M3D-C1 ZOOM Meeting

10/26/2020

Agenda

1. CS Issues
    1. GPU solve status and skeleton codes Jin Chen
    2. Local systems
    3. Other systems
    4. NERSC Time
    5. Changes to github master since last meeting
    6. Explicit method for Alfven Wave Simulation – Chang Liu
    7. Request to replace bf=f with bfp=df/d(phi)..
2. Physics Studies
    1. Status of first coupled M3D-C1/LP Simulation .. Lyons/Samulyak
    2. Grad-B drift in M3D-C1 -Jardin
    3. Sawtoothing discharge with RE – Chen Zhao / Jardin
    4. Status of other simulations
    5. Other?

GPU solve status – and Skeleton codes

Jin Chen to update

1. OpenACC skeleton code

Local Systems

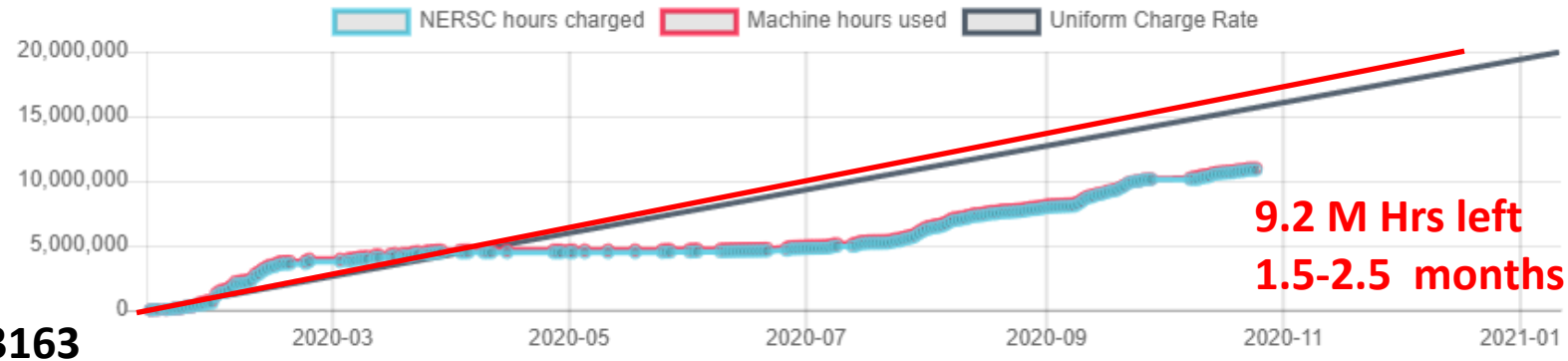
- PPPL centos7(10/26)
  - All 6 regression tests PASSED on centos7:
- PPPL greene (10/26)
  - 5 regression tests PASSED
  - No batch file found for pellet
- EDDY (10/26)
  - All 6 regression tests PASSED
- TRAVERSE(10/26)
  - Code compiles
  - Regression test failed: split_smb not found in PATH
  - Have not yet tried shipping .smb files from another machine

Other Systems

- Cori-KNL (10/26)
  - 6 regression tests passed on KNL
- Cori-Haswell (10/26)
  - 5 regression tests passed
  - KPRAD_RESTART did not pass, but differences are very small in velocity variables. All magnetic and thermal good. Similar difference as Cori-KNL
- 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)
  - I applied and received an account on cori-gpu

NERSC Time

mp288



m3163

Closed for general use

- Should be enough mp288 time to last until new PU/PPPL computer arrives in fall – red line is linear usage until Dec 15 (New estimated arrival date)
- John Mandrakes (DOE) has added ~ 8 M hours to mp288 on 10/21/2020.

