Multiple timescale calculations of sawteeth with M3D-*C*[1]

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PPPL PRINCETON PLASMA PHYSICS LABORATORY

Summary and Overview:

- M3D-C^1 can take very long time steps and can thus span timescales: ideal-MHD, magnetic reconnection, transport

- The implicit solution procedure is complicated by the fact that the multiple timescales present in the physics lead to a very ill-conditioned matrix equation that needs to be solved each time step.
    - Here we describe the techniques we use to deal with this in M3D-C^1

- Code now runs on Hopper: Scales well to > 10^4 processors

- We find two types of behavior at large S
    - High Viscosity: Periodic Sawteeth
    - Low Viscosity: Sawtooth Free Stationary State (SFSS)

- Comparison of SFSS solution with axisymmetric solution

Implicit solution of MHD equations requires evaluating the spatial derivatives at the new time level.

The advantage of an implicit solution is that the time step can be very large and still be numerically stable (no Courant condition)

If we discretize in space (finite difference, finite element, or spectral) and linearize the equations about the present time level, the implicit equations take the form:

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{A}_{13} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \mathbf{A}_{23} \\ \mathbf{A}_{31} & \mathbf{A}_{32} & \mathbf{A}_{33} \end{bmatrix} \bullet \begin{bmatrix} \mathbf{V} \\ \mathbf{B} \\ p \end{bmatrix}^{n+1} = \begin{bmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \mathbf{r}_3 \end{bmatrix}^{n}$$

How best to solve this?

Very large, ~ (10^7 x 10^7)
non-diagonally dominant,
non-symmetric, ill-conditioned sparse matrix (contains all MHD waves)

3 step physics-based preconditioner greatly improves iterative solve

Original matrix multiplying
$\mathbf{V}^{n+1}$, $\mathbf{B}^{n+1}$, p^{n+1}
- non-symmetric,
- non-diagonally dominant &
- large range of eigenvalues

(1) Split implicit formulation

Smaller matrix multiplying $\mathbf{V}^{n+1}$ only,
- nearly symmetric
- closer to diagonal
- still with large range of eigenvalues

(2) Apply annihilation operators

Matrix now consists of 3 dominant diagonal blocks, each with narrower range of eigenvalues.

(3) Apply block-Jacobi preconditioner by using SuperLU_dist on each poloidal plane independently

Now, range of eigenvalues in each block is greatly reduced.

GMRES

Preconditioned system converges in 10's of iterations

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→ [ ] → [[ ] [ ] [ ]] → [[ ] [ ] [ ]] → GMRES

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Preconditioned system converges in 10's of iterations

(1) Split implicit formulation eliminates $\mathbf{B}^{n+1}$ and p^{n+1} in favor of $\mathbf{V}^{n+1}$

As an example, consider the simple 1D wave equation for velocity V and pressure p

$$\left.\begin{aligned}\frac{\partial V}{\partial t} &= c\frac{\partial p}{\partial x}\\ \frac{\partial p}{\partial t} &= c\frac{\partial V}{\partial x}\end{aligned}\right\} \quad \frac{\partial^2 V}{\partial t^2} - c^2\frac{\partial^2 V}{\partial x^2} = 0$$

Implicit FD time advance evaluates spatial derivatives at the new time level

$$\frac{V_j^{n+1} - V_j^n}{\delta t} = c\left(\frac{\boxed{p_{j+1/2}^{n+1}} - p_{j-1/2}^{n+1}}{\delta x}\right)$$

$$\frac{\boxed{p_{j+1/2}^{n+1}} - p_{j+1/2}^{n}}{\delta t} = c\left(\frac{V_{j+1}^{n+1} - V_j^{n+1}}{\delta x}\right)$$

Now, algebraically eliminate new time pressure in favor of velocity

$$V_j^{n+1} = V_j^n + (\delta t c)^2\left(\frac{V_{j+1}^{n+1} - 2V_j^{n+1} + V_{j-1}^{n+1}}{\delta x^2}\right) + \delta t c\left(\frac{p_{j+1/2}^n - p_{j-1/2}^n}{\delta x}\right) \quad \longleftarrow$$

Symmetric & diagonally dominant!

$$p_{j+1/2}^{n+1} = p_{j+1/2}^n + \frac{\delta t c}{\delta x}\left(V_{j+1}^{n+1} - V_j^{n+1}\right)$$

These equations will give exactly the same answers, but can be solved sequentially!

Schematic of difference in matrices to be inverted after applying split implicit formulation

$$
2N \; \begin{bmatrix}
1 & -S & & & & & & & & & & \\
S & 1 & -S & & & & & & & & & \\
 & S & 1 & -S & & & & & & & & \\
 & & S & 1 & -S & & & & & & & \\
 & & & S & 1 & -S & & & & & & \\
 & & & & S & 1 & -S & & & & & \\
 & & & & & S & 1 & -S & & & & \\
 & & & & & & S & 1 & -S & & & \\
 & & & & & & & S & 1 & -S & & \\
 & & & & & & & & S & 1 & -S & \\
 & & & & & & & & & S & 1 & -S \\
 & & & & & & & & & & S & 1
\end{bmatrix}
\;\Longrightarrow\;
N \; \begin{bmatrix}
1+2S^2 & -S^2 & & & & \\
-S^2 & 1+2S^2 & -S^2 & & & \\
 & -S^2 & 1+2S^2 & -S^2 & & \\
 & & -S^2 & 1+2S^2 & -S^2 & \\
 & & & -S^2 & 1+2S^2 & -S^2 \\
 & & & & -S^2 & 1+2S^2
\end{bmatrix}
\quad
N \; \begin{bmatrix}
1 & & & & & \\
 & 1 & & & & \\
 & & 1 & & & \\
 & & & 1 & & \\
 & & & & 1 & \\
 & & & & & 1
\end{bmatrix}
$$

$$S = \frac{c\delta t}{\delta x} \gg 1$$

Coupled system multiplying V^{n+1} & p^{n+1}

Un-coupled system multiplying V^{n+1} & p^{n+1} separately

Substitution takes us from having to invert a 2N x 2N anti-symmetric system that has large off-diagonal elements to sequentially inverting a N x N symmetric system that is diagonally dominant + the identity matrix.

Mathematically equivalent → same answers! (but much better conditioned)

3 step physics-based preconditioner greatly improves iterative solve

(1) Split implicit formulation

(2) Apply annihilation operators

(3) Apply block-Jacobi preconditioner by using SuperLU_dist on each poloidal plane independently

Original matrix multiplying
V^{n+1}, **B**$^{n+1}$, p^{n+1}
- non-symmetric,
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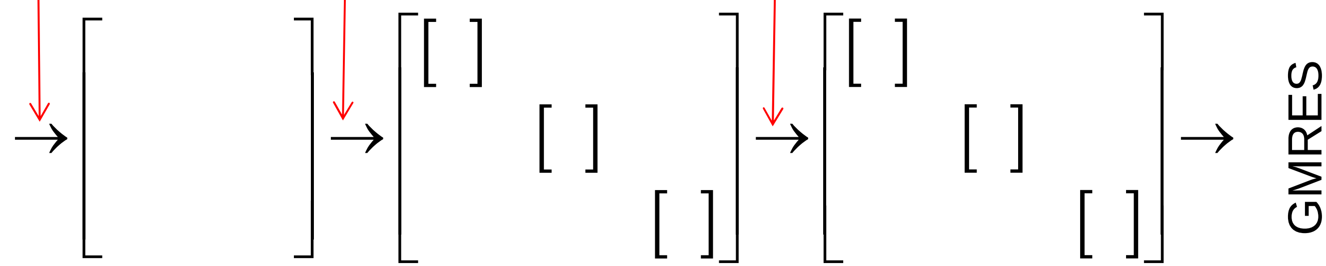
- large range of eigenvalues



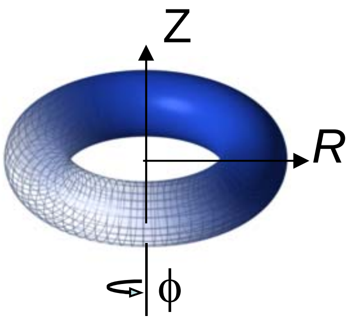
Smaller matrix multiplying **V**$^{n+1}$ only,
- nearly symmetric
- closer to diagonal
- still with large range of eigenvalues

Matrix now consists of 3 dominant diagonal blocks, each with narrower range of eigenvalues.

