Improvements to the PSI-TET Equilibrium Code

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Outline

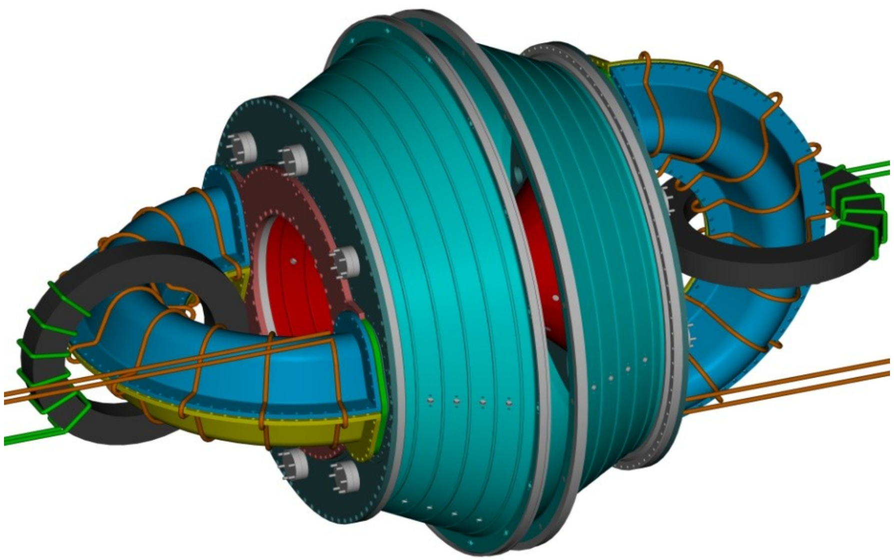
- Variable Lambda Solver
  - Modified the solvers to accommodate lambda profiles
  - Necessary for direct experimental comparison with HIT-SI
- Hybrid MPI/OpenMP parallelism
  - Original code was limited by OpenMP implementation
  - MPI provides access to higher resolution and more procs
  - Hybrid model provides higher mem/proc and looks to the many-core trend in future systems, ie Hopper.
- Some experimental comparison

Variable Lambda Solver

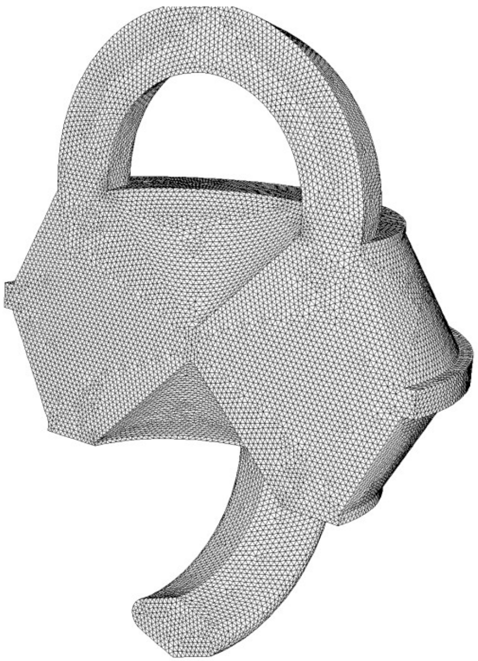
- The PSI-TET code has been modified to calculate full 3-D non-axisymetric equilibria with variable lambda on HIT-SI.
- For the first time equilibria have been calculated with injector driving and spatially variable lambda profiles.
- A new method to efficiently identify and tag magnetic surfaces has been created for use in the equilibrium solver.

Modeling HIT-SI in PSI-TET

- Copper wall with an insulating inner coating
- "Handles" (injectors) enforce vacuum field and current BCs
- PSI-TET employs a mimetic discretization on an unstructured tetrahedral mesh



HIT-SI Coil Schematic



HIT-SI mesh

Physical Problem

The code is designed to solve for solutions to the zero beta ideal MHD equilibrium equation with spatially variable lambda.

$$\vec{j} \times \vec{B} = 0 \rightarrow \vec{j} = \lambda(\vec{x})\vec{B}$$

Taking the divergence of this equation yields a limitation on the form of $\lambda(\vec{x})$.

$$\vec{B} \cdot \nabla\lambda = 0$$

Numerical approach to solving for equilibria

- Initialize the magnetic field with the Taylor state field at a specified $\Phi_{Tor}/\ \Phi_{INJ}$.
- With the magnetic field known, calculate a lambda profile as a function of position.
  - Locate magnetic surfaces and stochastic field regions.
  - Set lambda based on the surface structure.
- Using lambda fixed, recalculate the magnetic field holding the flux ratio fixed.
- Iterate until the solution converges.

New approach to locating magnetic surfaces

- Lambda is constrained to be constant along field lines and in stochastic regions by the physical problem.
- An artificial temperature is computed as the steady state solution to parallel diffusion along field lines.

$$\nabla \cdot (bb \cdot \nabla T) = 0$$

- Boundary conditions of T=1 at the magnetic axis and T=0 outside the separatrix are imposed.

Lambda profile specification

- Lambda is specified as a function of the artificial temperature.
- The resulting profile is constant along field lines as required for equilibrium.
- A smoothly transitioning two lambda model has been used for initial studies.
- Alpha is held fixed for a given simulation so that the normalized profile è remains constant.

$$\square = \square\square = \square 1 + \propto \; \rangle h(40\square^2)$$

Separating the solution into components simplifies the calculation

he goal is to solve the eigenvalue problem

$$[1] \quad \vec{\nabla} \times \vec{B} = \lambda(\vec{x})\vec{B}$$

eparating the homogeneous and inhomogeneous solutions allows solving using existing algorithms.

$$B = B^H + B^I_{cur} + B^I_{flux}$$

$$j = \nabla \times B^H + \lambda_{INJ} B^I_{flux}$$

Formulation of solvable system of equations

Rewriting Equation 1 using the separated forms

$$\frac{1}{\hat{\lambda}}\nabla \times B^H - \bar{\lambda}B^H = \bar{\lambda}B^I_{cur} + \left(\bar{\lambda} - \frac{\lambda_{INJ}}{\hat{\lambda}}\right)B^I_{flux}$$

Taking the curl

$$\nabla \times \left(\frac{1}{\hat{\lambda}}\nabla \times B^H\right) - \bar{\lambda}\nabla \times B^H = \bar{\lambda}\lambda_{INJ}B^I_{flux} - \nabla \times \frac{\lambda_{INJ}}{\hat{\lambda}}b^I_{flux}$$

A particular solution, B_P^H, is computed along with the minimum eigenvalue solution to the equation

$$\nabla \times \left(\frac{1}{\hat{\lambda}}\nabla \times B^H_e\right) = \bar{\lambda}\nabla \times B^H_e$$

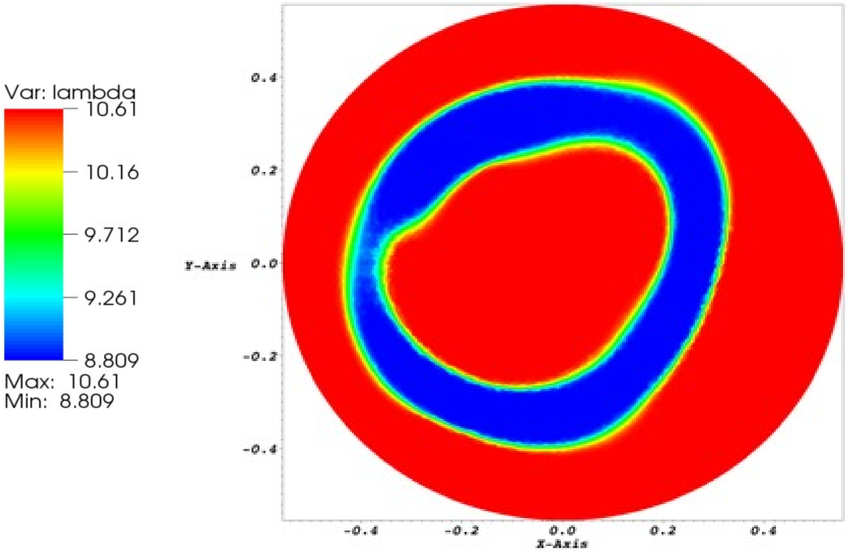
Final solution is a combination of the separated equations

The resulting solution is

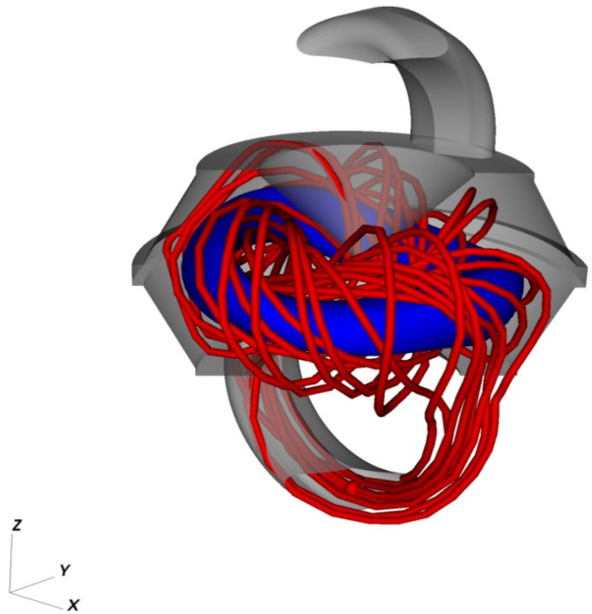
$$B = B_P^H + aB_e^H + B_{cur}^I + B_{flux}^I$$

- The value of *a* is then computed to hold the ratio of torodial flux to injector flux fixed at the specified value.
- Both alpha and the flux ratio are held fixed during iterations, while $\bar{\lambda}$ is determined by the lowest eignenvalue solution.

