M3D-C1 ZOOM Meeting 10/19/2020 Agenda

- 1. CS Issues
 - 1. Comments on GPU Solves...M. Shephard
 - 2. Status of GPU solves on Traverse and Cori-GPU
 - 3. Local systems
 - 4. Other systems
 - 5. NERSC Time
 - 6. Changes to github master since last meeting
 - 7. Restarting with a different number of planes...resolved
 - 8. Request to replace bf=f with bfp=df/d(phi).. Status and plans
- 2. Physics Studies
 - 1. Status of first coupled M3D-C1/LP Simulation .. Lyons/Samulyak
 - 2. Grad-B drift in M3D-C1?
 - 3. NSTX shot 134020 status of equilibrium
 - 4. Carbon Pellet Mitigation on NSTX C. Clauser
 - 5. 177053 case with Ar Chen Zhao
 - 6. Sawtoothing with RE Chen Zhao
 - 7. Other?

Mark Shephard on GPUs

GPU solve status – Cori GPU

Jin Chen to update

- 1. Code works now with solvers running on GPU nodes
- KSPSolve Timings for 2D real runs on CORI HASWELL, CORI KNL, and CORI GPU HASWELL=9.7s KNL=37.6s GPU=35.3s
- 3. KPS Solve Timings for 3D real runs on CORI HASWELL, CORI KNL, and CORI GPU HASWELL=117.15s KNL=240.22s GPU= 351.79

Local Systems

- PPPL centos7(10/18)
 - All 6 regression tests PASSED on centos7:
- PPPL greene (10/18)
 - 5 regression tests PASSED
 - No batch file found for pellet
- EDDY (10/09)
 - All 6 regression tests PASSED on eddy
- TRAVERSE(10/05)
 - Code compiles
 - Regression test failed: split_smb not found in PATH

Other Systems

- Cori-KNL (10/9)
 - 6 regression tests passed on KNL
- Cori-Haswell j(10/9)
 - 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 (10/19)
 - salloc: Job submit/allocate failed: Invalid account or account/partition combination specified
 - I have now requested an account on CORI-GPU (10/19)

NERSC Time

mp288



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 Nov 1
- John Mandrakes (DOE) has 45M hours to distribute, but got requests for 3x that. Says he will finalize allocations this week. We can expect ~ 5 M hours.

Changes to github master since last meeting

- J. Chen
 - 10/18/20: regression tests solvers fixed on CORI GPU
- S. Jardin
 - 10/13/20: removed changes from last commit (subtracting F0 for fp solve)
 - 10/15/20: committed corrected centos7.mk file from Seegyoung
 - 10/18/20: added capability for non-constant density for basicq cylinder (itor=0)
- N. Ferraro
 - 10/14/20: Fixed bug when changing nplanes on restart
 - 10/14/20: Minor tweak to coding for restarting with different numbers of planes to simplify and prepare for cases with nonuniform plane spacing

Jump in KE when restarting with increased planes -- NOW RESOLVED --

Brendan showed some slides on 9/28/20 of how there is a glitch in the kinetic energy when he restarts with additonal planes.

From Brendan: 10/12/20

With cori back up, I restarted a case that had 8 planes, once with the same 8 planes and again with 32, both from output slice 40 and then output every time step:

8-plane: /global/cscratch1/sd/blyons/C1_35007033/ 32-plane: /global/cscratch1/sd/blyons/C1_35007045/

The deviation is present at output slice 40, so it's in the mapping of the 8 Hermite cubics to 32 Hermite cubics. At the original plane locations (every 45 degrees), the fields are exactly the same, but they start varying in between, peaking halfway in between. I've attached a movie showing the difference in 'phi' at every integer toroidal angle.

I've submitted another run with 16 planes, to see if doubling will work properly. I'd appreciate your thoughts.

Error in increasing # of planes has been fixed!

Before



After



Kudos to Brendan and Nate!

