# M3D-C1 ZOOM Meeting

08/09/2021

#### **Announcements**

#### **CS** Issues

- 1. Intel-MPI on stellar
- 2. Mesh adaptation update
- 3. NERSC Time
- 4. Changes to githuon b master since last meeting
- 5. Regression tests
- 6. Progress on optimizing the matrix assembling on GPUs Chang Liu

#### **Physics Studies**

- 1. Energy conservation with itemp=0,1, ipres=0,1 -- Lyons
- 2. Resistive wall mode in a periodic Cylinder Strauss
- 3. Sawteeth with 50% runaways Chen Zhao

Note: meeting minutes posted on m3dc1.pppl.gov

# In attendance

Steve Jardin

Hank Strauss

Patrick Kim

Mark Shephard

Jin Chen

Adelle Wright

Nate Ferraro

**Andreas Kleiner** 

Chen Zhao

**Brendan Lyons** 

Chang Liu

Seegyoung Seol

Priyanjana Sinha

## **Announcements**

- Virtual Sherwood Meeting August 16-18
  - Registration until August 9 (Today)
  - No m3dc1 meeting August 16
- APS Nov 8-12
  - Meeting will be IN PERSON with virtual option
  - M3D-C1 Invited talks by C. Liu, A. Wingen
  - CTTS meeting? Will DOE allow travel?
- EPS 6/27 7/1 2022 in Maastricht, Netherlands
  - Nominate invited speakers by 29 October 2021

# stellar.princeton.edu

#### From Adelle Wright 8/5/2021:

I tested intelmpi on the stellarator version for a 3D fixed boundary case (24 planes, 6 nodes). There was no noticeable speedup but the memory usage was roughly halved.

While it's probably just that I did not configure everything correctly, I did have issues with post-processing (trace and IDL) when the modules needed for intelmpi were loaded.

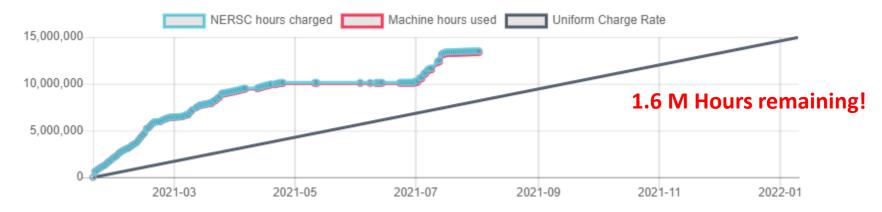
**Update?** 

# **Mesh Adaptation Update**

RPI?

## **NERSC Time**

#### mp288



- mp288 received 10M Hrs for CY 2021
- Initial allocation exhausted by May 1
- John Mandrekas (DOE) added 5M Hrs additional
- More time may be possible if this is exhausted
- Pearlmutter time will not be charged for this FY
- We are NESAP Tier 2. Machine not yet ready. Phase-I w GPUs

# Changes to github master since 08/02/21

No Changes!

# **Local Systems**

- PPPL centos7(08/02/21)
  - 6 regression tests PASSED on centos7:
- PPPL greene (08/02/21)
  - 5 regression tests PASSED on greene (m3dc1)
- STELLAR (08/02/21)
  - 6 regression tests PASSED on stellar
- TRAVERSE(03/29/21)
  - Code compiles
  - Regression test failed: split\_smb not found in PATH

# Other Systems

- Cori-KNL (2/08/2021)
  - 6 regression tests passed on KNL
- Cori-Haswell (6/29/2021)
  - 6 regression tests passed
- PERSEUS
  - All 6 regression tests PASSED on perseus (J. Chen, 9/04/20)
- MARCONI
  - All regression tests PASSED on MARCONI (J. Chen, 9/04/20)
- CORI GPU (10/26)
  - ??

