

M3D-C1 ZOOM Meeting

08/29/2022

Upcoming meetings and deadlines

CS Issues

1. Solver problem on Perlmutter_cpu
2. New Latex documentation
3. New meshing capabilities requested
4. Mesh adaptation update -
5. NERSC Time and NERSC policy change
6. Changes to github master since last meeting
7. Regression tests
8. isurface discussion
9. reproducibility problem

Physics Studies

1. Status of Chen Zhao paper
2. Chen DIII-D VDE case
3. Problem with BC in ITER problem
4. Stellarator version convergence
5. Anything else

In attendance

Steve Jardin

Dingyun Liu

Cesar Clauser

Andreas Kleiner

P. Sinha

Chen Zhao

Nate Ferraro

Brendan Lyons

Adelle Wright

Cesar Clauser

Mark Shephard

Seegyong Seol

Morteza

Usman

Upcoming Meetings

International Conference on Numerical Simulation of Plasma
August 30-September 2 2022 – online only

APS-DPP

Oct 17-21 In Spokane Washington

26th Workshop on MHD stability Control is on Oct 14-15

CTTS SciDAC meeting is on Sunday Oct 16 (TBA)

Solver Problems on Perlmutter_cpu

I have a large mesh (98K faces) with 128 partitions that I would like to run on Perlmutter_cpu. The base directory is:

/global/cfs/cdirs/mp288/Jardin/m3dnl/Perl_cpu/128-K

- Runs ok with mumps with 4 planes with 32 CPUs/NODE (Run01) and 64 CPUs/NODE (Run02)
- Same runs FAIL with superlu_dist (Run01a and Run02a)
- The following runs all failed with PETSc error

| Run | cpu/N | planes | solver |
|------------|--------------|---------------|---------------|
| Run03 | 64 | 36 | mumps |
| Run04 | 64 | 36 | superlu |
| Run05 | 64 | 8 | mumps |
| Run06 | 32 | 8 | mumps |
| Run07 | 32 | 32 | mumps |

New LaTeX Documentation

A cleaned version of M3DC1 user's guide is uploaded to M3DC1/doc and this version compiles on all machines using the command "pdflatex M3DC1.tex".

Updated since 8/01/22

mesh-gen.tex

doc.tex

Section 8: All C1input variables have been completed!

The LaTeX documentation has been added to the m3dc1.pppl.gov with the label NEW (in-progress). The old Word document is there as well.

Sill work to be done. Order of sections, obsolete sections, incomplete, etc.

New Meshing Capabilities Requested

3/28/22: Nate requested extension of M3DC1_meshgen with more regions

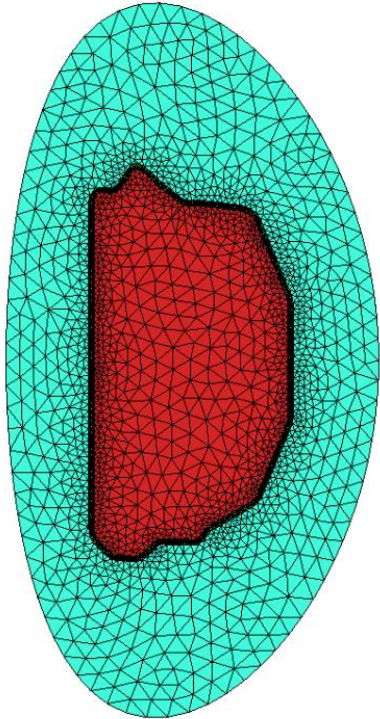
6/21/22: Mark suggested extending ToMMs (which XGC uses) instead

Nate noted that we need different info than XGC for electromagnetics

6/27/22: Mark proposed an extension to m3dc1_meshgen for an arbitrary # regions :