Results- $\Phi_{Tor} / \Phi_{INJ} = 2$



Lambda Profile

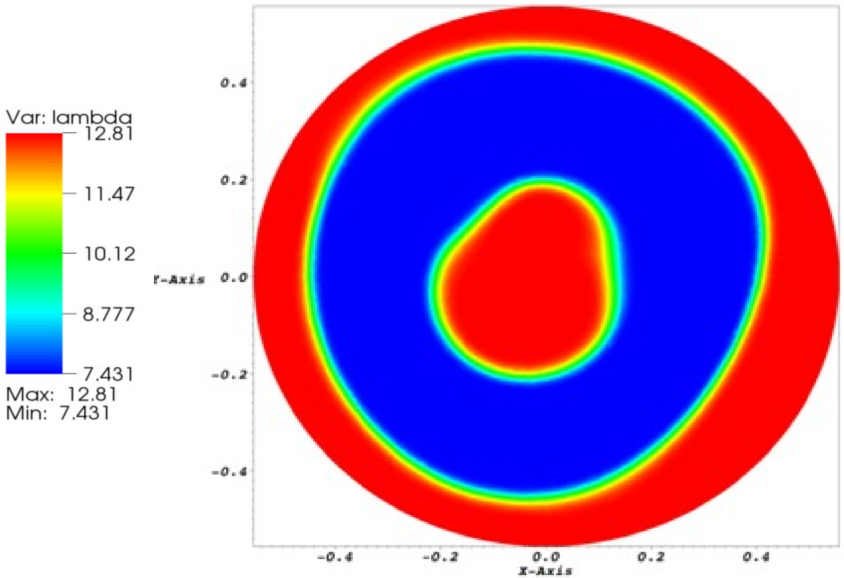


Separatrix Position

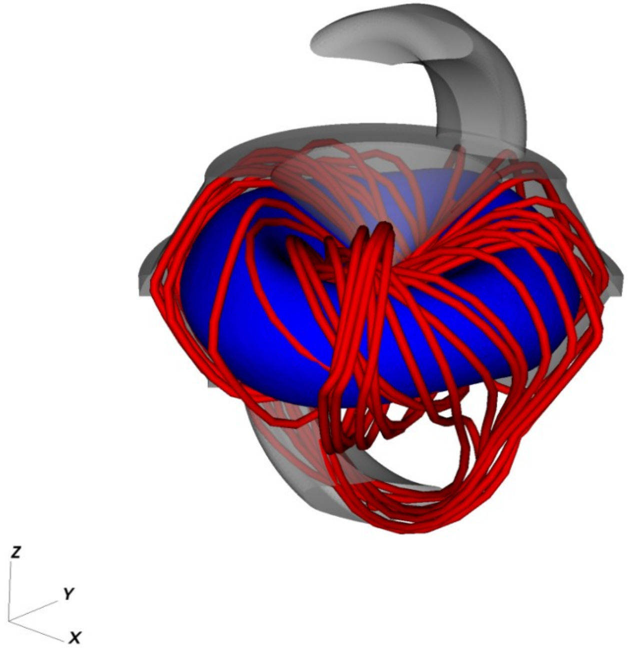
Injector Lambda = 10.61

Axis Lambda = 8.8

Results- $\Phi_{Tor} / \Phi_{INJ} = 5$



Lambda Profile

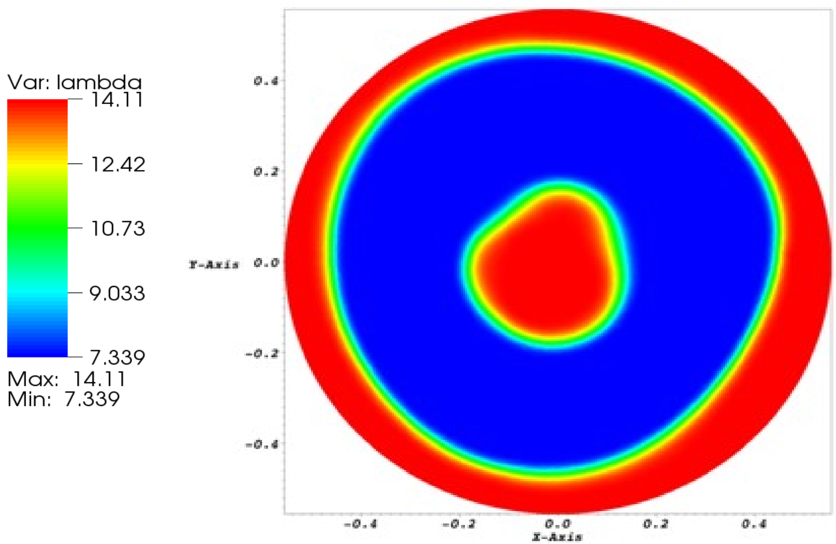


Separatrix Position

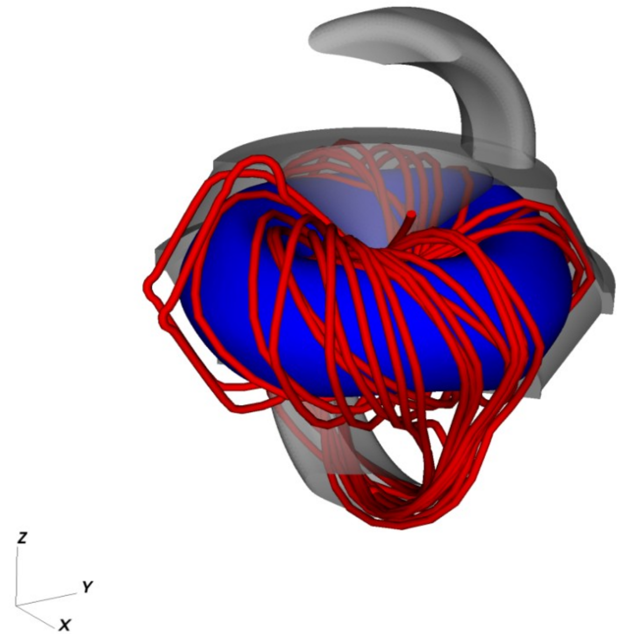
Injector Lambda = 12.81

Axis Lambda = 7.4

Results- $\Phi_{Tor} / \Phi_{INJ} = 10$



Lambda Profile

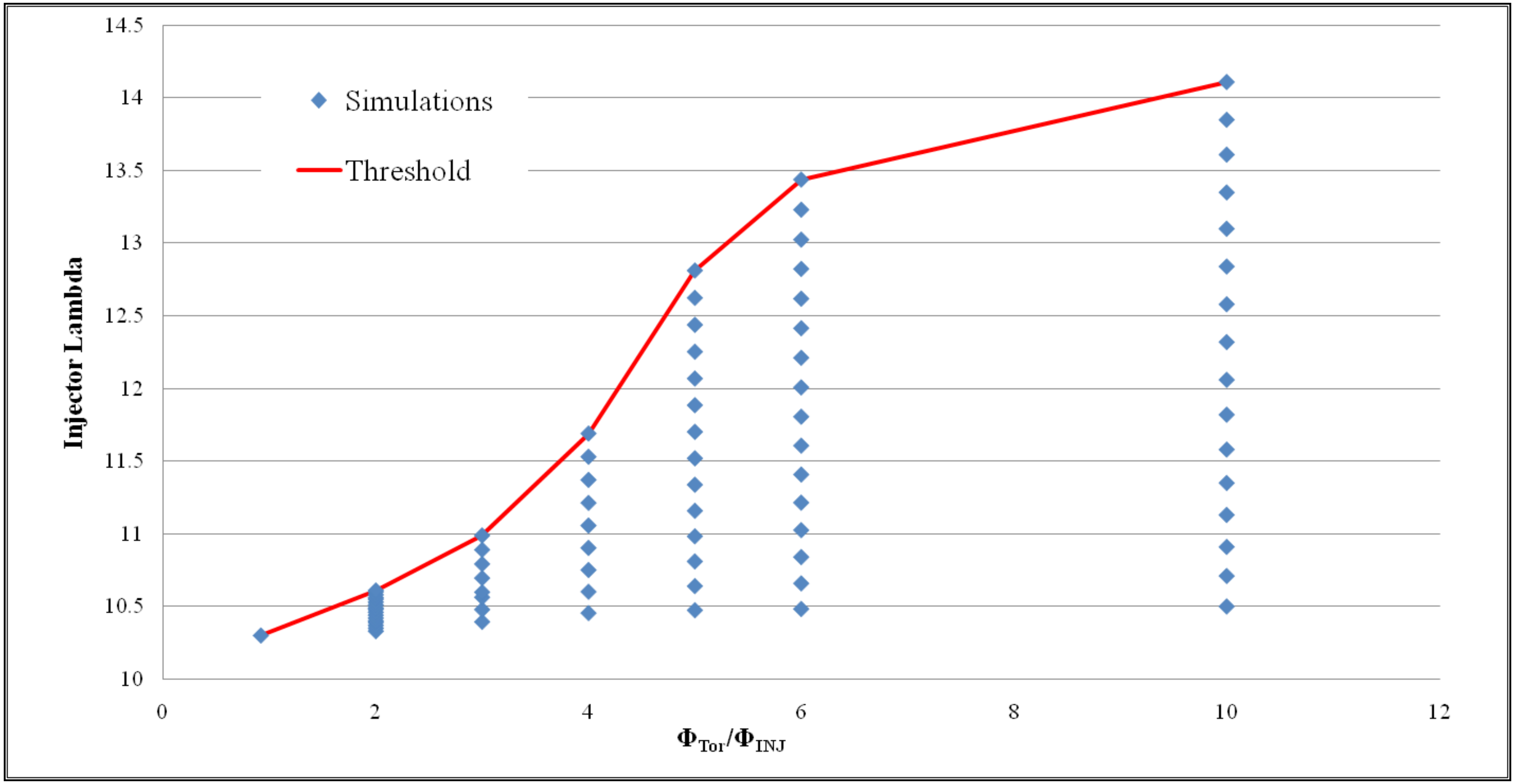


Separatrix Position

Injector Lambda = 14.11

Axis Lambda = 7.3

High flux ratios allows convergence at higher injector lambdas



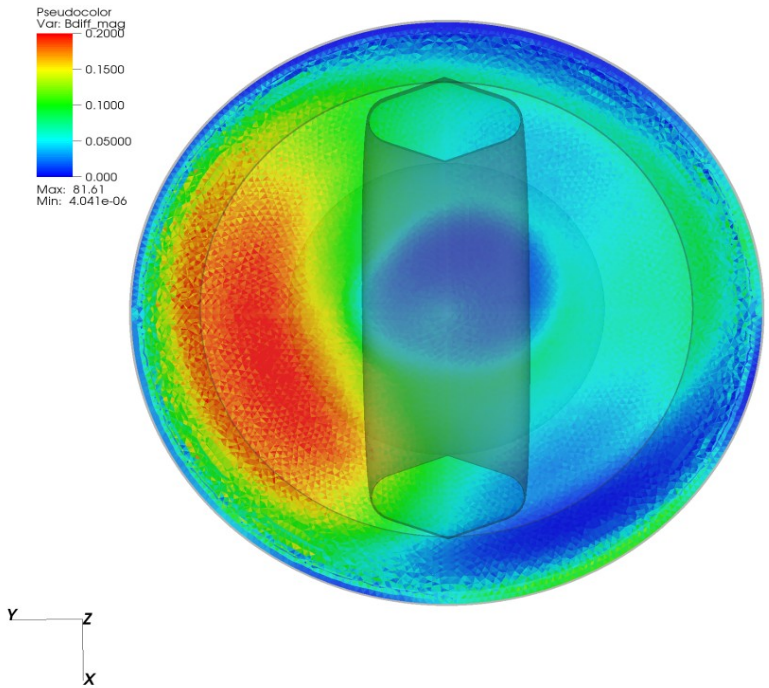
Stable solution space showing the maximal solution for each flux ratio

Limitations on convergence and accessibility of the solution space

- The maximum injector lambda, for a given flux ratio, is limited, with values above this point failing to converge.
- This threshold limits the maximum lambda gradient for a given flux ratio.
- Higher driving lambda values are accessible with increasing torodial flux and current.
- Resolution constraints with the current code are thought to limit the solution space.

Comparison With Taylor State (λ=10.3) shows the effect of variable lambda

- Localized deviation from the Taylor state is present in equilibrium solutions.
- Variations up to 30% in magnitude are present in high flux ratio cases.
- The bulk of the difference is aligned with the direction of the spheromak field.



Deviation from Taylor State $\Phi_{Tor}/\Phi_{INJ} = 10$

Equilibrium results highlight the need for higher resolution

- Initial simulations have shown promising results, with the successful calculation of 3-D equilibrium states in HIT-SI.