# Progress on optimizing the matrix assembling on GPUs

**Chang Liu** 

# Discrepancies in Heat Flux Diagnostic

by

**Brendan C. Lyons** 

August 2nd, 2021



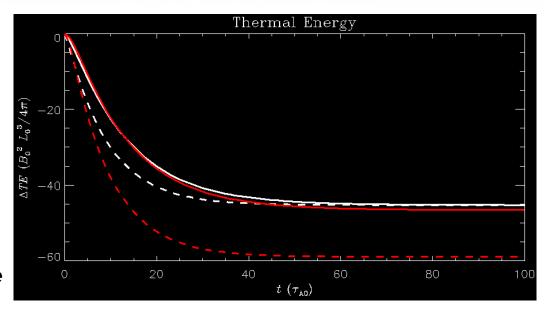
#### **General Comments**

- Based on a 2D ITER L-mode simulation
- Heat conduction should be the dominant source/sink
  - No ohmic heating: iohmic\_heating=0
  - No impurities
  - Kinetic energy << Thermal energy</li>
- In figures, white is the change thermal energy, red is the integrated flux\_thermal
- All folders in /pfs/nobackup/blyons/kappa\_test/ on portal
- "Perpendicular" dominant case: kappat=1e-1, kappar=1e-8
- "Parallel" dominant case: kappat=1e-1, kappar=1e+4
- Boundary conditions
  - itemp=1 cases use iconst\_t=1 with tebound=tibound=2e-5
  - itemp=0 cases use iconst\_p=1, since iconst\_t=1 doesn't work for pressure equations
- Lowering time step doesn't seem to make a qualitative difference in my tests



# Two Temperature Equations: ipres=1, itemp=1

- Perpendicular (solid)
  - kth\_krl\_ip1\_it1/
  - Not terrible, but not good
- Parallel (dashed)
  - kth\_krh\_ip1\_it1/
  - Significant excess in the calculated heat flux
- These discrepancies are what has made me look into this problem in the first place, since they mess up energy accounting



For itemp=1, ipres=1, larger error for  $\kappa_{11}$  large



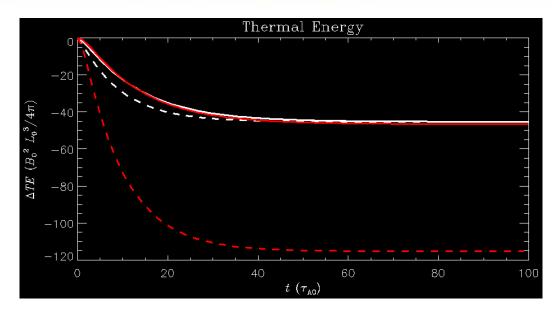
# Single Temperature Equation: ipres=0, itemp=1

#### Perpendicular (solid)

- kth\_krl\_ip0\_it1/
- Same as ipres=1

#### Parallel (dashed)

- kth\_krh\_ip0\_it1/
- Roughly double the heat flux even though thermal decay is only very slightly different
- Parallel heat flux appears to be double counted in flux\_heat()
- Maybe because it accounts for the ion and electron temperature gradients?



For itemp=1 ipres=0 gives larger error than ipres=1



# Single Pressure Equation: ipres=0, itemp=0

#### Very strange behavior

- Temperature becomes lower in core than edge
- Something wrong with heat flux implementation for open field lines?

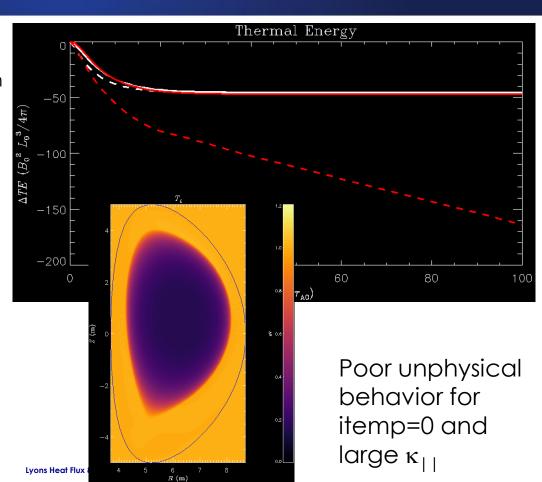
#### Perpendicular (solid)

