Shape optimization: theoretical, numerical and practical aspects

Habilitation à diriger les recherches

Beniamin Bogosel

CMAP, École Polytechnique

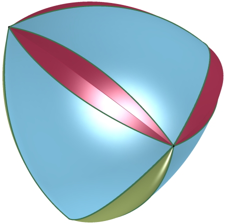
30/05/2024

Shape Optimization

$$\min_{\omega\in\mathcal{A}} J(\omega)$$

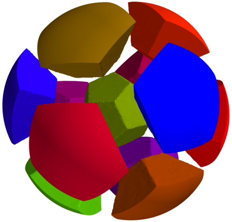
Theoretical aspects

- ⋆ existence, regularity
- ⋆ shape derivative
- ⋆ find optimal shapes
- ⋆ qualitative properties



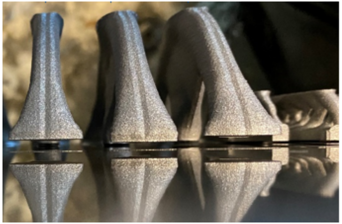
Numerical aspects

- ⋆ discretization choice
- ⋆ efficient computations
- ⋆ new theoretical ideas
- ⋆ solve theoretical gaps



Practical aspects

- ⋆ industrial problems
- ⋆ analysis
- ⋆ modelization
- ⋆ simulation

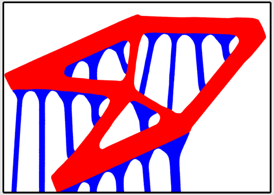


Structure of the memoir – purpose of using numerical tools

1. **Design optimization for additive manufacturing**	(practical applications)
2. **Numerical shape optimization for convex sets**	(test and find new ideas)
3. **Optimal partitioning and multiphase problems**	(test and find new ideas)
4. **The polygonal Faber-Krahn inequality**	(contributing to theoretical proofs)

Structure of the memoir – purpose of using numerical tools

1. **Design optimization for additive manufacturing** (practical applications)



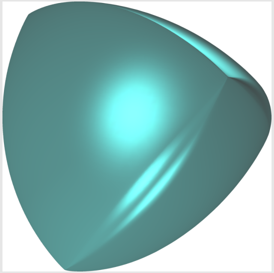
- Support optimization, overhang constraints
- Simplified simulation model [M. Bihr's PhD thesis]
- Imperfect part/support interface [M. Godoy's postdoc]
- **New: Accessibility constraints**

2. **Numerical shape optimization for convex sets** (test and find new ideas)
3. **Optimal partitioning and multiphase problems** (test and find new ideas)
4. **The polygonal Faber-Krahn inequality** (contributing to theoretical proofs)

Structure of the memoir – purpose of using numerical tools

1. **Design optimization for additive manufacturing** (practical applications)
2. **Numerical shape optimization for convex sets** (test and find new ideas)

- Parametrization using the support function
- Spectral vs discrete representation
- **New theoretical ideas – constant width constraint**

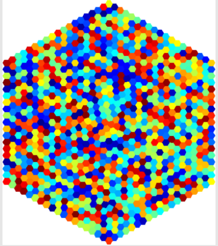


3. **Optimal partitioning and multiphase problems** (test and find new ideas)
4. **The polygonal Faber-Krahn inequality** (contributing to theoretical proofs)

Structure of the memoir – purpose of using numerical tools

1. **Design optimization for additive manufacturing** (practical applications)
2. **Numerical shape optimization for convex sets** (test and find new ideas)
3. **Optimal partitioning and multiphase problems** (test and find new ideas)

- Optimal partitions for spectral functionals
- Maximizing the length of minimal perimeter partitions
- Optimal Cheeger clusters

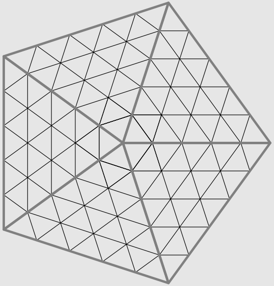


4. **The polygonal Faber-Krahn inequality** (contributing to theoretical proofs)

Structure of the memoir – purpose of using numerical tools

1. **Design optimization for additive manufacturing** (practical applications)
2. **Numerical shape optimization for convex sets** (test and find new ideas)
3. **Optimal partitioning and multiphase problems** (test and find new ideas)
4. **The polygonal Faber-Krahn inequality** (contributing to theoretical proofs)

- Second shape derivatives for polygons
- Explicit error estimates – $\mathbf{P}_1$ finite elements
- Validated computing: interval arithmetic
- **New: complete hybrid proof of local minimality.**



1. **Design optimization for additive manufacturing**

2. Convex shapes - constant width constraint

3. The polygonal Faber-Krahn inequality

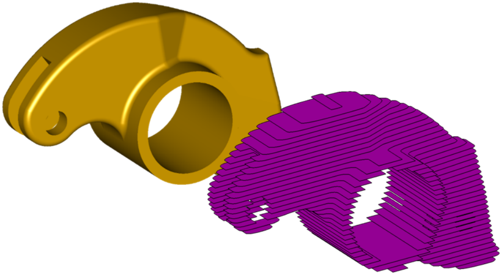
Additive Manufacturing

SOFIA The SOFIA project: Industrial partners: AddUp, Safran, Fusia, Zodiac, Volume

Collaboration with Grégoire Allaire, Martin Bihr, Matias Godoy

Material deposition:

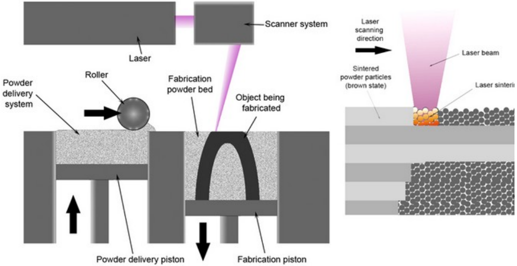
one slice at a time



[iti-global.com]

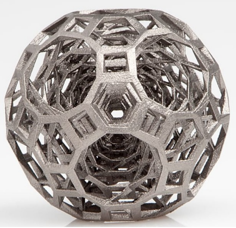
Technology of interest:

Selective Laser Melting (SLM)

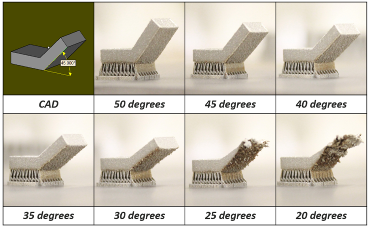


[Wikimedia]

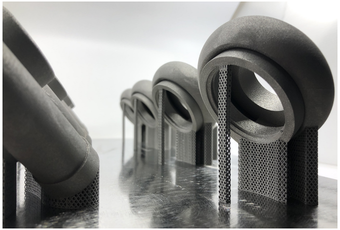
Arbitrary topology, but... other constraints



[robohub.org]



[insta3dp.com]



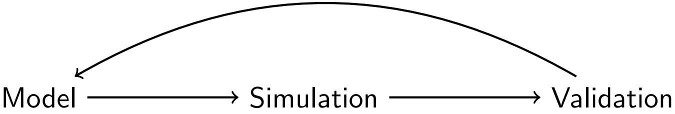
[szbiest.com]

- Inclined surfaces (overhangs) not realized correctly
- Large temperature gradients: thermal deformations as the metal contracts

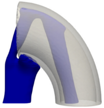
supports are added solve these problems ⟶ additional cost ⟶ optimize them

Regular exchanges with industrial partners: better understand the role of supports

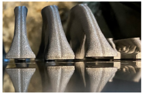
Works related to AM


Model → Simulation → Validation

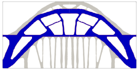
[B., G. Allaire, 18] gravity loads, simultaneous part/support optimization



[M. Bihr, B., G. Allaire, 20] optimizing the orientation, boundary loads, equivalent thermal loads



[M. Bihr et al., 22] simplified model simulation: reducing the stress and decreasing thermal deformations



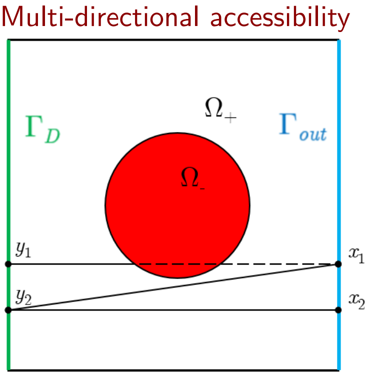
[M. Godoy, G. Allaire, B., 22] imperfect interfaces support/part

Most recent work: [G. Allaire, M. Bihr, B., M. Godoy] – **accessibility constraints**

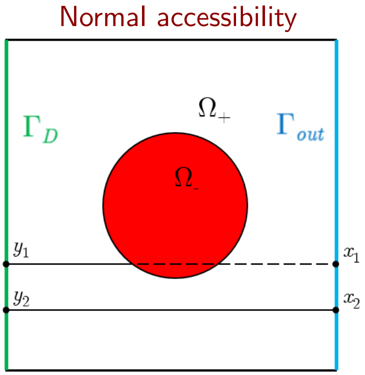
Accessibility constraints

⋆ **Why?** Supports removal: part still in the machine, supports need to be reached

⋆ **How?** For simplicity, in a straight line



natural choice, difficult



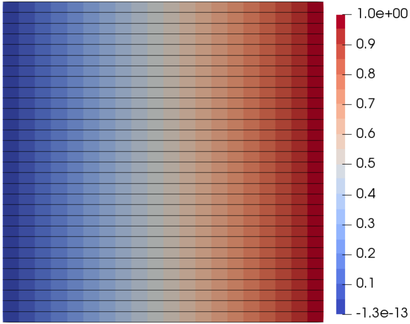
more restrictive, easy to evaluate

Distance functions: accessibility evaluation

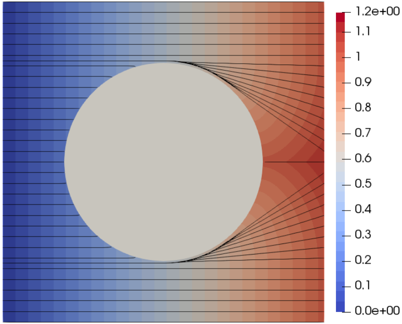
$\star$ $h_\varepsilon \longrightarrow$ regularized Heaviside function

Criteria: surface integral $\int_{\Gamma_{\text{out}}} h_\varepsilon(d - d_0)$, volume integral $\int_{\Omega_+} h_\varepsilon(d - d_0)$

