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Shape optimization of harmonic helicity in toroidal domains

Robin Roussel [1]
In collaboration with Rémi Robin [2]

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[1]Laboratoire Jacques-Louis Lions, Sorbonne Université, Inria, Paris

[2]Laboratoire de Physique de l'École Normale Supérieure, Mines Paris, Inria, CNRS, ENS-PSL, Sorbonne Université, PSL Research University, Paris, France

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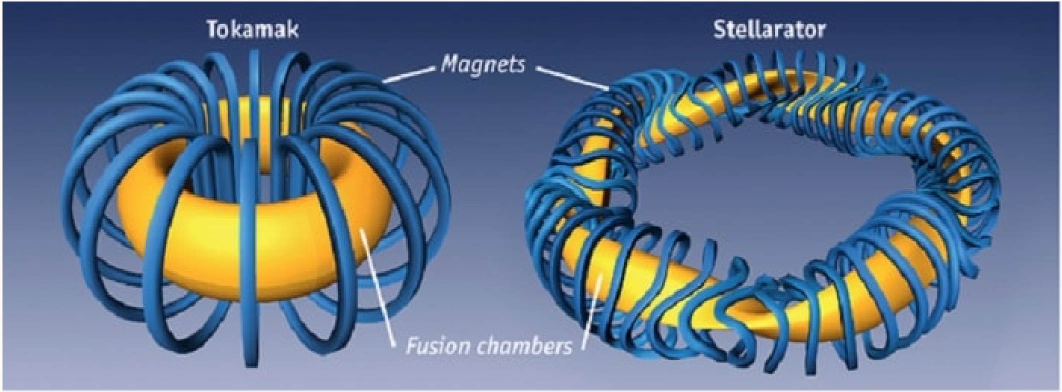
Tokamaks and Stellarators



Magnetic confinement reactors

- Tokamaks: axisymmetric, current inside the plasma
- Stellarators: non axisymmetric, no current inside the plasma

MHD and helicity

Ideal MHD

Fluid model describing interactions between a plasma and the electromagnetic field.

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Fluid model describing interactions between a plasma and the electromagnetic field.

- In ideal MHD, helicity is conserved.
- Helicity is related to the linkage of magnetic field lines.
- High helicity $\implies$ large magnetic topological structures.

The Biot–Savart operator and helicity

Ω bounded domain in $\mathbb{R}^3$.

$$\mathrm{BS}(V)(y) = \frac{1}{4\pi} \int_\Omega \frac{V(x) \times (y - x)}{|y - x|^3} dx$$

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If $\mathrm{div}\, V = 0$ and $V \cdot n = 0$ (V is a magnetic field), the helicity of V is

$$\mathrm{H}(V) = \langle V, \mathrm{BS}(V)\rangle$$

Previous works

For magnetic fields, we have $\operatorname{curl} \mathrm{BS}(V) = V$.
This implies that helicity maximizers for fixed energy are eigenfields of the curl.

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References:

- Theoretical study: J. Cantarella, D. DeTurck, H. Gluck, and M. Teytel. "Isoperimetric problems for the helicity of vector fields and the Biot–Savart and curl operators". In: *Journal of Mathematical Physics* (2000)
- Numerical methods: A. Alonso-Rodríguez et al. "Finite Element Approximation of the Spectrum of the Curl Operator in a Multiply Connected Domain". In: *Foundations of Computational Mathematics* (2018)

Harmonic fields

Ω bounded domain in $\mathbb{R}^3$. B is harmonic if

$$\operatorname{div} B = 0$$
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Harmonic fields

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$$\begin{aligned} \operatorname{div} B &= 0 \\ \operatorname{curl} B &= 0 \\ B \cdot n &= 0 \end{aligned}$$

- If Ω is diffeomorphic to $\mathbb{D}^2 \times S^1$, the set of harmonic fields is one dimensional.
- We get a unique field by fixing the circulation along a toroidal loop
- In general, the dimension is equal to the number of "holes" in Ω.

Our work

We want to study the helicity of the harmonic field as a shape functional

$$
\begin{tikzcd}
\Omega \arrow[r, "\text{Harmonic field}"'] \arrow[rr, bend left, "\text{Harmonic helicity}"] & B(\Omega) \arrow[r, "\text{Helicity}"'] & \mathrm{H}(B(\Omega)) =: \mathcal{H}(\Omega)
\end{tikzcd}
$$

- PDE formulation for the helicity
- Shape differentiation of harmonic helicity
- Numerical analysis and implementation

Contents

Differential operators

Usual differential operators of electromagnetism.

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We then have $\operatorname{curl} \nabla = \operatorname{div} \operatorname{curl} = 0$.

