A New Method for Computing the Magnetic Configuration of Toroidal Fusion Devices

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What is fusion?

Figure: ITER, Saint-Paul-lès-Durance, France

- ITER is one of the world largest and most expensive science experiments.
- Started in 2013, complete in 2027. Estimated cost > 20 billion Euro.

Why confinement?

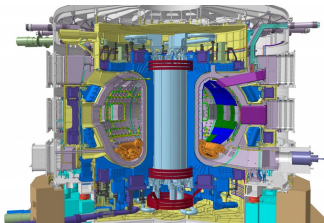Figure: A cutaway of the ITER Tokamak

- To extract energy from benign particle movements (analogy of Archimedes' Burning Mirror; don't want a hydrogen bomb), particles are tightly controlled under strong magnetic fields.

What about layers?

Figure: delicious Crêpe

- Design particle paths to be clustered and moving like fluid and in layers (flux surfaces are Laminar flows). In fact, want maximal layers.
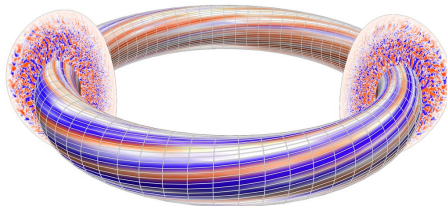
What are the layers?

Figure: stabilizing MHD instabilities in an axisymmetric toroid

$$\nabla p = J \times B \rightarrow B \cdot \nabla p = 0$$

- Particles are stick to (helically moving along) the flux surfaces. Layers are the pressure profiles (aka temperature profiles).

Confinement surfaces

- The ideal balanced force equation from previous slide is wrong. For a multi-particle system, it can be out of balance and still in quasi-static Magnetohydrodynamics (MHD) due to diffusion.

- Figuring out temperature profiles and confinement surfaces are two separated tasks. The discrepancy of the two provides insights of transport properties, such as relaxation time and diffusion length.

- The goal of this project is to produce images of magnetic confinement surfaces for given *B* fields, and from there to determine if the confinement is closed and if it forms layers.

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The challenges

- Unlike pressure profiles, magnetic confinement surfaces are not directly measured.
- Traditionally people take measurements of B and use field line tracing method:

$$\begin{cases} x'(t) = B_x(t) \\ y'(t) = B_y(t) \\ z'(t) = B_z(t) \end{cases} \implies \begin{cases} x'(z) = B_x/B_z \\ y'(z) = B_y/B_z \end{cases}$$

- For every t, use Runge-Kutta, solve it as initial value problem, so in literature, $z := \phi$ is often called the "time" coordinate.

The field line tracing algorithm

- Pick a cross section $z_0 = \phi_0$ and a point (x_0, y_0) on the cross section as the starting point. Choose a $n \in \mathbb{N}$, let $\Delta z = 2\pi/n$.
- After n forward steps, it will be back on that cross section. Record the point, and continue iterations.
- After many iterations, some shape will form on the cross section. It is called the Poincaré plot.
- On the next slide there is a Poincaré plot, with 3 different starting points on the same cross section. It used $n = 40$, and made 500 turns around the torus.
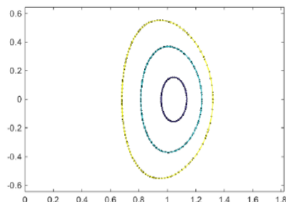
Figure: Poincaré plot

- The *B* field used in the plot was one of the known stable solutions to MHD equilibrium, with $d_{1,2}$ being parameters of the torus.

$$B_x = 8d_1 \rho y$$
$$B_y = \rho^2/2 + 2d_2 + 4d_1(\rho^2 - 2z^2)$$
$$B_z = 0.01/\rho$$

Why is the new method better?

- ode45 has a global 4th order accuracy, but it assumes that B is continuous and to be known everywhere on the tracing line. Otherwise a spline (3rd order polynomial interpolation) is required. In reality don't have an analytic B, and measurements are done on the grids points.
- In comparison, the new method doesn't need interpolations, and it achieves a global 3rd order accuracy, and similar run-time to field line tracing with interpolations.
- More importantly, unlike field tracing method is controlled by the initial value (stable if B is not turbulent), the new method takes all grid points into account.
- It utilizes the physics of confinement surfaces and allow information to propagate from one layer to the neighboring layers.