- kth\_krl\_ip0\_it0/
- No qualitative impact from temperature hole

#### Parallel (dashed)

- kth\_krh\_ip0\_it0/
- Shows persistent heat flux even after thermal energy is dissipated





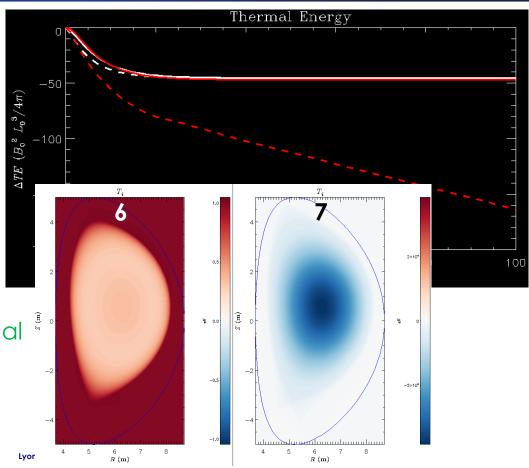
# Two Pressure Equations: ipres=1, itemp=0

#### Even stranger behavior

- Ion temperature because huge and negative between outputs 6 and 7
- No idea what to make of this
- Traces are basically identical to ipres=0
- Perpendicular (solid): kth\_krl\_ip1\_it0/
- Parallel (dashed): kth\_krh\_ip1\_it0/

Poor unphysical behavior for itemp=0 and large  $\kappa_{11}$ 





#### Conclusions

- Something is off with the flux\_heat() diagnostic
- Nature of discrepancy is dependent on the ipres and itemp
- There may be something wrong about how the heat flux itself, not just the diagnostic, is implemented in the code for itemp=0



## Do not use itemp=0 when kappar.ne.0

$$Itemp = 0$$

$$\frac{\partial p}{\partial t} = \dots + \nabla \cdot \kappa_{\parallel} \frac{\mathbf{B} \mathbf{B}}{B^{2}} \cdot \nabla \left( \frac{p}{n} \right)$$

$$= \dots + \nabla \cdot \kappa_{\parallel} \frac{\mathbf{B} \mathbf{B}}{B^{2}} \cdot \left( \frac{1}{n} \nabla p - \frac{p}{n^{2}} \nabla n \right)$$

This term is a problem since p and n are solved separately. Will cause very large errors and possibly numerical instability

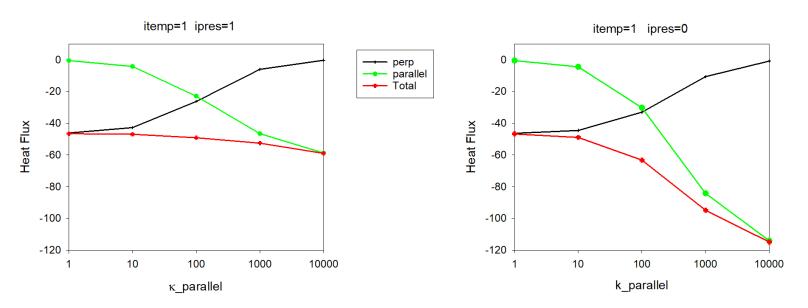
$$n\frac{\partial T}{\partial t} = \dots + \nabla \cdot \kappa_{\parallel} \frac{\mathbf{B}\mathbf{B}}{\mathbf{R}^2} \cdot \nabla (T)$$
 Well behaved, diagonally dominant

$$\frac{1}{R^{2}} \left[ \hat{n} \cdot \nabla T_{e} + \kappa_{i} \hat{n} \cdot \nabla T_{i} \right] \qquad \text{HF\_perp}$$

$$\frac{1}{R^{2}} \left[ \hat{n} \cdot \nabla \psi \times \nabla \varphi \right] \left[ \nabla \psi \times \nabla \varphi \cdot \left( \kappa_{\parallel} \nabla T_{e} + \kappa_{\parallel} \nabla T_{i} \right) \right] \qquad \text{HF\_par}$$