Now, range of eigenvalues in each block is greatly reduced.

Preconditioned system converges in 10’s of iterations

(2) Apply annihilation operators to separate eigenvalues into diagonal blocks



$$\nabla_\perp \equiv \hat{R}\frac{\partial}{\partial R} + \hat{Z}\frac{\partial}{\partial Z}$$

Velocity vector written in terms of 3 scalar fields:

$$\mathbf{V} = R^2 \nabla U \times \nabla \phi + R^2 \omega \nabla \phi + \frac{1}{R^2}\nabla_\perp \chi$$

Associated mainly with the shear Alfven wave: does not compress the toroidal field

Associated mainly with the slow wave: also does not compress the toroidal field

Associated mainly with the fast wave: does compress the toroidal field

To obtain scalar equations, we apply annihilation projections to isolate the physics associated with the different wave types in different blocks in the matrix

Alfven wave: $\nabla \varphi \bullet \nabla_\perp \times R^2$

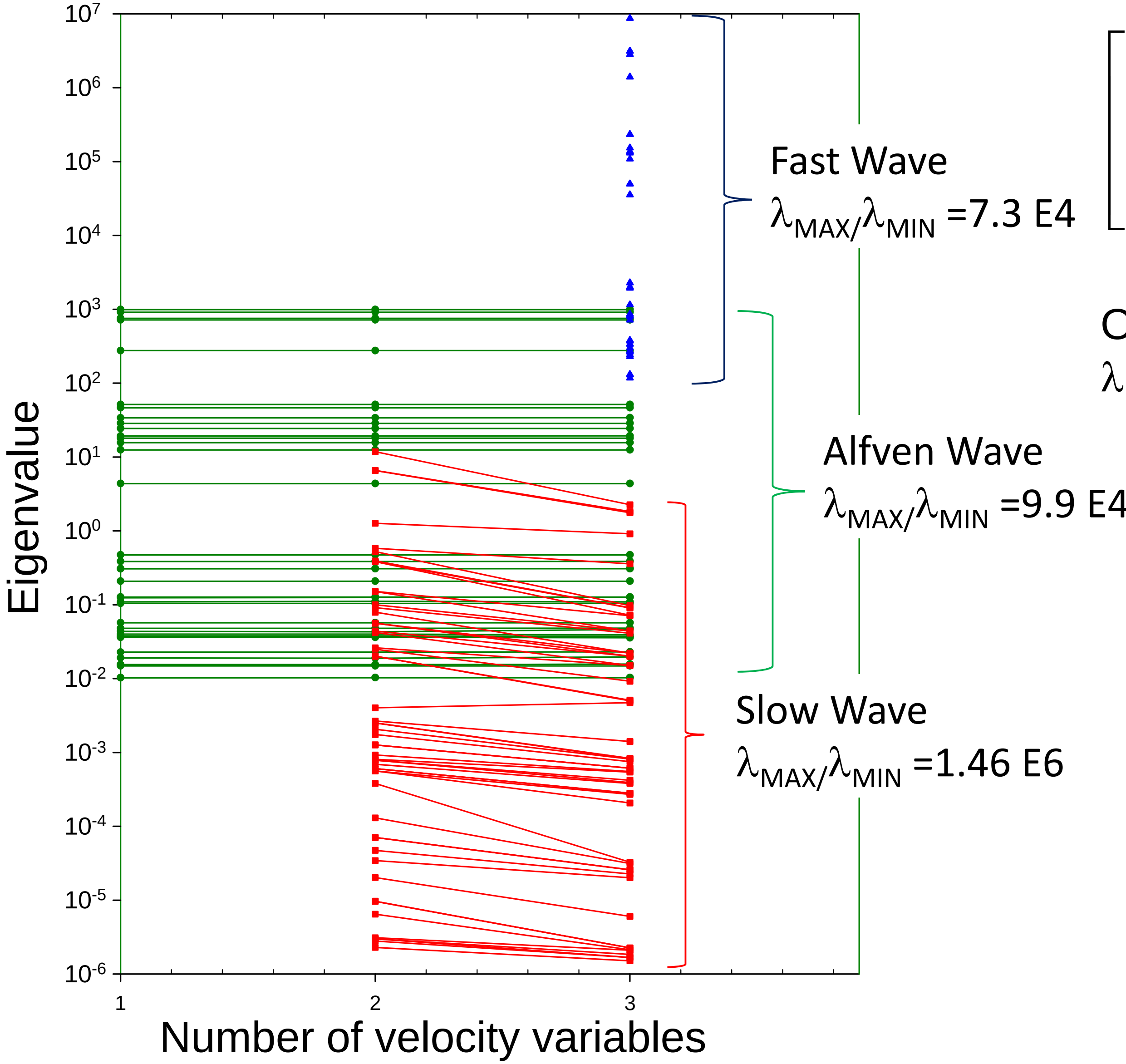
slow wave: $R^2 \nabla \varphi \bullet$

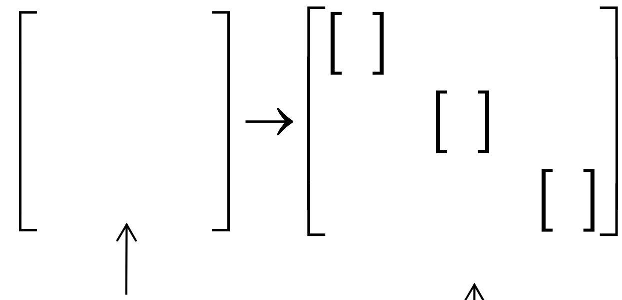
fast wave: $-\nabla_\perp \bullet R^{-2}$

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \bullet \nabla \mathbf{V} = \frac{1}{nM_i}\left[-\nabla p + \mathbf{J} \times \mathbf{B} - \nabla \bullet \mathbf{\Pi}_{GV} - \nabla \bullet \mathbf{\Pi}_\mu\right]$$

Code can be run with 1,2 (reduced MHD) or 3 (full MHD) velocity variables

M3D-C^1 can be run with 1, 2, or 3 velocity variables. Tracking the eigenvalues shows how they separate into 3 groups



