Equilibrium States via Simulated Annealing*

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Goal: Describe two versions 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.

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* 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:

\[
\frac{\partial Y}{\partial t} = J \frac{\delta H}{\delta Y} = \{Y, H\}
\]

\(Y\) state variables. e.g. for MHD \(u = \{v, B, \rho, p\}\)

- The Poisson operator \(J \Rightarrow\) Poisson bracket \(\{F, G\}\) satisfies

  * antisymmetry \(\{F, G\} = -\{G, F\}\) and Jacobi \(\{\{F, G\}, H\} + \text{cyc} = 0\)

  * degeneracy of \(J\) explains and allows discovery of mysterious Casimir invariants

\[J \frac{\delta C}{\delta Y} = 0\]

  e.g. for MHD \(\int A \cdot B\) & \(\int v \cdot B\)
Double Bracket Dynamics Uses $\mathcal{J}^2$

- Fake Dynamics:

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

* 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

\[ \min H \text{ at constant } C \]

* Choice of $C \rightarrow$ different equilibria.
Double Bracket Simulated Annealing for RMHD

M. Furukawa* and PJM

*Tottori University
Simulated Annealing (SA) is a method for obtaining stationary states (equilibria) of Hamiltonian systems as energy extrema.


- 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.
Ideal, low-beta reduced MHD in cylindrical geometry

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

- Cylindrical coordinate system \((r, \theta, z)\), as well as \( \zeta := \frac{z}{R_0} \) is used.

- Ideal, low-beta reduced MHD (normalized) is written as

\[
\begin{align*}
\frac{\partial U}{\partial t} &= [U, \varphi] + [\psi, J] - \varepsilon \frac{\partial J}{\partial \zeta} \\
\frac{\partial \psi}{\partial t} &= [\psi, \varphi] - \varepsilon \frac{\partial \varphi}{\partial \zeta}
\end{align*}
\]

where

\[
\begin{align*}
v &= \hat{z} \times \nabla \varphi & \text{: fluid velocity} \\
B &= \hat{z} + \nabla \psi \times \hat{z} & \text{: magnetic field} \\
U &= \Delta_{\perp} \varphi & \text{: vorticity (z component)} \\
J &= \Delta_{\perp} \psi & \text{: current density (\(-z\) component)}
\end{align*}
\]

\( \varepsilon := \frac{a}{R_0} \)

Normalization

- \( a \) : length
- \( B_0 \) : typical magnetic field
- \( \rho_0 \) : typical mass density
- \( v_A := \frac{B_0}{\sqrt{\mu_0 \rho_0}} \) : velocity
- \( \tau_A := \frac{a}{v_A} \) : time

Normalization

\( \Delta_{\perp} \) : Laplacian in \( r - \theta \) plane

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

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

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

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

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

\[
\tilde{\varphi}(x) := \int_D d^3x' K_{1j}(x, x') f^j(x')
\]

\[
\tilde{J}(x) := \int_D d^3x' K_{2j}(x, x') f^j(x')
\]

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

\[ U(x, 0) = U_{-2/1}(r) \sin(-2\theta + \zeta) \]
\[ \psi(x, 0) = \psi_{0/0}(r) + \psi_{-2/1}(r) \cos(-2\theta + \zeta) \]

- 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 \( n = 1 \) (\( \Delta' \approx 22.4 \))
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

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

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

with \( r_s = \frac{1}{2} \), \( L = \frac{1}{10} \), \( \tilde{\varphi}_{-2/1} = 10^{-3} \), \( \tilde{J}_{-2/1} = 10^{-3} \)
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 equilibria
Metriplectic Simulated Annealing for Beltrami

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

*Garching
Fundamental Structure of Dissipative Dynamics: 
Metriplectic Dynamics

- Metriplectic Systems:

\[
\frac{\partial Y}{\partial t} = J \frac{\delta H}{\delta Y} + G \frac{\delta S}{\delta Y}
\]

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

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

\[
\frac{dH}{dt} = 0 \quad \text{and} \quad \frac{dS}{dt} \geq 0
\]
Dissipative generalisation of Hamiltonian dynamics\textsuperscript{1,2}

\[
\frac{dY}{dt} = \{Y, H\} + (Y, S) \quad \forall Y = Y(u), \quad (u = u(t) \text{ state variable, } u_0 = u(0))
\]

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

\[
\{Y, S\} = 0, \quad (S, S) \leq 0, \quad (Y, H) = 0 \quad \forall Y
\]

**Relaxation:**

\[
\frac{d}{dt}H = 0, \quad \frac{d}{dt}S = (S, S) \leq 0
\]

**Variational principle:**

\[
u_* = \arg\min_u \{S(u) : H(u) = H(u_0)\}
\]
Application to Variational Problems

Variational Problem:

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

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

\[ u(t) \to u_\star \text{ for } t \to \infty \]

**Challenges:**

- This requires \((S, S) = 0 \iff \frac{\delta S}{\delta u} = \lambda \frac{\delta H}{\delta u}.\)
- 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\(^3\)

\[^3\text{Bressan C et al 2018, J. Phys. Conf. Ser., 1125 012002}\]
Application to Beltrami Fields (Force-free MHD Equilibria)

Linear Beltrami fields: \( B : \Omega \rightarrow \mathbb{R}^3, \lambda \in \mathbb{R}, \) such that
\[
\nabla \times B = \lambda B, \quad \nabla \cdot B = 0, \quad \text{in } \Omega
\]

Variational formulation:\(^4\)
\[
S(B) = \frac{1}{2} \int_{\Omega} |B|^2 \, dx, \quad \mathcal{H}(B) = \frac{1}{2} \int_{\Omega} A \cdot B \, dx, \quad \begin{cases} 
\nabla \times A = B \text{ in } \Omega \\
A \times n = 0 \text{ on } \partial \Omega 
\end{cases}
\]
\[
\frac{\delta S}{\delta B} = \lambda \frac{\delta \mathcal{H}}{\delta B} \iff B = \lambda A \Rightarrow \nabla \times B = \lambda B
\]

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.