Problem seems to be with the parallel heat flux with ipres=0

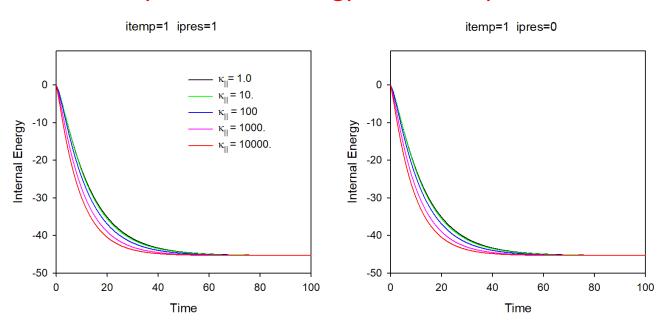
## Parallel heat flux is much larger for ipres=0



#### Note:

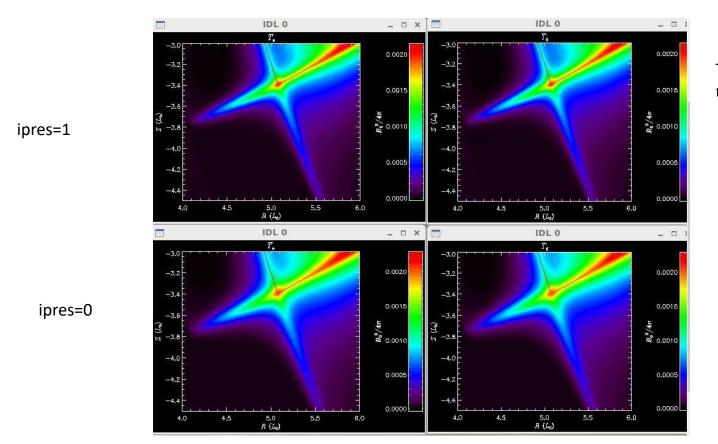
- Red line (total heat lost) should be horizontal if energy conserved for all  $\kappa_{11}$
- Perpendicular heat loss almost the same for ipres=1 and ipres=0
- Parallel heat loss at large  $\kappa_{||}$  slightly too large for ipres=1, much too large for ipres=0

# Decay of internal energy similar for ipres=1,0



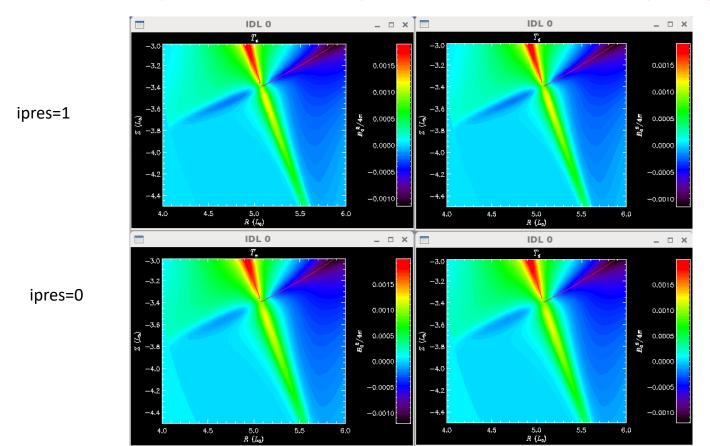
Only weakly dependent on  $\kappa_{\vert\vert}$  for both cases, and very similar