Request to replace bf = f with bfp = df/d ϕ

$$\mathbf{A} = R^{2} \nabla \varphi \times \nabla f + \psi \nabla \varphi - F_{0} \ln R \hat{Z}$$
$$\mathbf{B} = \nabla \psi \times \nabla \varphi - \nabla_{\perp} f' + F \nabla \varphi$$
$$F \equiv F_{0} + R^{2} \nabla \bullet \nabla_{\perp} f \qquad \text{(note: } f' \equiv \partial f / \partial \varphi)$$

Presently,

$$\dot{F} = \dots$$
$$R^2 \nabla \bullet \nabla_{\perp} f = F - F_0$$

Proposed (by Yao) to eliminate one derivative on f

$$\dot{F} = \dots$$

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

PHASE I: Just solve for fp to compare with f' but don't use it

- 1. In M3Dmodules.f90
 - 1. Add: type(field_type) :: bfp_field(0:1), bfp_ext
 - 2. Remove: integer, parameter :: bf_mat_rhs_index = 39 (never used)
 - 3. Add: integer, parameter :: bfp_mat_rhs_index = 39
- 2. In module newvar_mod
 - 1. integer, parameter :: NV_IP_MATRIX = 8
 - 2. type(newvar_matrix) :: mass_mat_rhs_bfp
- 3. In subroutine set_newvar_indices
 - 1. call set_matrix_index(mass_mat_rhs_bfp%mat, bfp_mat_rhs_index)
- 4. In subroutine create_newvar_matrices
 - 1. If (if bound.eq.1) then
 - 2. call create_newvar_mat(mass_mat_rhs_bfp, NV_DC_BOUND, NV_IP_MATRIX,0)
 - 3. else if (ifbound.eq.2) then
 - 4. call create_newvar_mat(mass_mat_rhs_bfp, NV_NM_BOUND, NV_IP_MATRIX,0)
 - 5. endif
- 5. In subroutine create_newvar_matrix
 - 1. case(NV_IP_MATRIX)
 - 2. Temp(:,:,1,1) = intxx2(mu79(:,:,OP_1),nu79(:,:,OP_DP))
- 6. In subroutine space
 - call create_field(bfp_field(0)
 - call create_field(bfp_field(1)
 - call create_field(bfp_ext)

- 7. In subroutine derived_quantities
- 8. . In output.f90:

call output_field: fp_plasma, fp_plasma_i, fp, fp_i

Status: Phase 1 implemented and committed



I restarted a 3D NL calculation and ran 1 time step with the new coding

The top and bottom curves should be identical but they are not. There is an error I would like someone else to look at the coding and do tests

-- NOW RESOLVED --

df/f ϕ from f, OP=11 and fp, OP=1 vs NPLANES



Converges if enough planes are used!

Thanks to Yao Zhou

Phase II: replace f with fp in calculations

In subroutine derived_quantities
! vector potential stream function
if(imp_bf.eq.0 .or. ilin.eq.0 .or. ntime.eq.0) then
if((i3d.eq.1 .or. ifout.eq.1) .and. numvar.ge.2) then
if(myrank.eq.0 .and. iprint.ge.2) print *, "f", ilin
if((ilin.eq.0 .and. eqsubtract.eq.1) .or. eqsubtract.eq.0) then
if(itor.eq.0) then
temp = bzero
else
temp = bzero*rzero
end if
call add(bz_field(ilin),-temp)
endif
call solve_newvar1(bf_mat_lhs,bf_field(ilin),mass_mat_rhs_bf, &
bz_field(ilin), bf_field(ilin))
if((ilin.eq.0 .and. eqsubtract.eq.1) .or. eqsubtract.eq.0) call add(bz_field(ilin), temp)
endif
end if

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 add h5r_read_field for bfp_field, bbfp_ext

backward compatibility?

5. In particle.f90

Need Help. Can we replace bf_field with fbp_field? What else needs to be changed?

