# Equilibrium States via Simulated Annealing*

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**Goal:** Describe two version of Simulated Annealing, a relaxation method for the numerical calculation of equilibria. **Here, calculate MHD equilibria** with **islands** and **chaos**, to the extent they exist.

**Thanks** to DOE, Humboldt Foundation, NMPP, MPI Garching

* With Masaru Furukawa, Tottori University, Japan and Camilla Bressan, M. Kraus, and O. Maj, NMPP, Max Planck Institute, Garching, Germany

## Numerical Relaxation Methods

- Many numerical techniques known: friction, conjugate gradient, etc.

- What's new? The fundamental structure of dynamics used.

## Two Simulated Annealing Methods

- Double Bracket Dynamics with M. Furukawa
- Metriplectic Dynamics with C. Bressan, M. Kraus, and O. Maj

# Fundamental Structure of Nondissipative Dynamics

- **All** (correct) nondissipative plasma evolution equations have the split form:

$$\frac{\partial \mathcal{Y}}{\partial t} = \mathcal{J}\,\frac{\delta H}{\delta \mathcal{Y}} = \{\mathcal{Y}, H\}$$

$\mathcal{Y}$ state variables. e.g. for MHD $u = \{\boldsymbol{v}, \boldsymbol{B}, \rho, p\}$

- The Poisson operator $\mathcal{J}$ $\Rightarrow$ Poisson bracket $\{F, G\}$ satisfies
  - ⋆ antisymmetry $\{F, G\} = -\{G, F\}$ and Jacobi $\{\{F, G\}, H\} + \text{cyc} = 0$
  - ⋆ degeneracy of $\mathcal{J}$ explains and allows discovery of mysterious Casimir invariants

$$\mathcal{J}\,\frac{\delta C}{\delta \mathcal{Y}} = 0$$

e.g. for MHD $\int \boldsymbol{A} \cdot \boldsymbol{B}$ & $\int \boldsymbol{v} \cdot \boldsymbol{B}$

# Double Bracket Dynamics Uses $\mathcal{J}^2$

- Fake Dynamics:

$$\frac{\partial \mathcal{Y}}{\partial t} = \mathcal{J}^2 \frac{\delta H}{\delta \mathcal{Y}}$$

  - ⋆ The operator $\mathcal{J}^2$ is positive definite $\Rightarrow$ relaxation.

  - ⋆ The operator $\mathcal{J}^2$ has null space of $\mathcal{J}$.

- The fake dynamics solves the variational principle

$$\min H \quad \text{at constant } C$$

  - ⋆ Choice of $C \to$ different equilibria.

# Double Bracket Simulated Annealing for RMHD

M. Furukawa* and PJM

*Tottori University

# Motivation

- Simulated Annealing (SA) is a method for obtaining stationary states (equilibria) of Hamiltonian systems as energy extrema

  G. R. Flierl, P. J. Morrison, Physica D **240**, 212 (2011).

  - In the SA, we solve a system of artificial evolution equations derived from an original Hamiltonian system so that the energy (Hamiltonian) changes monotonically
  - Casimir invariants are preserved in the SA for noncanonical Hamiltonian systems
- If an equilibrium is an energy minimum state, which is stable, SA will recover the equilibrium when started from a perturbed state
  - SA can be used as a stability analysis tool

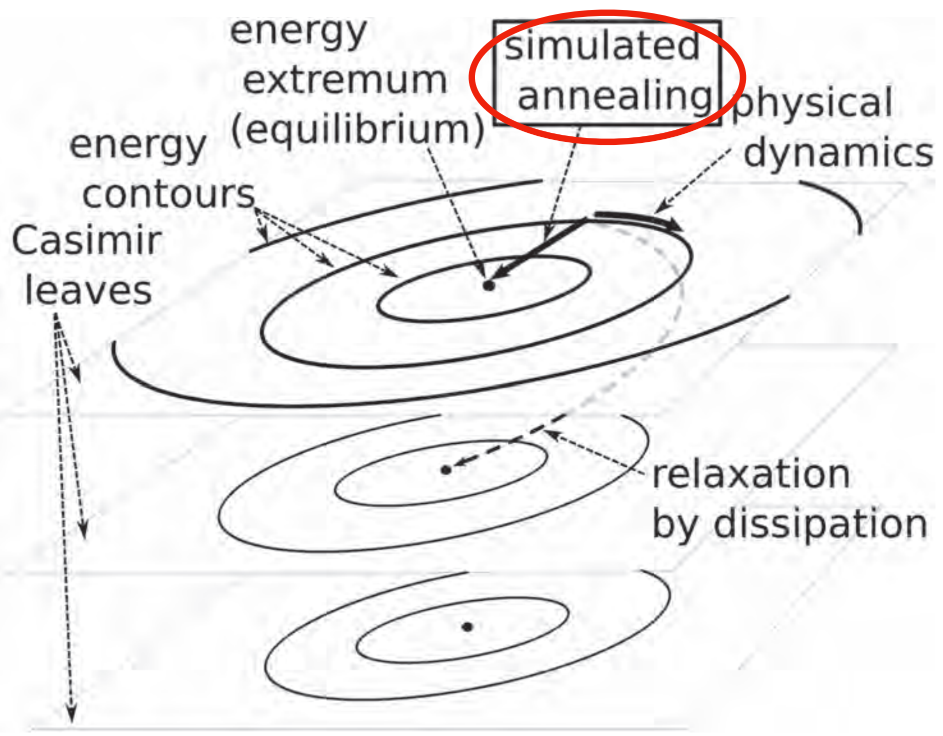



**Figure 1.** Schematic picture explaining Casimir leaf, physical and artificial dynamics.

Cited from: M. Furukawa and P. J. Morrison, Plasma Phys. Control. Fusion **59**, 054001 (2017).

