MRX: A differentiable 3D MHD equilibrium solver without nested flux surfaces

Tobias Blickhan*, Julianne Stratton, Alan A. Kaptanoglu

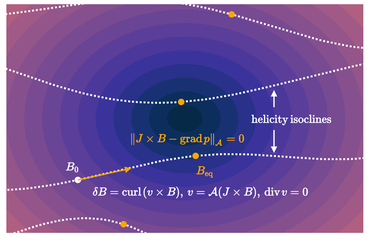
Courant Institute of Mathematical Sciences, New York University

Overview

We introduce a structure-preserving magnetic-relaxation solver that can handle arbitrary field-line topology.

- Through **structure-preserving mixed finite-elements**, we guarantee $\operatorname{div} B = 0$ to machine precision, energy-dissipation and helicity preservation.
- **High-order** B-Spline bases and tools from isogeometric analysis allow exhibit rapid convergence for regular solutions as well as non-uniform meshes.
- The code is **pure Python (JAX)**, making it very easy to install, run, and extend, as well as performant on GPUs. It is also fully differentiable for future inverse design and optimization applications.

Magnetic relaxation



$$\mathcal{E}(B) = \frac{1}{2}\int |B|^2, \qquad \text{(magnetic energy)}$$

$$\delta_v B = \operatorname{curl}(v \times B) \quad \text{(admissible variations)}$$

$$\delta_v \mathcal{E}(B) = -\int (J \times B) \cdot v$$

set $v = J \times B - \operatorname{grad} p$, $\operatorname{div} v = 0$:

$$\delta_v \mathcal{E}(B) = -\int |J \times B - \operatorname{grad} p|^2 \leq 0$$

$$\text{and } = 0 \Leftrightarrow v = J \times B - \operatorname{grad} p = 0$$

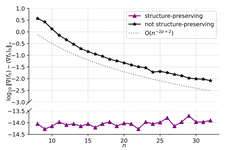
Dynamics approach equilibrium.

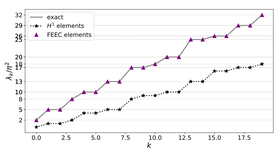
Crucial ingredient: preservation of helicity $\int B \cdot \operatorname{curl}^{-1} B$ guarantees a lower bound on $\mathcal{E}(B)$.

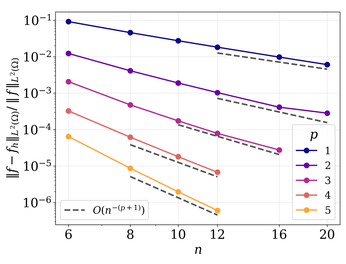
Structure-preserving finite elements

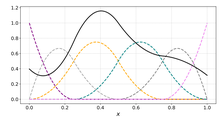
We build on the Finite Element Exterior Calculus framework [1] to combine approximation spaces. Some equations hold point-wise ($\operatorname{div} B = 0$) and some in a L^2 sense: $(B, \operatorname{curl} \Lambda) = (J, \Lambda)\ \forall \Lambda$.

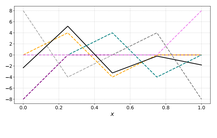
- Discrete helicity is preserved.
- Discrete energy is dissipated.
- $\operatorname{div} B = 0$ to machine precision.
- $\operatorname{curl} \operatorname{grad} = \operatorname{div} \operatorname{curl} = 0$.
- inf sup stability is guaranteed.







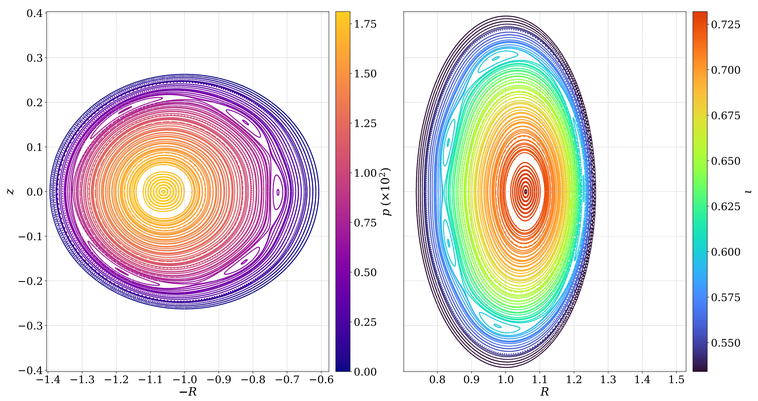




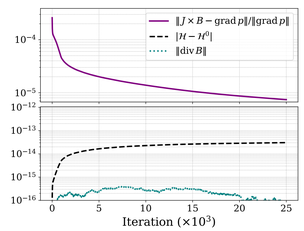
(top) Continuous and discrete derivatives coincide.
(top right) No spurious Laplacian eigenvalues.
(left) Error convergence for $-\Delta f = g$ on a toroid.
(bottom) Quadratic splines and their derivatives.