6. rmp.f90 Need Help: 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	
auxiliary_fields		
bootstrap.f90	bootstrap.f90	
diagnostics.f90		
electric_field.f90	electric_field.f90	
ludef_t.f90	ludef_t.f90	
m3dc1_nint.f90	m3dc1_nint.f90	
metricterms_new.f90		
temperature_plots.f90		
transport.f90		

bf179 auxiliary_fields.f90

electric_field.f90 ludef_t.f90 m3dc1_nint.f90 metricterms_new.f90 temperature_plots.f90

bftx79

diagnostics.f90 electric_field.f90 ludef_t.f90 m3dc1_nint.f90 metricterms_new.f90 temperature_plots.f90 transport.f90

parallel_heat_flux.f90

Make these substitutions in all of the above routines

init_basicj.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.

metricterms new.f90 v1psif(x, x,f) b1psifn1(x,x,f,x) v1bf(x,x,f) b1psifn2(x,x,f,x) v1huf(x,x,f)b1bfn1(x,x,f,x)v1hvf(x,x,f)b1bfn2(x,x,f,x)v1hchif(x,x,f) bipsifd1(x,x,f,x) v2psif1(x,x,f) b1psifd2(x,x,f,x) v2psif2(x,x,f) b1bfd1(x,x,f,x)v2bf(x,x,f) b1bfd2(x,x,f,x)v2ff(x,f,f)b2feta(x,f,x) v2huf(x,x,f) b2jrefeta(x,x,f,x,x) v2hvf(x,x,f)b2fv(x,f,x)v2hchif(x,x,f) b2psifn(x,x,f,x) v3psif(x,x,f) b2bfn(x,x,f,x)v3bf(x,x,f) b2psifd(x,x,f,x) v3huf(x,x,f) b2bfd(x,x,f,x)v3hvf(x,x,f)b3psifeta(x,x,f,x,x) v3hchif(x,x,f)b3bfeta(x,x,f,x,x) b1jrefeta(x,x,f,x,x) b3ffeta(x,f,f,x,x) B1feta(x,f,x) b3pefd(x,x,f,x) b1fu(x,f,x)tepsifkappar(x,x,f,x,x,x) b1fv(x,f,x)tebfkappar(x,x,f,x,x,x) b1fchi(x,f,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

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 10/7/20 – need to decide where to evaluate the electron density, temperature, and magnetic field. In the m3dc1 pellet cloud, or upstream.

DIII-D 171322 @ 2730 ms



Grad-B drift in M3D-C1?

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

Add density source to cylindrical equilibrium



Difference in final density and initial density at some given time.

Compare results between single-fluid and 2F run at a given time



Is this difference due to the grad-B drift?

NSTX shot 134020

Fast ion transport with coupled kink and tearing modes J. Yang, C. Liu



q-profile as calculated from M3D-C1 does not agree with that from geqdsk at the origin!



NSTX shot 134020 (cont)

Fast ion transport with coupled kink and tearing modes

- J. Yang, C. Liu
- Plasma limited by mesh boundary!
- Mid-plane current density very jagged



NSTX shot 134020 (cont)



Central value of q depends on limiter position. This geqdsk had a left boundary of 0.185 instead of 0.01 as in earlier geqdsk files. Also, mesh needs to be extended.

Meeting held 10/6 to discuss. Devon will provide coil and vessel currents and we will re-computer the free boundary equilibrium

Carbon Pellet Mitigation on NSTX

C. Clauser and S. Jardin met with Roger Raman on 10/7 to discuss Cesar's Carbon mitigation runs

- Roger wants to model a carbon powder filled shell pellet, that deposits the carbon uniformly when the pellet reaches the plasma center
- To do long time simulations of the current quench, Cesar wants to reduce the number of toroidal planes once the impurity is mixed. Is this possible?
- How best to model the carbon deposition from the shell pellet?