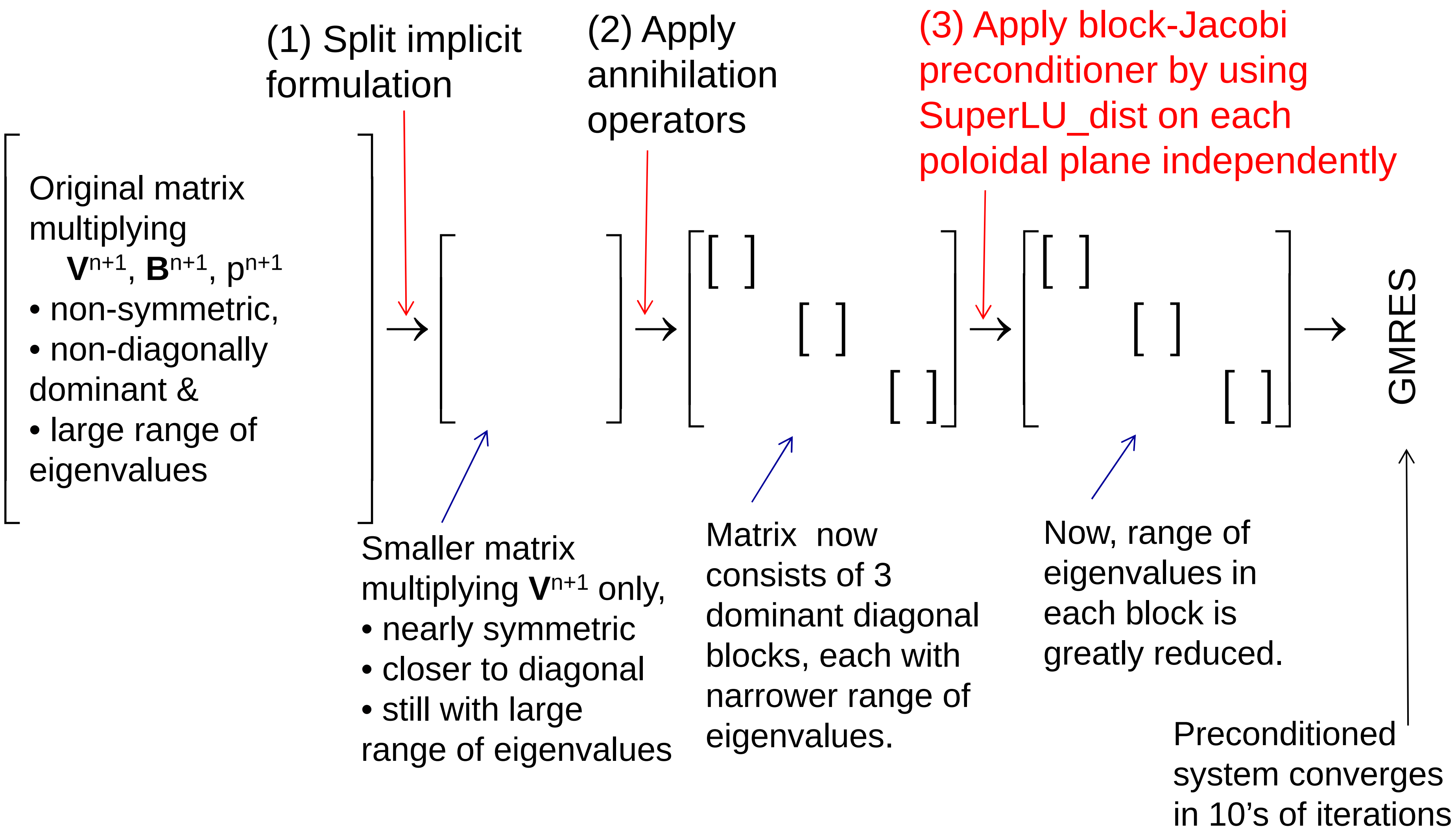


Original matrix:
$\lambda_{MAX}/\lambda_{MIN} = 10^{13}$

Annihilation operators split this into 3 loosely connected matrices, each with a condition number much less than original matrix

U $\quad$ $U+\omega$ $\quad$ $U+\omega+\chi$

3 step physics-based preconditioner greatly improves iterative solve

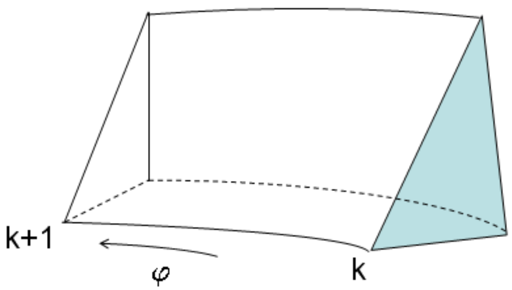


(3) Apply block-Jacobi preconditioner by using SuperLU_dist on each poloidal plane independently

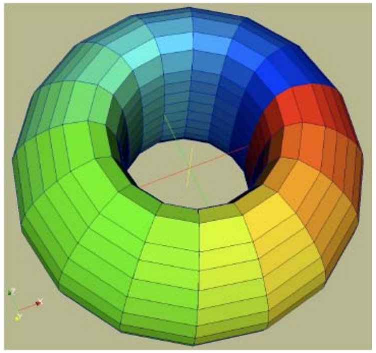
M3D-*C¹* uses a triangular wedge high order finite element

- Continuous 1st derivatives in all directions … *C¹ continuity*
- Unstructured triangles in (R,Z) plane
- Structured in φ

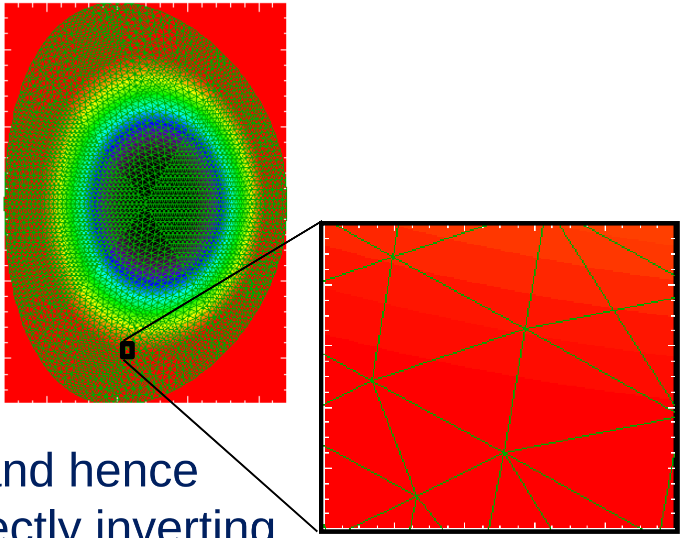
Triangular wedge integration volume



Top view: 16-32 toroidal prisms



Slice view: ~ 10^4 nodes/plane



Because of the small zone size within the plane, and hence strong coupling, we precondition the matrix by directly inverting the components within each poloidal plane simultaneously.

Block Jacobi Preconditioner: reduces condition number by $\left(\frac{\Delta x_{\varphi}}{\Delta x_{R,Z}}\right)^2 \sim 4000$

(3) Apply block-Jacobi preconditioner by using SuperLU_dist on each poloidal plane independently (cont)

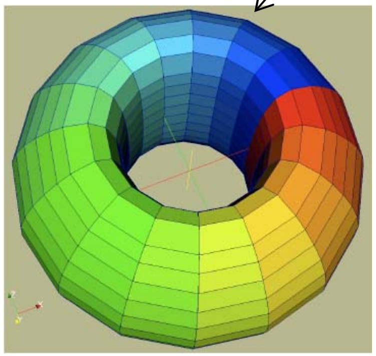
- All the nodes on each poloidal plane are coupled only to their nearest neighbors. This leads to block triangular structure

$$\begin{bmatrix} B_1 & C_1 & & & & & & A_1 \\ \bullet & \bullet & \bullet & & & & & \\ & \bullet & \bullet & \bullet & & & & \\ & & A_j & B_j & C_j & & & \\ & & & \bullet & \bullet & \bullet & & \\ & & & & \bullet & \bullet & \bullet & \\ & & & & & \bullet & \bullet & \bullet \\ C_N & & & & & & A_N & B_N \end{bmatrix} \bullet \begin{bmatrix} V_1 \\ . \\ V_{j-1} \\ V_j \\ V_{j+1} \\ . \\ . \\ V_N \end{bmatrix}^{n+1} = \begin{bmatrix} y_1 \\ . \\ y_{j-1} \\ y_j \\ y_{j+1} \\ . \\ . \\ y_N \end{bmatrix}^{n}$$

A_j, B_j, C_j

are 2D sparse matrices at plane j

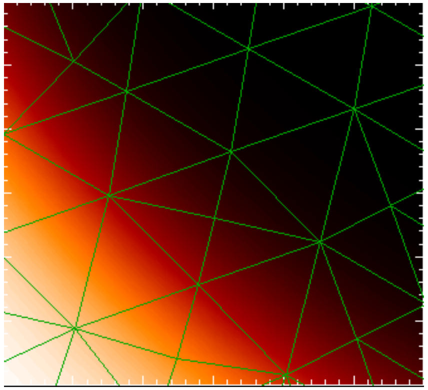
V_j denotes all the velocity variables on plane j



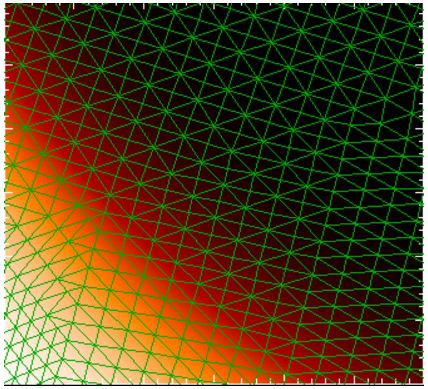
Block Jacobi preconditioner corresponds to multiplying each row by inverse of diagonal block B_j^{-1}