- # of nested closed loops
- The geometric definition of the first being the vacuum loop that is an indicated analytic expression and its parameters
- The geometry of the remaining loops will be a set of discrete points one loop at a time going from the outside to the inside
- # of island loops
- For each island loop indicate the two nested loops it lies between. Give its geometry in terms of a discrete set of points

Mesh adaptation update

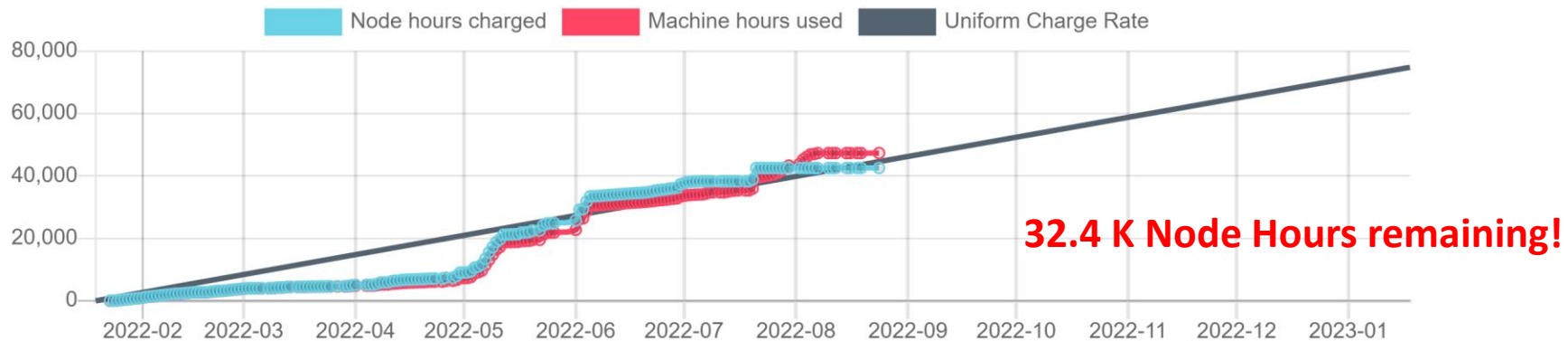


Mark Shephard: 8/22/22 As part of the development of the multi-face (also known as multi-region) capability Usman has added a new option for the finite wall thickness case that supports generating an anisotropic mesh between the two wall curves. In this case, a wall loop and a finite element wall thickness is provided. The finite thickness wall is defined in such a way that we can apply a "lofting" meshing function in Simmetrix that allows us to have a given number of elements between the two wall loops while having a different (most likely larger) node spacing on the wall loops. This can address Hanks request for having high through the wall resolution between the wall curves while not having the rest of the mesh be too fine. The attached figures demonstrate the application of this procedure.

The multi-face meshing and this new finite thickness wall feature and documentation of its use in the new M3D-C1 documentation will be available in the near future (hopefully within two weeks).

NERSC Time

mp288



- MP288 usage is on track. Both value and rate are ok.
- All users now have access to Perlmutter_cpu.
 - Some issues for large problems...see future slide
- We have 7000 GPU node hours as well.

NERSC Policy

- Perlmutter scratch file system down 8/22 – 8/31
- On 8/31, the “free of charge” phase on Perlmutter will end
- After this time, Perlmutter jobs will be charged to existing repos (mp288)
- Some free time will remain available, but it will have very low priority. (m3984)
- Energy Research Computing Allocations Process (ERCAP) proposals are due Oct 3, 2022
 - Separate proposals for Perlmutter _GPU and Perlmutter CPU
- Large users (Stellarator?) might consider requesting a ALCC award. (ASCR Leadership Computing Challenge). These are awarded in July.

