M3D-C1 ZOOM Meeting

07/11/2022

Upcoming meetings and deadlines

CS Issues

1. LBL Report
2. 1D Hermite Cubic Finite Element Test Problem
3. New Latex documentation
4. New meshing capabilities requested
5. Mesh adaptation update -
6. NERSC Time
7. Changes to github master since last meeting
8. Regression tests
9. Segmentation error on Cori Haswell
10. SUBPC error on Perlmutter_cpu
11. Convert_polar now polar_meshgen

Physics Studies

1. PPPL Theory Seminar on ultra-high beta plasmas
2. Status of Chen Zhao paper
3. Upgrade to impurity radiation model – Brendan Lyons
4. Problem with BC in ITER problem

In attendance

Steve Jardin
Jin Chen
Hank Strauss
Adelle Wright
Chang Liu
Chen Zhao
Nate Ferraro
Brendan Lyons
P. Sinha
Andreas Kleiner

Mark Shephard
Seegyoung Seol
Morteza

Sam Williams
Sherry Li
Yang Liu

Upcoming Meetings

OpenACC and Hackathons Summit 2022
        August 02-04
        C. Liu to present talk on M3D-C1
        J. Chen to attend

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

APS-DPP
        Oct 17-21 In Spokane Washington
        Jardin & Kleiner to give invited (only ones in PPPL theory?)
        26th Workshop on MHD stability Control is on Oct 14-15
        CTTS SciDAC meeting is on Sunday Oct 16 (TBA)

LBL Progress on Solvers

Iterative Solver for Hermite-Cubic Elements

Sam Williams asked for a simple 1D problem using Hermite Cubic Elements so they could experiment with preconditioners:

I sent him a small F90 program I have that solves:

$$\frac{\partial \Phi}{\partial t} + V \frac{\partial \Phi}{\partial x} = \alpha \frac{\partial^2 \Phi}{\partial x^2} - \varepsilon \frac{\partial^4 \Phi}{\partial x^4}$$

Or, in finite element form:

$$\left[\mathbf{M} + \delta t \theta \left[V\mathbf{N} + \alpha \mathbf{P} + \varepsilon \mathbf{Q} \right] \right] \bullet \mathbf{Y}^{n+1} = \left[\mathbf{M} - \delta t (1 - \theta) \left[V\mathbf{N} + \alpha \mathbf{P} + \varepsilon \mathbf{Q} \right] \right] \bullet \mathbf{Y}^{n}$$

I now solve this with a direct solver, but he (or one of his students) will try and solve this iteratively with a preconditioner.

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 6/20/22
M3DC1.tex
app-paraview.tex
idl-postproc.tex
mesh-gen.tex
score-api.tex
doc.tex

       8.1 Model Options

       8.2 Initial Conditions Options

       other C1input sections being worked on

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 (and make update)

Any update?

NERSC Time

mp288

36.7 K Node Hours remaining!
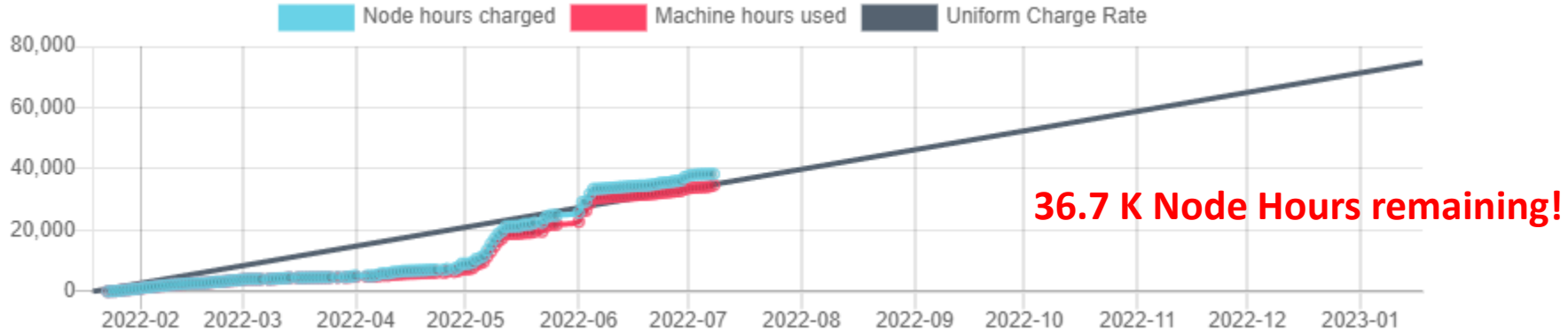
- MP288 usage is on track.   Both value and rate are ok.
- All users now have access to Perlmutter_cpu. There is no charge for the year!
    - Some issues for large problems…see future slide
- NERSC Checkpoint/Restart Requirements Gathering Workshop, July 12-13
    - Is anyone attending?   Does M3DC1 Restart capability meet requirement?