- It is believed that limitations in code accuracy are limiting the maximum lambda gradient.
- Attempts to integrate finite beta into the equilibrium solver further highlighted this issue when attempting to calculate the pressure driven current contribution.

OpenMP -> MPI/OpenMP

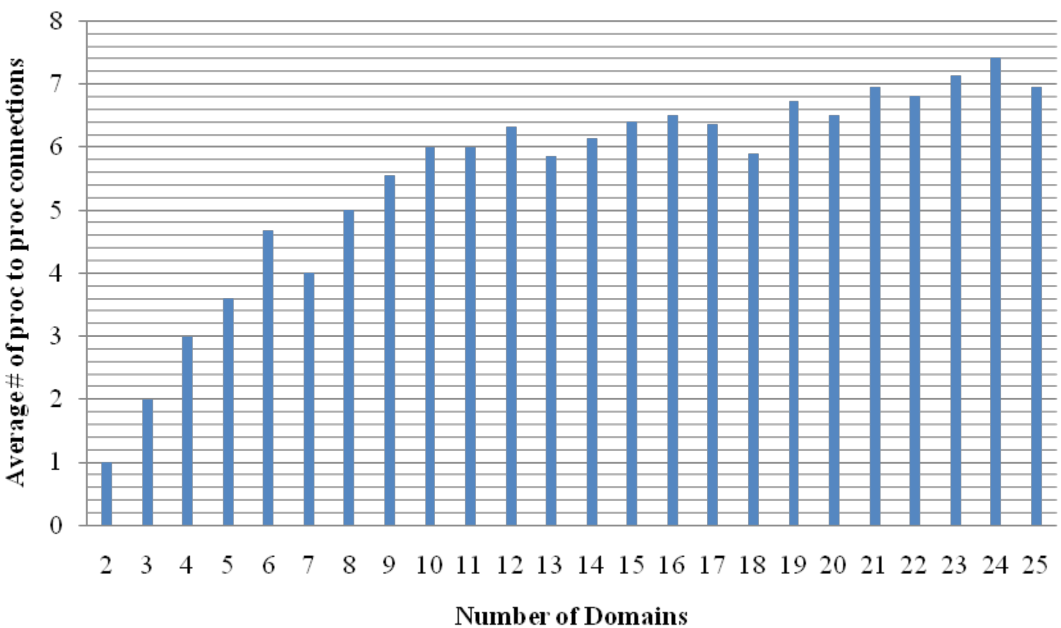
- The PSI-TET code has been modified to use a hybrid MPI/OpenMP parallelization scheme.
- Good initial scaling in both a strong and weak sense has been seen on the ICE cluster.
- Scaling to larger system sizes, 100's of millions of degrees of freedom on 100's of procs has been demonstrated.
- Restart and output I/O using Parallel HDF5

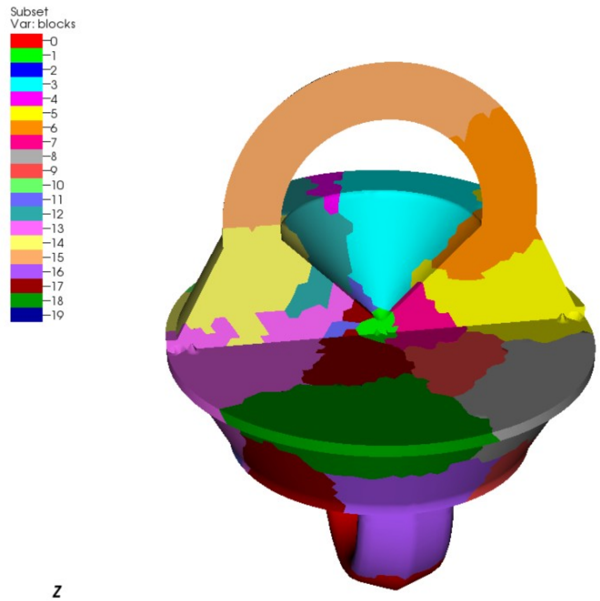
MPI Methodology

- Local mesh construction is performed on each processor
- Proc to proc linkage is determined for stitching and reduction operations
- Reduction using MPI_REDUCEALL calls
- Stitching using MPI_ISEND and MPI_RECV
- Unstructured mesh leads to a question of comm optimization

Linkage Scaling

- Domain decomposition is performed using the METIS library
- The number of domains, processes, each processor connects to approaches a constant.
- This limits the number of communications required per stitch





Stitching operations on an unstructured mesh can decrease efficiency

- The use of an unstructured mesh and complicated geometries like HIT-SI leads to a difficulty with comm optimization.
- For stitching each processor must share its boundary information
- Ring architecture (Basic)-
  - Very parallel transfers, but lots of wasted communications
- MPI_SENDRECV (mh4d)-
  - Only required transfers are made, but lots of wait time due to cyclic dependencies