Changes to github master since last meeting

- J. Chen
  - 10/22/20: Added skeleton code and its openacc variation
- Yao Zhou for Chen Zhao
  - 10/21/20: corrected the wrong fp terms in b3bfeta and b3ffeta
- N. Ferraro
  - 10/22/20: Added “phi” array to mesh data in 3D calculation
  - 10/22/20: Added function to read vector attributes from hdf5 file
  - 10/22/20: updated toroidal restart to work with arbitrary number of planes / packing
  - Fixed compile time error in 2D case

Explicit Method for Alfven Wave Simulation

Chang Liu to present

Request to replace bf = f with bfp = df/dφ

$$\mathbf{A} = R^2 \nabla \varphi \times \nabla f + \psi \nabla \varphi - F_0 \ln R \hat{Z}$$

$$\mathbf{B} = \nabla \psi \times \nabla \varphi - \nabla_\perp f' + F \nabla \varphi$$

$$F \equiv F_0 + R^2 \nabla \bullet \nabla_\perp f \qquad \text{(note: } f' \equiv \partial f / \partial \varphi\text{)}$$

Presently,

$$\dot{F} = \ldots$$

$$R^2 \nabla \bullet \nabla_\perp f = F - F_0$$

Proposed (by Yao) to eliminate one derivative on f

$$\dot{F} = \ldots$$

$$R^2 \nabla \bullet \nabla_\perp f' = F'$$

Phase II: replace f with fp in calculations

1. In subroutine derived_quantities

```
789  ! vector potential stream function
790  if(imp_bf.eq.0 .or. ilin.eq.0 .or. ntime.eq.0) then
791    if((i3d.eq.1 .or. ifout.eq.1) .and. numvar.ge.2) then
792      if(myrank.eq.0 .and. iprint.ge.2) print *, "  f", ilin
793      if((ilin.eq.0 .and. eqsubtract.eq.1) .or. eqsubtract.eq.0) then
794        if(itor.eq.0) then
795          temp = bzero
796        else
797          temp = bzero*rzero
798        end if
799        call add(bz_field(ilin),-temp)
800      endif
801      call solve_newvar1(bf_mat_lhs,bf_field(ilin),mass_mat_rhs_bf, &
802          bz_field(ilin), bf_field(ilin))
803      if((ilin.eq.0 .and. eqsubtract.eq.1) .or. eqsubtract.eq.0) call add(bz_field(ilin), temp)
804    endif
805  end if
```

Remove

2. In m3dc1_nint.f90: Change

call eval_ops(itri,bf_ext,bfx79,rfac) → call eval_ops(itri,bfp_ext,bfpx79,rfac)

call eval_ops(itri,bf_field(1),bf179,rfac) → call eval_ops(itri,bfp_field(1),bfp179,rfac)

call eval_ops(itri,bf_field(0),bf079) → call eval_ops(itri,bfp_field(0),bfp079)

3. In time_step.f90, time_step_split.f90, time_step_unsplit.f90: Change

bf_field → bfp_field everywhere

4. In restart_hdf5.f90

no need to add h5r_read_field for bfp_field. We can recompute bfp from F'

bfp_ext ?

5. In particle.f90

Can we replace continue to use bf_field (at least for the time being)

7. In ludef_t.f90

In bf_equation_lin, change:

```
ssterm(:,bz_g) = intx2(trial(:,:,OP_1),lin(:,OP_1))
```

With

```
ssterm(:,bz_g) = intx2(trial(:,:,OP_1),lin(:,OP_DP))
```

In bf_equation_nolin, just replace coding with

```
r4term = 0
return
```

bft79	bf079	bf179	bftx79
auxiliary_fields		auxiliary_fields.f90	
bootstrap.f90	bootstrap.f90		
diagnostics.f90			diagnostics.f90
electric_field.f90	electric_field.f90	electric_field.f90	electric_field.f90
ludef_t.f90	ludef_t.f90	ludef_t.f90	ludef_t.f90
m3dc1_nint.f90	m3dc1_nint.f90	m3dc1_nint.f90	m3dc1_nint.f90
metricterms_new.f90		metricterms_new.f90	metricterms_new.f90
temperature_plots.f90		temperature_plots.f90	temperature_plots.f90
transport.f90			transport.f90
electrostatic.potential.f90	init_basicj.f90		
gyroviscosity.f90			
			parallel_heat_flux.f90

bft79(:,OP_DZP) → bfpt79(:,OP_DZ)
bft79(:,OP_DRP) → bfpt79(:,OP_DR)
bft79(:,OP_DZPP) → bfpt79(:,OP_DZP)
bft79(:,OP_DRPP) → bfpt79(:,OP_DRP)
bft79(:,OP_DRRP) → bfpt79(:,OP_DRR)
bft79(:,OP_DZZP) → bfpt79(:,OP_DZZ)
bft79(:,OP_DRZP) → bfpt79(:,OP_DRZ)
bft79(:,OP_LPP) → bft79(:,OP_LP)
bft79(:,OP_GSP) → bft79(:,OP_GS)

Etc for bf079, bf179, bftx79.