Changes to github master --after 2022-8-01

Steve Jardin:

08/21/22: Completed documentation of C1input variables in Latex documentation

Nate Ferraro

08/10/22: Added get lcfs.pro for reading lcfs ppath: updated plot_lcfs and calling functions as appropriate

08/12/22: Simplified and modified method for assigning types to boundary nodes in preparation for new multiregion model with arbitrary number of zones

08/12/22: Allow user to set boundary type and zone type

08/23/22: Added error message when trying to restart a com. run from a 3D run

08/23/22: Improvement to create_map.pro for plotting stellarator fields

08/23/22: Blocked off coding in stellarator version that was causing hyperi to fail

08/23/22: Blocked off coding causing hyper to fail in stellarator version

08/25/22: Overhauled hyperviscosity coding to be compatible with mixed BC

08/23/22: More cleanup of old hyperv coding

08/25/22: Added hypervisc.f90

Changes to github master --after 2022-8-01

Riaz Usman

8/02/22: Updated work on MultiRegion Mesh Development

8/08/22 : Updates on MultiRegion Mesh Development. Vacuum Region is optional in this update

8/09/22: Minor changes in example cases

8/09/22: Function to put aligned vertices on two loops has been added

Seegyong Seol

08/04/22: Minor change in multi region mesh gen not to generate vacuum wall

08/10/22: adding sanity check and some minor changes in multi meshgen

08/15/22: Users Guide modified to reflect new m3dc1_meshgen development

08/15/22: fixing hard-coded mesh sizes for multi region model

08/15/22: removing files from doc/figures

08/25/22: minor clean-up for m3dc1_meshgen & M3dc1_mfmgen

Local Systems

- PPPL centos7(08/26/22)
 - 7 jobs **PASSED**
- PPPL greene (08/26/22)
 - 5 jobs **PASSED**
- STELLAR (08/26/22)
 - 7 regression tests **PASSED** on stellar
- TRAVERSE_gpu(08/26/22)
 - Compilation error

NERSC

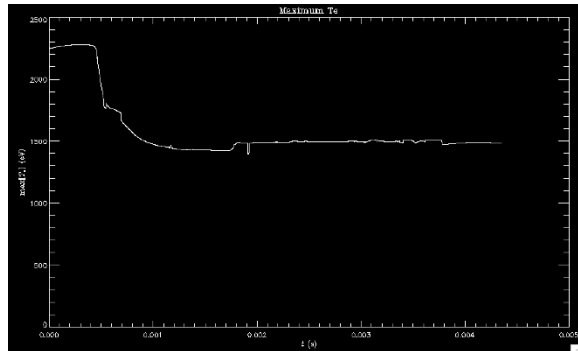
- Cori-KNL (08/27/2022)
7 regression tests **PASSED**
- Cori-Haswell (08/27/22)
7 regression tests **PASSED**
- Perlmutter (08/28/2022)
6 regression tests **PASSED**
NCSX **FAILED** with very small difference in C1ke
- Perlmutter_cpu (08/28/22)
all jobs **FAILED** with segmentation fault!

isurface

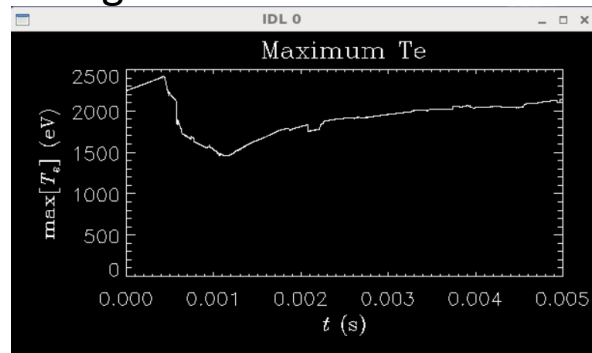
- `isurface=1` retains the surface terms from the integration –by-parts for the boundary terms: `isurface=0` neglects them
- Are there any problems where setting `isurface=1` leads to a better solution than `isurface=0`
- There are problems where `isurface=1` leads to a worse solution (numerical instability)
- Should we remove this option? It would lead to simplified code.