PETSc now has the capability of doing this using SuperLU_Dist concurrently on each plane

Parallel Scaling Studies have been performed from 96 to 12288 p

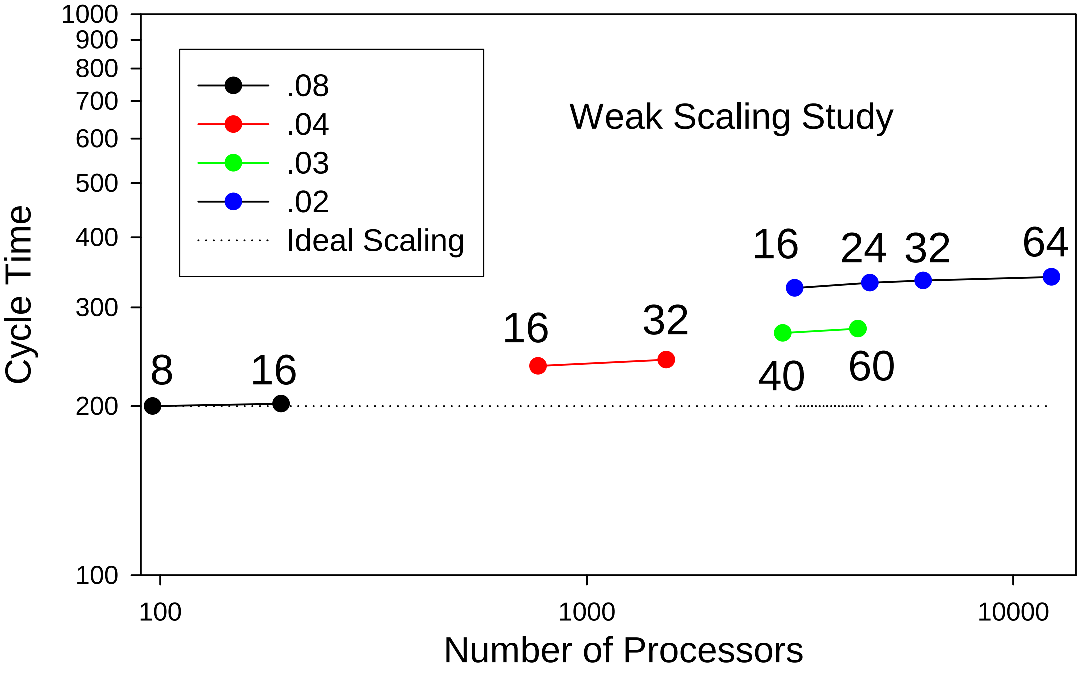


.08



.02

Triangle linear dimension varied by factor of 4



Number of toroidal planes varied from 8 to 64

Transport Timescale simulations in which stability is important: with $\Delta t = 40\ \tau_A$

Resistivity: $\eta = n^{3/2} p^{-3/2}$

Thermal Conductivity: $\kappa_\perp = n^{3/2} p^{-1/2}$

$$\kappa_\parallel = 10^6 \kappa_\perp$$

Viscosity: uniform (~η)

Current controller provides loop voltage to maintain plasma current at initial value.

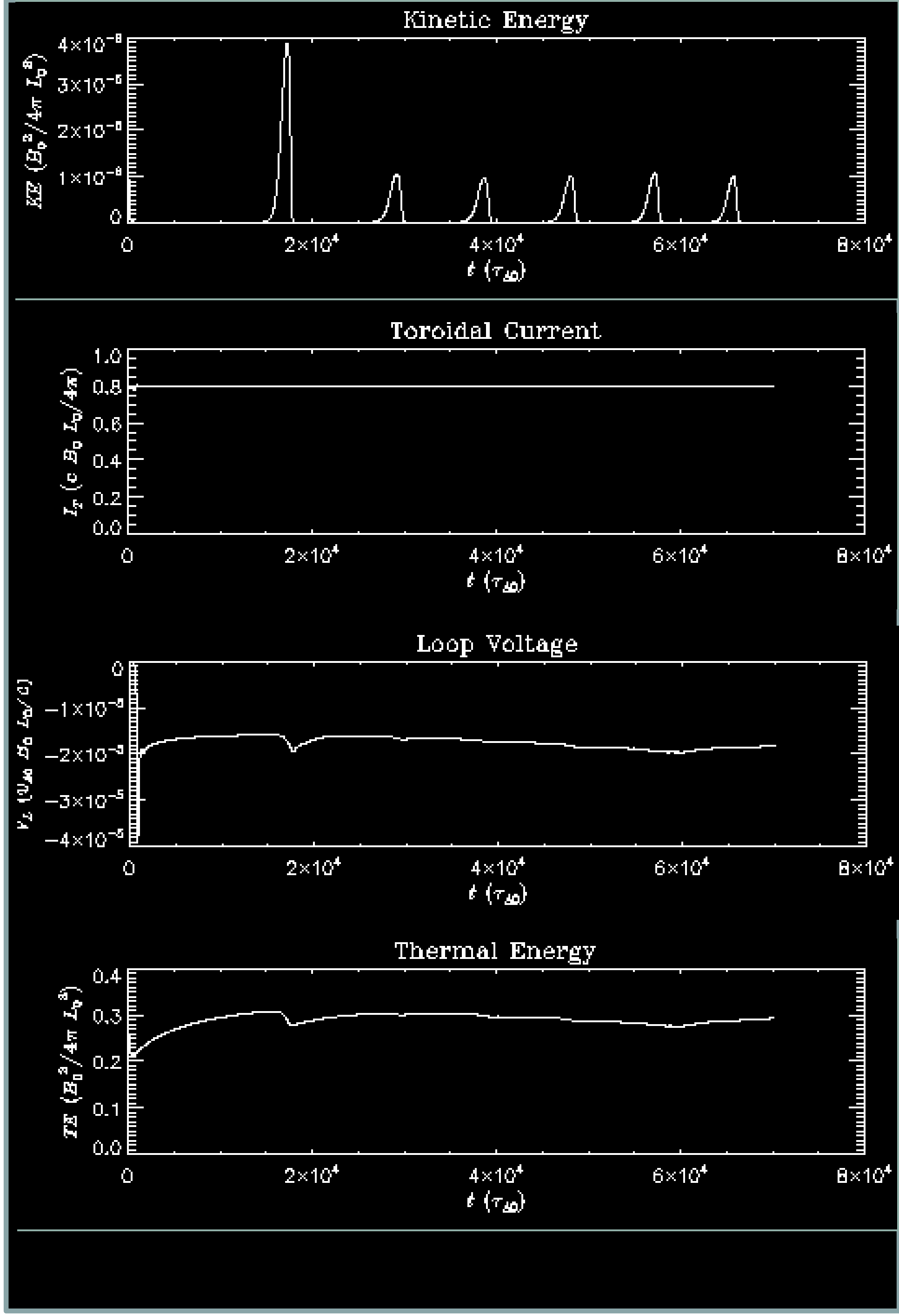
Loop voltage provides thermal energy through Ohmic heating

Two types of behavior seen:

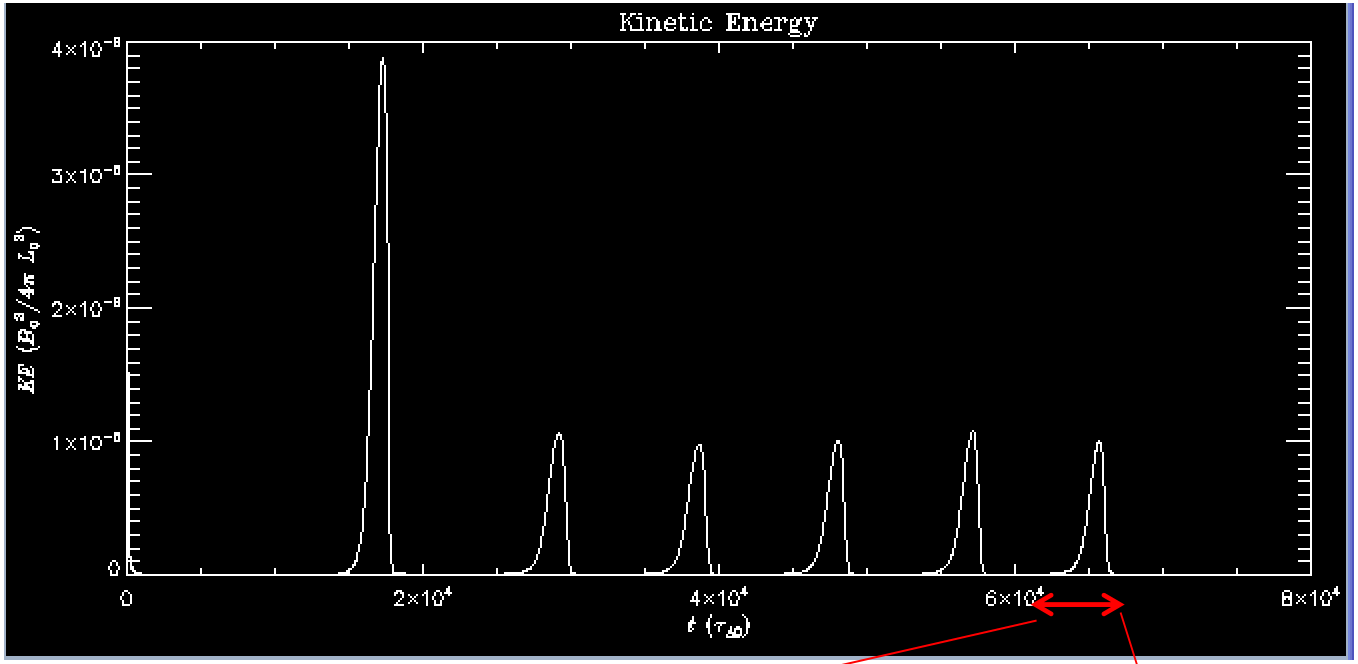
(1) Periodic sawteeth

or

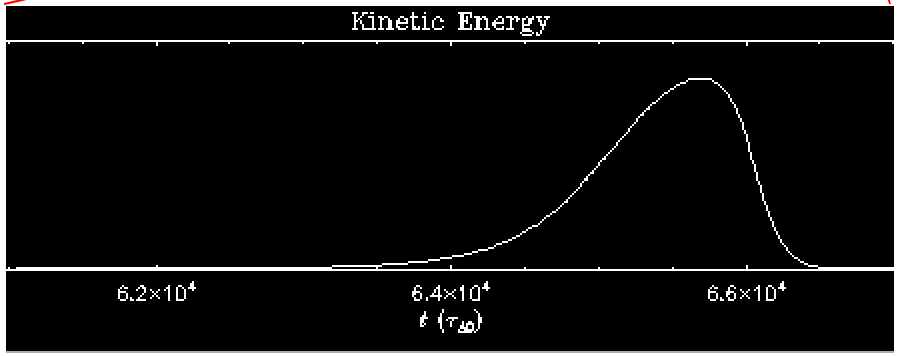
(2) Stationary states with flow



Typical result: 1st sawtooth event depends on initial conditions.
After many events, system reaches steady-state or periodic behavior