Make these substitutions in all of the above routines

metricterms_new.f90

v1psif(x, x,f)
v1bf(x,x,f)
v1huf(x,x,f)
v1hvf(x,x,f)
v1hchif(x,x,f)
v2psif1(x,x,f)
v2psif2(x,x,f)
v2bf(x,x,f)
v2ff(x,f,f)
v2huf(x,x,f)
v2hvf(x,x,f)
v2hchif(x,x,f)
v3psif(x,x,f)
v3bf(x,x,f)
v3huf(x,x,f)
v3hvf(x,x,f)
v3hchif(x,x,f)
b1jrefeta(x,x,f,x,x)
B1feta(x,f,x)
b1fu(x,f,x)
b1fv(x,f,x)
b1fchi(x,f,x)

b1psifn1(x,x,f,x)
b1psifn2(x,x,f,x)
b1bfn1(x,x,f,x)
b1bfn2(x,x,f,x)
bipsifd1(x,x,f,x)
b1psifd2(x,x,f,x)
b1bfd1(x,x,f,x)
b1bfd2(x,x,f,x)
b2feta(x,f,x)
b2jrefeta(x,x,f,x,x)
b2fv(x,f,x)
b2psifn(x,x,f,x)
b2bfn(x,x,f,x)
b2psifd(x,x,f,x)
b2bfd(x,x,f,x)
b3psifeta(x,x,f,x,x)
b3bfeta(x,x,f,x,x)
b3ffeta(x,f,f,x,x)
b3pefd(x,x,f,x)
tepsifkappar(x,x,f,x,x,x)
tebfkappar(x,x,f,x,x,x)
teffkappar(x,f,f,x,x,x)

bootstrap.f90

bs_b1psibf(x,x,x,f)
bs_b2psibf(x,x,x,f)

In each of these routines, remove the last P in OP_XP for only the argument marked f

S. Jardin and Y. Zhou plan to independently make these changes in new branches on Oct 27 and to compare files

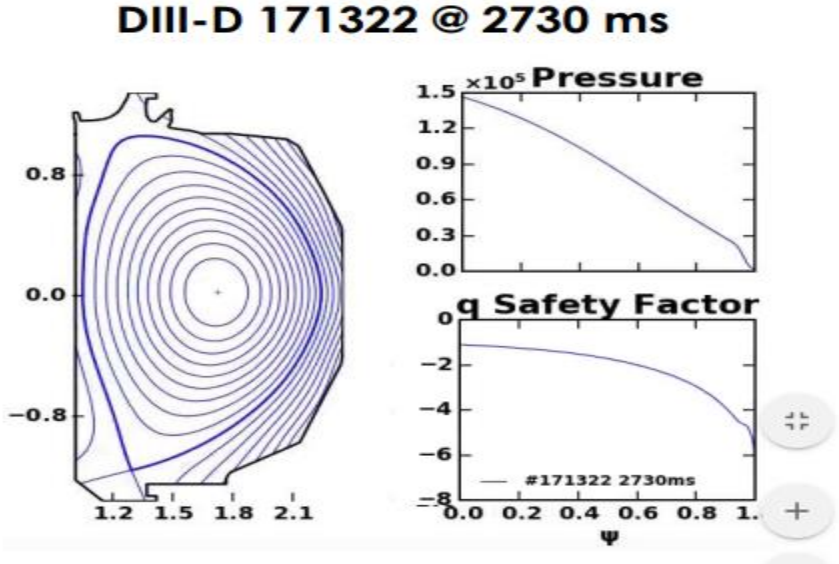
Comments from Yao Zhou 10/21

(1) bftx79 in helicity (diagnostics.f90) cannot be replaced, and hence bf079 etc should be kept and evaluated in m3dc1_nint.f90.