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Mathematical Formulation of the problem

Theorem

If the flux surface of a B field inside of a torus is closed and a B field is not zero everywhere, then there is a ψ such that $B \cdot \nabla \psi = 0$ and the contour of ψ is the flux surface of B.

Proof.

In 2D, it is clearly true. In 3D, not so fast, because in 3D two vectors that are both perpendicular to a third vector are not necessary coincide to each other. Luckily the underlying structures are two surfaces. Assume flux of *B* is closed and combine with the fact that magnetic lines have no crossings, the two surfaces have to agree. □

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Mathematical Formulation of the problem

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Overview

Corollary

If there is no such ψ can be found though the algorithm, then the confinement surface of B is not closed.

This is the first showcase of how strong the interconnection is between the algorithm and the underlying physical system. The rest of the talk will continue to explore those ideas:

- Show the stability of the algorithm (CFL) relates to the underlying physical MHD stability;
- Show the up winding scheme in the algorithm has a conservative flow, which correlates to the physical *B* field.

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Lax-Friedrichs

Let's demonstrate why Lax-Friedrichs was chosen.
Consider the three Hamiltonian equations,

$$H(q, p) = E(t) = p^2/2m + V(q)$$
$$\frac{dq}{dt} = \frac{\partial H}{\partial p}$$
$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

In the first equation q, p are treated as if they were
independent. The next two equations add in their relations.
Separating variables is the key success to Hamilton mechanics.

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Lax-Friedrichs Deviation

For simplicity, let's start from 1D, $H(q, p) = E$, want to solve for $q(t)$. Treating $q, p = q_t$ as independent, first order Taylor to linearize H,

$$
\begin{aligned}
H\left(q, \frac{q_t^+ + q_t^-}{2}\right) &= H(q, q_t^+) - \left(\frac{\partial H}{\partial q_t}\right)_{q_t = q_t^+} \frac{q_t^+ - q_t^-}{2} \\
&= H(q, q_t^-) + \left(\frac{\partial H}{\partial q_t}\right)_{q_t = q_t^-} \frac{q_t^+ - q_t^-}{2}
\end{aligned}
$$

where $q_t^{\pm}$ are the right/left derivatives, thus in term of mesh grids, q_i means at the ith grid,

$$
\frac{q_t^+ - q_t^-}{2} = \frac{q_{i+1} - 2q_i + q_{i-1}}{2\Delta t}
$$

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Lax-Friedrichs Assumption: going with the flow

Define viscosity,

$$\sigma = \frac{\partial H}{\partial q_t}$$

The reason why it is called will become apparent soon. Thus

$$q_i = \frac{\Delta t}{\sigma}(H(q, q_t^+) - H(q, \frac{q_{i+1} - q_{i-1}}{2\Delta t})) + \frac{q_{i+1} + q_{i-1}}{2}$$
$$= \frac{\Delta t}{-\sigma}(H(q, q_t^-) - H(q, \frac{q_{i+1} - q_{i-1}}{2\Delta t})) + \frac{q_{i+1} + q_{i-1}}{2}$$

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Lax-Friedrichs Assumption: going with the flow and its algorithm

Here is the meat of Lax-Friedrichs: How to precede iterations. If $\sigma > 0$, use the 1st equation, replace $H(q, q_t^+)$ by E. Elif $\sigma < 0$, use the 2nd equation, replace $H(q, q_t^-)$ by E. Symbolically

$$q_i \leftarrow \frac{\Delta t}{|\sigma|} \left(E - H(q_i, \frac{q_{i+1} - q_{i-1}}{2\Delta t}) \right) + \frac{q_{i+1} + q_{i-1}}{2}$$

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Lax-Friedrichs algorithm explanation

- The replacement of $H(q, q_t^{\pm})$ by E means that in the early stage of iterations, if $q_i, q_{i\pm 1}$ were used to compute $H(q, q_t^{\pm})$, they wouldn't give E. In other words, early q didn't satisfy the equation of motion.

- The choice of choosing $H(q, q_t^{\pm})$ depends on the sign of σ made by LF was a delicate one. As it will be shown, it follows the direction of the flow of the hyperbolic system (in connection to conservation law).