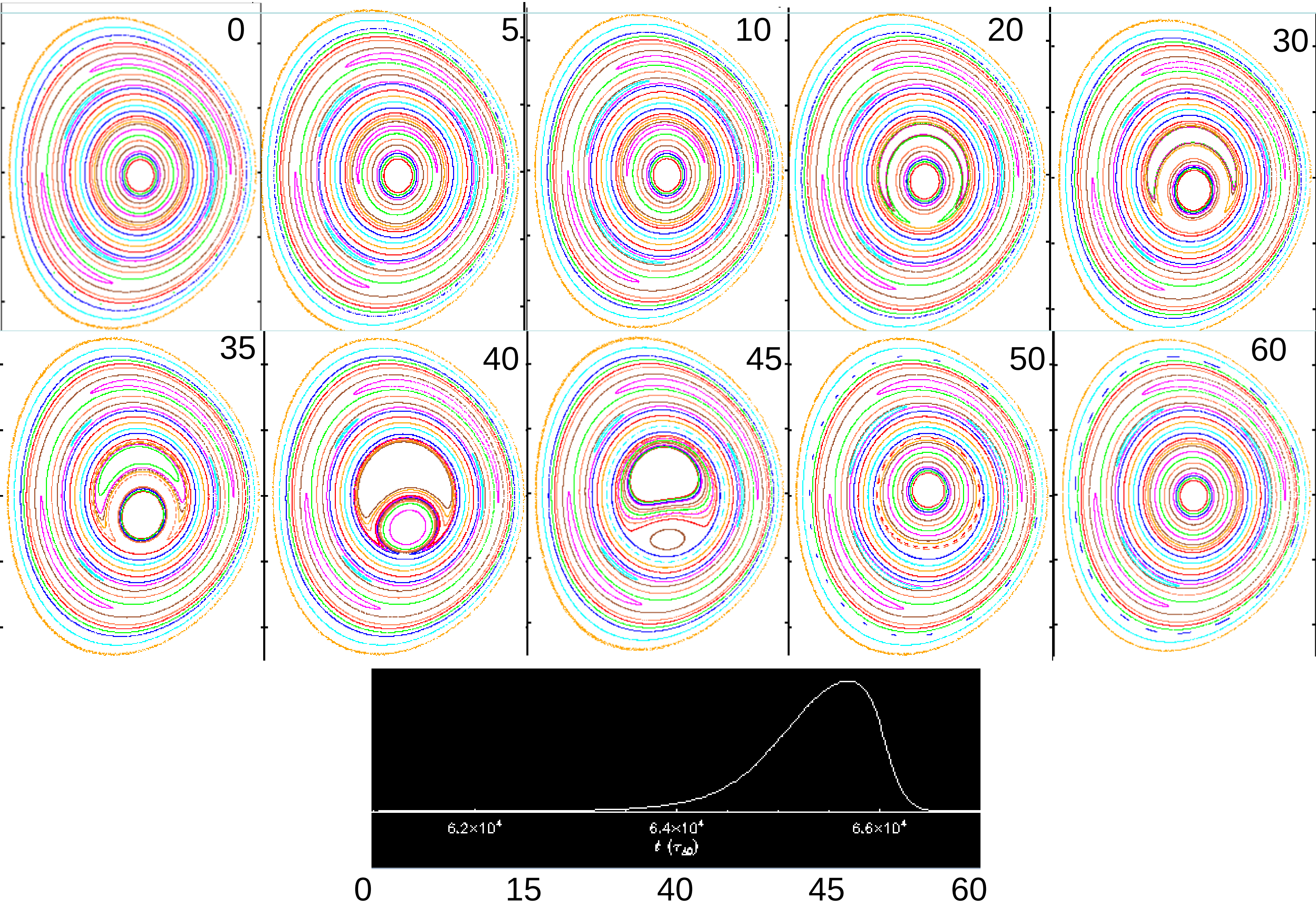


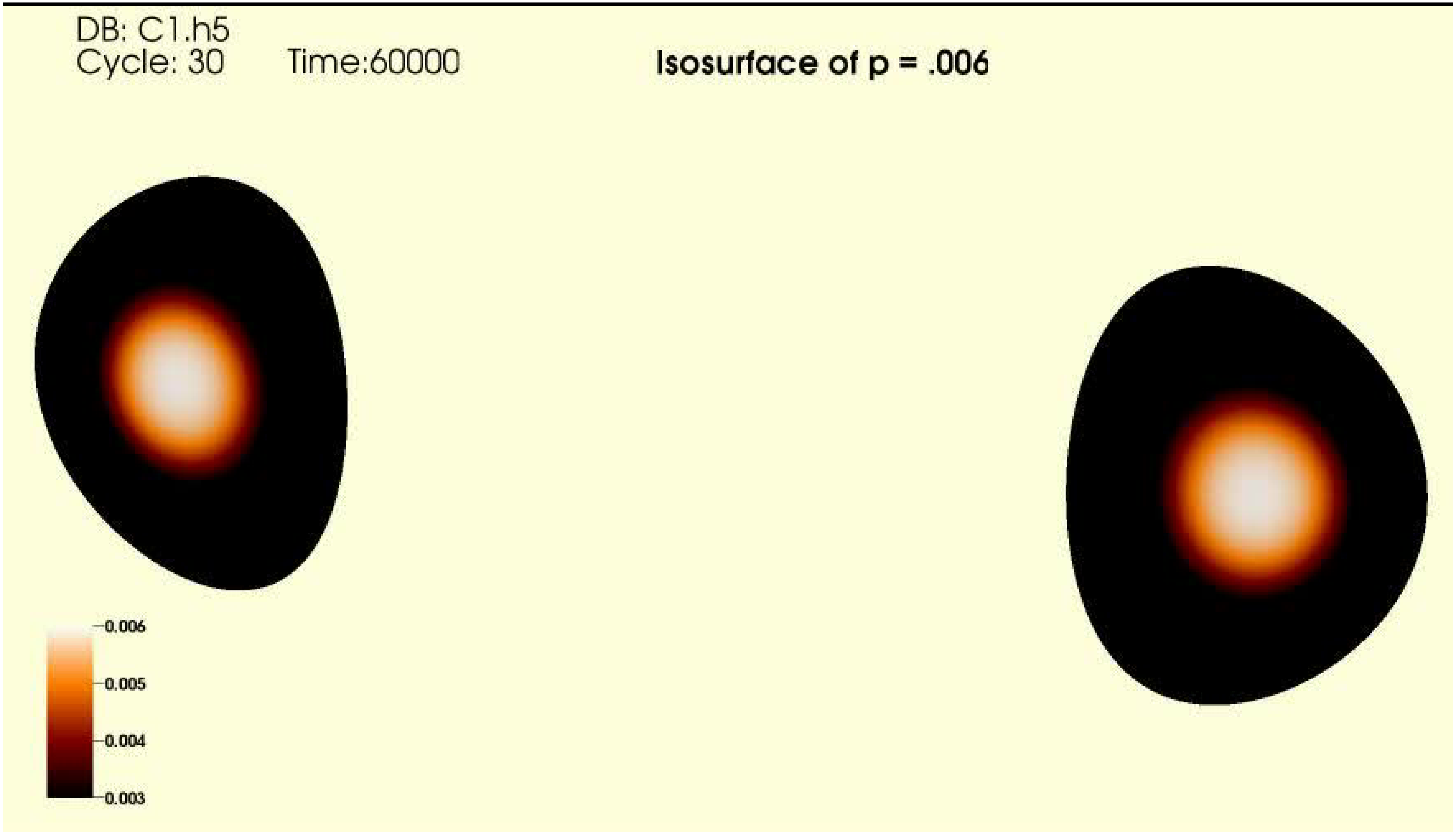
Repeating sawtooth cycle



Precursor phase Crash phase

Poincare plots during a single sawtooth cycle

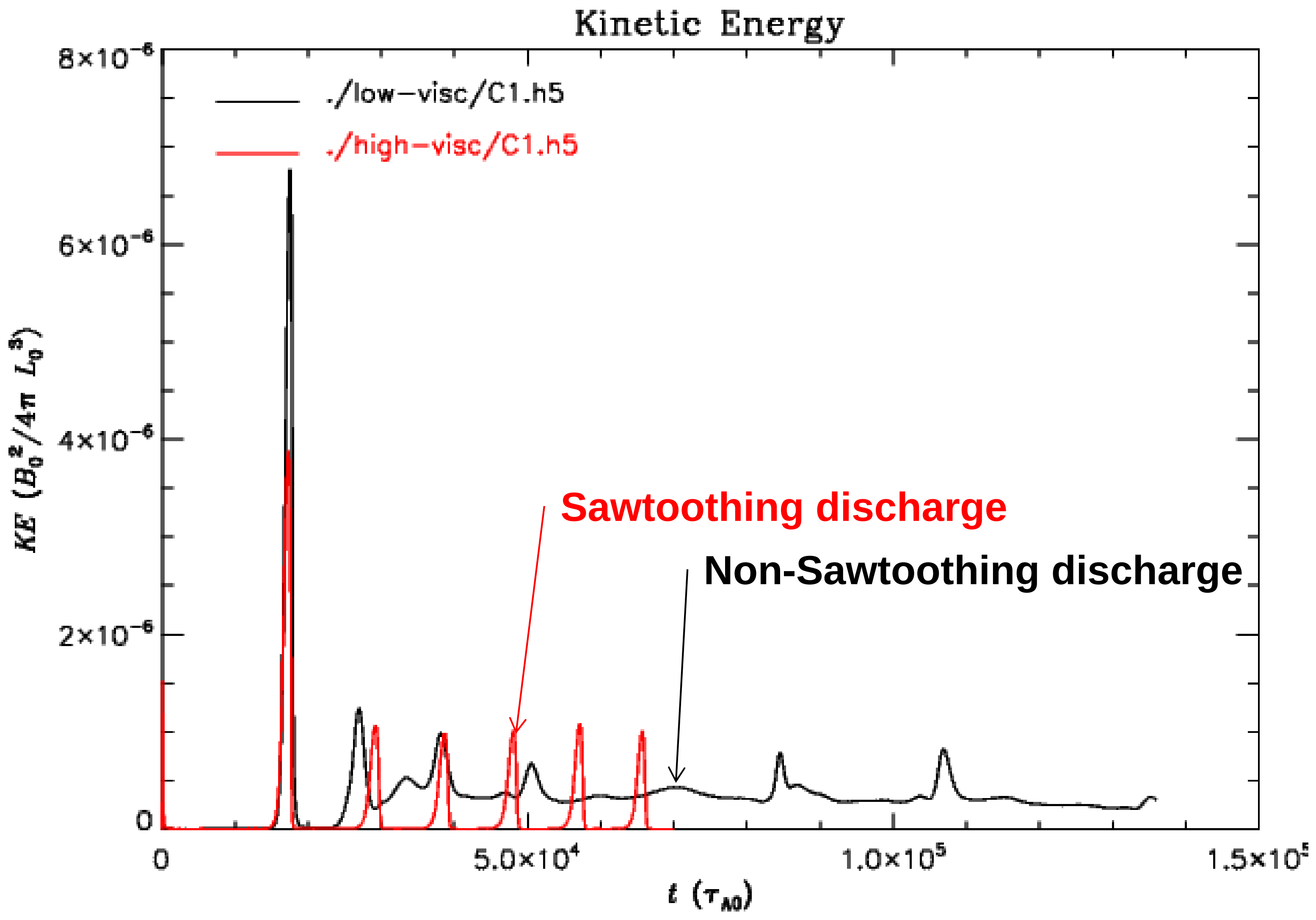



DB: C1.h5
Cycle: 30
Time:60000
Isosurface of p = .006
0.006
0.005
0.004
0.003

Stationary States with Flow

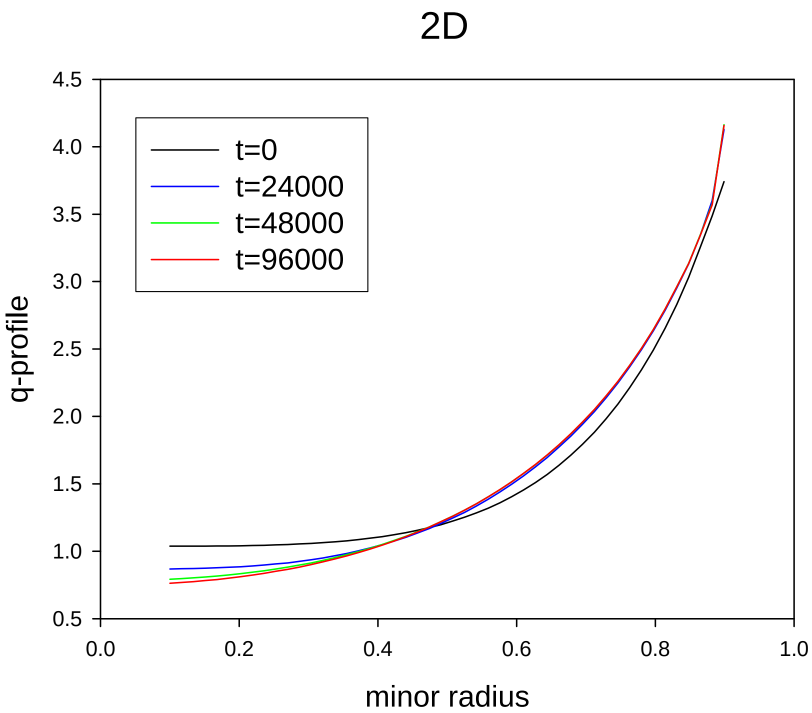
In lower viscosity cases, the sawtooth behavior stops after a few cycles, and a central helical (1,1) structure forms with flow.