(2) Terms using bf but missing from previous page
b1fj b1psi2bfpe
b2fj
b2psi2bfpe
p1psifkappar
p1psifpnkappar
p1bfkappar
p1bfpnkappar
p1ffkappar
p1ffpnkappar
p1qfkappar
q1pf
j1b2ipsif
j1b2ifb
j1b2iff

Status of First Coupled M3D-C1 / LP Simulation

- **Iterate independent simulations of MHD and LP codes**
  - Run pellet injection in MHD code with analytic, Parks ablation formula
  - Send plasma states along pellet path to LP code to compute ablation rate at each point
  - Rerun MHD codes with LP ablation rates
  - Iterate between codes until convergence
- **Test case for DIII-D modeling**
  - 1 mm Ne pellet using extruder parameters
  - 160606, standard case for SPI modeling
  - 171322, super-H target for upcoming small-pellet ablation experiment
  - Latter will be used for predict-first of experiment



8/10/20 – proposed

10/5/20 – Brendan sent data from a 2D run

10/7/20 – Roman requested more concise data from around pellet vs time

10/20/20 – Brendan developed and documented postprocessor for LP ablation code. Will be posted today on m3dc1.pppl.gov

Grad-B drift in M3D-C1—HF side

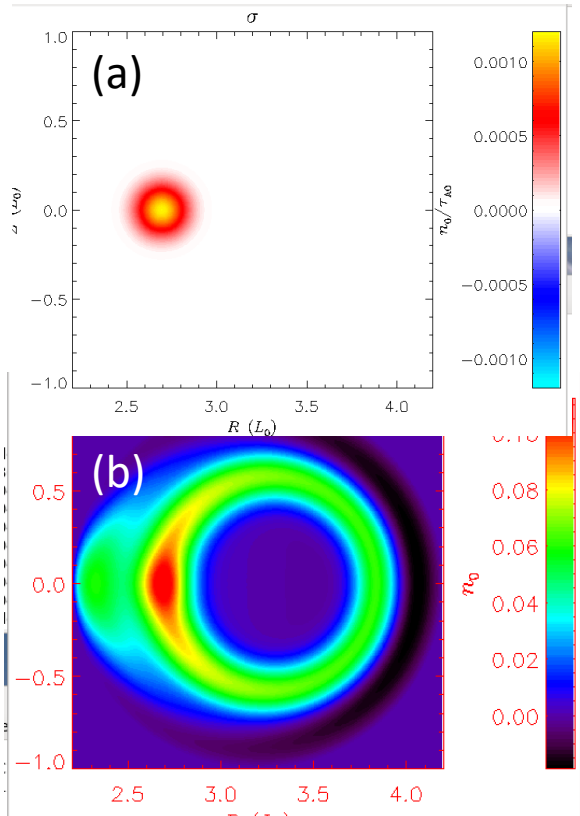
Request to calculate grad-B drift in M3D-C1 and to compare with that being put into the LP Code

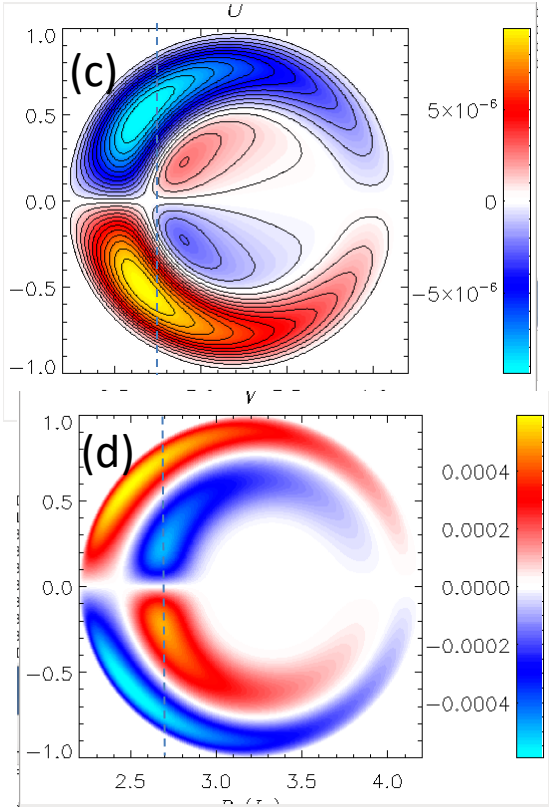
(a) Density source in 1F toroidal equilibrium