- The convergence of LF requires as iterations go on,

$$H\left(q_i, \frac{q_{i+1} - q_{i-1}}{2\Delta t}\right) \to E$$

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Lax-Friedrichs stability

Write the iteration in matrix form, and greatly simplify things (otherwise numerical analysis of stability can never work $\ddot\smile$), drop q dependence of H, and assume $H \approx \sigma q_t, E = 0$

$$q^{(n+1)} = A q^{(n)}$$

where

$$
A = \begin{bmatrix}
\ddots & & & & & \\
\ddots & & \ddots & & & \\
& \frac{|\sigma| - \sigma}{2|\sigma|} & & \frac{|\sigma| + \sigma}{2|\sigma|} & & \\
& & \ddots & & \ddots & \\
& & & & \ddots &
\end{bmatrix}
$$

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Tailor to the problem

The matrix A from previous slide showed how the data propagated. It either copied its left or right element, depending on the sign of q_t; q^{n+1}.

Tailor to the problem, $H = B \cdot \nabla \psi = 0$, with the corresponding substitutions $q = \psi, \sigma = B, q_t = \nabla \psi, E = 0$,

$$\psi^{(n+1)}(x_i, y_j) = \begin{cases} \dfrac{\frac{|B_x|}{\Delta x} \psi^{(n)}(x_{i-1}, y_j) + \frac{|B_y|}{\Delta y} \psi^{(n)}(x_i, y_{j-1})}{\frac{|B_x(x_i, y_j)|}{\Delta x} + \frac{|B_y(x_i, y_j)|}{\Delta y}} & B_x > 0, B_y > 0 \\[3ex] \dfrac{\frac{|B_x|}{\Delta x} \psi^{(n)}(x_{i+1}, y_j) + \frac{|B_y|}{\Delta y} \psi^{(n)}(x_i, y_{j-1})}{\frac{|B_x(x_i, y_j)|}{\Delta x} + \frac{|B_y(x_i, y_j)|}{\Delta y}} & B_x < 0, B_y > 0 \\[3ex] \dfrac{\frac{|B_x|}{\Delta x} \psi^{(n)}(x_{i-1}, y_j) + \frac{|B_y|}{\Delta y} \psi^{(n)}(x_i, y_{j+1})}{\frac{|B_x(x_i, y_j)|}{\Delta x} + \frac{|B_y(x_i, y_j)|}{\Delta y}} & B_x > 0, B_y < 0 \\[3ex] \dfrac{\frac{|B_x|}{\Delta x} \psi^{(n)}(x_{i+1}, y_j) + \frac{|B_y|}{\Delta y} \psi^{(n)}(x_i, y_{j+1})}{\frac{|B_x(x_i, y_j)|}{\Delta x} + \frac{|B_y(x_i, y_j)|}{\Delta y}} & B_x < 0, B_y < 0 \end{cases}$$

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Error to LF

- To test accuracy and convergence, need a definition of error. Recall

$$q_i \leftarrow \underbrace{\frac{\Delta t}{|\sigma|}\left(E - H(q_i, \frac{q_{i+1} - q_{i-1}}{2\Delta t})\right)}_{\text{convergence error}} + \frac{q_{i+1} + q_{i-1}}{2}$$

- The linearized LF converges to a linear function: $q_i = a \cdot i + b$. This shows the first part can be consider as the error, and the viscosity $|\sigma|$ is the speed of convergence.

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Error to the problem

The error after n iterations in 2D is

$$error^{(n)}(x_i, y_j) = \frac{\left| B_x \frac{\psi(x_{i+1}, y_j) - \psi(x_{i-1}, y_j)}{2\Delta x} + B_y \frac{\psi(x_i, y_{j+1}) - \psi(x_i, y_{j-1})}{2\Delta y} \right|}{\frac{|B_x|}{\Delta x} + \frac{|B_y|}{\Delta y}}$$

which is proportional to $B \cdot \nabla^c \psi$, using the central difference, thus it's proportional to the angle between B and $\nabla^c \psi$. Thus define the error on the domain to be

$$error^{(n)} = \frac{1}{D} \iint_D \frac{B \cdot \nabla^c \psi}{\|B\| \|\nabla^c \psi\|}$$

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Stability & CFL

- Previously for 1D, the stability matrix A is just 0/1 off-diagonal.