PSI-TET Stitching Solution

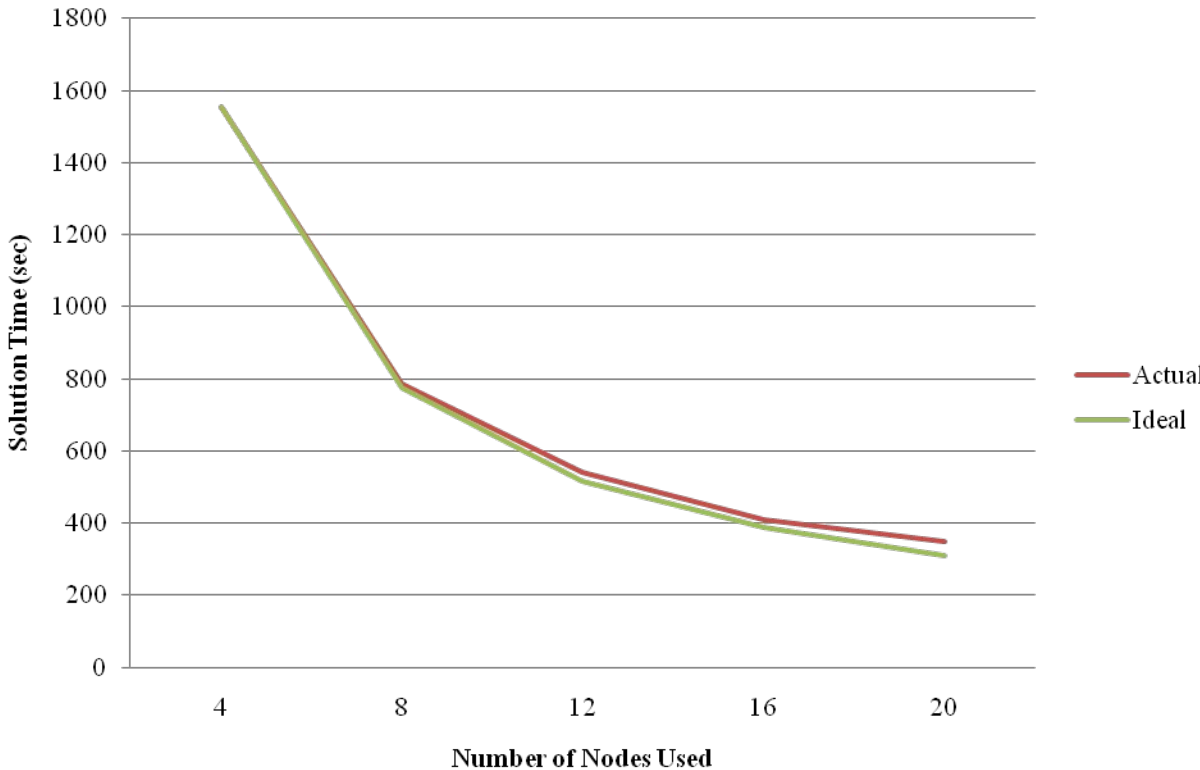
```
do j=1,nproc_con
  call MPI_ISEND(tmptrans(j)%lp, …)
enddo

do j=1,nproc_con
      call MPI_RECV(lptmp, …)
      perform stitching
enddo
call MPI_WAITALL
```

- An array of pointers is created, all pointing to the same array in memory, and filled with the local boundary data
- Non-blocking sends are established to each processor
- Data is then received for each process and stitched
- Allows for smallest number of communications in parallel

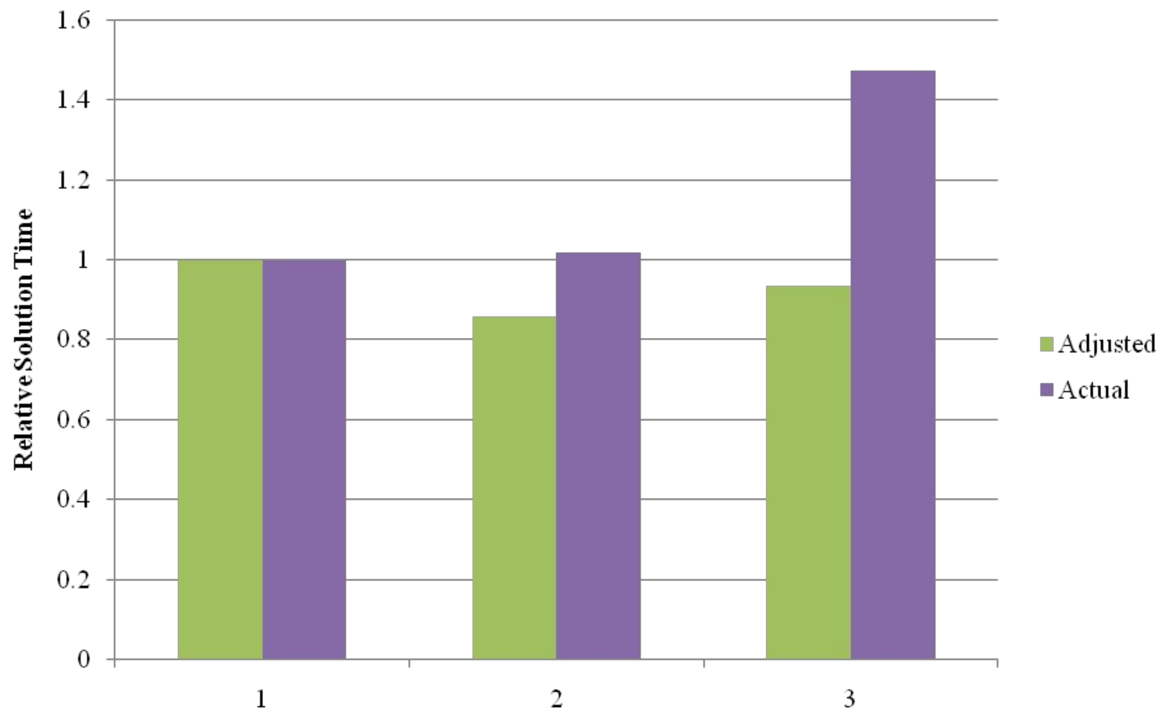
Strong Scaling (ICE)

- Strong scaling performed on the ICE cluster with flat MPI
- Maximum deviation from ideal scaling at 20 nodes is 11%



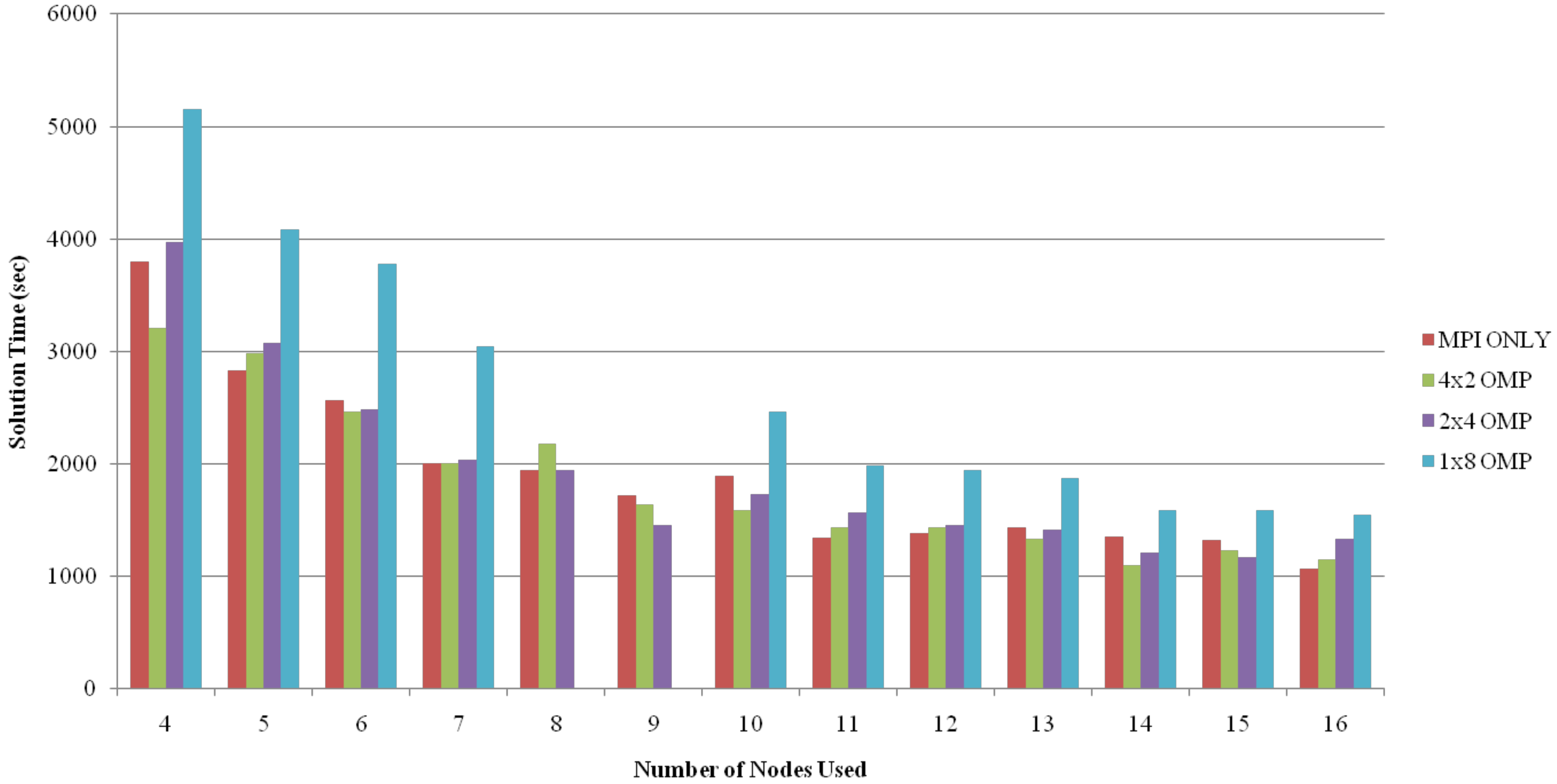
Weak Scaling (ICE)