# Ideal, low-beta reduced MHD in cylindrical geometry

- Cylindrical plasma is considered
  - Minor radius $a$
  - Length $2\pi R_0$

inverse aspect ratio $\varepsilon := \dfrac{a}{R_0}$

- Cylindrical coordinate system $(r, \theta, z)$ , as well as $\zeta := \dfrac{z}{R_0}$ is used
- Ideal, low-beta reduced MHD (normalized) is written as

$$\frac{\partial U}{\partial t} = [U, \varphi] + [\psi, J] - \varepsilon \frac{\partial J}{\partial \zeta}$$

$$\frac{\partial \psi}{\partial t} = [\psi, \varphi] - \varepsilon \frac{\partial \varphi}{\partial \zeta}$$

H. R. Strauss, Phys. Fluids **19**, 134 (1976).

where

$\boldsymbol{v} = \hat{\boldsymbol{z}} \times \nabla \varphi$ : fluid velocity

$\boldsymbol{B} = \hat{\boldsymbol{z}} + \nabla \psi \times \hat{\boldsymbol{z}}$ : magnetic field

$U := \triangle_\perp \varphi$ : vorticity ( $z$ component)

$J := \triangle_\perp \psi$ : current density ( $-z$ component)

$\hat{\boldsymbol{z}}$ : unit vector in $z$ direction

$\triangle_\perp$ : Laplacian in $r - \theta$ plane

$[f, g] := \hat{\boldsymbol{z}} \cdot \nabla f \times \nabla g$ : Poisson bracket for two functions $f$ and $g$

**Normalization**

$a$ : length

$B_0$ : typical magnetic field

$\rho_0$ : typical mass density

$v_A := \dfrac{B_0}{\sqrt{\mu_0 \rho_0}}$ : velocity

$\tau_A := \dfrac{a}{v_A}$ : time

## Evolution equations for SA have same form as those of low-beta reduced MHD but different, artificial convection fields

- For the low-beta reduced MHD

$$\frac{\partial U}{\partial t} = [U, \varphi] + [\psi, J] - \varepsilon \frac{\partial J}{\partial \zeta} \qquad =: f^1$$

$$\frac{\partial \psi}{\partial t} = [\psi, \varphi] - \varepsilon \frac{\partial \varphi}{\partial \zeta} \qquad =: f^2$$

the explicit form of the artificial evolution equation of SA by the symmetric bracket is

M. Furukawa and P. J. Morrison, Plasma Phys. Control. Fusion **59**, 054001 (2017).

$$\frac{\partial U}{\partial t} = [U, \tilde{\varphi}] + [\psi, \tilde{J}] - \varepsilon \frac{\partial \tilde{J}}{\partial \zeta} \qquad \tilde{\varphi}(\boldsymbol{x}) := \int_{\mathcal{D}} \mathrm{d}^3 x' \, K_{1j}(\boldsymbol{x}, \boldsymbol{x}') f^j(\boldsymbol{x}')$$

$$\frac{\partial \psi}{\partial t} = [\psi, \tilde{\varphi}] - \varepsilon \frac{\partial \tilde{\varphi}}{\partial \zeta} \qquad \tilde{J}(\boldsymbol{x}) := \int_{\mathcal{D}} \mathrm{d}^3 x' \, K_{2j}(\boldsymbol{x}, \boldsymbol{x}') f^j(\boldsymbol{x}')$$

- The advection fields are replaced by the artificial ones
- $(K_{ij})$ is chosen to be positive definite so that the energy decreases monotonically
- Casimir invariants, such as magnetic helicity, are preserved since the Poisson bracket is same

# Initial condition

- Initial condition is given by a summation of cylindrically symmetric state plus a perturbation opening a small magnetic island at the rational surface

$$U(\boldsymbol{x},0) = U_{-2/1}(r)\sin(-2\theta+\zeta)$$

$$\psi(\boldsymbol{x},0) = \psi_{0/0}(r) + \psi_{-2/1}(r)\cos(-2\theta+\zeta)$$

  - Cylindrically symmetric state

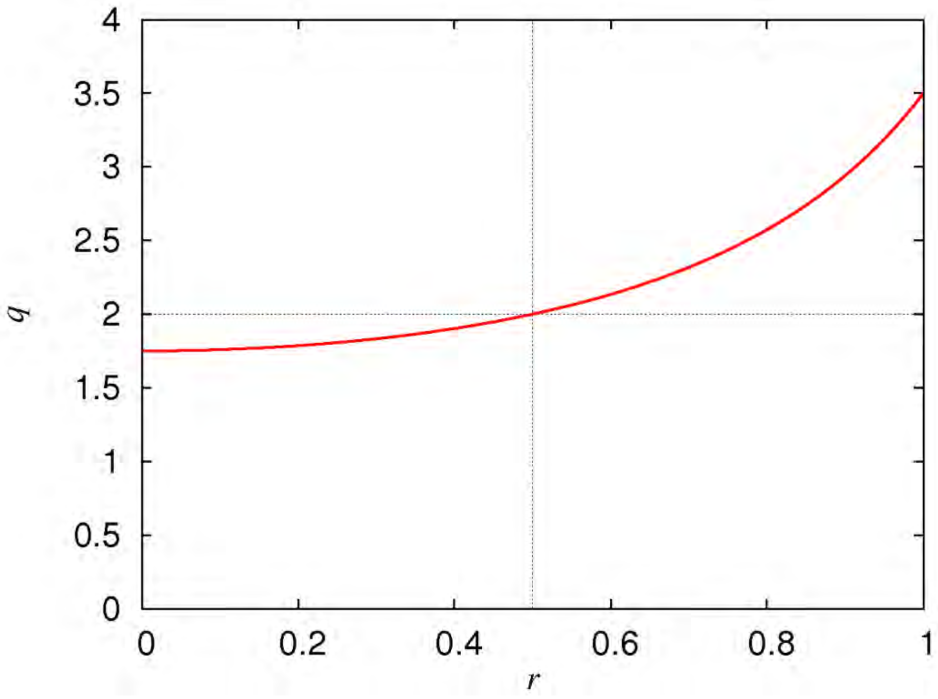
$$J_{0/0}(r) = \tilde{J}_{0/0}(1-r^2) \quad \text{with} \quad \tilde{J}_{0/0} = -\frac{4}{35}$$

Inverse aspect ratio $\varepsilon = \frac{1}{10}$

$q = 2$ surface at $r = \frac{1}{2}$

No plasma rotation

Unstable against tearing mode with $m = -2$ and $n = 1$ ( $\Delta' \simeq 22.4$ )