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Local Collision-like Bracket for Beltrami Fields

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

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

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\textsuperscript{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. $B = 0$)

\textsuperscript{5}Chodura, Schlüter, *J. Comp. Phys.*, 41, 68-88
Numerical example

Structure-preserving Discretization I

- **Finite Element Exterior Calculus** for incompressible ideal MHD \(^6\)
  
  (implemented in FEniCS\(^7\))

\[
egin{align*}
H_0^1(\Omega) & \xrightarrow{\text{grad}} H_0(\text{curl}, \Omega) & \xrightarrow{\text{curl}} H_0(\text{div}, \Omega) & \xrightarrow{\text{div}} L^2(\Omega) \\
V_h^n & \xrightarrow{\text{grad}} V_h^1 & \xrightarrow{\text{curl}} V_h^2 & \xrightarrow{\text{div}} V_h^3.
\end{align*}
\]

\[
\begin{align*}
E_{h}^{n+1/2} & \simeq E_{h}(t_n + \Delta t/2) \in V_h^1 \\
J_{h}^{n+1/2} & \simeq J_{h}(t_n + \Delta t/2) \in V_h^1 \\
H_{h}^{n+1/2} & \simeq H_{h}(t_n + \Delta t/2) \in V_h^1 \\
B_{h}^{n} & \simeq B_{h}(t_n) \in V_h^2.
\end{align*}
\]

\(^6\)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

\[
(\partial^h_t B^n_h, C_h) + (\nabla \times H_{h}^{n+1/2}, C_h) = 0 \quad \forall \ C_h \in V_2^h
\]
\[
(H_{h}^{n+1/2}, G_h) - (B_{h}^{n+1/2}, G_h) = 0 \quad \forall \ G_h \in V_1^h
\]
\[
(J_{h}^{n+1/2}, K_h) - (B_{h}^{n+1/2}, \nabla \times K_h) = 0 \quad \forall \ K_h \in V_1^h
\]
\[
(E_{h}^{n+1/2}, F_h) - (H_{h}^{n+1/2} \times J_{h}^{n+1/2}, H_{h}^{n+1/2} \times F_h) = 0 \quad \forall \ F_h \in V_1^h
\]

with notation
\[
\partial^h_t B^n_h = \frac{1}{\Delta_t}(B_{h}^{n+1} - B_{h}^{n}), \quad B_{h}^{n+1/2} = \frac{1}{2}(B_{h}^{n+1} + B_{h}^{n})
\]

• 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
   \[ \nabla \cdot B_h^n = 0 \quad \forall n \geq 0 \quad \text{if} \quad \nabla \cdot B_h^0 = 0 \]

2. The chosen entropy functional is dissipated
   \[ S(B_h^{n+1}) = S(B_h^n) - \Delta t \| H_h^{n+1/2} \times J_h^{n+1/2} \|^2, \quad \text{and thus} \quad S(B_h^{n+1}) \leq S(B_h^n) \]

3. The chosen Hamiltonian functions is preserved
   \[ H(B_h^{n+1}) = H(B_h^n) \quad \forall \quad n \geq 0 \]
Numerical Results

Properties of the Scheme

\[ N = 32 \]
\[ nt = 25000 \]
\[ dt = 10^{-8} - 10^{-6} \]
\[ t_f = 0.1 \]
Poincarè plot of the analytical condition
Numerical Results

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

$t=1.5e-08$  \hspace{1cm}  t=7.16e-02
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 represent an alternative approach; they dissipate $\mathcal{H}$ while preserving all the Casimirs of the system.

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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 \( u : \Omega \to \mathbb{R}^n \),

\[
(A, B) = - \int \int L_i \left( \frac{\delta A}{\delta u} \right) \cdot T_{ij} L_j \left( \frac{\delta B}{\delta u} \right) dx dx'
\]

\[
L(h) = \nabla h(x) - \nabla h(x'), \quad h : \Omega \mapsto \mathbb{R}^n, \quad (\nabla h)_{ij} = \frac{\partial h_{ij}}{\partial x_i} \quad T_{ij}(x, x') = T_{ji}(x', x)
\]

The kernel of the metric bracket is defined as:

\[
T_{ij}(x, x') \propto |g(x, x')|^2 \mathbb{I} - g(x, x') \otimes g(x, x'), \quad g = L \left( \frac{\delta \mathcal{H}}{\delta u} \right)
\]

such that \( \mathcal{H} \) is conserved and \( S \) 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.

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:

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

\[D(x) = |g(x)|^2 I - g(x) \otimes g(x), \quad g(x) = \nabla \left( \frac{\delta H}{\delta u} \right)\]

Remarks:
- conservation of \( H \) and dissipation of \( S \) proven as in the integral case