Reproducibility problem

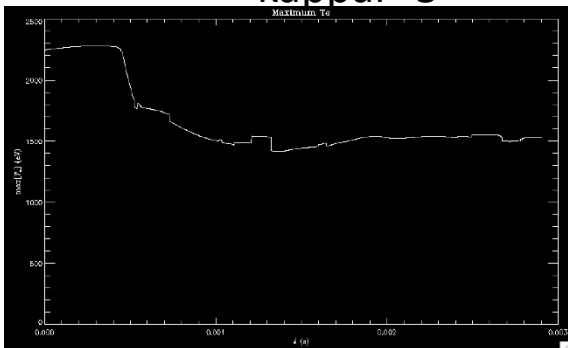
Dingyun, eta_fac=264, beam_rate=1.6E23, kappar=10



Original run from 2018



kappar=5



Possible explanation: new coding was added:

```
if((ipres.eq.0 .and. numvar.ge.3) .or. (ipres.eq.1 .and. numvar.lt.3))  
then
```

! Add ion heat flux

$$\text{tempx} = (1. + \text{kappai_fac} * (1. - \text{pefac}) / \text{pefac}) * \text{tempx}$$

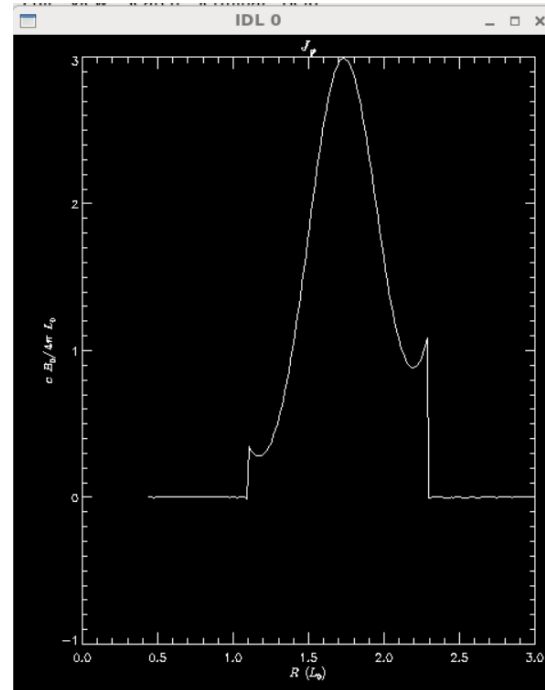
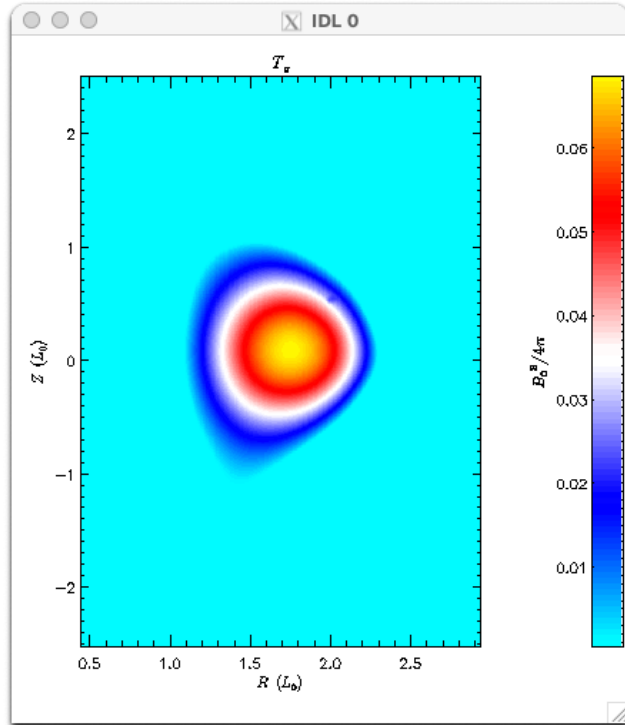
For both kappa and kappar