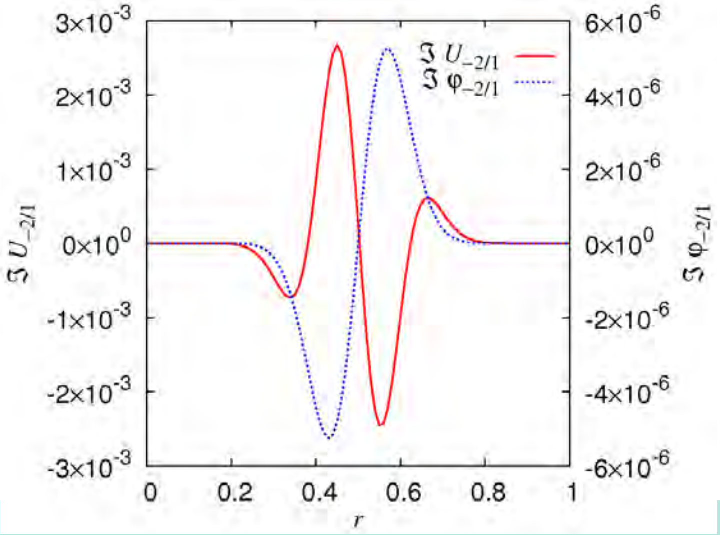
# Initial condition – cnt'd

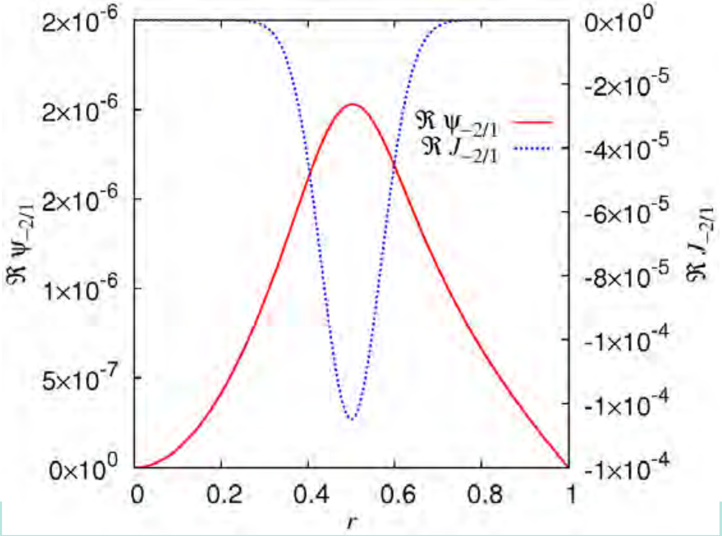
- Initial condition is given by a summation of cylindrically symmetric state plus a perturbation opening a small magnetic island at the rational surface
  - Perturbation part

$$\varphi_{-2/1}(\boldsymbol{x},0) = -\tilde{\varphi}_{-2/1}(r-r_{\mathrm{s}})r(1-r)\,\mathrm{e}^{-(\frac{r-r_{\mathrm{s}}}{L})^2}\sin(-2\theta+\zeta)$$

$$J_{-2/1}(\boldsymbol{x},0) = -\tilde{J}_{-2/1}r(1-r)\,\mathrm{e}^{-(\frac{r-r_{\mathrm{s}}}{L})^2}\cos(-2\theta+\zeta)$$

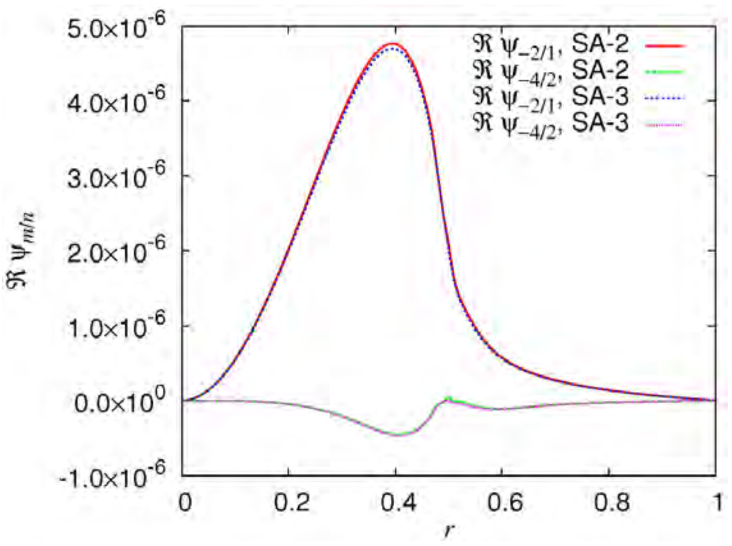
with $r_{\mathrm{s}} = \frac{1}{2}$ , $L = \frac{1}{10}$ , $\tilde{\varphi}_{-2/1} = 10^{-3}$ , $\tilde{J}_{-2/1} = 10^{-3}$