$$A = \begin{bmatrix} 0 & \ddots & & \ddots & & & & & & & & & \\ \ddots & 0 & \ddots & & & \ddots & & & & & & & \\ & \ddots & 0 & \ddots & & & \ddots & & & & & & \\ & & \ddots & 0 & \ddots & & & \ddots & & & & & \\ \ddots & & & \ddots & 0 & \ddots & & & \ddots & & & & \\ & & & & \ddots & 0 & & & & & & & \\ \frac{|B_y|-B_x}{2\Delta y} & & \frac{|B_y|-B_y}{2\Delta y} & 0 & \frac{|B_y|+B_y}{2\Delta y} & & \frac{|B_x|+B_x}{2\Delta y} & & & & & \\ \frac{|B_x|}{\Delta x}+\frac{|B_y|}{\Delta y} & & \frac{|B_x|}{\Delta x}+\frac{|B_y|}{\Delta y} & & \frac{|B_x|}{\Delta x}+\frac{|B_y|}{\Delta y} & & \frac{|B_x|}{\Delta x}+\frac{|B_y|}{\Delta y} & & & & & \\ & & & & & & 0 & \ddots & & & & \\ & & & & & \ddots & & \ddots & 0 & \ddots & & & \ddots \\ & & & & & & \ddots & & \ddots & 0 & \ddots & & \\ & & & & & & & & \ddots & & 0 & \ddots & \\ & & & & & & & & & \ddots & & 0 & \ddots \\ & & & & & & & & & & \ddots & & 0 \end{bmatrix}$$

- Above is A in 2D. Restricting its eigenvalue (CFL) < 1 implies $|B_x|/\Delta x, |B_y|/\Delta y$ should be on the same order.

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Conservation & Hyperbolicity

- Recall the connection between hyperbolic system and conservation laws. Generally speaking Lax-Friedrichs works well for hyperbolic equations.

- The physical understand of this connection is that there is a general flow in the system that is conversed. In the problem, the B field serves as the general flow and it is conversed.

- Because hyperbolic equation has two branches, one is bounded below and the other bounded above, the closed magnetic confinement surface guarantees that the contour of Hamiltonian is well structured, i.e. it has a min or max; the data flow conservation guarantees that updating formula will follow the path that goes to the min or max.

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Boundary Value & Initial Value problem

- General LF algorithm will require:
  1. Fix the boundary during iterations. Typically choose constant values. That is because the constant function is a solution to the linearized Hamiltonian.
  Does't mean it will get a constant answer? Yes, but it takes infinite number of steps. Before it gets to that, it will return a reasonable solution. Since only interested in the contour of ψ, the exact scale doesn't matter.
  This also suggest that since information flows from the boundary to inside, pick

  number of iterations $\approx \sqrt{3} \cdot$ number of cubic grids

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Boundary Value & Initial Value problem

- General LF algorithm will require:
  2. After fix the constant boundary, say K, then typically choose a constant, say M, for the interior points as initial values.
  If $K > 0$, set $M > B$. If $K < 0$, set $M < B$. During the iterations, only update in increasing or deceasing order, i.e. for $K > 0$

$$\psi^{(n+1)} = min\{\psi^{(n)}, \textit{whatever LF computes}\}$$

  Change to *max* for $K < 0$. That is to force the hyperbolic to converge to its min/max, depending on the branches.

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Existence & Uniqueness

- As it was shown in the corollary, if LF returns no sensible solutions, it means
  1. either there is no closed magnetic confinement surfaces,
  2. or the LF algorithm hasn't converge yet due to lack of iterations,
  3. or unable to converge due to instability with violation of CFL.

- What about uniqueness? Although both ψ and ψ^2 are satisfied, soon as the boundary was chosen to be a constant, only that constant will be the solution.

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What about the new method?

- The new method requires nothings:
  1. Not fix the boundary during iterations.
  2. Nor does it force the updating to go monotone.
- It instead:
  picks random values as initial values (we call them dopings) and update to whatever LF computes.
- Why?
  1. Each layer of closed confinement surfaces is separated and shielded. Acting like a boundary, what's inside remains inside; what is outside remains outside, because B field has no crosing.
  2. The data flow direction is already conservative, the path is on the convergence path. Don't need additional convergence imposition.