(b) Change in density after 10^3 τ_A

(c) Poloidal velocity stream function

(d) Toroidal velocity contours





Grad-B drift in M3D-C1– LF source

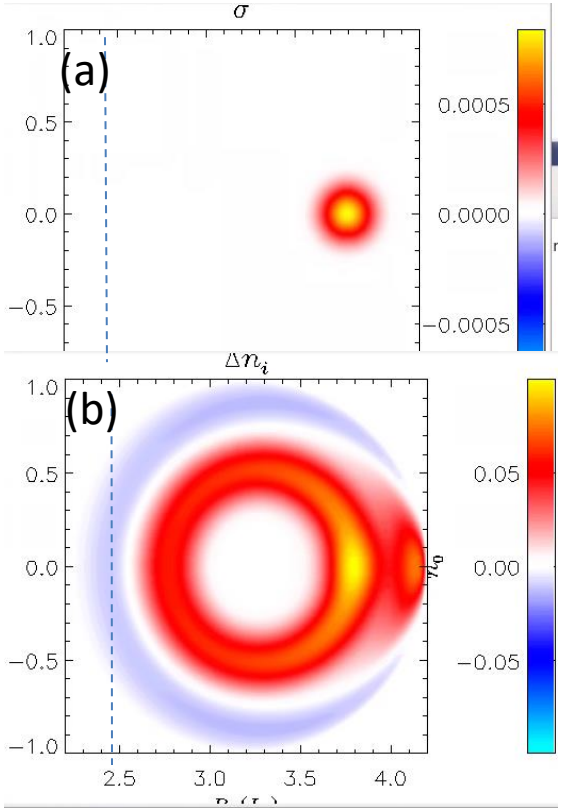
Request to calculate grad-B drift in M3D-C1 and to compare with that being put into the LP Code

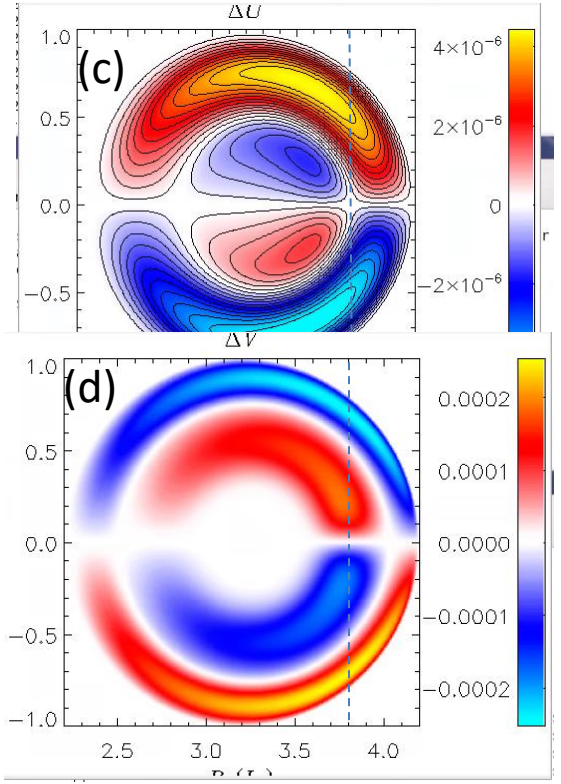
(a) Density source in 1F toroidal equilibrium