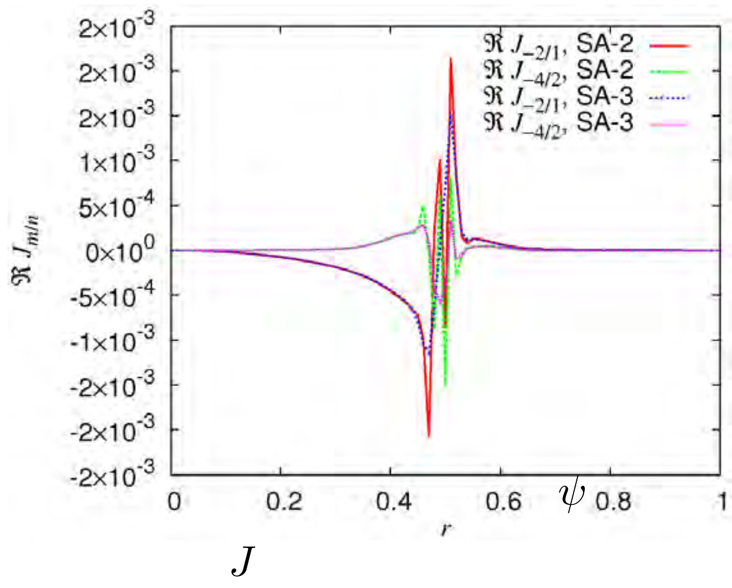


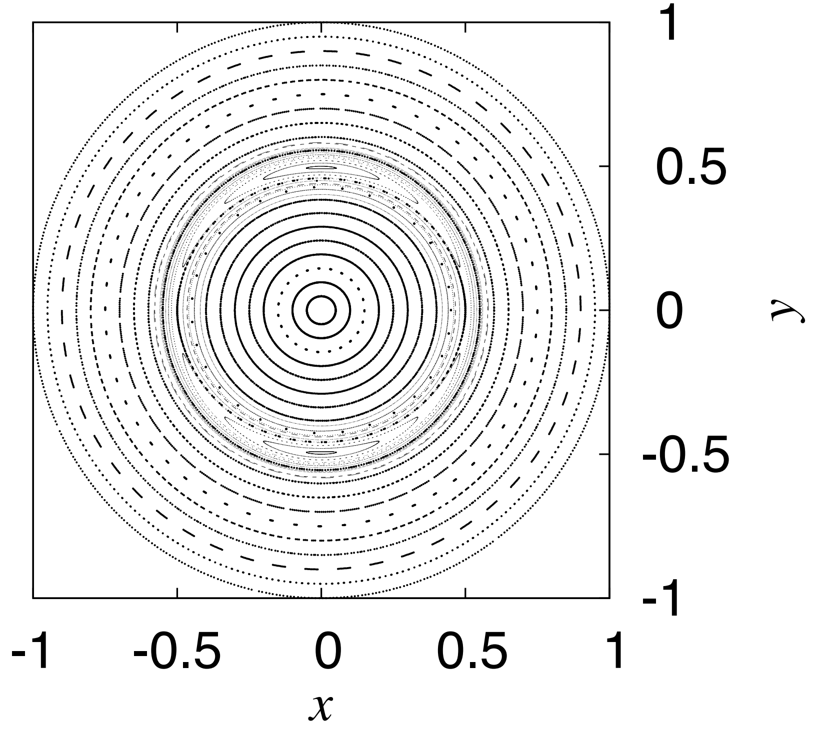



# Equilibrium with magnetic islands obtained

- Radial profiles of $\Re\psi_{m/n}$ and $\Re J_{m/n}$ at the final state (left, center)
- Poincaré plot (right)



# Recent Work

- Method to find desired initial conditions
- Tailoring operator to find optimal decent paths
- Adapted SA to create a stability method: convergence implies stable equilibra

# Metriplectic Simulated Annealing for Beltrami

C, Bressaan, M. Kraus, O. Maj* and PJM

*Garching

# Fundamental Structure of Dissipative Dynamics: Metriplectic Dynamics

- Metriplectic Systems:

$$\frac{\partial \mathcal{Y}}{\partial t} = \mathcal{J}\,\frac{\delta H}{\delta \mathcal{Y}} + \mathcal{G}\,\frac{\delta S}{\delta \mathcal{Y}}$$

Here $\mathcal{G}$ a metric operator, $H =$ energy, and $S =$ entropy. Casimirs are candidate entropies.

- Encapsulates dynamically the $1^{st}$ and $2^{nd}$ laws of thermodynamics:

$$\frac{dH}{dt} = 0 \qquad \text{and} \qquad \frac{dS}{dt} \geq 0$$

# Metriplectic Dynamics

Dissipative generalisation of Hamiltonian dynamics[1,2]

$$\frac{d\mathcal{Y}}{dt} = \{\mathcal{Y}, \mathcal{H}\} + (\mathcal{Y}, \mathcal{S}) \quad \forall \mathcal{Y} = \mathcal{Y}(u), \qquad (u = u(t) \text{ state variable}, \quad u_0 = u(0))$$

where $\{\ \}$=Poisson bracket, $(\ )$=Metric bracket, $\mathcal{H}$=Hamiltonian, $\mathcal{S}$=Entropy, s.t.

$$\{\mathcal{Y}, \mathcal{S}\} = 0, \quad (\mathcal{S}, \mathcal{S}) \leq 0, \quad (\mathcal{Y}, \mathcal{H}) = 0 \qquad \forall \mathcal{Y}$$

**Relaxation:**

$$\frac{d}{dt}\mathcal{H} = 0, \qquad \frac{d}{dt}\mathcal{S} = (\mathcal{S}, \mathcal{S}) \leq 0$$

**Variational principle:**

$$u_\star = \arg\min_u \{\mathcal{S}(u) : \mathcal{H}(u) = \mathcal{H}(u_0)\}$$

[1] Morrison P J 1984, *Phys. Lett. A*, **100**, 423-7
[2] Morrison P J 1986, *Physica D*, **18**, 410-9

# Application to Variational Problems

**Variational Problem:**

$$u_\star = \arg\min_u \{\mathcal{S}(u) : \mathcal{H}(u) = \mathcal{H}(u_0)\}$$

**Problem**: Find a metric bracket ( ) s.t. the solution $u = u(t)$, with $u(0) = u_0$, satisfies

$$u(t) \to u_\star \quad \text{for } t \to \infty$$

**Challenges**:

- This requires $(\mathcal{S}, \mathcal{S}) = 0 \iff \frac{\delta \mathcal{S}}{\delta u} = \lambda \frac{\delta \mathcal{H}}{\delta u}$.
- The null space of the metric operator has to be "properly tuned

**Proposed solution:** Generalisation of Landau collision operator

- General form amounts to an integrodifferential operator
- Local (simplified) version is also available which leads to partial differential equations
- Tested in 2D[3]

[3] Bressan C et al 2018, *J. Phys. Conf. Ser.*, **1125** 012002

# Application to Beltrami Fields (Force-free MHD Equilibria)

**Linear Beltrami fields**: $B:\Omega\to\mathbb{R}^3$, $\lambda\in\mathbb{R}$, such that

$$\nabla\times B=\lambda B,\quad \nabla\cdot B=0,\quad \text{in}\quad \Omega$$

**Variational formulation:**[4]

$$\mathcal{S}(B)=\frac{1}{2}\int_\Omega |B|^2\,dx,\quad \mathcal{H}(B)=\frac{1}{2}\int_\Omega A\cdot B dx,\quad \begin{cases}\nabla\times A=B\,\text{in}\quad \Omega\\ A\times n=0\ \text{on}\quad \partial\Omega\end{cases}$$

$$\frac{\delta S}{\delta B}=\lambda\frac{\delta H}{\delta B}\iff B=\lambda A\Rightarrow \nabla\times B=\lambda B$$

**Remark**: If $\mathcal{H}(B)=0$, then $B=0$ is a (trivial) solution.

**Aim**: Find a metric bracket that relaxes an initial condition to a solution of the original variational principle.

[4]Woltjer, 1958, *Proc. National Academy of Sciences*, **44**, 6

# Local Collision-like Bracket for Beltrami Fields

The simplest version of the local metric collision-like bracket gives

$$\begin{cases} \partial_t B + \nabla \times E = 0, \text{ in } \Omega \\ E = -B \times (B \times \nabla \times B), \text{ in } \Omega \\ B \cdot n = 0, \quad E \times n = 0, \text{ on } \partial\Omega \end{cases}$$

which is equivalent to the Lie-dragging of B by an effective velocity field $V$:

$$\partial_t B - \nabla \times (V \times B) = 0, \quad V = (\nabla \times B) \times B$$

$\Rightarrow$ the “field-line topology” is preserved

$\Rightarrow V = 0,\ B \neq 0 \iff \nabla \times B \propto B$

This is the method of Chodura-Schlüter[5]specialised to Beltrami fields and is recovered as a special case of the collision-like metric brackets.