Papers in Preparation

- Chen Zhao, C. Liu, et al, “Simulation of DIII-D disruption with pellet injection and runaway electron beam”
 - ***Chen is rerunning this now with a lower isotropic thermal conductivity***

Note: May want to plot total thermal energy vs time to compare with experiment....not T_{e_max}

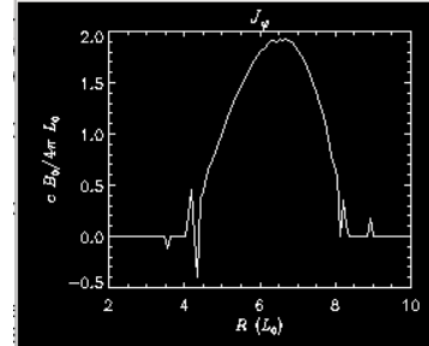
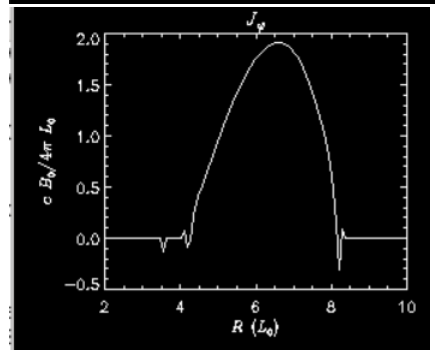
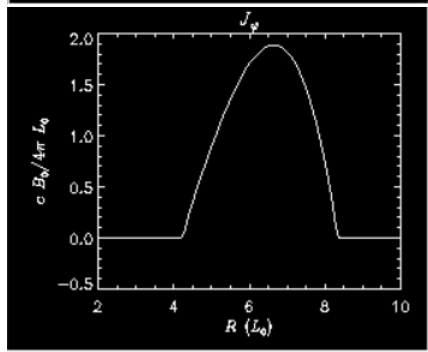
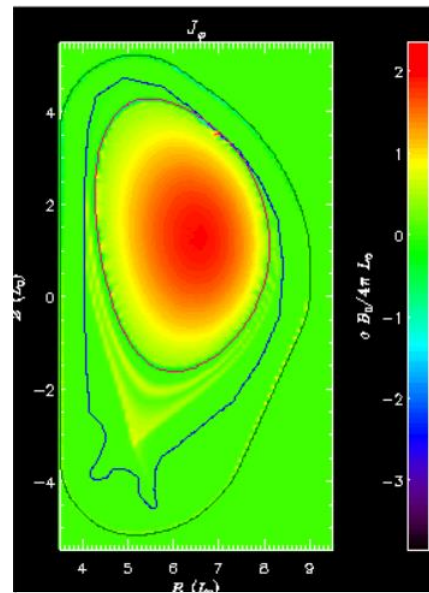
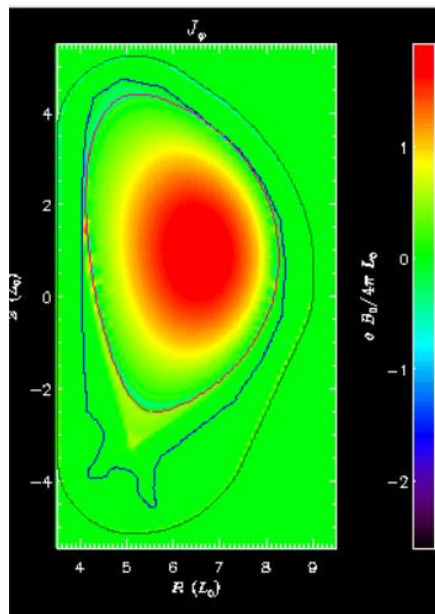
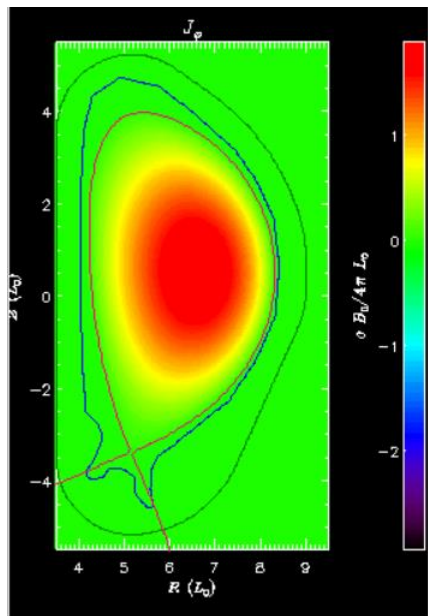
Chen DIII-D VDE case