Proposed solution:

```
Restart with a new value of ipellet_abl = 0
pellet_rate(ip) = .....
```

Izzo & Parks, Phys. Plasma (2017)

The neutral Ar is deposited on axis with a 2D Gaussian profile in the poloidal plane having a 15 cm half width and is elongated in the toroidal direction with a 1.5 m half width. A 3D rendering of the shape of the deposited neutral Ar plume is shown in Fig. <u>1.</u>



FIG. 1. 3D rendering of an isosurface of neutral Ar density (plotted in two views along with two poloidal planes) shortly after the simulation is initiated. With a 1.5 m half-width, the initial plume extends about 1/3 of the way around the torus.

Chen Zhao

- DIII-D shot 177053 with Ar injection
- Sawteeth with RE

That's All I have

Anything Else ?

RE Fluid Modeling of DIII-D shot 177040

Carlos Paz-Soldan email 9/14/20 (not he had this in his talk last week!!)

- 1) Dependence of RE current carriers (or not) on saturated mode amplitude (dB/B)?
- 2) Dependence of saturated dB/B on absolute B&I (fixed a, all q=2). —> ITER extrapolation
- 3) Dependence of saturated dB/B on absolute I (fixed B, smaller a, all q=2).





Dependence of Growth Rate on Plasma and Vacuum resistivity





Growth Rate vs q(a)



Batemanscale modifies F(1) but keeps p' and FF' fixed.

We should ask MARS to make a similar plot.

177053 case with Argon

10/12/20



This only happened in DIII-D geometry, not in cylinder. If no runaways, the plasma current also did not shift

The growth rate of plasma current was at about 6ms larger than 0 and both the runaway current and the plasma current increased.

•

The reason is that the the plasma current shifted towards so that at last the runaway current at the low field side was higher than plasma current and caused an increasing of plasma current





Sawtooth case with Isabel's Equlibrium

10/12/20

No runaways





The temperature was dropped when the 1/1 mode growing, and since the runaway current do not have ohmic heating effect, the temperature would not come back to the previous value when the 1/1 mode disappear, the resistivity become larger, and because the resistive kink mode do not have the resistivity correction effect, the growth rate will become higher, and finally the case crashed when the temperature was too low.

I think after the first sawtooth phase, the current drive should disappear by the large runaway current effect according to Cai & Fu paper's opinion.

9/18/20 Chen Zhao: Shot 177040 with RE









With ExB drift terms removed



DIII-D Shot 177053 (with RE sources) – Chen Zhao



Code changes now committed to GIT NEXT Steps:

- 1. Study of sensitivity to κ_{\perp} ?
- 2. Comparison with shot results
- 3. Presentation at DIII-D disruption meeting

177053 Exp. Traces (Lyons 06/08/20)



Test of Boozer Theory for Cold VDE (Clauser)

- Boozer's analytic theory that if ITER suffers a disruption on the mid-plane, such that the current decreases to I = 0.83 I₀, vertical stability will be lost, even for an ideally conducting wall.
- Cesar has tried to verify this, and finds the plasma is still VDE stable with I = $0.3 I_0$
- Difference is likely the wall model, Cesar to confirm.



Boozer, "Halo currents and vertical displacements after ITER disruptions", Phys. Plasmas 26, 114501 (2019)

DIII-D Neon pellet mitigation simulation (for KORC)



/global/cscratch1/sd/blyons/C1_33984065



Mid-plane Electron Temperature and Electric Field



Magnetic Surface Breakup



Partial Surfaces Reforming



32 plane rerun now in progress



8 planes

32 planes

32 plane case crashed with negative density



Near the end, dt > dx / V in the toroidal direction, which can lead to oscillations. Recommendations: (1) iupstream=1, (2) smaller dt, (3) increase hyperv, (4) increase denm

Energy conservation

6% error does not depend on:

- dt=0.5, 1.0, 2.0
- inocurrent_pol=0,1
- inocurrent_tor=0,1
- Itemp = 0.1
- jadv = 0,1
- etar = 1.e-7, 1.e-9
- idens = 0,1
- Now checking dependence on magnetic boundary conditions and form of Poyting Flux divergence: ∇•(E×B)