**Remark:** if the numerical scheme breaks the constraint on the conservation of the magnetic helicity, the solution is trivial (i.e. $B = 0$)

[5] Chodura, Schlüter, *J. Comp. Phys.*, **41**, 68-88

## Structure-preserving Discretization I

- **Finite Element Exterior Calculus** for incompressible ideal MHD [6]

(implemented in FEniCS[7])

$$
\begin{array}{ccccccc}
H_0^1(\Omega) & \xrightarrow{\text{grad}} & H_0(\text{curl},\Omega) & \xrightarrow{\text{curl}} & H_0(\text{div},\Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \\
\downarrow & & \downarrow & & \downarrow & & \downarrow \\
V_h^0 & \xrightarrow{\text{grad}} & V_h^1 & \xrightarrow{\text{curl}} & V_h^2 & \xrightarrow{\text{div}} & V_h^3 .
\end{array}
$$

$$
\begin{aligned}
E_h^{n+1/2} &\simeq E_h(t_n + \Delta t/2) \;\in\; V_h^1 \\
J_h^{n+1/2} &\simeq J_h(t_n + \Delta t/2) \;\in\; V_h^1 \\
H_h^{n+1/2} &\simeq H_h(t_n + \Delta t/2) \;\in\; V_h^1 \\
B_h^{n} &\simeq B_h(t_n) \;\in\; V_h^2
\end{aligned}
$$

[6] Hu et. al., 2021, *J. Comp. Phys.*, **436**

[7] Alnaes M S et. al., 2015, *Archive of Numerical Software*, **3**

# Structure-preserving Discretization II

- Crank-Nicolson discretisation in time

$$
\begin{aligned}
(\partial_t^h B_h^n, C_h) + (\nabla \times H_h^{n+1/2}, C_h) &= 0 \quad \forall\, C_h \in V_h^2 \\
(H_h^{n+1/2}, G_h) - (B_h^{n+1/2}, G_h) &= 0 \quad \forall G_h \in V_h^1 \\
(J_h^{n+1/2}, K_h) - (B_h^{n+1/2}, \nabla \times K_h) &= 0 \quad \forall K_h \in V_h^1 \\
(E_h^{n+1/2}, F_h) - (H_h^{n+1/2} \times J_h^{n+1/2}, H_h^{n+1/2} \times F_h) &= 0 \quad \forall F_h \in V_h^1
\end{aligned}
$$

with notation $\partial_t^h B_h^n = \frac{1}{\Delta t}(B_h^{n+1} - B_h^n), \quad B_h^{n+1/2} = \frac{1}{2}(B_h^{n+1} + B_h^n)$

- Picard iterations with block back-substitution reduce the problem to a symmetric positive-definite linear system which can be solved efficiently with a matrix-free iterative solver.

# Properties of the scheme

The numerical scheme satisfies:

1. The magnetic field is divergence-free

$$\nabla \cdot B_h^n = 0 \quad \forall n \geq 0 \qquad \text{if} \quad \nabla \cdot B_h^0 = 0$$

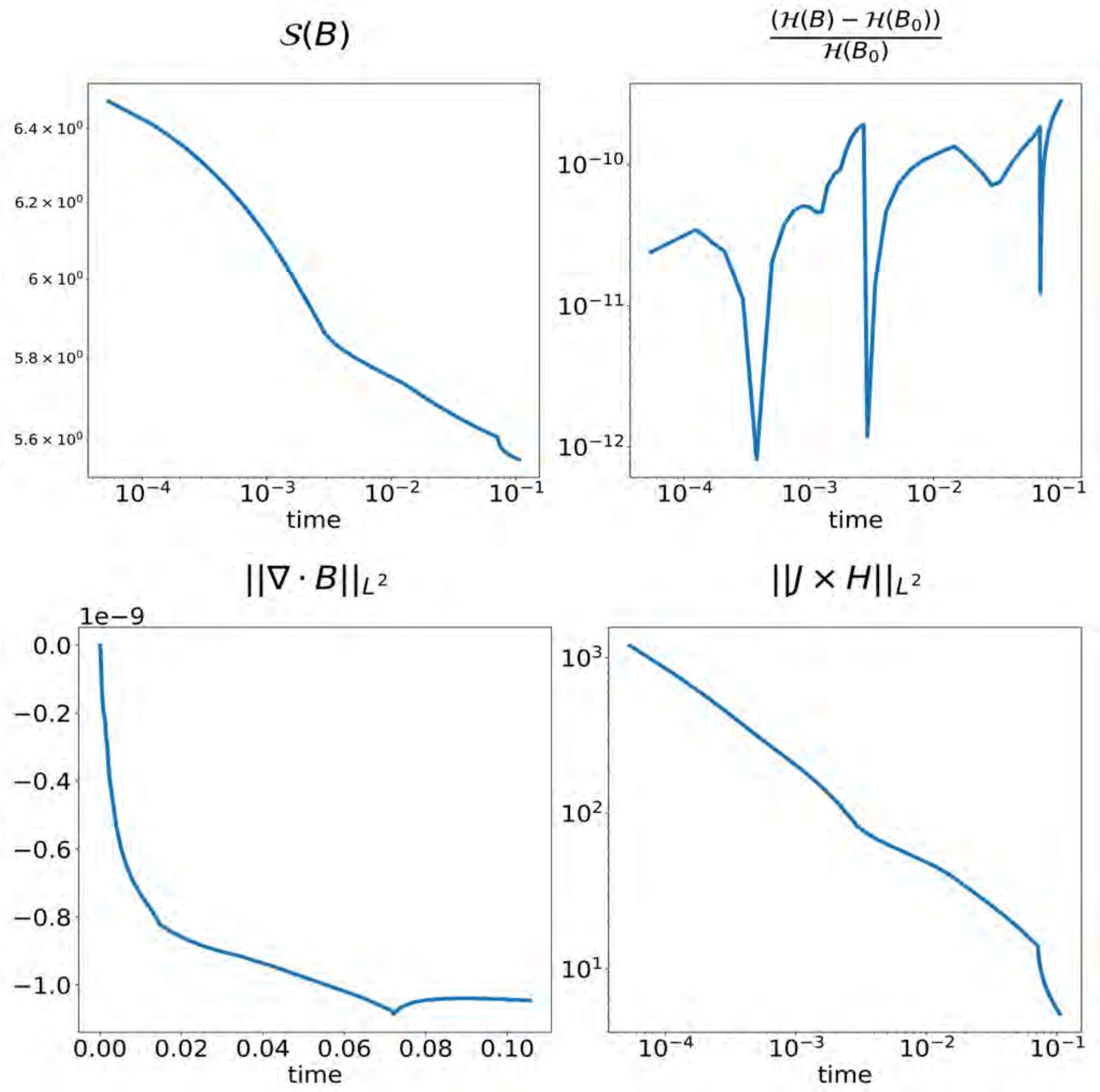
2. The chosen entropy functional is dissipated

$$\mathcal{S}(B_h^{n+1}) = \mathcal{S}(B_h^n) - \Delta t ||H_n^{n+1/2} \times J_h^{n+1/2}||^2, \quad \text{and thus} \quad \mathcal{S}(B_h^{n+1}) \leq \mathcal{S}(B_h^n)$$