This current profile will not work for a VDE case.
Current density must go smoothly to zero!!

ITER 2D VDE

/scratch/gpfs/sjardin/ITER2D/ITER-03NM-H-64




ITER Boundary Conditions

6/27/22 Brendan Lyons

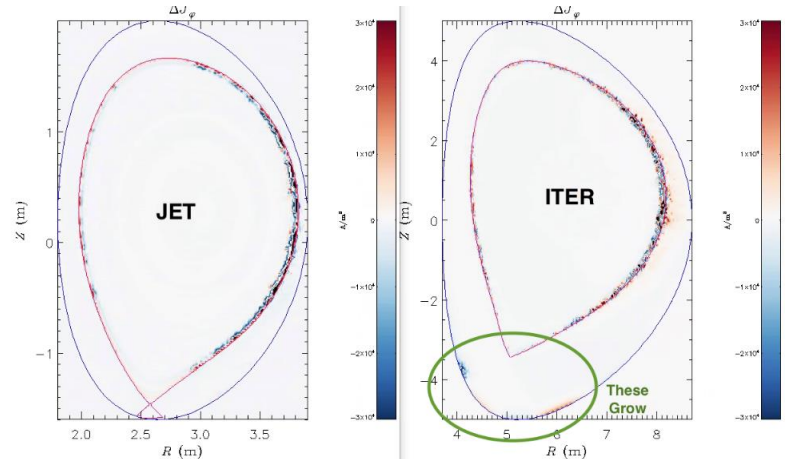
I'm still struggling to get an ITER case to run with the new inoslip_pol=2 boundary condition. I can use it in DIII-D, JET, and KSTAR runs without too much of a problem, but ITER develops an instability at the boundary right away. This is hindering our ability to bring M3D-C1 to bear on ITER SPI modeling,

7/11/22 S. Jardin

Only solution I have found is to set inoslip_pol=1. Is this acceptable? 