- Weak scaling performed on the ICE cluster with flat MPI
- The current solver implementation is not scalable
- Adjusting for the solver by normalizing to the number of iterations shows good scalability



Strong Hybrid Scaling (Hopper)

- Strong scaling performed on Hopper with hybrid
- The NERSC advised 2x4 configuration scales well

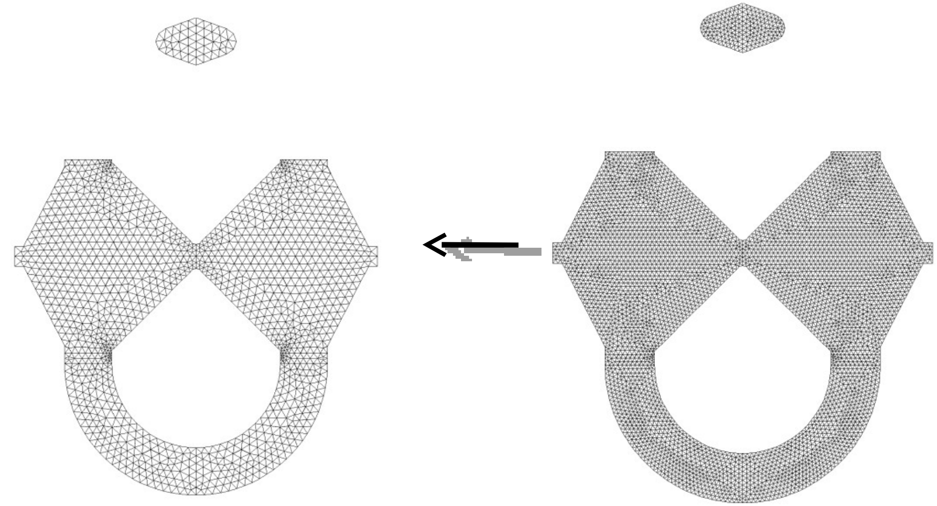


Comments on scaling

- Scaling studies on ICE have shown promise for the scalability of the implementation.
- The number of comms required plateaus with the number of domains using our stitching method.
- OpenMP does not appear to buy us any speed advantage over flat MPI.
  - Number of connections is the same so latency floor is the same
- Scalable scalar solvers are already in place and work on vector solvers is progressing using geometric multigrid.

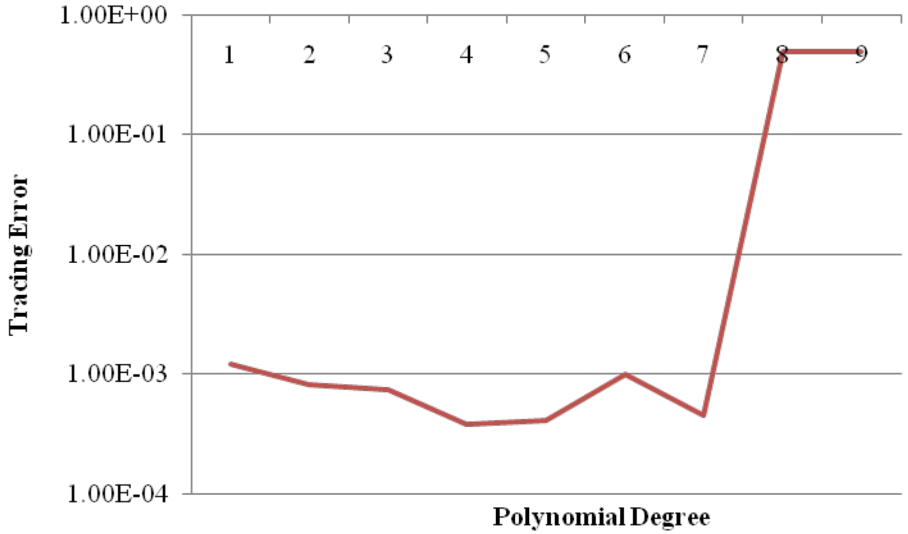
Tracing on high resolution meshes

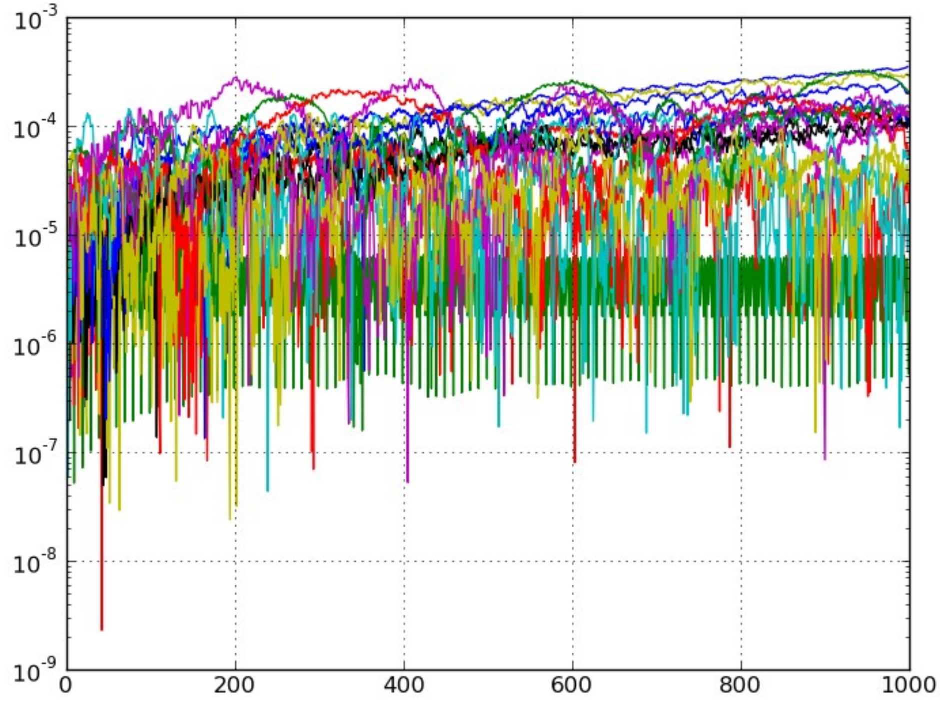
- Tracing is required for surface tagging in the equilibrium solver
- Domain based tracing parallelism is too slow
- Polynomials are used to interpolate the magnetic field onto a coarser mesh, of the full domain, on each proc for tracing
- Hybrid with OpenMP allows this “base” mesh to be finer resulting in higher accuracy



Interpolation tracing error

- Tracing error for coarsening 2 levels.
- Optimum tracing error is 3rd – 5th order polynomials