Changes to github master --after 2022-6-19

Mark Shephard
06/21/22: Minor edits to meshing section

Steve Jardin:
06/24/22: added input sections 8.1 and 8.2 to Latex document

Jin Chen
06/22/22: petsc library update
07/05/22: account name change on Perlmutter for cpu-only job scripts
Nate Ferraro
06/27/22: updated documentation for building M3D-C1
06/29/22: Added capability to change x-axis of plot_scalar with versus
Seegyoung Seol
06/20-21/22: Updates on User's Guide
06/22/22: Steve's updates on User's Guide?
06/27/22: adding mesh generation source code except Simmetrix part
            removing meshgen related files, meshgen cleaned up for PPPL

Local Systems

- PPPL centos7(07/09/22)
  - 7 jobs PASSED

- PPPL greene (07/09/22)
  - 5 jobs PASSED

- STELLAR (07/09/22)
  - 7 regression tests **PASSED** on stellar

- TRAVERSE_gpu(07/09/22)
  - 5 regression tests **PASSED**
  - KPRAD_2D, KPRAD_restart FAILED due to 0.001 fractional diff in C1ke

NERSC

- Cori-KNL (07/09/2022)
  7 regression tests **PASSED**
  KPRAD_2D failed on first try

- Cori-Haswell (07/09/2022)
  7 regression tests **PASSED**

- Perlmutter (07/09/2022)
  6 regression tests **PASSED**
  NCSX **FAILED** with "PC failed due to SUBPC_ERROR"

- Perlmutter_cpu (07/09/22)
  6 regression tests **PASSED**
  NCSX failed due to small differences in C1ke file (0.00102)

Segmentation error on Cori-Haswell at end

Adelle Wright: (5/12/2022}
Currently, my stellarator runs on cori-haswell are completing but not exiting cleanly. Jin identified the issue as that mentioned below.

Jin Chen: (4/21/2022)
The segfault is caused by line
 613   call MPI_Finalize(ier)
In file "newpar.f90". So you don't have to worry about it for now. I'll look into the cause of it.

Jin Chen: (6/22/2022)
PETSc library is updated on CORI HASWELL, PERLMUTTER GPU & CPU. The error that @Adelle Wright had on haswell should be fixed. Her test case finished with no complaining errors anymore. Please check. Please use superlu_dist instead of MUMPS

SUBPC error on Perlmutter_cpu

Runs with 8 planes and 36 planes failed due to either:
"PC failed due to SUBPC ERROR" (These runs did not fail immediately but after a few time steps, at which point NaN were generated.) or just hanging during the first GS solve. You can view failed cases at:

/global/cfs/cdirs/mp288/Jardin/m3dnl/Perl_cpu/128-K/Run03   (36 planes)
/global/cfs/cdirs/mp288/Jardin/m3dnl/Perl_cpu/128-K/Run05   (8 planes)

A 4-plane case that worked ok is at
/global/cfs/cdirs/mp288/Jardin/m3dnl/Perl_cpu/128-K/Run02
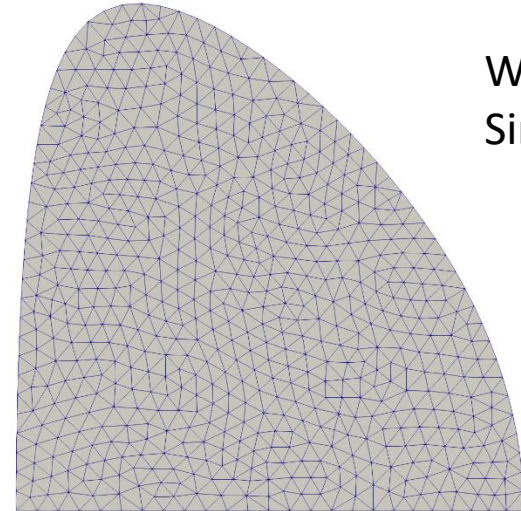
convert_polar

6/27/22 S. Seol: The program "convert_polar" (the mesh generator with "POLAR" file; an equilibrium transffered from the PPPL JSOLVER code) doesn't use the Simmetrix so it doesn't provide any mesh control nor nice a quality mesh. And furthermore, you mentioned that M3DC1 cannot load the generated mesh files so you had to use a workaround to make it work in M3DC1.