3. The chosen Hamiltonian functions is preserved

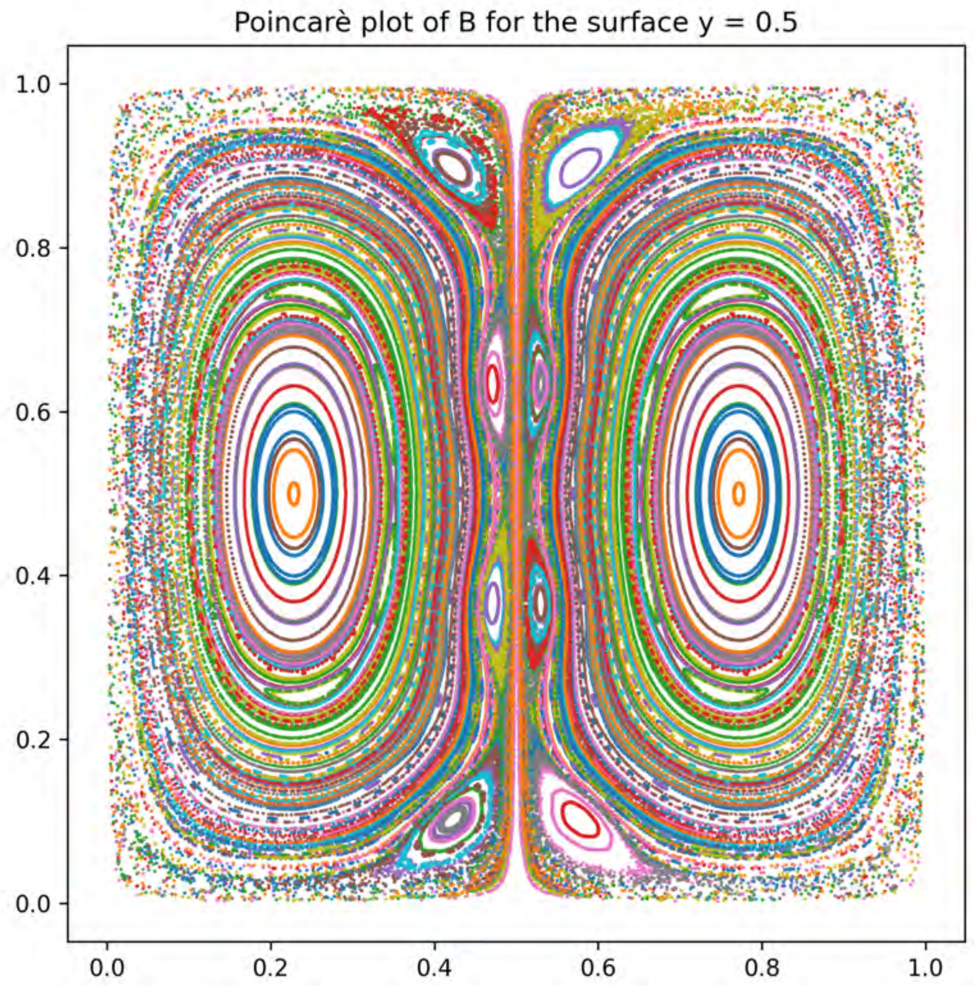
$$\mathcal{H}(B_h^{n+1}) = \mathcal{H}(B_h^0) \quad \forall \quad n \geq 0$$

# Properties of the Scheme



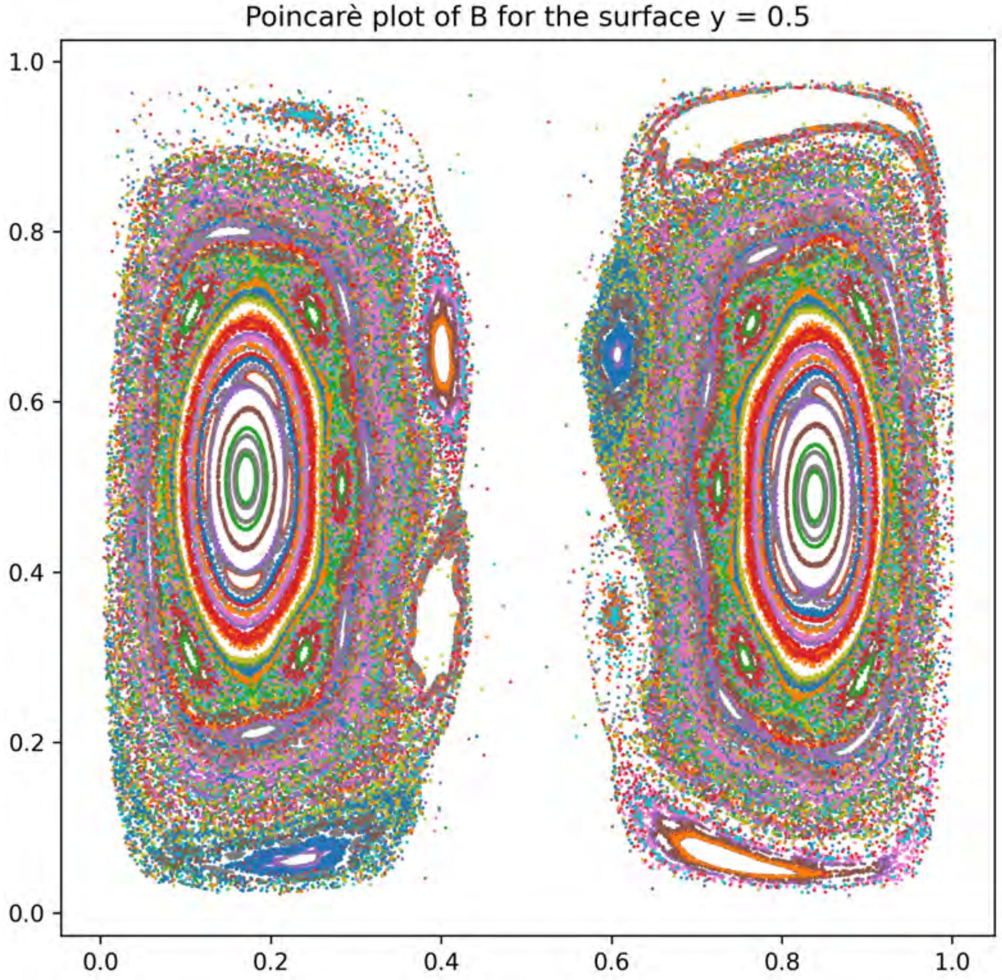

| | |
|---|---|
| **N** | 32 |
| **nt** | 25000 |
| **dt** | $10^{-8} - 10^{-6}$ |
| $t_f$ | 0.1 |