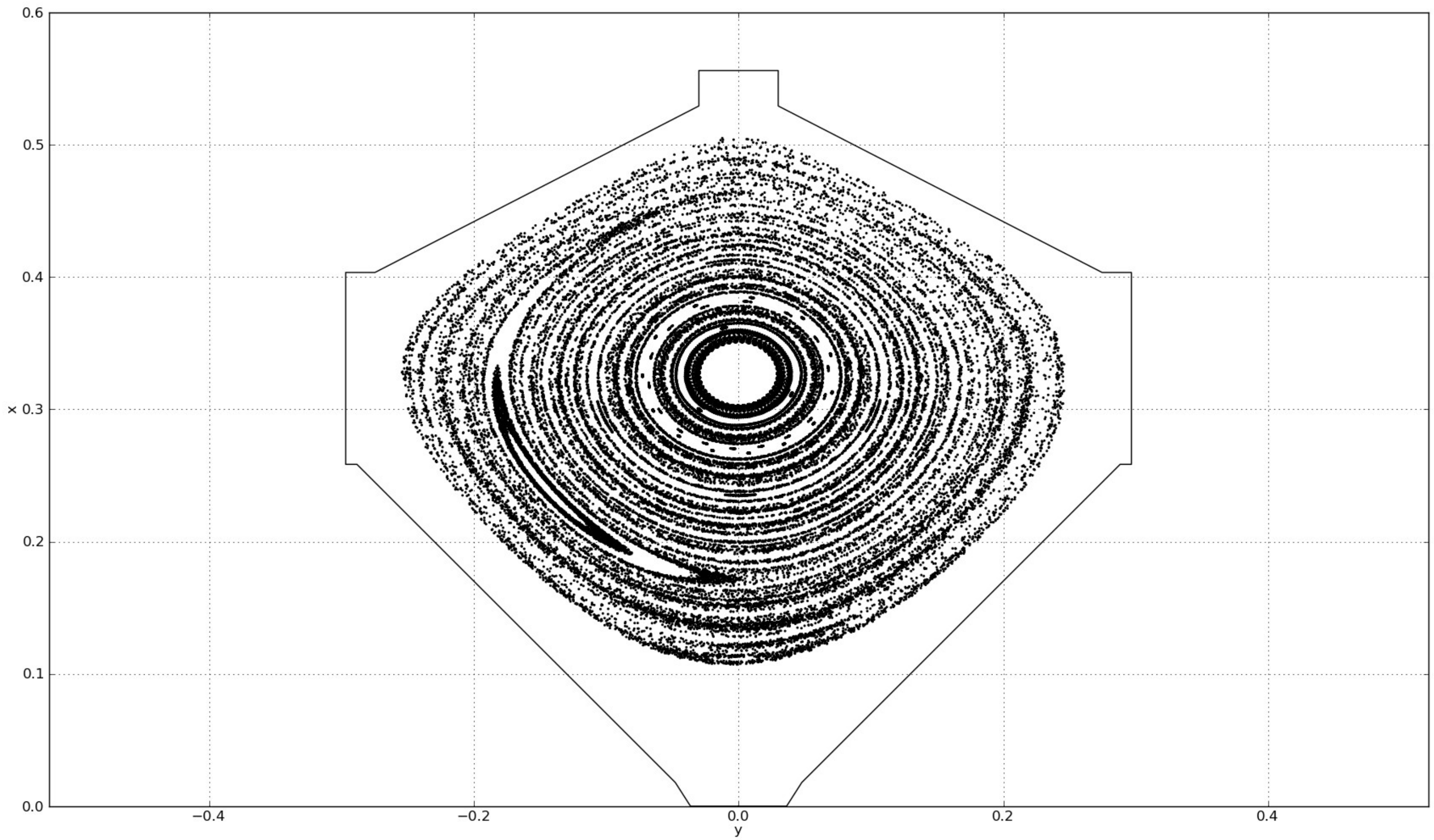




Tracing Error vs Trace Length (np=4)

High Resolution Taylor State

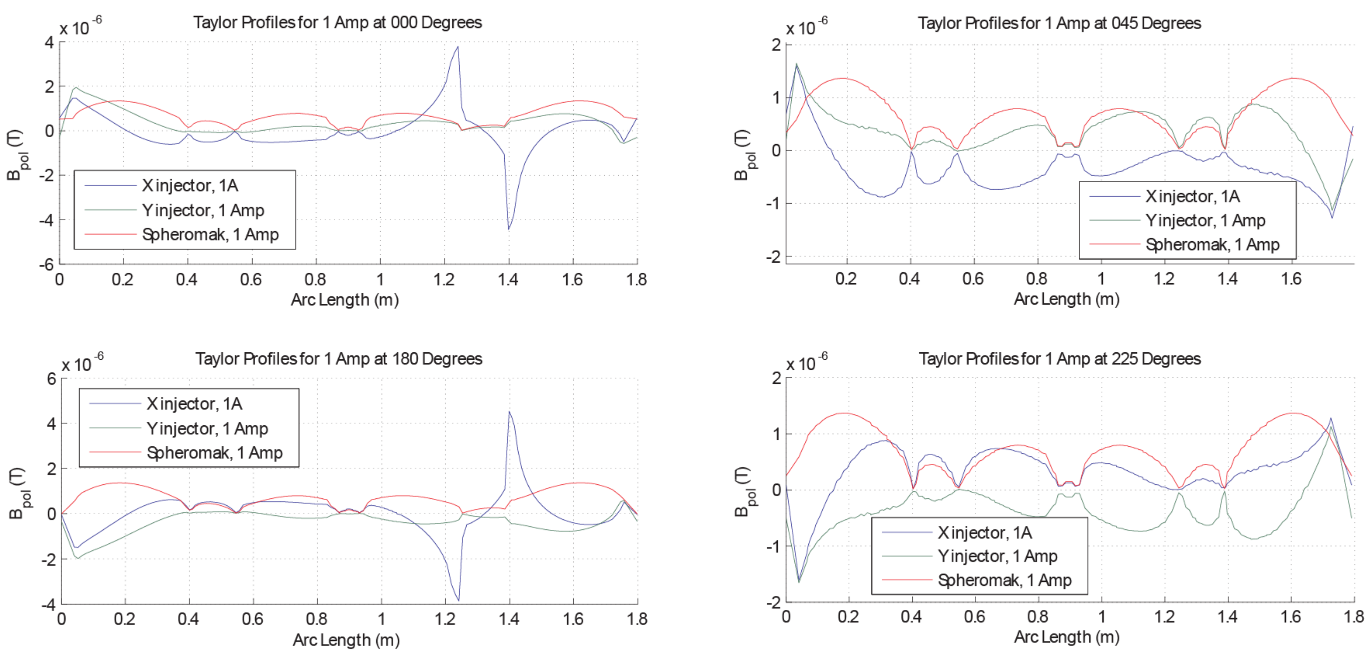
Poincare plot 1/8" resolution, traced on ½" resolution mesh using 4th order polynomials, 155 million DOF



Experimental Comparison HIT-SI

- Throughout the last year extensive comparison between experimental and computed Taylor states has been done
- The injector and spheromak states are super imposed based on torodial current to get a combined field for comparison

Surface Magnetic Fields Calculated Using Uniform Taylor Equilibria for Lambda = 10.3/m

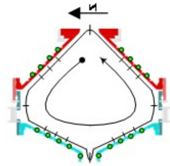


Surface Probes

- An array of surface magnetic probes embedded in the HIT-SI flux conserver resolves plasma dynamics from 10 Hz – 200 kHz.
- Amperian loops are formed by the array at toroidal angles of 0°, 45°, 180°, and 225°
- 18 probes compose each amperian loop
- Magnetic field profiles, shown on the previous slide, have been computed along the boundary at each toroidal slice.
- Comparison between Taylor equilibrium and probe data is shown in the next 3 slides.

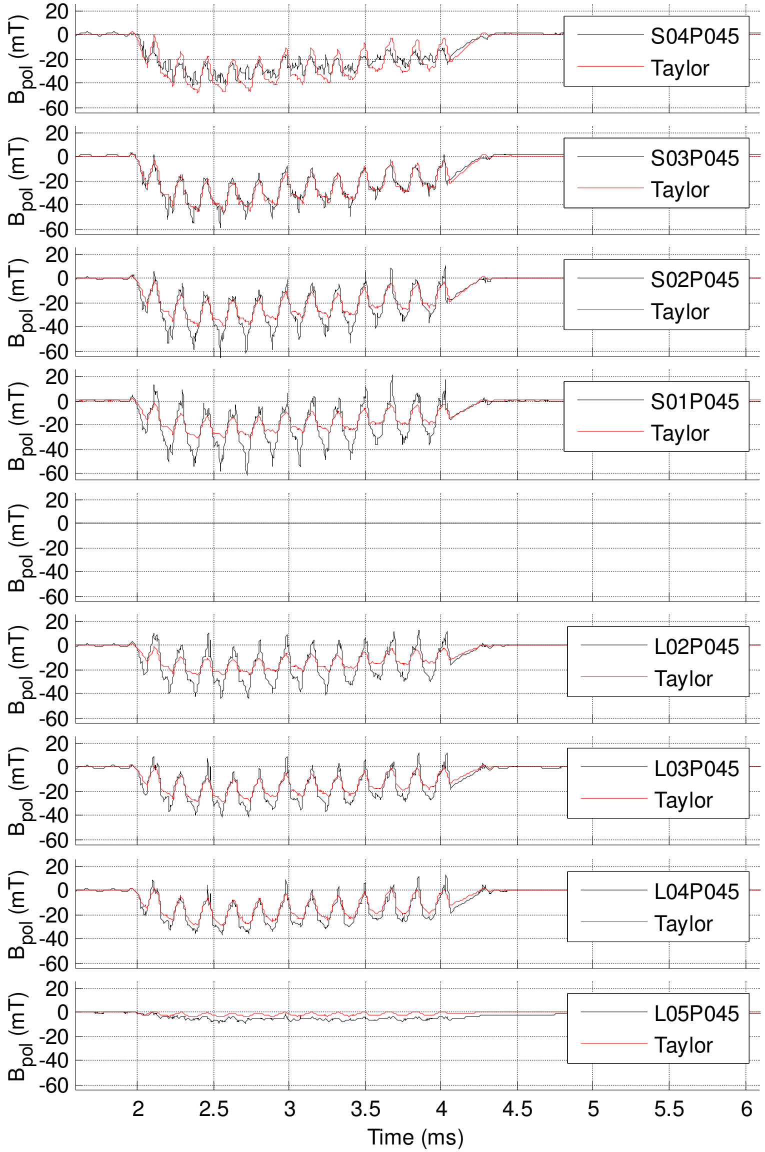
Data and figures courtesy of Jonathon Wrobel, HIT-SI Group

