

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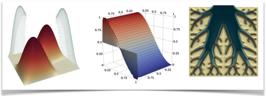
LVPP-Saddle Point Problem



$$\alpha J'(u) + \Lambda^* \psi = \Lambda^* \nabla f(\Lambda v)$$
$$\Lambda u - \nabla f^*(\psi) = 0$$

Figure: The LVPP nonlinear saddle point subproblem. Similar saddle point formulations are **not** available in interior point, quadratic penalty, or augmented Lagrangian approaches.

After discretization, the solution $(\overline{u}_h, \overline{\psi}_h)$ provides a latent solution: $\nabla f^*(\overline{\psi}_h)$, which is always in C. This *guarantees* a *globally feasible discrete* approximation of $\Lambda \overline{u}$.

This is what is going on at the core of the Proximal Galerkin method!