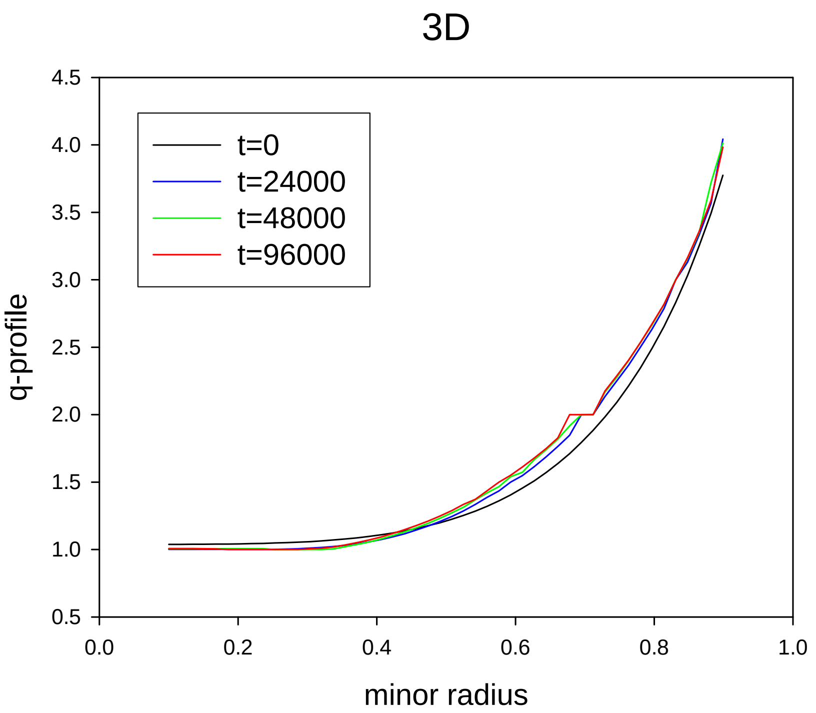
This flow is such as to flatten the central pressure and temperature. This flattening causes the current density to also flatten near the center, keeping $q_0 \sim 1$ in the central region.



Kinetic Energy
./low-visc/C1.h5
./high-visc/C1.h5
Sawtoothing discharge
Non-Sawtoothing discharge
8×10⁻⁶
6×10⁻⁶
4×10⁻⁶
2×10⁻⁶
0
0
5.0×10⁴
1.0×10⁵
1.5×10⁵
KE (B₀²/4π L₀³)
t (τ_A0)

Comparison of 3D Sawtooth Free Helical Stationary State (SFHSS) with 2D configuration with same transport parameters