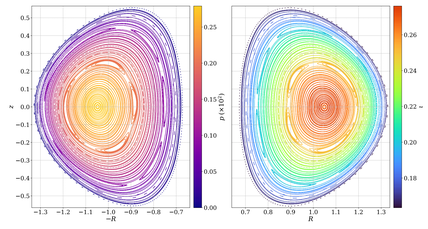
https://github.com/ToBlick/mrx

Island chains



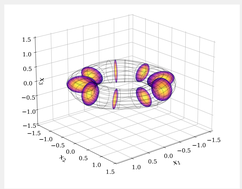
(top) Rotating ellipse: Magnetic field after 2.5×10^4 iterations colored by pressure and rotational transform. A $(3,5)$ island chain formed at the $\iota = 3/5$ surface. (bottom left) Force decay and preservation of force/helicity for the rotating ellipse. (bottom right) A simulation in a Tokamak geometry. Applying radial perturbations to B leads to the formation of islands at $\iota \in \{1/5, 1/4\}$.





Geometries

Computations in MRX are done on a logical domain $\hat{\Omega}$, where the geometry of the physical domain Ω is encoded by a map $\Phi : \hat{\Omega} \to \Omega$. **This map does not need to be flux-aligned, but it can be chosen to be.**
The structure-preserving properties hold for all such maps, including those with a polar singularity [3]. We currently enforce C^1 regularity at the $\hat{x}_1 = 0$ axis. The $\hat{x}_1 = 0$ axis only coincides with the magnetic axis for very specific choices of Φ.



For example, when $x = \Phi(\hat{x})$ and $\hat{u}(\hat{x}) = u(\Phi(\hat{x}))$, a scalar Laplace operator is given by

$$\int_\Omega \operatorname{grad}_x u(x) \cdot \operatorname{grad}_x v(x)\, \mathrm{d}x = \int_{\hat{\Omega}} \operatorname{grad}_{\hat{x}} \hat{u}(\hat{x}) \cdot \left(D\Phi(\hat{x})^T D\Phi(\hat{x}) \right)^{-1} \operatorname{grad}_{\hat{x}} \hat{v}(\hat{x}) \det D\Phi(\hat{x})\, \mathrm{d}\hat{x}.$$

67th Annual Meeting of the APS Division of Plasma Physics

Connecting to existing solvers

The optimization objective of VMEC, DESC, and GVEC is a map $\Phi : \hat{x} \mapsto x$ that defines the magnetic field with given magnetic fluxes. This formulation is limited to nested flux surfaces.

In MRX, the map from logical to physical domain is fixed for the entire relaxation process. We can use an initially flux-aligned map to start from nested equilibrium configurations and study island formation by running the relaxation from there. **The preservation of global helicity does not rule out local reconnection and changes in field-line topology.**

A first interface with GVEC is implemented.

Compared to the most mature modern relaxation code SIESTA [2], the main differences are:

- Language: Fortran90 $\rightarrow$ Python/JAX for ease of use and differentiability.
- Discretization: Finite differences and Fourier expansions
  $\rightarrow$ Spline finite elements for structure-preservation and non-uniform meshes.
- Pressure treatment: Dynamical variable with equation of state $p = \rho^\gamma$
  $\rightarrow$ Incompressibility condition $\Delta p = \operatorname{div}(J \times B)$ to simplify the relaxation formulation.

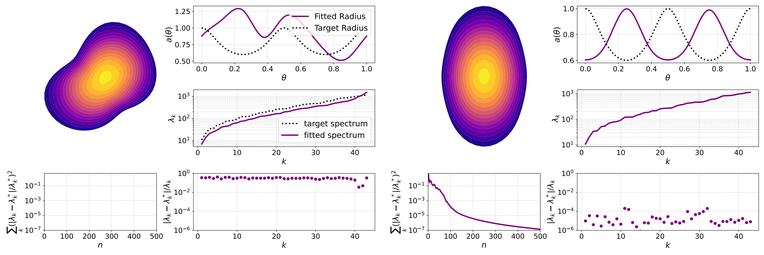
Outlook: shape optimization

The end-to-end differentiability provides interesting opportunities.

Consider the map $(r, \theta) \mapsto (r a_\alpha(\theta)\cos(\theta), r a_\alpha(\theta)\sin(\theta))$. a_α is parametrized by coefficients α. Denote the Laplacian spectrum on $\Phi_\alpha(\hat{\Omega})$ by $\{\lambda_k^\alpha\}_k$. Then, solve the **inverse problem** $\{\lambda_k^\alpha\}_k \mapsto \alpha$:

$$\min_\alpha \textstyle\sum_k |\lambda_k^\alpha - \lambda_k^*|^2 / \lambda_k^{*2} \quad \text{such that} \quad \{\lambda_1^\alpha, \lambda_2^\alpha, \dots\} = \operatorname{eig}(-\Delta_a).$$

The forward problem $\alpha \mapsto \{\lambda_k^\alpha\}_k$ consists of assembling $\mathbb{L}$, $\mathbb{M}$, followed by solving $\mathbb{L}\mathbf{x}_k = \lambda_k \mathbb{M}\mathbf{x}_k$ for the eigenvalue/vector pairs $\{\lambda_k, \mathbf{x}_k\}_k$. We compute $\partial_\alpha \{\lambda_k^\alpha\}_k$ by differentiating through this process and find α^* using an off-the-shelf ADAM optimizer starting from a random initial guess.



References

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This work was supported through a grant from the Simons Foundation under award 560651.

tobias.blickhan@nyu.edu