## dTe,i/dy profiles look nearly the same in SOL for itemp=1, ipres=0,1



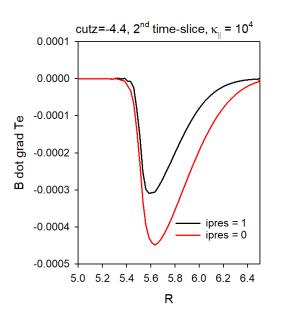
Time slice 2  $\kappa_{||} = 10^4$ 

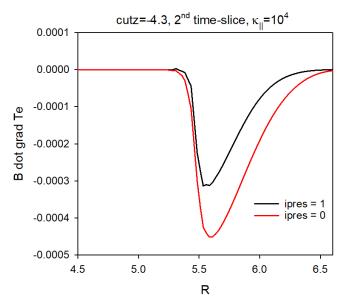
# dTe,i/dx profiles look nearly the same in SOL for itemp=1, ipres=0,1



Time slice 2  $\kappa_{||} = 10^4$ 

# B $\cdot \nabla$ Te along z=-4.4, 4.3 much larger for ipres=0





## Perpendicular temperature equation for ipres=0

$$n_{e} \dot{T}_{e} = \nabla \cdot \kappa \nabla T_{e}$$

$$n_{i} \dot{T}_{i} = \nabla \cdot \kappa (\text{kappai\_fac}) \nabla T_{i}$$

$$T_{i} = \frac{(1 - \text{pefac})}{\text{pefac}} T_{e}$$

$$(1)$$

$$n_i \frac{\text{(1-pefac)}}{\text{pefac}} \dot{T}_e = \nabla \cdot \kappa (\text{kappai\_fac}) \frac{\text{(1-pefac)}}{\text{pefac}} \nabla T_e$$
 (2)

Equation for  $T_e$  that conserves energy is obtained by adding (1)+(2)

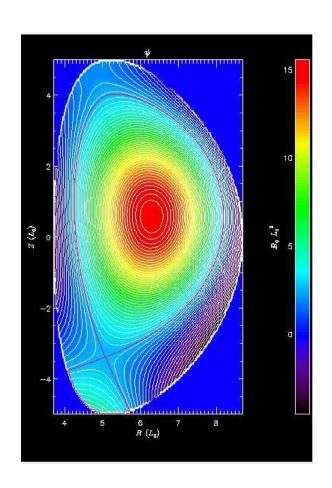
$$\left[n_e + n_i \frac{(1\text{-pefac})}{\text{pefac}}\right] \dot{T}_e = \nabla \bullet \left[1 + (\text{kappai\_fac}) \frac{(1\text{-pefac})}{\text{pefac}}\right] \kappa \nabla T_e$$

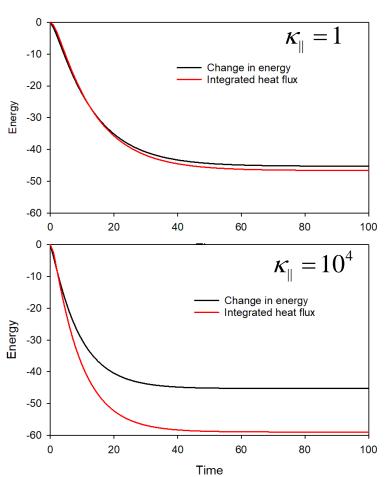
#### Same needs to be done for parallel heat conduction for ipres=0!

for ipres=0, replace (in temperature\_lin)

kappar --> 
$$\left| 1 + \text{kappai\_fac} \frac{(1 - \text{pefac})}{\text{pefac}} \right|$$
 kappar  $\leftarrow$  This needs to be changed

## Parallel heat flux term requires high resolution





Now, exactly the same results for ipres=1 and ipres=0 for itemp=1.

Much better energy conservation at small values of  $\kappa_{\text{II}}$ 

Large  $\kappa | |$  energy conservation may improve if mesh is refined

# Problem Solved!

- 1. Do not use itemp=0 if kappar .ne. 0
- 2. To make itemp=1, ipres=1 and itemp=1, ipres=0 identical

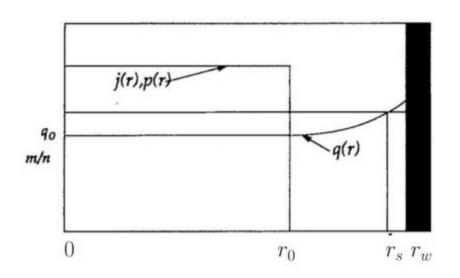
for ipres=0, replace (in temperature\_lin)

$$kappar --> \left[1 + kappai\_fac \frac{(1 - pefac)}{pefac}\right] kappar$$

- 3. To get more precise energy balance for large kappar, may need to increase spacial resolution in SOL:
- I have not yet committed the change as it makes one of the regression tests fail (RMP\_nonlin)

# Resistive Wall Mode in Periodic Cylinder

H. Strauss, 8/9/21



Plasma resistivity? What is *f* ?