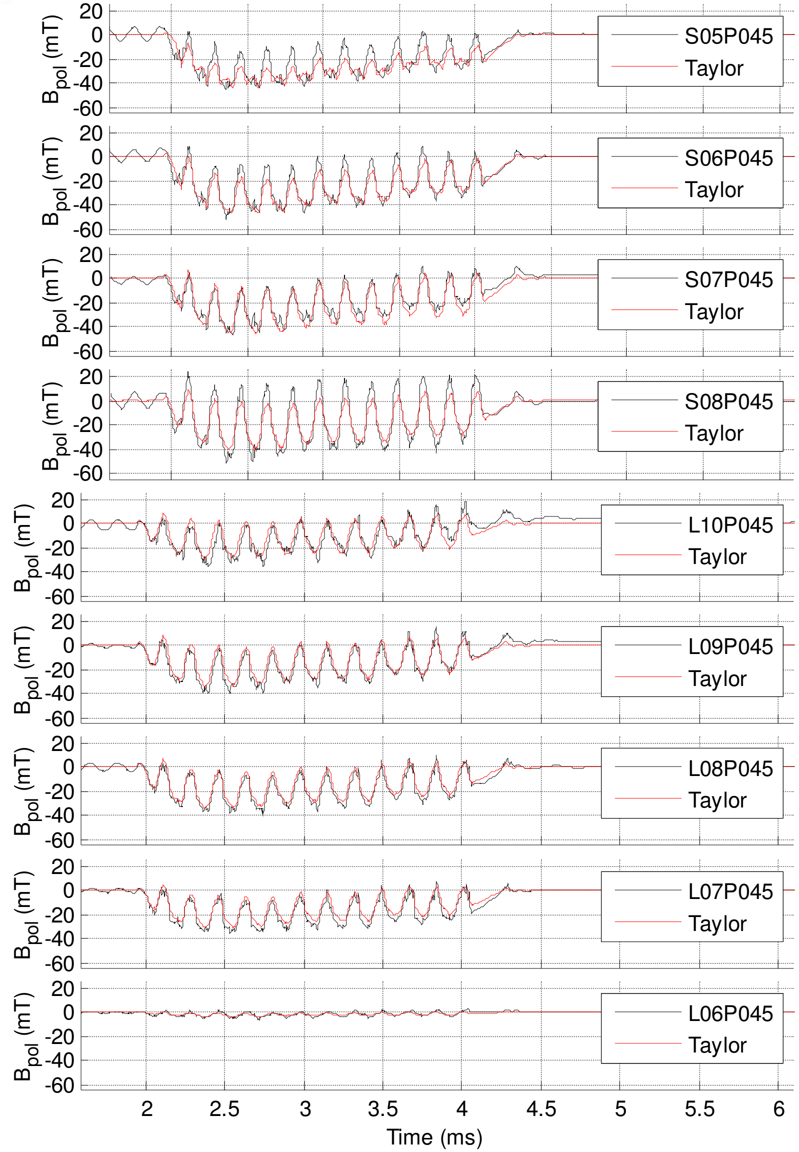
- Surface Probe Field
- Taylor Equilibrium Field