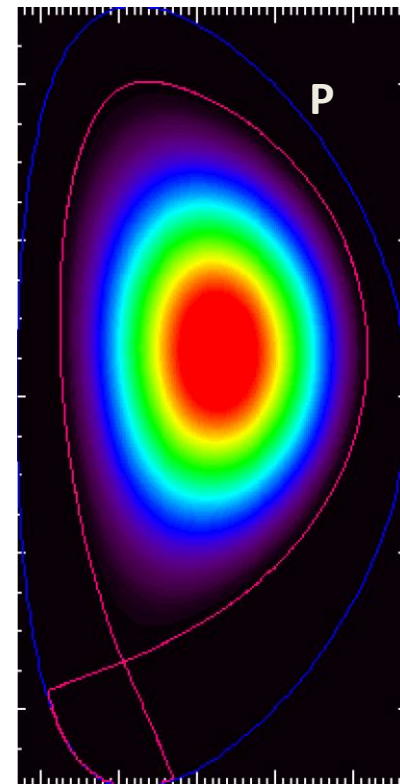
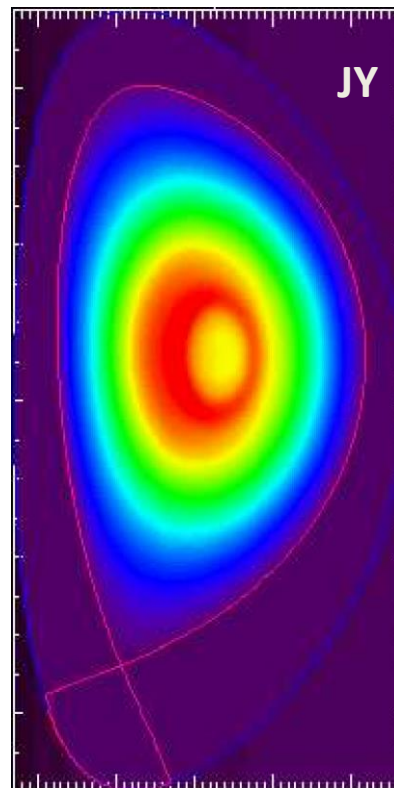
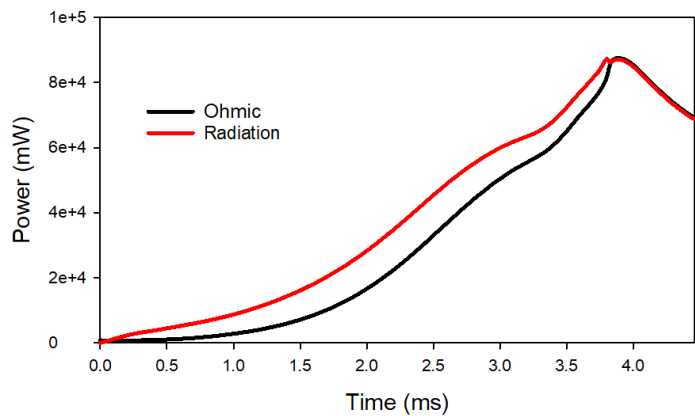
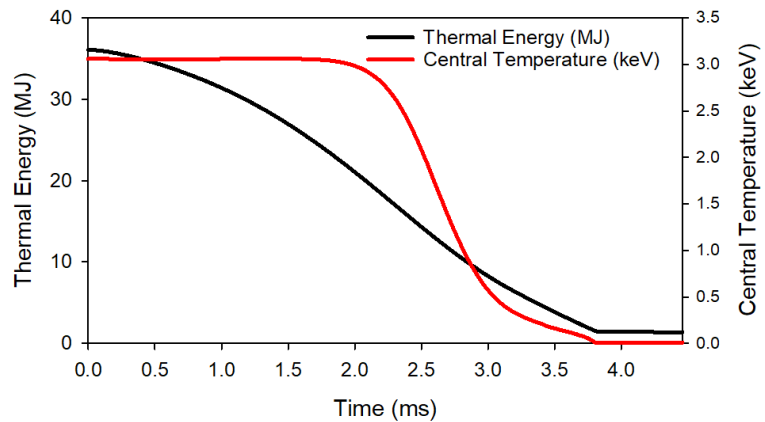
From Michael Lehnen to Brendan 8/24/22

The boundary condition problem is a severe one and maybe you can communicate with Steve Jardin about how to solve it.