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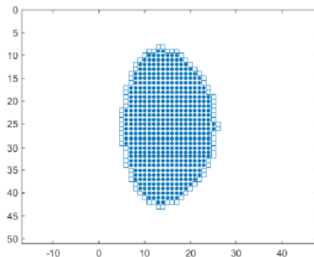The New Modified Lax-Friedrichs
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Experimental results
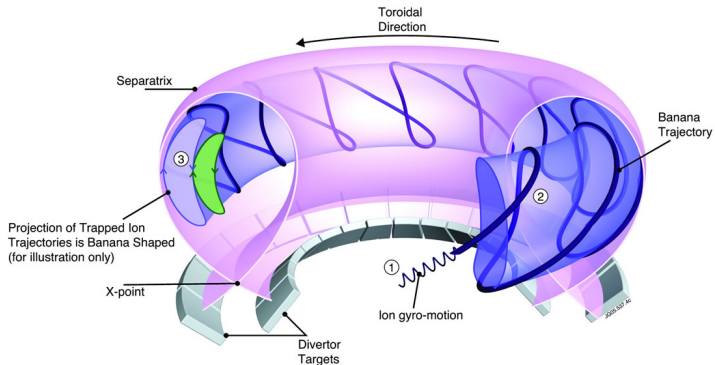
Figure: From Doughnuts to Banana Orbits

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Experimental results

Discretization: The square dots are the boundary. There are only about $20 \times 20 = 400$ points in the domain and it is impressive to learn that this is enough to get good results.

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Experimental results

Both graphs used traditional LF. One started with positive initial values; the other started with negative values.
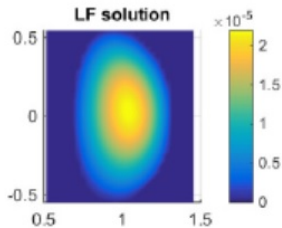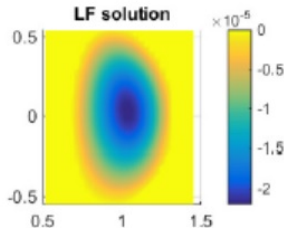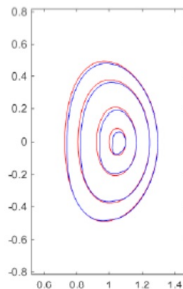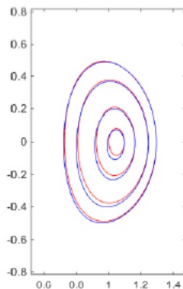

$M > 0$ $M < 0$

Figure: 2D surface plots

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Experimental results

Red lines are exact solutions; blue lines are LF solutions. Left graph used traditional LF & right graph used the new modified LF.

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Experimentally test the hypotheses

Hypotheses:

1. The underlying flow of the system is the *B* field.

2. That the flow is conservative provides super convergence so that is no need for imposing the monotonic convergence requirement as for the traditional LF.

3. That the flux surface is closed provides a build-in boundary so that there is no need for fixed boundary.

4. An violation of CFL will return no sensible solutions. Such instability is linked to the physical instability of MHD.

Having those properties turn out to be critical for the 3D islands example, where contours are no longer monotonically nested.

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Experimentally test the hypotheses

Test hypothesis 1.

Take the example where B fields are approximately concentric circles. Don't use the matrix, use loops for the LF updating formula, i.e. let it sweep like a wedding cake. Then flip $B \rightarrow -B$. Observed indeed while sweeping in the direction of B, got better convergence and required less iterations.

Figure: spiral like a wedding cake

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Experimentally test the hypotheses

Test hypothesis 2.
Change the Hamiltonian to

$$\frac{B \cdot \nabla \psi}{\|\nabla \psi\|} = 0$$

so that $\sigma \neq B$, then computed the new updating rules and found the new rule would depend on all 4 neighboring points, thus the elegant data propagation direction didn't exist. Found the spiral on wedding cake method were no longer effective, and increasing iterations would no longer always decreased errors.

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Experimentally test the hypotheses

Test hypothesis 3.