# Poincarè plot of the analytical condition

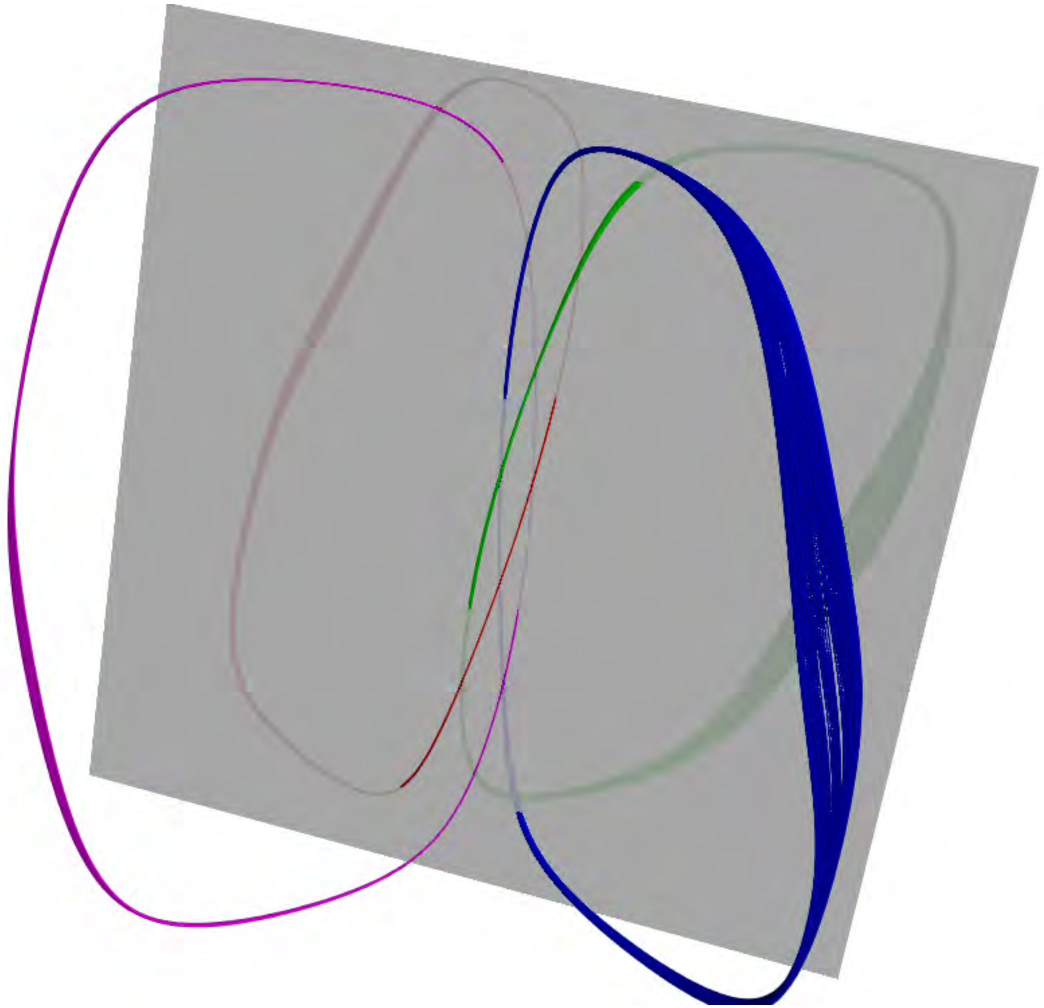


# Time evolution of the Poincarè plot

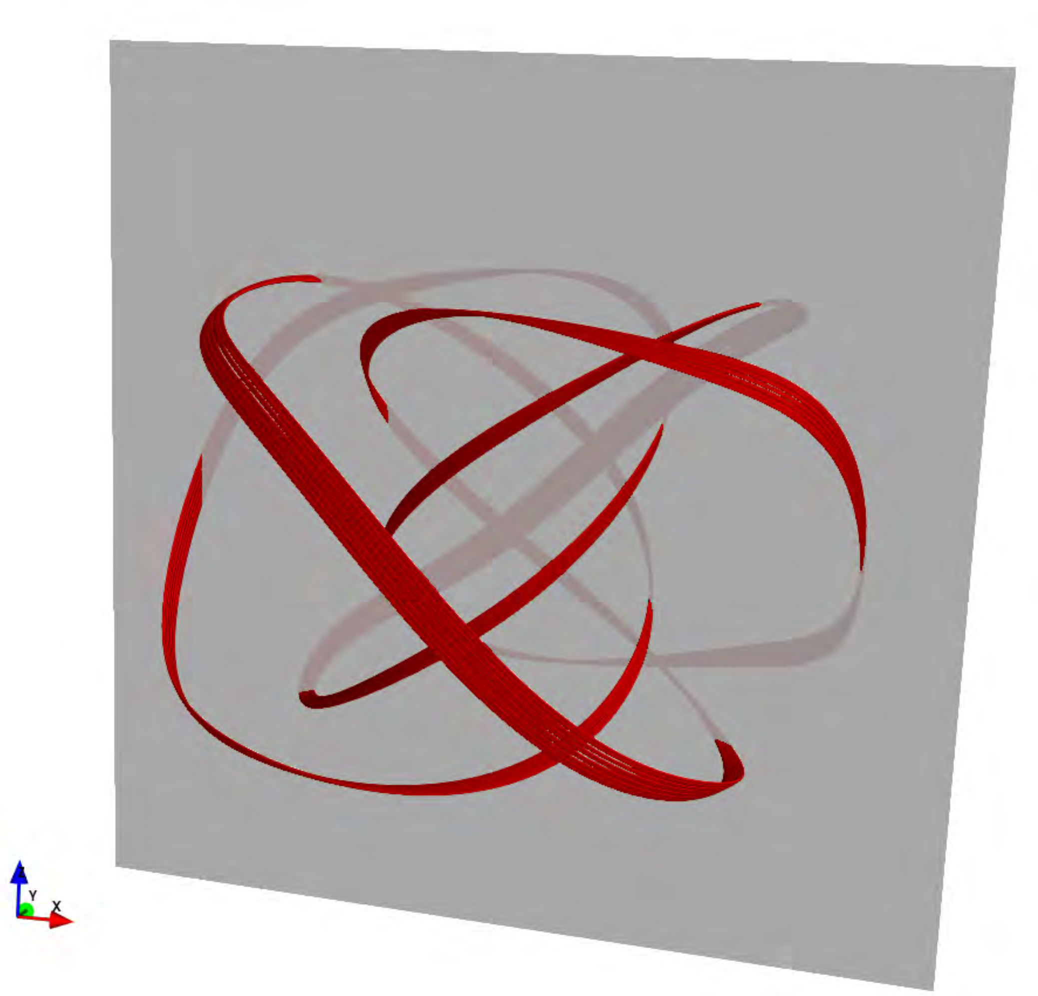
## Final state (t=0.1)