Normal accessibility



d_0 = distance from Γ_D without obstacle



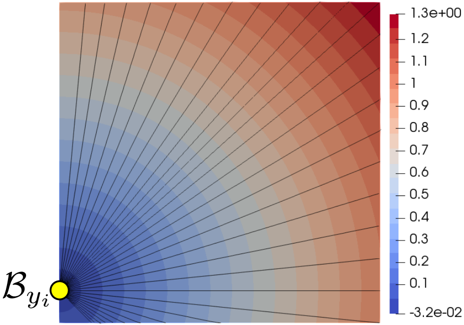
d = distance from Γ_D with obstacle

Distance functions: accessibility evaluation

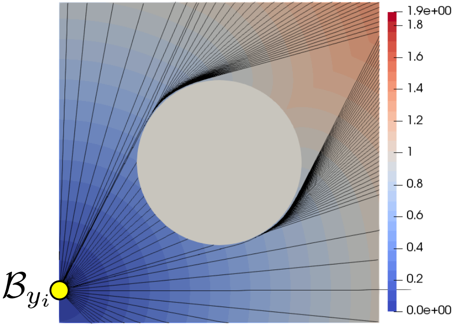
$\star$ $h_\varepsilon \longrightarrow$ regularized Heaviside function

Criteria: surface integral $\int_{\Gamma_{\text{out}}} h_\varepsilon(d-d_0)$, volume integral $\int_{\Omega_+} h_\varepsilon(d-d_0)$

Multi-directional accessibility



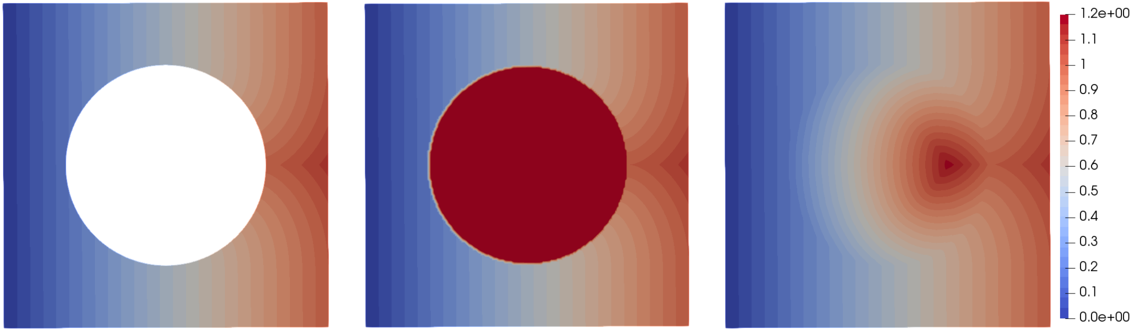
d_0 = distance from $\mathcal{B}_{y_i}$ without obstacle



d = distance from $\mathcal{B}_{y_i}$ with obstacle

Variable speed

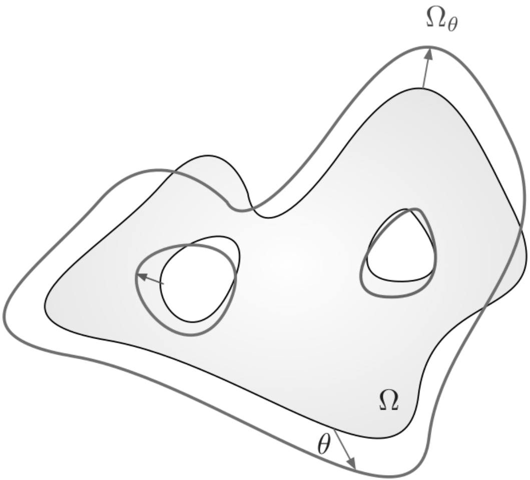
$$\text{Define } V(x) = \begin{cases} V_+ \equiv 1 & \text{in } \Omega_+, \\ V_- < 1 & \text{in } \Omega_-, \end{cases} \quad \text{and solve} \quad \begin{cases} V(x)|\nabla d(x)| = 1 & \text{in } \Omega, \\ d = 0 & \text{on } \Gamma_D. \end{cases}$$



Pure obstacle $\quad V_- = 0.01 \quad V_- = 0.5$

- ⋆ V_- small enough does not change d outside the obstacle Ω_-
- ⋆ fixed mesh, differentiability

Shape derivative



[image source: C. Dapogny]

- ⋆ perturb the domain using a vector field θ
- ⋆ $J((I+\theta)(\Omega)) = J(\Omega) + J'(\Omega)(\theta) + o(\|\theta\|)$
- ⋆ **Standard form:** under regularity assumptions we can write $J'(\Omega)(\theta) = \int_{\partial\Omega} \mathbf{f}\, \theta \cdot \mathbf{n}$
- ⋆ **Numerical application**: $\theta = -\mathbf{f}\ \mathbf{n}$ is a descent direction for the objective function

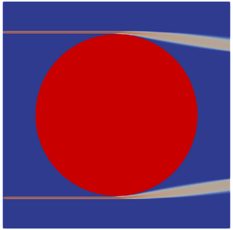
Differentiating the accessibility criterion

$\star$ The interface Σ between Ω_- and Ω_+ is perturbed by the vector field θ; $d = d(\Sigma)$

$$J(\Sigma) = \int_\Omega j(d) + \int_{\Gamma_{\text{out}}} k(d) \text{ gives } J'(\Sigma)(\theta) = \int_\Omega j'(d) d'(\theta) + \int_{\Gamma_{\text{out}}} k'(d) d'(\theta).$$