(b) Change in density after 10^3 τ_A

(c) Poloidal velocity stream function

(d) Toroidal velocity contours





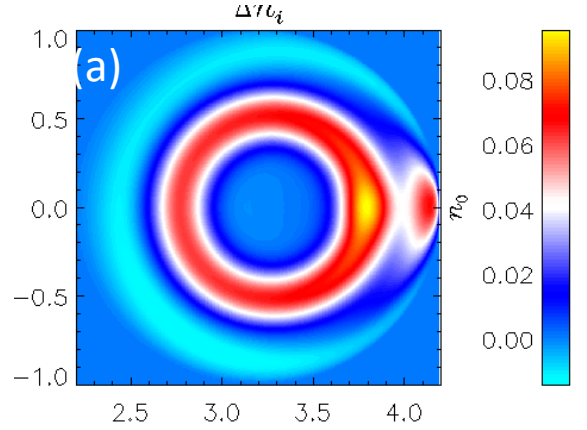
Grad-B drift in M3D-C1—2F effects

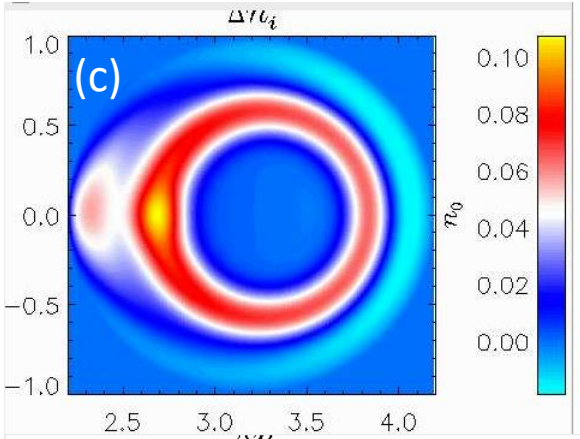
(a) 2F density change after 10^3 τ_A for LF side source

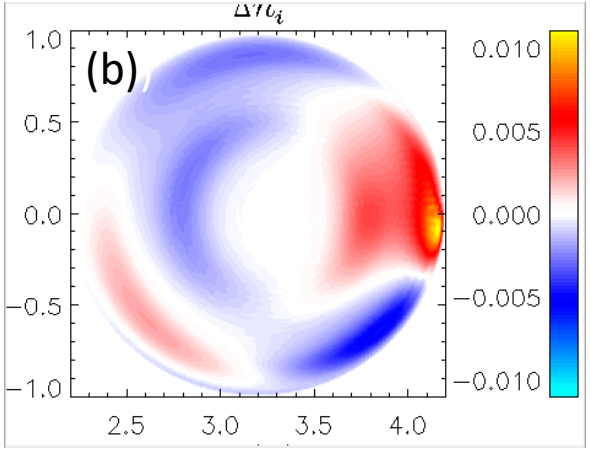
(b) Difference in 1F and 2F density (LF)

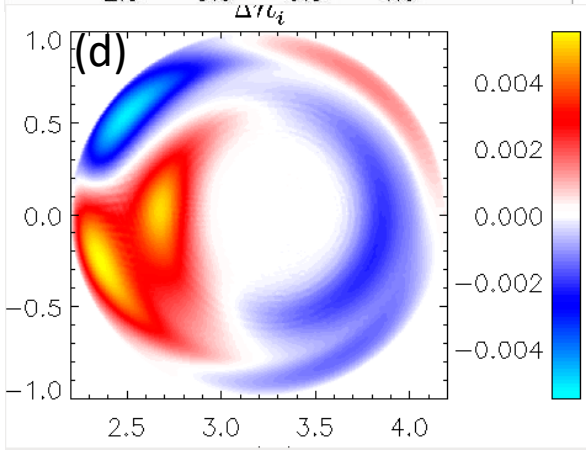
(c) 2Fdensity change after 10^3 τ_A for HF side source

(d) Differencein 1F and 2F density (HF)