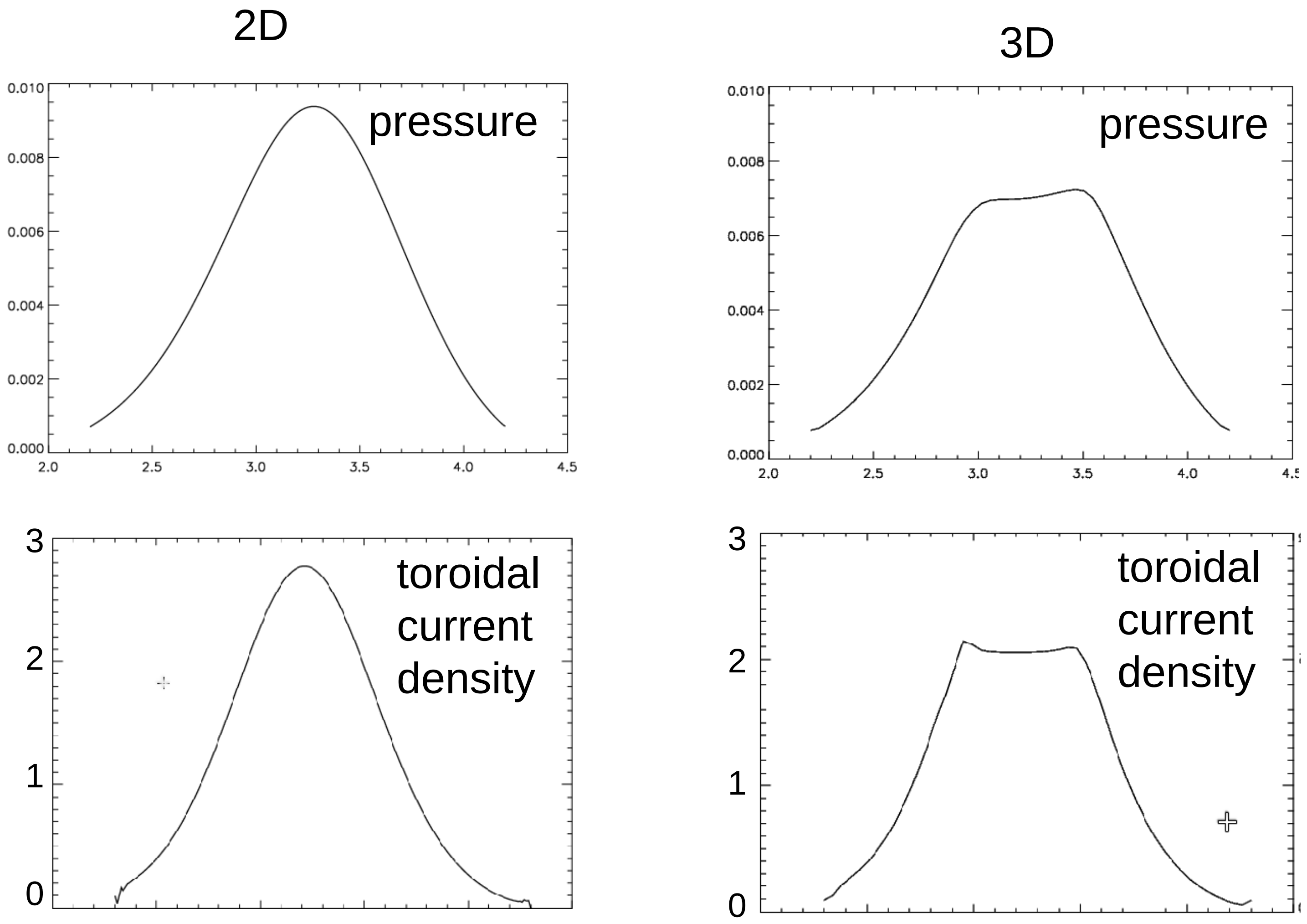




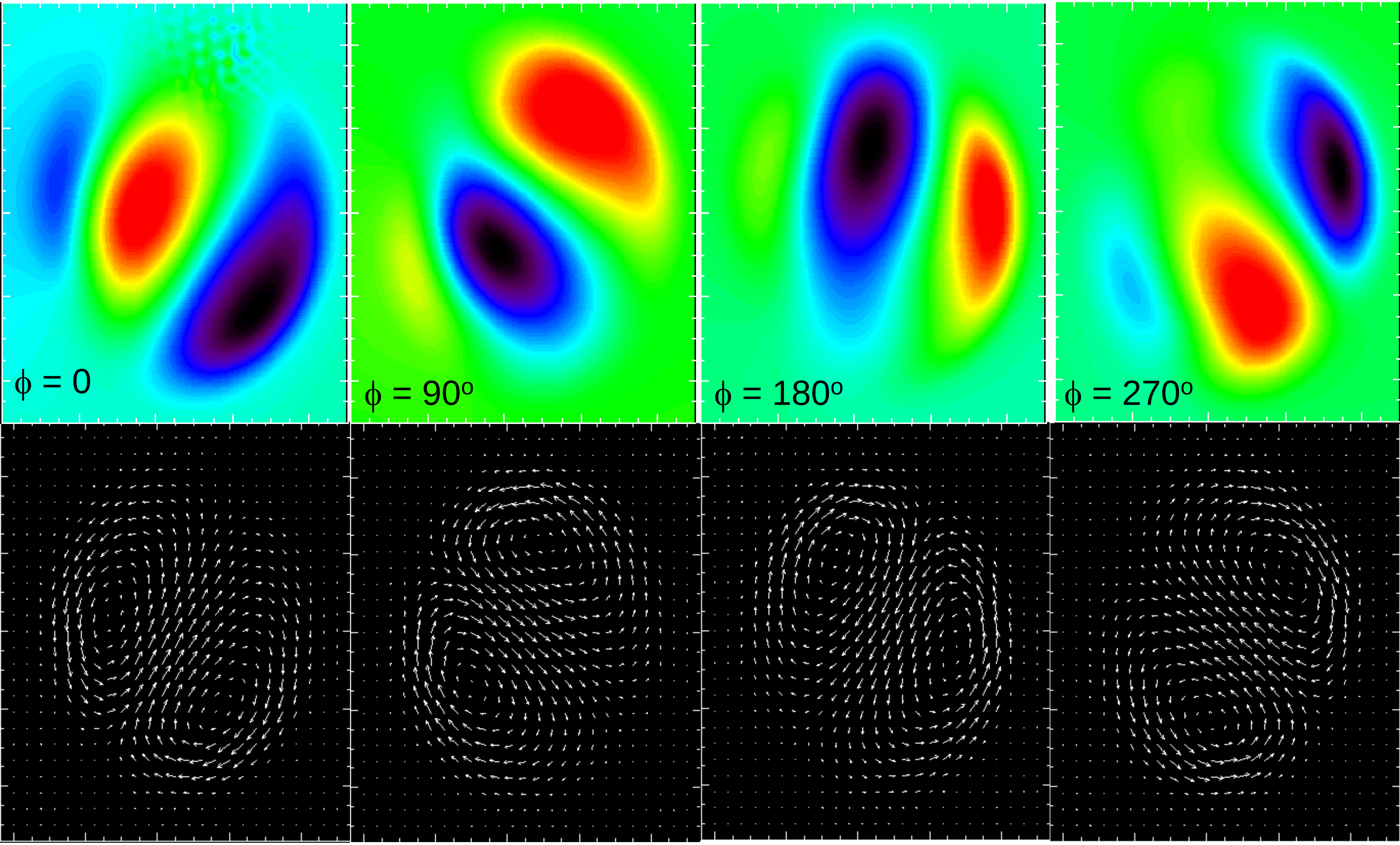
Exact same case was run with M3D-C^1 in 2D and in 3D.

- In 2D, q_0 drops to about 0.7.
- In 3D, it is clamped at 1.0

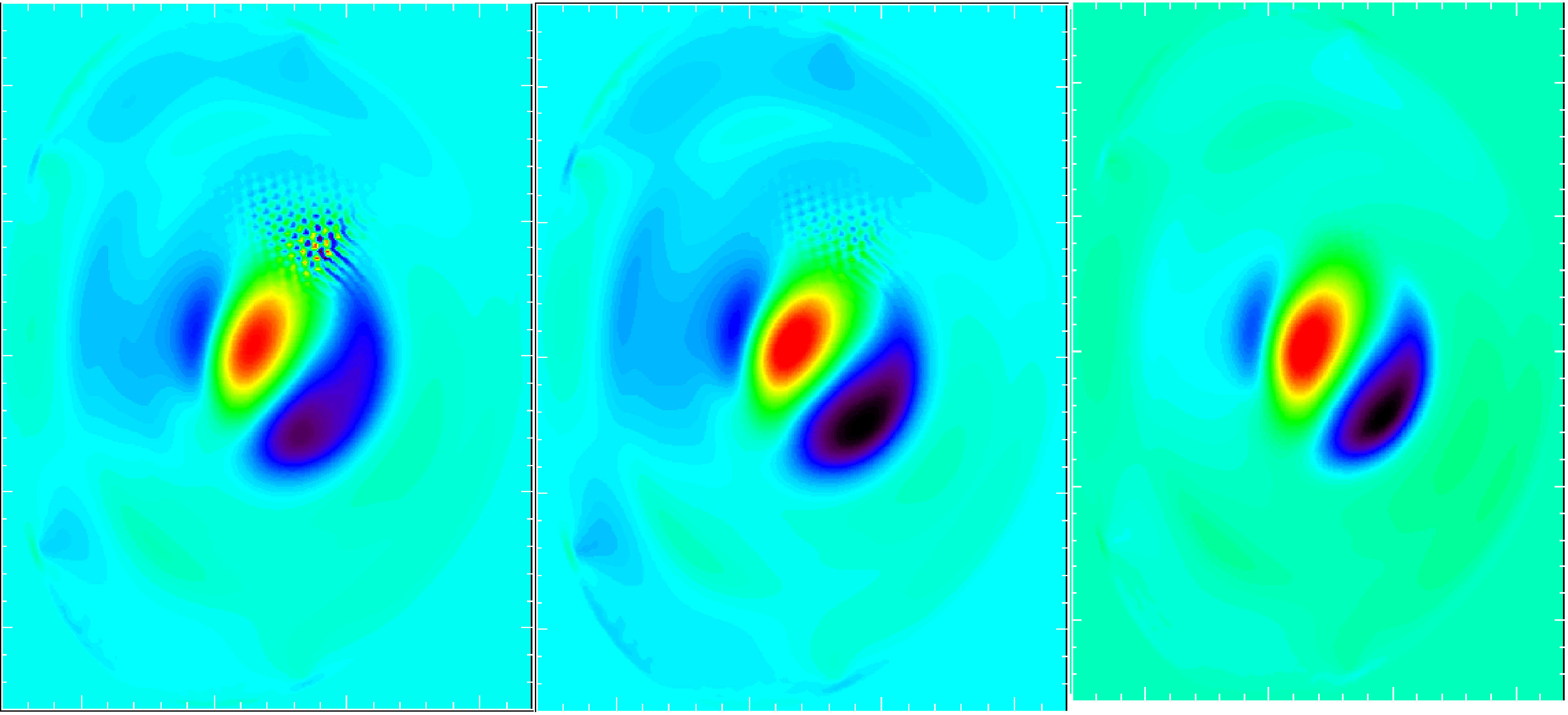
Comparison of 3D Sawtooth Free Helical Stationary State (SFHSS) with 2D configuration with same transport parameters



In 3D, pressure and toroidal current density are much less peaked.



Close up of central toroidal velocity contours (top) and poloidal velocity vectors for stationary state $V_T(\max) \sim 0.0004$ $V_P(\max) \sim 0.0002$



Note: Adding a small hyperviscosity term to toroidal velocity and hyper-resistivity term to toroidal field removed grid-scale oscillations

hyperi = 2.0
hyperv = 2.0

ihypeta = 1
Ihypamu = 1

hyperi = 4.0
hyperv = 4.0

ihypeta = 1
Ihypamu = 1

Summary

- 3-step physics based preconditioner employed
  - Split implicit method reduces matrix size by 2 and makes matrix near symmetric and diagonally dominant
  - Annihilation operators approximately split matrix into 3 diagonal blocks, each with a greatly reduced condition number
  - Block Jacobi preconditioner dramatically reduces the condition number of each of the diagonal blocks
  - Final preconditioned matrix given to GMRES converges in 10s of iterations for fine zoned problem

- Recent Results
  - Repeating sawtooth demonstrate multiple timescale calculations
  - For some parameters, the sawtooth dies out, and a helical stationary state with flow forms