This was easy. Cut the domain in half and kept the upper half so that there would be no closed flux surfaces, then observed no convergence at all. Next tested a non-smooth boundary domain which had a X-divertor (e.g. separatrix of magnetic islands), and it handled very well.
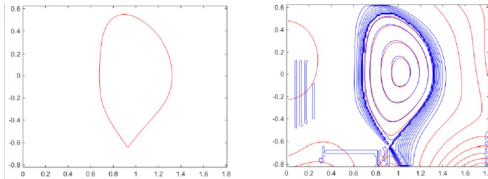
Left graph shows the boundary. On the right, red lines are exact solutions, blue are LF solutions.

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Experimentally test the hypotheses

Test hypothesis 4.

Recall CFL condition says the order of $B_x/\Delta x$, $B_y/\Delta y$ and $B_z/\Delta z$ should be the same, so that the eigenvalues of the matrix A is at minimal.

Suppose same B, but B_z is amplified

$$B_x = 8d_1\rho y$$
$$B_y = \rho^2/2 + 2d_2 + 4d_1(\rho^2 - 2z^2)$$
$$B_z = 0.01/\rho \rightarrow B_z = 1/\rho$$

Traditional field line tracing will return the same plot. For it, this change means rotation in azimuthal direction 100 times faster; but for the LF, the result is chaos, which is also unstable for the physical MHD system.

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Is high order necessary?

Is the higher the better?

- Recall from the X-divertor example, the simple central difference didn't capture the sharp turn very well, which motivates to use high order method.

- However recall from testing hypothesis 2, when H depended on all 4 neighbors, i.e. lost its elegant conservation flow, convergence would be in jeopardy. High order will depend on more than 4 neighbors. It turns out that it is still reasonably but not strictly convergent, i.e. tails can grow.

- As will be shown, a hybrid method, that combines 1st order and high order LF, works the best.

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The New Modified LF
The Hybrid LF

High order LF

A well-known method for high order derivatives is the high order ENO and WENO schemes. For sake of speed, ENO was used. It replaces left/right derivatives by the following. E.g. to compute $d^+q(t)$. First compute $d^2q_i := (q_{i+1} - 2q_i + q_{i-1})/(\Delta t)^2$, and d^2q_{i+1}, which are by themselves high order. If $|d^2q_i| \gg |d^2q_{i+1}|$, then

$$d^+q_i \leftarrow \frac{-q_{i+2} + 4q_{i+1} - 3q_i}{2\Delta t}$$

There is another replacement for case $|d^2q_i| \ll |d^2q_{i+1}|$ and a third replacement formula for the rest. They all look like high order runge kutta, but they only use values at grid points.

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Use Guang-Shan Jiang, Chi-Wang Shu's paper, "Efficient Implementation of Weighted ENO Schemes". High order derivatives were added to the algorithm and only the diffusion term was modified, because that term was what the solution would converge to

$$\frac{q_{i+1} + q_{i-1}}{2}$$

Replacing each q_{i+1}, q_{i-1} there, and using ENO for $d^{\pm}q_i$,

$$q_{i+1} \leftarrow q_i + d^+ q_i \cdot \Delta t, \quad q_{i-1} \leftarrow q_i - d^- q_i \cdot \Delta t$$

The hybrid LF algorithm spends first half of iterations in the modified 1st order LF, then the second half in the high order LF.

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The hybrid LF results

Use hybrid LF for the X-divertor. Compared to previous results, it improves sufficiently. The average angle error is 0.4046 degrees.

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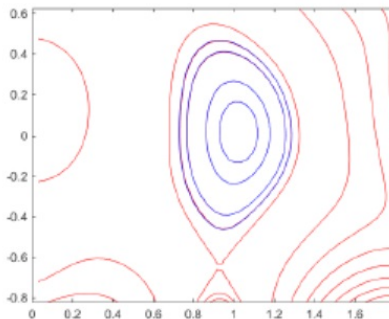
The hybrid LF accuracy test

- For the accuracy test, increased grids points and increased iterations. As mentioned before, high order LF is not strictly convergent, the tail will grow. The table below recorded the number of iterations that gave the minimal errors.

grids	iterations	angle error (deg)	run-time (s)
15×25	50	0.5511	0.1596
29×50	400	0.0402	5.3741
44×75	2000	0.0142	65.7846

- Thus the new method is about 3rd order global accurate. Most of the error happened in the middle of the graph, where B turned sharply and there weren't many grid points to support it.
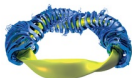
Outline