Functional spaces

$$H(\mathrm{curl}\,,\Omega) = \left\{U \in L^2(\Omega)^3 \mid \mathrm{curl}\, U \in L^2(\Omega)^3\right\},$$
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$$H^1(\Omega) \xrightarrow{\ \nabla\ } H(\mathrm{curl}\,,\Omega) \xrightarrow{\ \mathrm{curl}\ } H(\mathrm{div}\,,\Omega) \xrightarrow{\ \mathrm{div}\ } L^2(\Omega).$$

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$$H(\operatorname{curl}, \Omega) = \left\{ U \in L^2(\Omega)^3 \mid \operatorname{curl} U \in L^2(\Omega)^3 \right\},$$
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$$H^1(\Omega) \xrightarrow{\nabla} H(\operatorname{curl}, \Omega) \xrightarrow{\operatorname{curl}} H(\operatorname{div}, \Omega) \xrightarrow{\operatorname{div}} L^2(\Omega).$$

Tangential trace of $H(\operatorname{curl}, \Omega)$ in $H^{-1/2}(\partial\Omega)^3$ and normal trace of $H(\operatorname{div}, \Omega)$ in $H^{-1/2}(\partial\Omega)$.

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Invariance under adding gradients

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No invariance under adding harmonic fields

Gauge invariance of helicity

We modify the helicity formula to have invariance on the choice of potential vector (Bevir-Gray formula)

$$\mathrm{H}(B) = \int_\Omega B \cdot A - \int_\gamma A \cdot dl \int_{\gamma'} A \cdot dl.$$

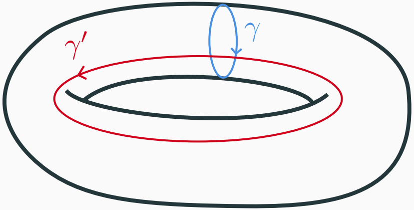

Figure 1: Diagram of the domain with a toroidal loop γ' and a poloidal loop *gamma*.

PDEs for the potential vector

We set

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Additional constraint for WP

$$\langle A, B \rangle = 0, \quad \text{or} \int_{\gamma'} A \cdot dl = 0.$$

Comments on well posedness

Harmonic field:

- Two variational formulations:
    - Classical formulation: harmonic field is strongly curl free.
    - Mixed formulation: harmonic field is strongly divergence free and tangent to the boundary.

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Using functional injections, we get Poincaré inequalities and Hodge decompositions.
Well posedness by inf–sup inequalities.

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What is shape differentiation ?

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- Ω bounded Lipschitz domain
- θ small Lipschitz vector field on $\mathbb{R}^3$ such that $(\mathrm{I}+\theta)$ is a diffeomorphism.
- Question: What is the volume of $\Omega_\theta = (\mathrm{I}+\theta)(\Omega)$ up to first order ?

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We have

$$\begin{aligned}\det(\mathrm{I} + D\theta) &= 1 + \mathrm{tr}(D\theta) + o(||\theta||_{W^{1,\infty}}), \\ &= 1 + \mathrm{div}\,\theta + o(||\theta||_{W^{1,\infty}}),\end{aligned}$$

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so that

$$\begin{aligned}\mathrm{Vol}(\Omega_\theta) &= \int_{\Omega} dx + \int_{\Omega} \mathrm{div}\,\theta dx + o\left(||\theta||_{W^{1,\infty}}\right),\\ &= \mathrm{Vol}(\Omega) + \int_{\partial\Omega} \theta \cdot n + o\left(||\theta||_{W^{1,\infty}}\right).\end{aligned}$$

What is shape differentiation ?

We therefore have

$$\mathrm{Vol}(\Omega_\theta) = \mathrm{Vol}(\Omega) + \mathrm{Vol}'(\Omega;\theta) + o(||\theta||_{W^{1,\infty}}),$$

where

$$\mathrm{Vol}'(\Omega;\theta) = \int_{\partial\Omega} \theta \cdot n$$

is the shape derivative of the volume.

Formula of shape differential

Theorem (R., Robin, 2023)
Let Ω be a Lipschitz toroidal domain. Then, the harmonic helicity is differentiable at Ω under $W^{1,\infty}$ deformations. Furthermore, if Ω is s-regular for $s > 1/2$, we have for all θ in $W^{1,\infty}(\mathbb{R}^3)^3$

$$\mathcal{H}'(\Omega;\theta) = 2\int_{\partial\Omega} B(\Omega)\cdot A(\Omega)\theta\cdot n.$$

Vector fields pullbacks

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$$\begin{array}{ccccccc}
H^1(\Omega_\theta) & \xrightarrow{\nabla} & H(\mathrm{curl}\,, \Omega_\theta) & \xrightarrow{\mathrm{curl}} & H(\mathrm{div}\,, \Omega_\theta) & \xrightarrow{\mathrm{div}} & L^2(\Omega_\theta) \\
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\end{array}$$

where the Φ^k_θ are the Piola transformations from FEEC.