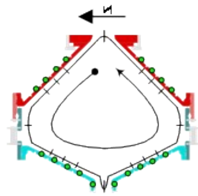
Poloidal Probes

Shot: 118373

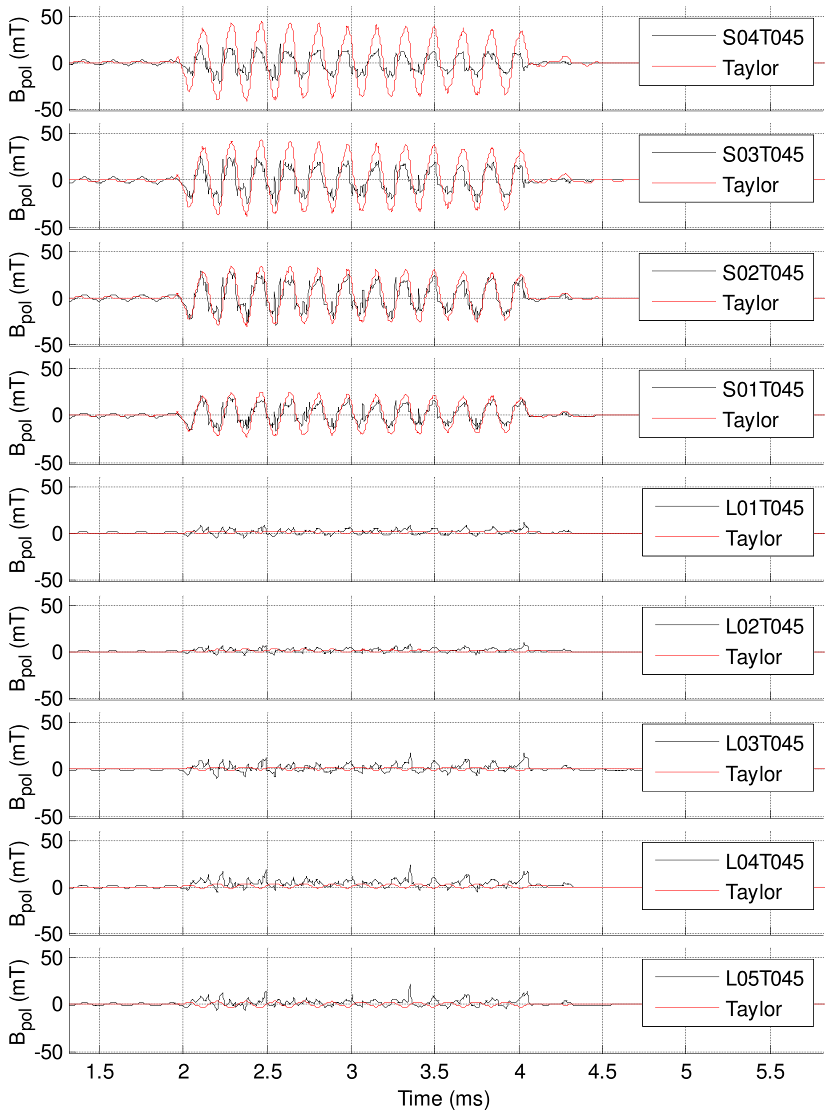


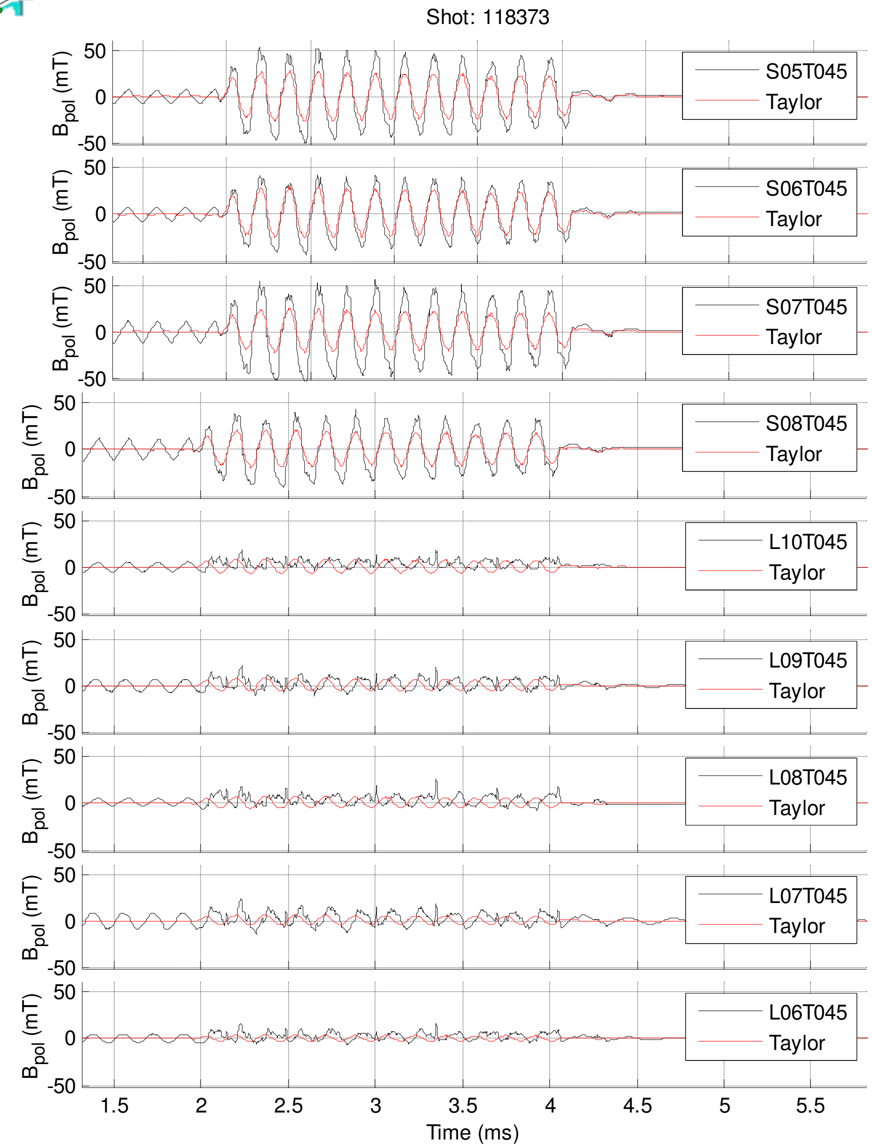


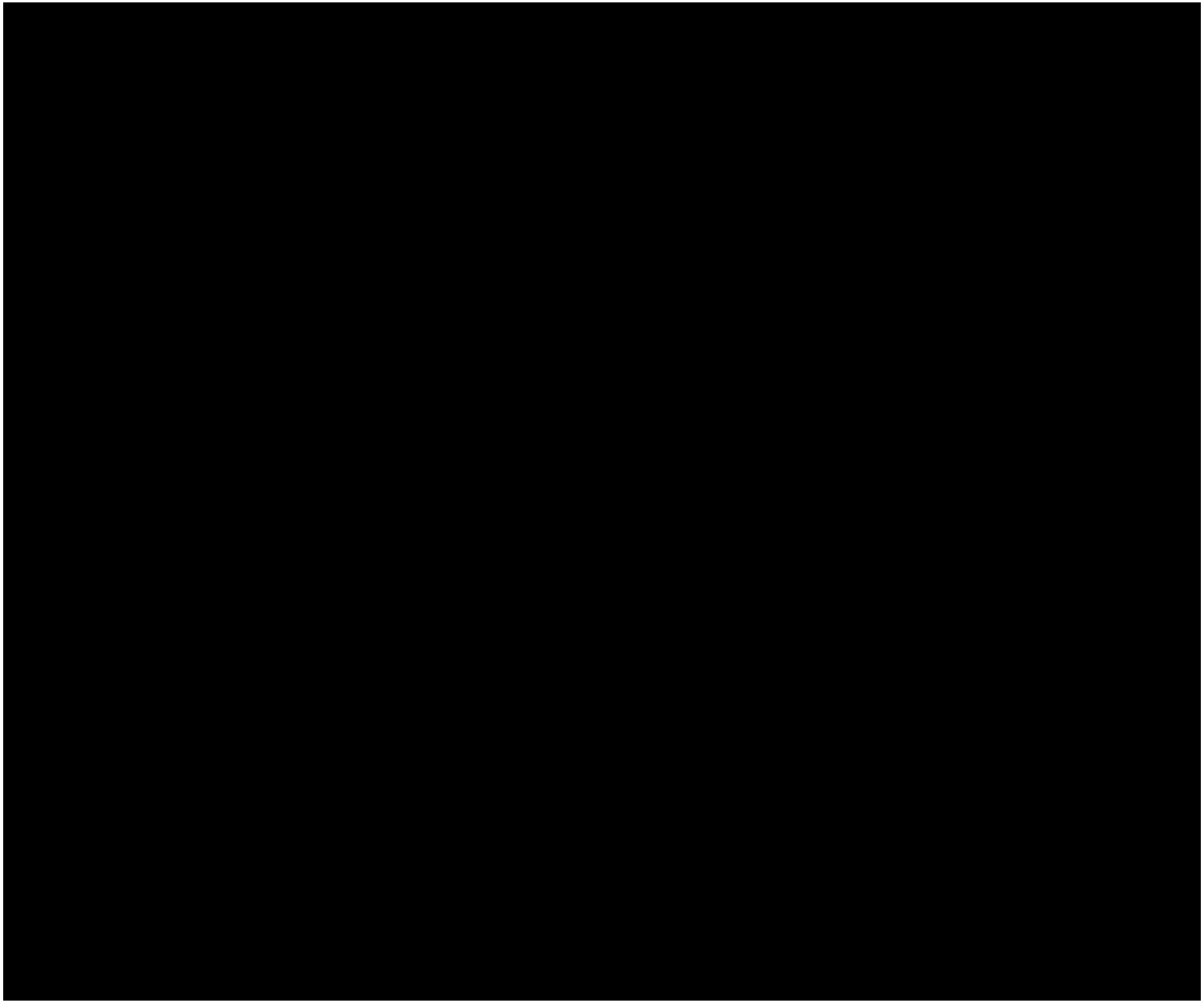
- Surface Probe Field
- Taylor Equilibrium Field



Toroidal Probes







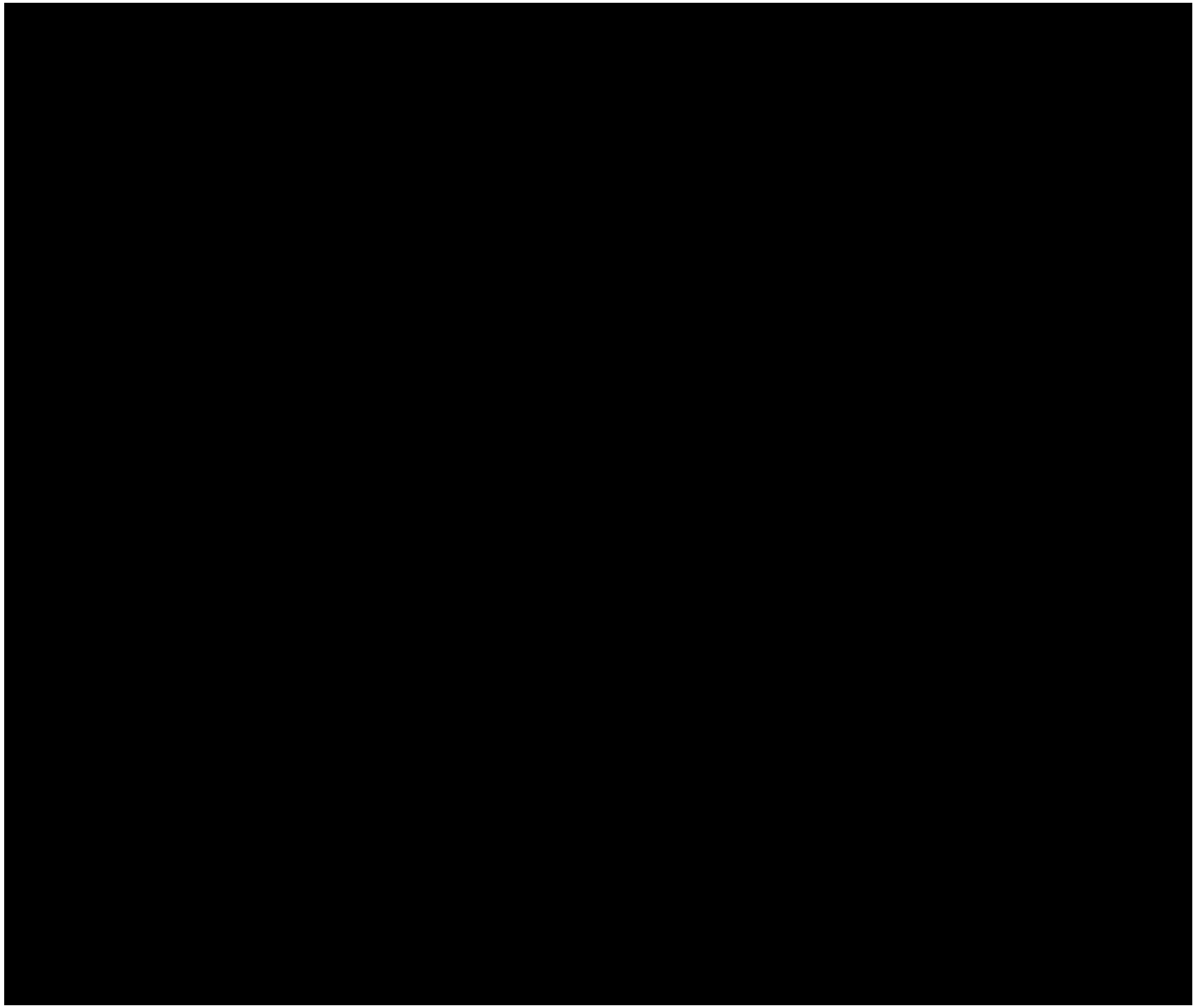
Internal Magnetic Probe

- A three-stem internal magnetic probe is positioned at the midplane of the confinement volume.
- Each stem contains an array of three-axis pickup coils and is insertable to a minimum major radius of 33.1 cm.
- Profiles were calculated along the probe chord for each injector and the spheromak and used for comparison.
- The following two movies show the field comparison throughout a shot at 5.8 kHz and 14.7 kHz operation.
- The top plot shows the field comparison, while the bottom plot shows the time in the shot and torodial current history.

Data and figures courtesy of Brian Victor, HIT-SI Group

Comparison at 5.8 kHz

Comparison at 14.7 kHz



Summary and Future Work

- Improvements to the PSI-TET equilibrium code have increased its speed, accuracy and solution space.
- The use of a hybrid MPI/OpenMP programming model shows scalability to large system sizes.
- Modification of solvers to accommodate variable lambda will move toward equilibria with injector BCs closer to the experiment.
- Scalable vector solvers using geometric multigrid are under development for full code scalability.
- Studies at higher resolutions on NERSC systems will be conducted