Adjoint state: active where geodesics of d touch the obstacle

$$\begin{cases} -\operatorname{div}(V_+\nabla d_+ p_+) & = & j'(d_+) & \text{in } \Omega_+, \\ -\operatorname{div}(V_-\nabla d_- p_-) & = & j'(d_-) & \text{in } \Omega_-, \\ p_+ & = & k'(d)/(V\nabla d \cdot \mathbf{n}) & \text{on } \Gamma_{\text{out}}, \\ p_+ & = & 0 & \text{on } \partial\Omega \setminus (\Gamma_{\text{out}} \cup \Gamma_D), \\ V_+(\nabla d_+ \cdot \mathbf{n})p_+ & = & V_-(\nabla d_- \cdot \mathbf{n})p_- & \text{on } \Sigma. \end{cases}$$



Shape derivative

$$J'(\Sigma)(\theta) = \int_\Sigma V_+(\nabla d_+ \cdot \mathbf{n})p_+ \left[(\nabla d_+ - \nabla d_-) \cdot \mathbf{n}\right] (\theta \cdot \mathbf{n})\, ds$$

Remarks, Implementation

$\star$ The framework applies to both normal and (discrete) multi-directional accessibility

$\star$ the obstacle bounded by Σ and the target Γ_{out} can be considered as shape variables

Numerical aspects:

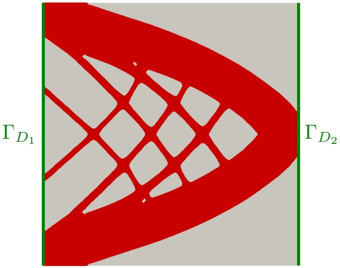
$\star$ compute d with variable speeds $V_\pm$: classical schemes, fast marching (`scikit-fmm`)
$\star$ computing the adjoint: first-order upwind scheme
$\star$ shape representation: level-set in FreeFEM
$\star$ volume constraints: projection
$\star$ other constraints: augmented Lagrangian

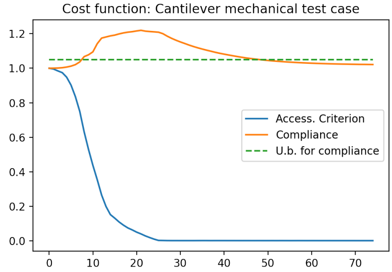
Example 1: Rendering a cantilever accessible

- ⋆ a classical cantilever shape is not normally accessible from the left boundary
- ⋆ minimize the accessibility criterion w.r.t two lateral sides $\Gamma_{D_1}, \Gamma_{D_2}$

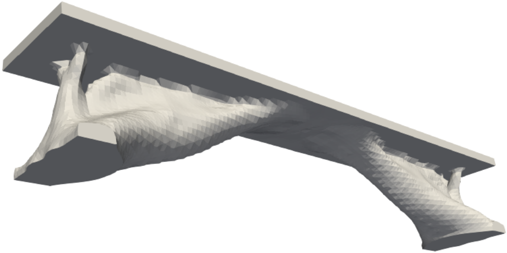
$$J(\Sigma) = \int_{\Omega_+} h_\varepsilon \left(\min_{i=1,2} (d_i(\Sigma) - d_{0,i}) \right) ds$$

- ⋆ constant area (projection), upper bound on the compliance (Augmented Lagrangian)

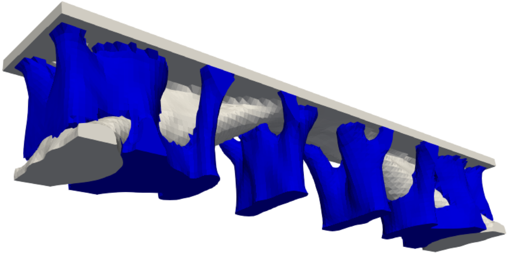




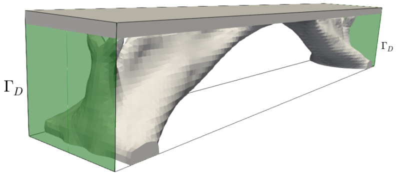
Example 2: Simultaneous optimization of part and supports



ω – one PDE for modeling final usage



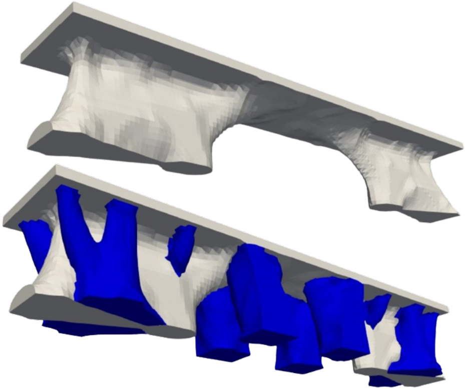
S – supports – one PDE for gravity loads

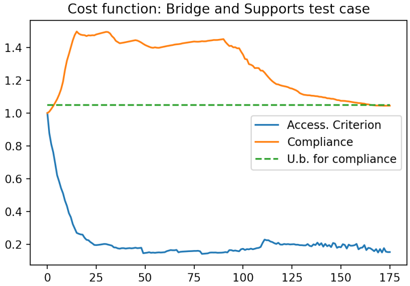


- Accessibility: $J(\omega, S) = \int_S h_\varepsilon \left(d(\omega) - d_0\right)$
- Volume constraints – projection
- Compliance constraints – Aug. Lag.