ITER 2D inoslip_pol=1 ...cont

L-mode profiles



ITER 2D inoslip_pol=1

kprad_rad

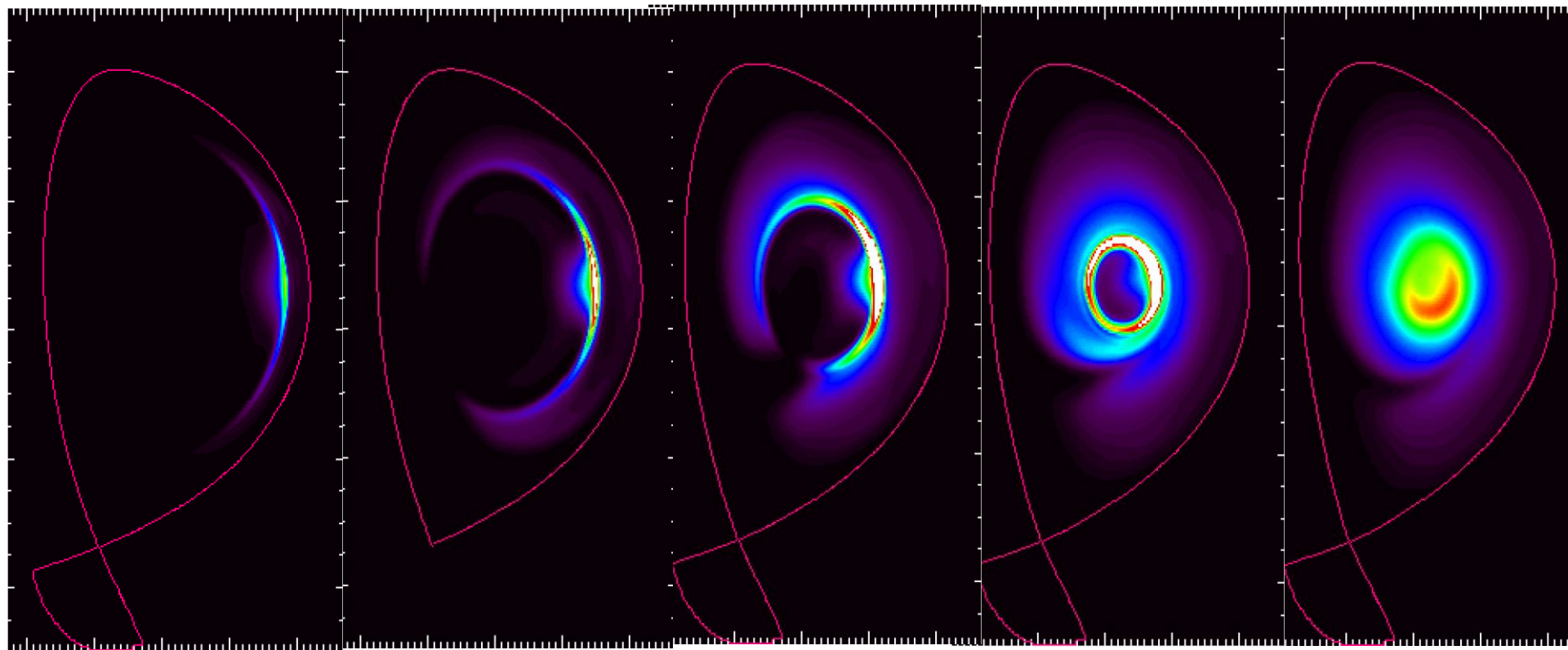
0.89 ms

1.78 ms

2.67 ms

3.56 ms

4.46 ms



Stellarator Version Convergence

Adelle posted on SLAC on 7/14/22:

We're running into a bit of an issue with the stellarator version, and I was wondering if someone could please take a look.

- In the stellarator version, we have more difficulty getting the velocity solve to converge. In practice, this means we run at viscosities that are 1-2 orders of magnitude higher than in tokamaks. The thought is that the preconditioner is not as effective.
- Based on the fact that quasihelically symmetric (QH) cases are proving much more difficult to run than quasiaxisymmetric (QA) cases (although those are very challenging too), the issue might be specifically related to the non-quasiaxisymmetric terms in the velocity equation.
- If there is a way to improve the preconditioning, I think that would really improve the performance of the stellarator version, especially if it allows us to decrease the viscosity.

That's All I have

Anything Else ?

No Meeting Sept 5 (Labor Day)

I will be on vacation until Sept 16

Meeting with LBL on Oct 3

Upgrade to impurity radiation Routines

Brendan Lyons wrote to martin.omullane at ADAS on 6/22/22

Any Response?