**RWM** 

$$\gamma \tau_{wall} = -m \frac{1 - (m - nq)}{1 - (m - nq) - (r_0/r_w)^{2m}}$$

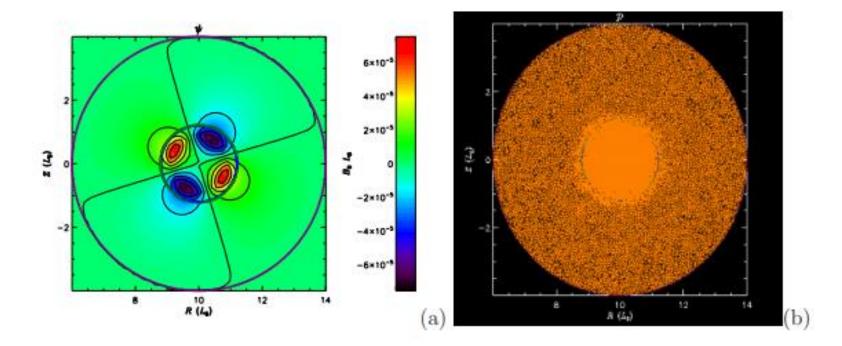
**RWTM** 

$$\gamma \tau_A = \frac{c_0}{S^{1/3} S_{wall}^{4/9}}$$

$$c_0 = 2.46 \left(\frac{q'r_s}{q}\right)^{2/9} f^{4/9} = 2.46 f^{4/9}$$

$$f = \frac{(r_s/r_w)^{2m}}{[1 - (r_s/r_w)^{2m}]^2}$$

-



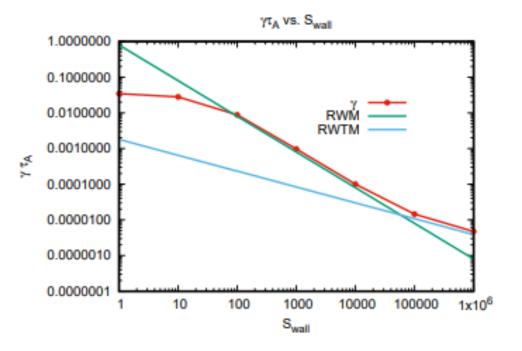


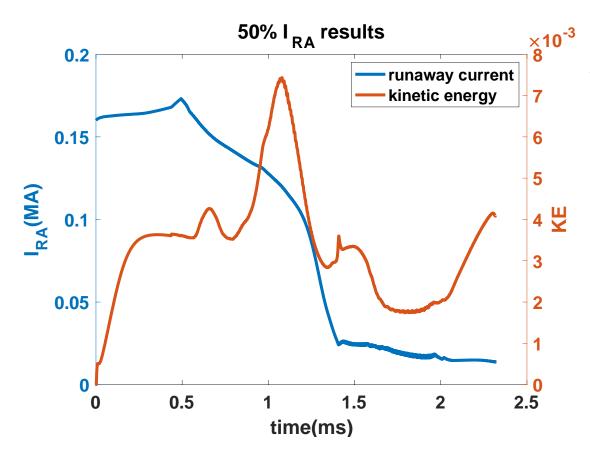
Fig.2(a) shows linear  $\psi$  for the case  $S_{wall} = 10^4$ . Fig.2(b) shows the adapted mesh used in all the cases. The mesh has a thin wall,  $\delta = 0.02$ . Fig.3 shows growth rate  $\gamma$  as a function of  $S_{wall}$ . For  $S_{wall} \ge 10^5$ , the most ustable mode appears to be a RWTM. The straight line fits are to  $S_{wall}^{-1}$  for a RWM and  $S_{wall}^{-4/9}$  for a RWTM.