Giving a taste of the computations

Using the following formulas

- $\Phi_\theta^3 u = \det(\mathrm{I} + D\theta) u \circ (\mathrm{I} + \theta)$,
- $\Phi_\theta^3 (U \cdot V) = \Phi_\theta^2 U \cdot \Phi_\theta^1 V$,

we get

$$\mathcal{H}(\Omega_\theta) = \int_{\Omega_\theta} B_\theta \cdot A_\theta,$$

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If

$$\Phi^2_\theta B_\theta = B_0 + B'(\Omega;\theta) + o(||\theta||),$$
$$\Phi^1_\theta A_\theta = A_0 + A'(\Omega;\theta) + o(||\theta||),$$

we get

$$\mathcal{H}'(\Omega;\theta) = \int_\Omega B'(\Omega;\theta)\cdot A_0 + \int_\Omega B_0 \cdot A'(\Omega;\theta).$$

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To conclude the proof

- We pull the VF for B and A back onto Ω using the Φ_θ^k

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- We differentiate the VF, and plug the result into the last formula

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Discretization of the De Rham complex

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Now that we can view the computation of the harmonic helicity and its shape derivative using PDEs, we can design a scheme to compute numerical solutions.

We construct finite element spaces to have the following commutative diagram (FEEC)

$$\begin{tikzcd}
H^1(\Omega) \arrow[r, "\nabla"] \arrow[d, "\Pi_h^0"'] & H(\mathrm{curl}\,, \Omega) \arrow[r, "\mathrm{curl}"] \arrow[d, "\Pi_h^1"'] & H(\mathrm{div}\,, \Omega) \arrow[r, "\mathrm{div}"] \arrow[d, "\Pi_h^2"'] & L^2(\Omega) \arrow[d, "\Pi_h^3"'] \\
V_h^0(\Omega) \arrow[r, "\nabla"] & V_h^1(\Omega) \arrow[r, "\mathrm{curl}"] & V_h^2(\Omega) \arrow[r, "\mathrm{div}"] & V_h^3(\Omega)
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- Convergence of A_h and B_h in L^2

$$\|B - B_h\|_{L^2} \leq Ch^s \|B\|_{L^2},$$
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- Convergence in L^2 implies convergence of the harmonic helicity

Issues for the convergence of the shape derivative

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- If Ω is s–regular with $s > 1/2$, A and B have traces in $L^2(\partial\Omega)^3$.

Problem: A_h and B_h do not have the same regularity, and the convergences found earlier do not give $L^2(\partial\Omega)^3$ convergence directly.

Contents

Numerical implementation

The numerical scheme was implemented in python.
Libraries

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- dolfinx for FEM
- petsc4py for matrix manipulation and system solving
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Surfaces parametrized with Fourier coefficients.

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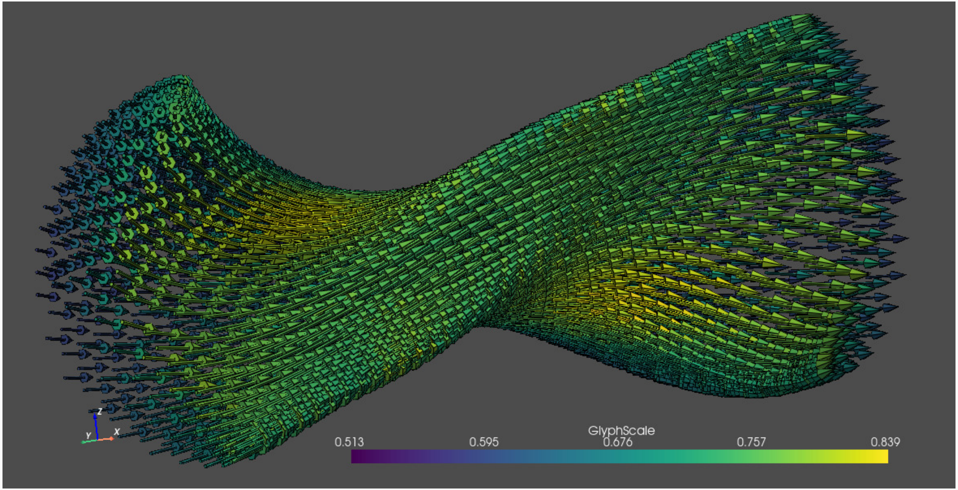