Summary of Past Work
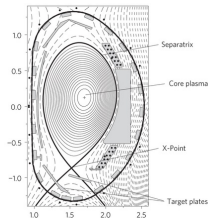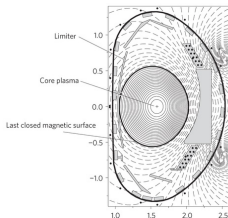
J. Ongena, R. Koch, R. Wolf H. Zohm, *Magnetic-confinement fusion*,
Nature Physics 12, 398â410 (2016) doi:10.1038/nphys3745

- After successfully simulated the limiter and divertor configurations (shown respectively in above pictures), the hybrid LF method is being applied to magnetic islands.

3D Islands
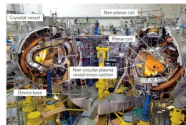
pictures source is the same as the previous slide.

- One example of magnetic islands is created by twisted flux tubes, which are periodic around the azimuthal direction.
- In term of the Toroidal coordinates, the period around the big circle is in commensurate to the period around the small circle. Such flux surfaces are called rational surfaces.
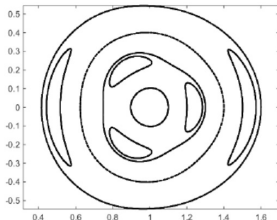- They are the center of turbulence, because as getting closer to their centers, collisions are unavoidable. Laminar flow is destroyed.

3D Islands

Figure: Poincaré Plot, used field line tracing

- The picture shows a 2-paired and a 3-paired islands. The 2-paired (3-paired) island makes $2 \cdot 2\pi$ ($3 \cdot 2\pi$) polar angle to come back to the initial cross section. They are nested layers too, i.e. there are smaller 2-paired or 3-paired islands inside of them.

Hybrid FL applied to 3D Islands

Hybrid FL Algorithm

- Use cylindrical coordinate, and glue $z = 0$ and $z = 2\pi$. They are amount to replace

$$\nabla \rightarrow \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{1}{z}\frac{\partial}{\partial z} \text{ and } z[k] \rightarrow z[(k \bmod (length(z)-1))+1]$$

- Set initial values constant everywhere with some dopings. Those dopings will create hills and valleys. If one were used the traditional LF, i.e. fixing the boundary and use monotonic updates, then he would not be able see hills and valleys.

- Choose Δz wisely. If it is small, there will be too many cross sections, consume time. If it is too big, violate CFL.

Outline

Things to try in the near future

- Recognized that at least a 20×20 grid is required on each cross section for each island, for a single island it takes about 20 minutes to run, thus a complete picture like above of 5 independent islands will take $20 \times 5^3 = 40$ hours, using looping fashion.
- The size of the matrix A is 2000×2000. Using sparse matrix multiplication and parallelism may speed it up.
- Obviously moving from 1st to 3rd order will dramatically increase computations, but it also boosts accuracy, which may mean that we can try to move to 5th order but reduce grid points so that to attain same accuracy with less grid.

Conclusions

- We revitalized conventional LF method so that there is no fixed boundary (by the boundary value problem) nor structured initial values (by the initial value problem), and there is no imposed monotonicity.

- We gave a coherent derivation of Lax-Friedrichs. We recognized its hidden assumptions and its connections to the conservation law. Because of its universal appealing assumption and our added values to it, made it maybe applicable to not only *B* fields, but many other physical models with different flows: streamline flow, Poincaré flow, Ricci flow, renormalization flow...

- The new hybrid LF has maximal connection to the physical systems. (next slide)

Conclusions

1. The conservative data flow structure diagnoses the closeness of confinement surfaces.
2. CFL stability links to the stability of magnetic flux configurations.
3. The number of iterations manifests causality. That is because data flow from one point to another through one iteration. Every point will depend on all its neighbors, unlike field line trace who depends on its one preceding point, so one bad measurement of B will fall everything. Moreover if field line trace hits the Cantor fields (fields contain $B = \infty$ point), it will stop progressing, so points who are far distance from it will suffer too. In contrast, LF will treat $B = \infty$ point as just one of its neighbors and points who are far distance from it won't be affect by it.

ITER is set to give:

In 2027

an <u>infinitely</u> amount of,

<u>clean</u> (with no radiation wastes)

energy

at <u>no-cost</u>

and it lasts <u>forever</u>.