# Central Period-2



# Green Period-10

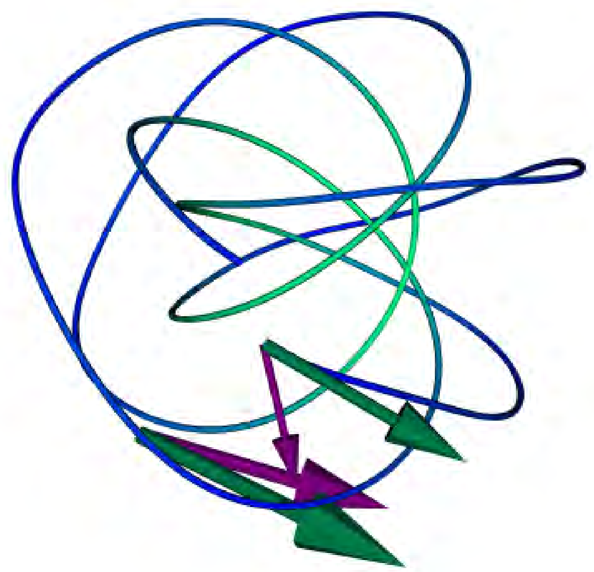


# Relaxation to a Beltrami Field

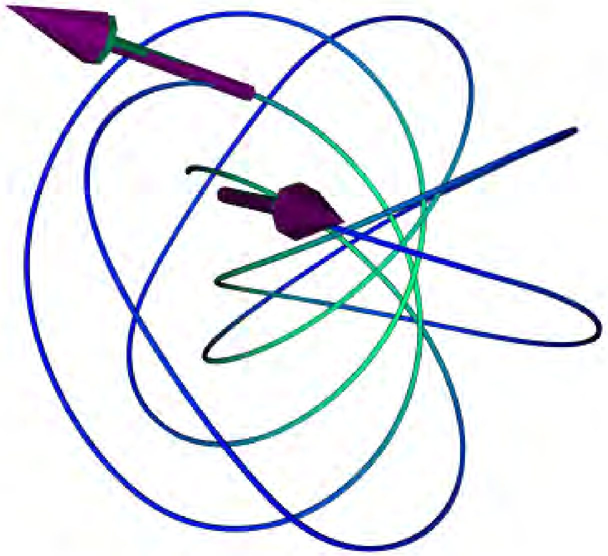
**Evaluation of the fields H (green) and J (violet) along a selected streamline**

• the angle between the vectors $H$ and $J$, projected on a $H^1$-conforming space and evaluated on a selected streamline, decreases

**t=1.5e-08**



**t=7.16e-02**



# Outlook

- A metric bracket, if suitably constructed, yields a relaxation method to compute solutions to variational problems.
- We propose a generalization of the Landau collision operator which yields a class of metric bracket with "good" relaxation dynamics.
- The method of Chodura-Schlüter for linear Beltrami fields is obtained as a special case of such a construction.
- Structure-preserving discretization is crucial to obtain non-trivial solutions (i.e. $B \neq 0$).
- The Double Brackets[8] represent an alternative approach; they dissipate $\mathcal{H}$ while preserving all the Casimirs of the system.

[8] Chikasue Y and Furukawa M 2015, *Phys. Plasmas*, **22**

END

## Collision-like metric bracket

- The Landau operator for Coulomb collisions can be written as a metric bracket.
- its generalisation leads to a collision-like metric bracket s.t., for $u : \Omega \to \mathbb{R}^n$,

$$(\mathcal{A}, \mathcal{B}) = -\int\int L_i\Big(\frac{\delta \mathcal{A}}{\delta u}\Big) \cdot T_{ij} L_j\Big(\frac{\delta \mathcal{B}}{\delta u}\Big) dx dx'$$

$$L(h) = \nabla h(x) - \nabla h(x'), \quad h\colon \Omega \mapsto \mathbb{R}^n, \quad (\nabla h)_{ij} = \frac{\partial h_j}{\partial x_i} \quad T_{ij}(x, x') = T_{ji}(x', x)$$

The kernel of the metric bracket is defined as:

$$T_{ij}(x, x') \propto |g(x, x')|^2 \mathbb{I} - g(x, x') \otimes g(x, x'), \qquad g = L\Big(\frac{\delta \mathcal{H}}{\delta u}\Big)$$

such that $\mathcal{H}$ is conserved and $\mathcal{S}$ is dissipated.

- No general rigorous proof of relaxation. Beneficial properties were observed in numerical experiments [9]
- To reduce the computational cost of an integro-differential operator a local version was developed.

[9] Bressan C et al 2018, *J. Phys. Conf. Ser.*, **1125** 012002

# The local metric collision operator

The suggested metric operator is integro-differential ⇒ Implemented for 2D fluid theories, in 3D is **computationally prohibitive**

Local class of brackets ⇒ **diffusion-like operators**:

$$(\mathcal{A}, \mathcal{B}) = -\int \left(\nabla \frac{\delta \mathcal{A}}{\delta u}\right) \cdot D_{ij} \left(\nabla \frac{\delta \mathcal{B}}{\delta u}\right) dx$$

$$D(x) = |g(x)|^2 \mathbb{I} - g(x) \otimes g(x), \qquad g(x) = \nabla \left(\frac{\delta \mathcal{H}}{\delta u}\right)$$

**Remarks**:

- conservation of $\mathcal{H}$ and dissipation of $\mathcal{S}$ proven as in the integral case