Figure 2: Plot of B_h

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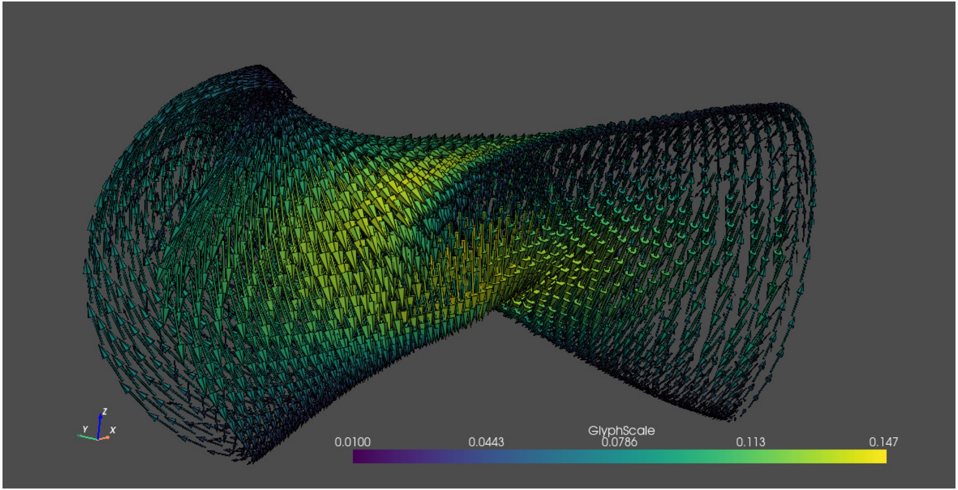

Figure 3: Plot of A_h

Numerical implementation

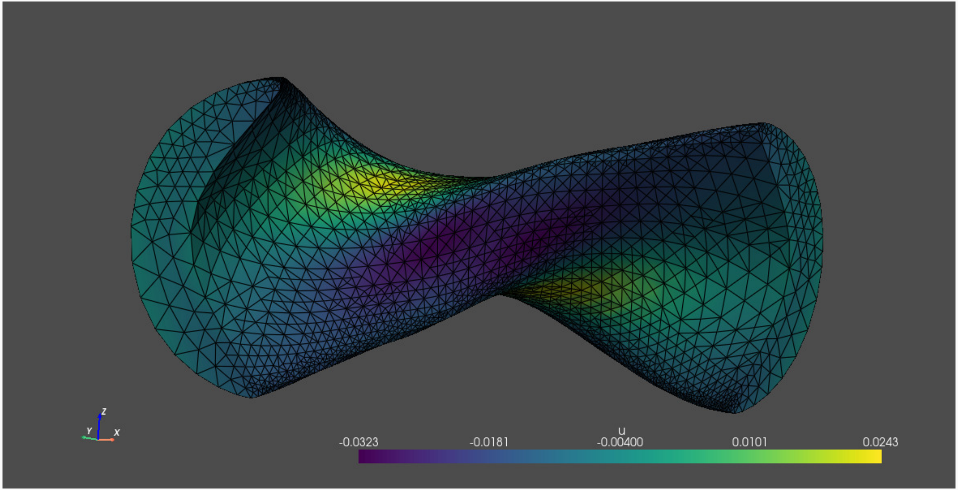

Figure 4: Plot of $B_h \cdot A_h$ on the boundary

Numerical implementation

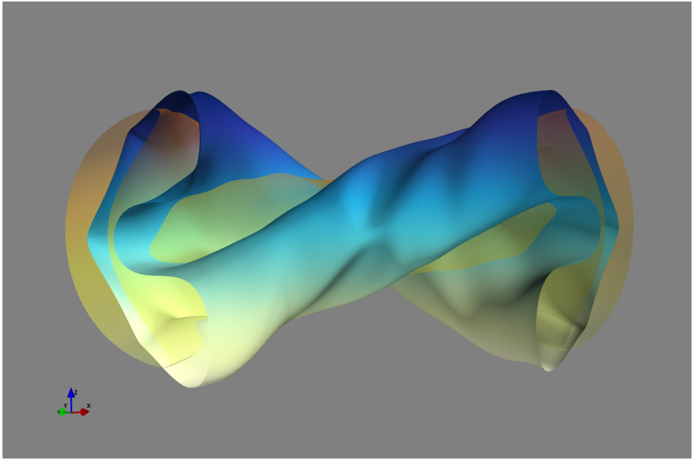

Figure 5: Original NCSX shape in orange, new shape in blue after a few steps of gradient descent (volume and curvature constraint)

Conclusions and perspectives

Conclusions:

- Introduction of the harmonic helicity shape functional, and formulation through solutions of PDEs.
- Derivation of a shape gradient formula for domains with low regularity using vector field pullbacks.
- Numerical analysis and implementation of a numerical scheme to compute shape helicity and perform numerical optimization.

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Perspectives:

- Convergence of B_h and A_h in $L^2(\partial\Omega)$
- Existence of optimal shapes: strong regularity (reach constraints) or low regularity (Lipschitz domains)

THANK YOU FOR YOU ATTENTION