Numerical Result

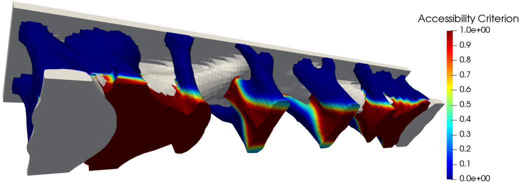
⋆ both the part and the supports are modified significantly by the optimization algorithm to try and respect the accessibility constraint

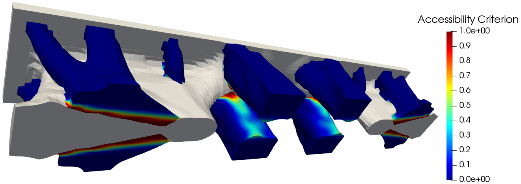


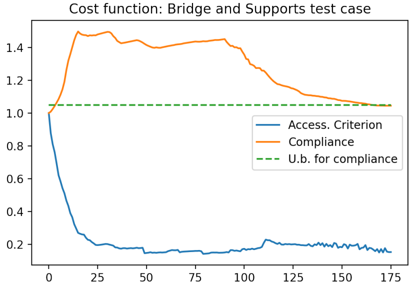


Numerical Result

⋆ both the part and the supports are modified significantly by the optimization algorithm to try and respect the accessibility constraint







Conclusions and perspectives

$\star$ More examples and tests in our paper:

[*Accessibility constraints in structural optimization via distance functions*, Allaire, Bihr, B., Godoy, 23]

Accessibility constraint – motivated by applications in AM:
New ideas explored: differentiating distance functions, non-standard adjoint equations

Open questions:
1. Justify rigorously the theoretical aspects related to the shape derivative: existence of solution for the adjoint (discontinuous speed across Σ) [Bouchut, James, 98, 1D]
2. Understand the limit case $V_- \to 0$: pure obstacle case.

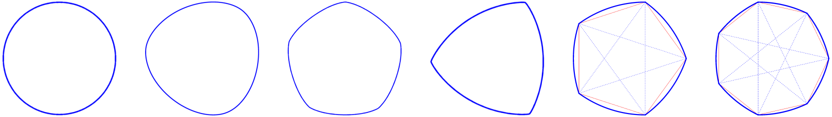
1. Design optimization for additive manufacturing

2. **Convex shapes - constant width constraint**

3. The polygonal Faber-Krahn inequality

Motivation: examples

1. Blaschke-Lebesgue Theorem. Among planar shapes of constant width the Reuleaux triangle minimizes the area.



2. Blaschke-Lebesgue Problem in 3D (open). The three dimensional body of constant width with the minimal volume is one of the Meissner tetrahedra.

Numerics: better understand the constant width constraint, general functionals in 2D, 3D

Co-authors: P. Antunes, A. Henrot, I. Lucardesi, F. Nacry, A. Al Sayed, M. Michetti

Support function: functional setting encoding all difficulties

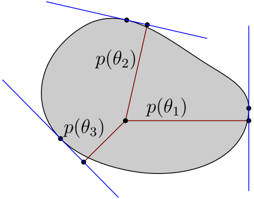
[Schneider, *Convex bodies*], [Bayen, Henrion], many others

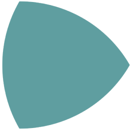
Definition: $p(\theta) = \max_{x\in\omega}(x\cdot\theta)$

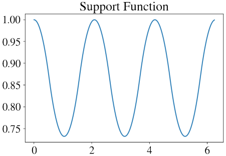
Width: $w(\theta) = p(\theta) + p(\theta+\pi)$

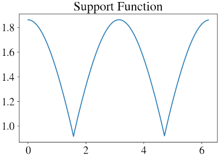
Parametrization: $\mathbf{x}(\theta) = p(\theta)\mathbf{r}(\theta) + p'(\theta)\mathbf{t}(\theta)$

Convexity: $p(\theta) + p''(\theta) \geq 0$ (the hard part...)









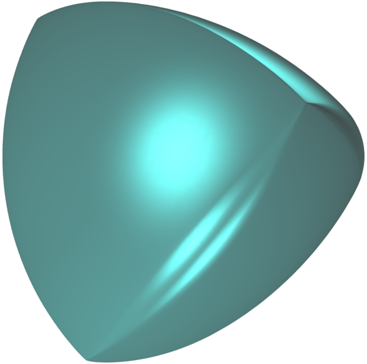
Knowing p, p', p'' gives a parametrization of ω and characterizes convexity:

- spectral decomposition: direct access to p, p', p'' - limited to strictly convex sets!
- direct choice of values for some angle discretization: how to choose p', p'' rigorously?

Some numerical results: constant width constraint

Minimizing the volume

[Antunes, B.]



Maximizing $\lambda_k(\Omega)$

$$-\Delta u_k = \lambda_k(\Omega) u_k, \ u_k \in H_0^1(\Omega)$$

[B., Henrot, Lucardesi], [B., 23]

Conjecture

Reuleaux triangle – optimal for $1 \leq k \leq 10$.

Why is the Reuleaux triangle optimal for so many functionals?