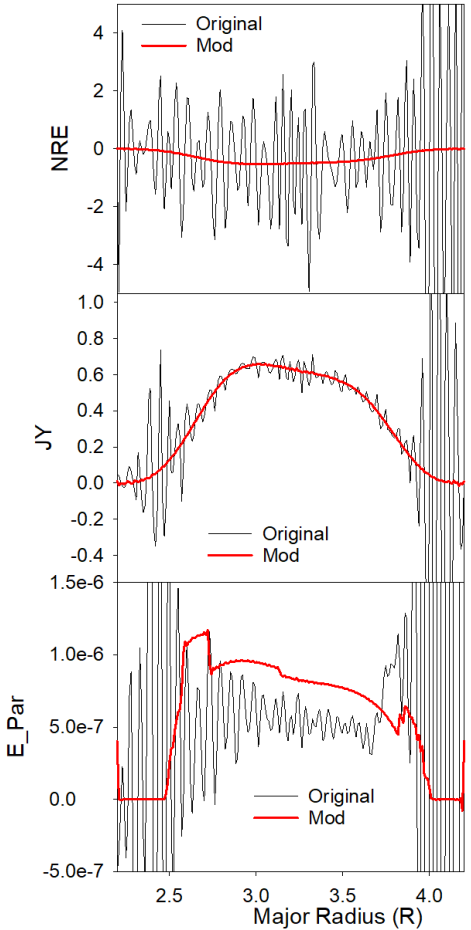








Sawtoothing discharge with runaway electrons

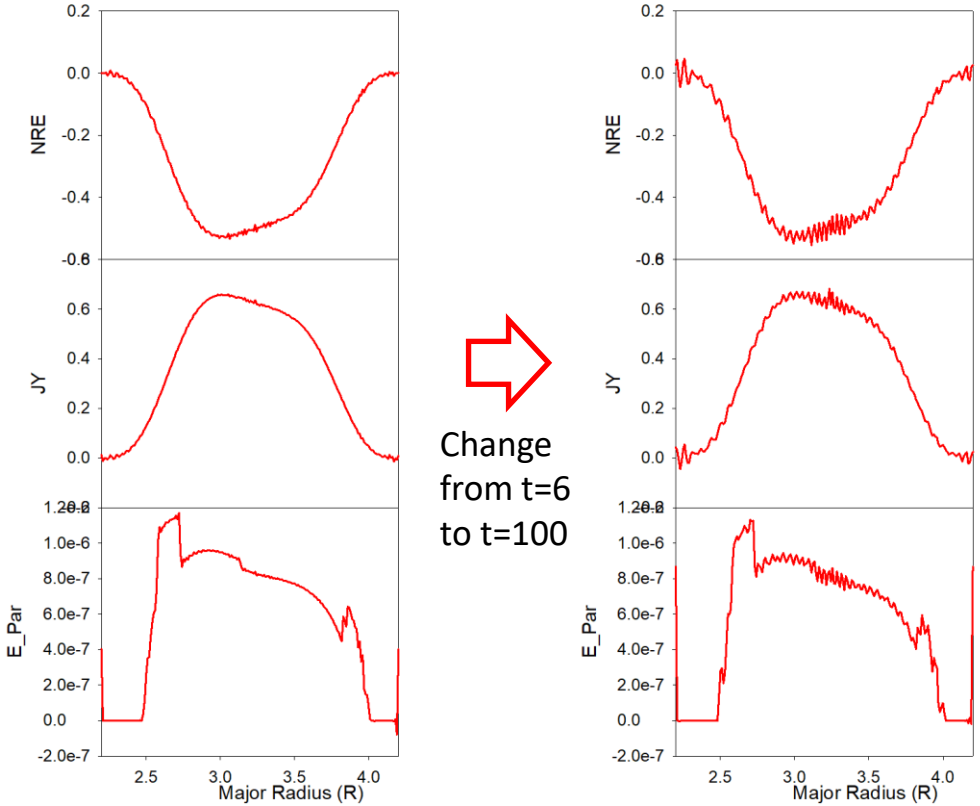


Profiles of nre, jy, and E_par after 30 timesteps

Original: /p/tsc/m3dnl/Isabel/Chen2D
Mod: /p/tsc/m3dnl/Isabel/Chen2D-mod1

Changed:
mesh size
"regular"
"integration points"
ipres=1
cre
pedge
viscosity
denm
equilibrium density

Longer times develops oscillations



- Short wavelength oscillations occur first in nre and then in other quantities (jy, e_par)
- Could we add some smoothing?

Progress on other shots?

NSTX shot 1224020 – Fast ion transport with coupled kink and tearing modes

- J. Yang, C. Liu. N. Ferraro … status of equilibrium reconstruction

DIII-D shot 177053 – Runaway generation with Ar injection

- Chen Zhao

DIII-D shot 177040 – saturated mode amplitude of (2,1) mode with runaways

- Chang Liu, Chen Zhao

DIII-D Neon pellet mitigation simulation for KORC

- Brendan Lyons

SPARK ?

That’s All I have

Anything Else ?