Dependence on η?
Does mode structure change?

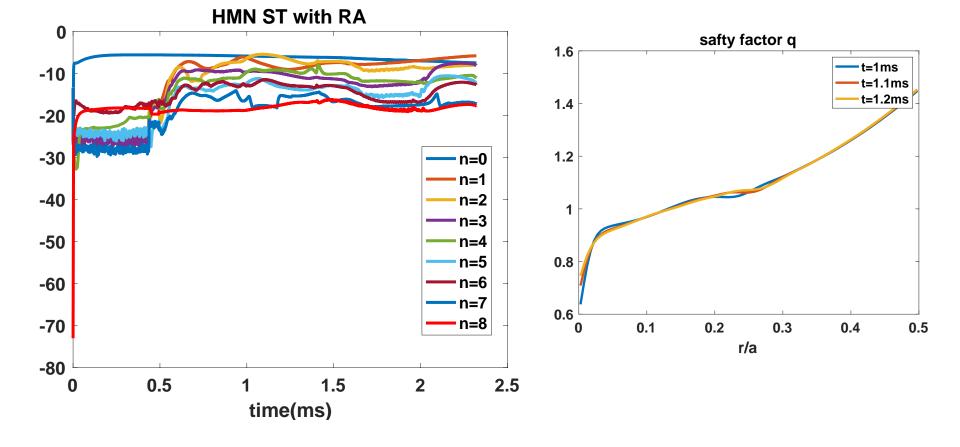
# Sawteeth with 50% runaway

08092021

current

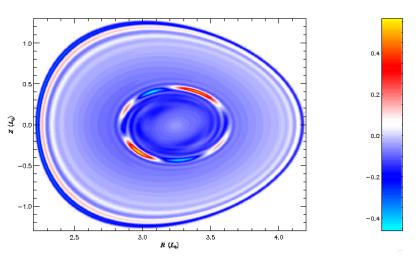


 The runaway electron current dropped dropped to nearly 0 at about t=1.1ms by the MHD instability during ST.



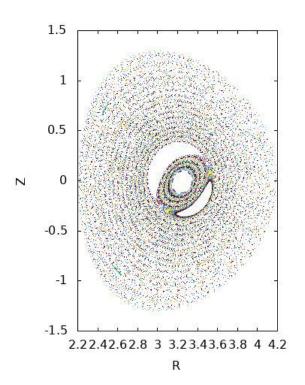
The highest is n=2 at t=1.1ms

#### Runaway current density profile at t=1.1ms

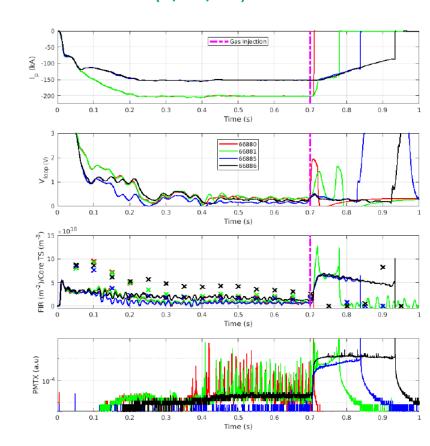


Maybe n=2 m=3 mode

#### Poincare plot at t=1.1ms



- Sawteeth expel Res
  - Seed population lost HXR spikes
  - No RE beam after MGI
- Lower I<sub>p</sub> removed Sawteeth
  - HXR spikes gone
- Stable RE beams produced
- Sharp drop in I<sub>p</sub> indicates larger Ohmic current contribution
  - Sharp drop in I<sub>D</sub> if fewer REs (green)
  - Significant RE current before MGI



From Umar Sheikh

(7/22/21)

# That's All I have

Anything Else?