⋆ optimal for: the area, inradius, perimeter and area of inner parallel sets, the Cheeger constant [Henrot, Lucardesi, 20], [B. 23], Dirichlet-Laplace eigenvalues (numerics)

Questions:

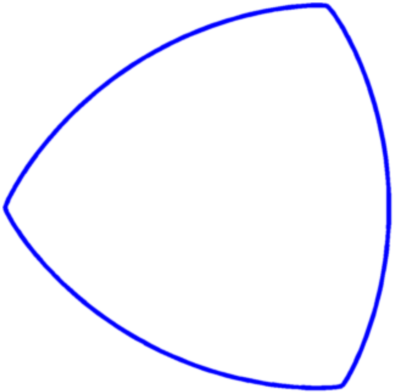
1. Unifying reason for optimality of the Reuleaux triangle the cases above?
⋆ Concavity for Brunn-Minkowski type inequalities?
⋆ The Reuleaux triangle: the only Reuleaux polygon which cannot be perturbed?

2. None of the current proofs for the minimality of the area in 2D generalize to 3D.
⋆ Find new ones which also work in 3D?

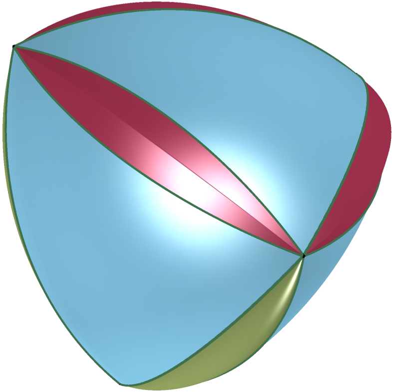
New idea in 3D: Meissner polyhedra

- ⋆ finite dimensional constant width family in 3D: analogue of Reuleaux polygons in 2D
- ⋆ [Montejano, Roldan-Pensado, 18], [Hynd, 23]

2D: Reuleaux triangle



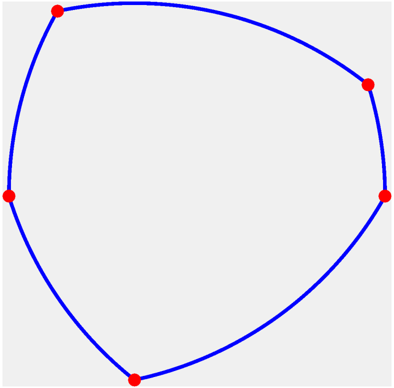
3D: Meissner tetrahedron



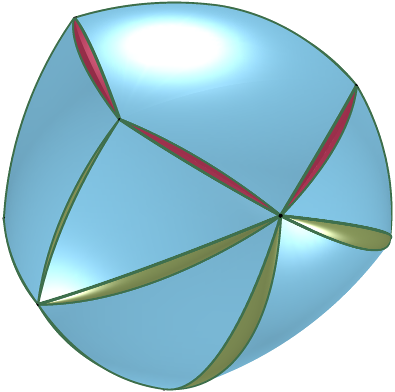
New idea in 3D: Meissner polyhedra

- ⋆ finite dimensional constant width family in 3D: analogue of Reuleaux polygons in 2D
- ⋆ [Montejano, Roldan-Pensado, 18], [Hynd, 23]

2D: Reuleaux polygon



3D: Meissner polyhedron



Meissner polyhedra

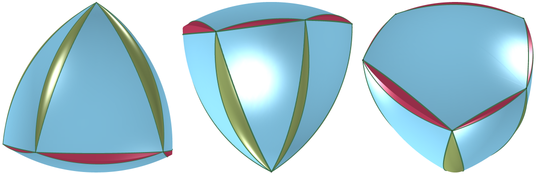
- ⋆ Explicit formula for area and volume [B. *Volume computation for Meissner polyhedra...*, 23]
- ⋆ Missing ingredient for solving 3D case: better understand extremal finite sets of diameter 1

Conjecture

No Meissner polyhedron is a local minimizer for the area. The tetrahedra are minimizers because **they cannot be perturbed** preserving constant width without adding extra vertices.

Tetrahedron: best among pyramids

Among all Meissner pyramids the tetrahedron minimizes the area/volume.



New proof in 2D

Dimension 2

$$\max_{B(1/2)\subset S\subset B(\sqrt{3}/3)} \frac{1}{2}\,\mathrm{Per}(S) - \mathrm{Area}(S)$$

Solution: regular hexagon [Bianchini, Henrot]

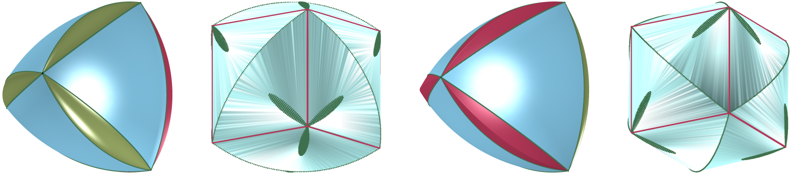
Relaxation of Blaschke-Lebesgue in 2D

Dimension 3

$$\max_{B(1/2)\subset S\subset B(\sqrt{3/8})} \frac{1}{2}\mathrm{Mean\ Width}(S) - \mathrm{Area(S)}$$

Solution: conv$(M, -M)$??

Relaxation of the 3D problem??



⋆ **Challenge for numerics:** Optimal shapes should have plenty of segments in the boundary! The non-smooth framework is needed in 3D!

[B. *Mixed volumes and the Blaschke-Lebesgue theorem*, 23]

Perspectives

- ⋆ Extend the numerical discrete approach to the 3D case: non-smooth support functions

- ⋆ Further study the geometry of Meissner polyhedra and extremal finite sets of diameter 1

- ⋆ Local minimality for the volume of Meissner polyhedra
    - numerical test for local minimality?
    - second order optimality conditions?

1 Design optimization for additive manufacturing

2 Convex shapes - constant width constraint

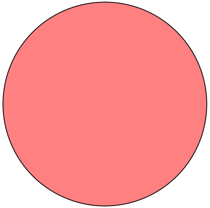
3 **The polygonal Faber-Krahn inequality**

The isoperimetric problem

$$\min_{|\Omega|=c} \operatorname{Per}(\Omega).$$

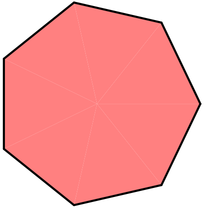
Ω: **General Shape**

$\star$ the solution is the disk



Ω: ***n*-gon**

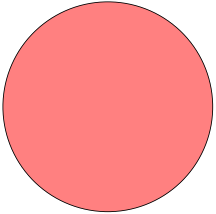
$\star$ the solution is the regular n-gon



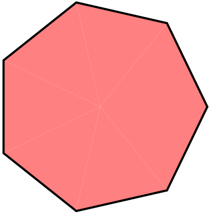
The first Dirichlet eigenvalue: Polyà-Szegö Conjecture

$$-\Delta u_1 = \lambda_1(\Omega) u_1, u_1 \in H_0^1(\Omega), \qquad \min_{|\Omega|=c} \lambda_1(\Omega).$$

Ω: **General Shape** (Faber-Krahn $\sim$ 1920)
Theorem: the solution is the disk



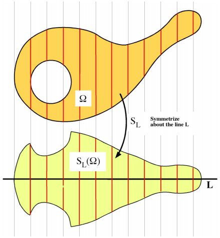
Ω: *n*-**gon** (Polyà-Szegö 1951, $n \in \{3, 4\}$)
Conjecture: the solution is the regular *n*-gon



Heuristic argument

If the optimal shape **among general shapes** is the disk then, when restricting to *n*-gons **the regular one should be optimal**.

Works on the subject



[source: A. Treibergs]

Theory:

⋆ Polyà-Szegö 1951: Steiner symmetrization decreases λ_1

only works for $n \in \{3, 4\}$

⋆ $n \geq 5$: Steiner symmetrization may increase the number of sides

⋆ An optimal n-gon exists and has precisely n sides

[Henrot, *Extremum problems for eigenvalues*, Chapter 3]

⋆ other works [Fragala, Velichkov, 19], [Indrei, 22]

Numerical evidence:

[Antunes, Freitas, 06], [B., PhD thesis, 15], [Dominguez, Nigam, Shahriari, 17]

Starting point for our work:

[Laurain, 19]: computes second shape derivative for the **Dirichlet energy** on polygons, deduces an explicit formula for the associated Hessian matrix

Hybrid proof strategy: use numerical tools when needed

⋆ the optimization variables are the coordinates of the polygon
⋆ finite dimensional optimization problem - classical optimality conditions

1. Explicit computation of the Hessian matrix of $P \mapsto \lambda_1(P)|P|$
2. **Proof of the local minimality** of the regular n-gon: numerical proof for $n \leq 8$
3. Computation of a neighborhood around the regular polygon where minimality occurs
4. Analytic estimate for geometric features of an optimal polygon
5. Reduce the conjecture for a given $n \geq 5$ to a finite number of certified numerical computations.

[B., Bucur, *On the polygonal Faber-Krahn inequality*, 22]

Local minimality: Key points learned

- Shape derivatives: volumic form is well defined for less regular domains

$$\left(-\int_{\partial\Omega}(\partial_n u)^2\theta\cdot\mathbf{n}=\right)\lambda'(\Omega)(\theta)=\int_\Omega \mathbf{S}_1^\lambda : D\theta \text{ with } \mathbf{S}_1^\lambda=[|\nabla u|^2-\lambda(\Omega)u^2]\,\mathbf{Id}-2\nabla u\otimes\nabla u$$

- Hessian matrix of $(\mathbf{x}_0,\mathbf{x}_1,...,\mathbf{x}_{n-1})\mapsto\lambda_1(P)|P|$ is explicit in terms of $2n+1$ PDEs
- For the regular n-gon the Hessian eigenvalues can be computed explicitly:
  4 of them are 0, the rest depend on 3 PDEs.
- If the remaining $2n-4$ are strictly positive then
  the local minimality of the regular *n*-gon holds

Problem

Proving the positivity of the eigenvalues of the Hessian is not obvious (for us, for now...).

Computing the eigenvalues numerically indicates they are positive.

How to turn this into a proof?

Reliable computing: Interval arithmetic

$\star$ floating point arithmetic is reliable (when used correctly): BUT a floating point computation is **not a proof**

$\star$ interval arithmetic replaces floating point numbers x with intervals $[x]$.

$\star$ operations on intervals are defined such that $\tilde{x} \in [x], \tilde{y} \in [y] \Longrightarrow \tilde{x} * \tilde{y} \in [x] * [y]$

$\star$ toolboxes like INTLAB in Matlab implement these operations rigorously [Rump]

Challenges

$\star$ many operations $\longrightarrow$ large intervals $\longrightarrow$ useless results

$\star$ Use any theoretical and practical tool available to pre-compute information.

$\star$ Nothing can be taken for granted: e.g. one needs to prove that the first eigenvalue found numerically is indeed the first eigenvalue!

Goal: Show that a Hessian eigenvalue $\mu = \mathcal{F}(\lambda_1, \nabla u_1, \nabla U^1, \nabla U^2)$ is strictly positive.

A priori estimates: continuous vs (exact) discrete solutions

$\mathbf{P}_1$ finite elements: simple, explicit estimates

Explicit *a priori* error estimates [Liu, Oishi, 13]

- $|\lambda - \lambda_h| \leq C_1 h^2$
- $\|u - u_h\|_{L^2} \leq C_2 h^2$
- $\|\nabla u - \nabla u_h\|_{L^2} \leq C_3 h$ (interpolation error dominates $\|\nabla(u - \Pi_{1,h} u)\|_{L^2} \leq Ch|u|_{H^2}$)

where C_1, C_2, C_3 are **explicit** for a given mesh.

Strategy: $\star$ $a(u, \varphi) = (f, \varphi)_{H^{-1},H^1}$ in $H_0^1(\Omega)$ (continuous problem)
$\star$ $a(v, \varphi) = (f, \varphi)_{H^{-1},H^1}$ in $\mathcal{V}^h$ (same RHS, but discrete; controlled by the interpolation error)
$\star$ $a(v_h, \varphi) = (f_h, \varphi)_{H^{-1},H^1}$ in $\mathcal{V}^h$ (actual FEM solution; continuous vs discrete RHS)

$\star$ easy to see how to choose h in order to achieve a desired precision

Search for an Equilibrium

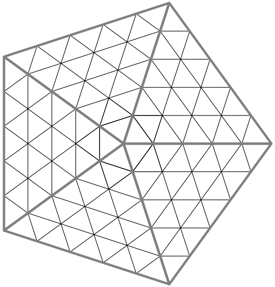
high precision → small h → big discrete linear systems → bad control of machine errors

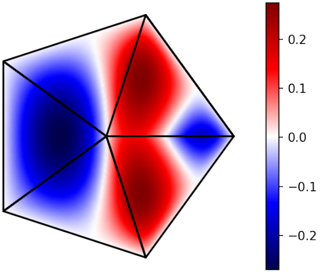
Our contribution

Explicit *a priori* estimates for problems of the form

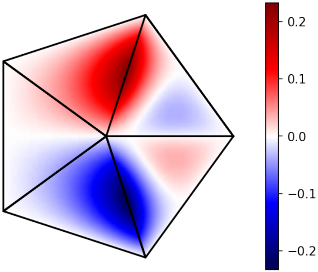
$$\int_\Omega (\nabla U \cdot \nabla v - \lambda_1(\Omega) U v) = \int_\Omega f v + \int_S g v, \quad \forall v \in H_0^1(\Omega), \int_\Omega U u_1 = 0$$

- ⋆ $f \in L^2(\Omega)$, S represents the rays $[\mathbf{oa}_i]$, $g \sim \partial_r u_1 \in H^{1/2}(S)$.
- ⋆ explicit estimates: $\|\nabla U - \nabla U_h\|_{L^2(\Omega)} = O(h)$ if segments in S are meshed exactly
- ⋆ **key idea:** U is not in $H^2(\Omega)$ but is piece-wise H^2 [Grisvard, Chapter 4]


Symmetric mesh



U_0^1



U_0^2

Validation strategy

A) Solve the FEM problems using interval arithmetics.

Control machine errors for the discrete problems

- ⋆ solve in floating point; validate afterwards (INTLAB, residual)
- ⋆ explicit assembly – all triangles in the mesh are congruent
- ⋆ modify `verifyeig` in INTLAB: replace matrix inversion with 3 verified linear systems

B) Compute the eigenvalues of the Hessian matrix.

Interval arithmetic is used in all computations

- ⋆ replace all FEM variables in the formulas and obtain $\mu_h = [\underline{\mu_h}, \overline{\mu_h}]$.

C) Add the a priori estimates.

Control errors between continuous and (exact) discrete problems

- ⋆ use optimal interpolation constants: mesh contains congruent triangles
- ⋆ the actual eigenvalue μ is guaranteed to belong to $[\underline{\mu_h} - Ch, \overline{\mu_h} + Ch]$

If $2n - 4$ of the intervals obtained are contained in $(0, +\infty)$ the **proof of local minimality succeeds**.

Preliminary results

- ⋆ Complete validation of local minimality for $n \leq 8$
- ⋆ Key points: improved error estimates, optimal interpolation constants

n	[B., Bucur, 22]			[B., Bucur, soon]		
	h	DoF	Intervals	h	DoF	Intervals
5	9.8e-4	2.5 million	✗	0.0125	16200	✓
6	4.2e-4	17 million	✗	0.0095	33390	✓
7	1.9e-4	97 million	✗	0.0055	114030	✓
8	1.35e-4	220 million	✗	0.0037	292680	✓

Conclusions

Polygonal Faber-Krahn inequality – academic problem:

New ideas explored: shape derivatives on polygons, explicit FEM estimates, validated numerics for local minimality

What's next? Continue the program proposed in [B., Bucur, 22]

⋆ Convexity of the optimal *n*-gon would surely help a lot.

⋆ *A posteriori* error estimates for the singular problem?

⋆ in preparation: The boundary structure theorem also holds for λ'' on convex polygons.

Numerics in shape optimization:

- practical applications
- guiding the theoretical study
- contribute to theoretical proofs

Thank you!