Lately, I have developed a mesh generator "polar_meshgen" to generate mesh with "POLAR" using Simmetrix. In addition to a quality mesh, this new "polar_meshgen" will allow basic mesh controls such as adjacency-based reordering, mesh size, etc.   I have attached two mesh pictures with and without Simmetrix for your reference.
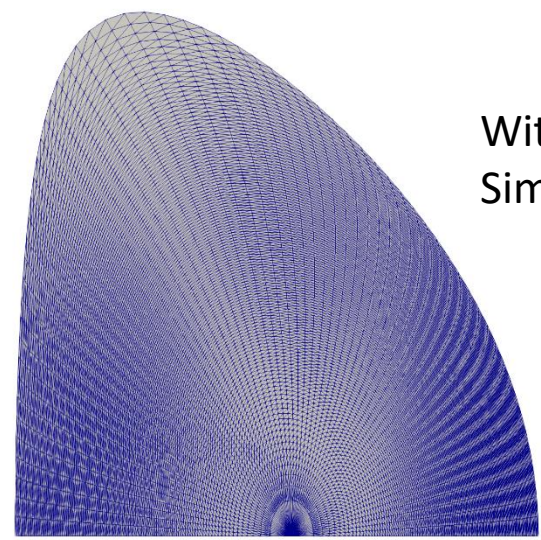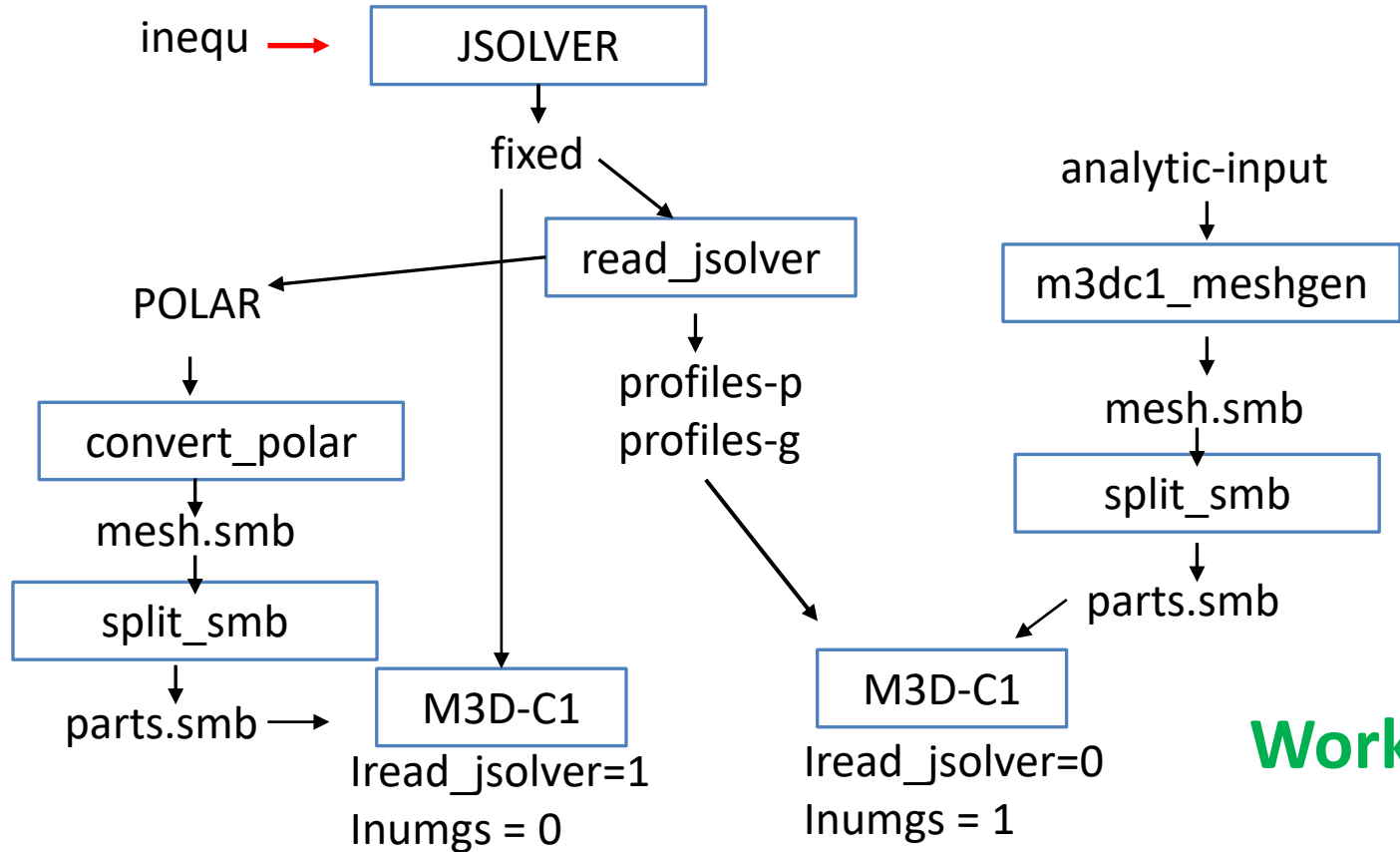

Without Simmetrix

With Simmetrix

convert_polar-2

6/27/22 S. Seol: To proceed further, I have a couple of questions:

1. "convert_polar" generates a file "norm_curv" and I wonder if you still need "norm_curv".

    1. **I don't think so.   Does anyone think different?**

2. what is the workaround that you used to load the mesh from "convert_polar"? It's nothing to do with "polar_meshgen" but I would like to know for curiosity.

    2. **See the next slide.   Posted 04/25/22**

3. would you please send me a test case of M3DC1 which uses the mesh file generated from POLAR?

    3. **See the case in /p/tsc/m3dnl/NSTX/Jsolver/A=3.0/A=3.0D**

4. Are you ok with the name "polar_meshgen"? If not, please suggest a better name.

    4. **ok**

5. I will keep "polar_meshgen" for now but it will be eventually merged to "m3dc1_meshgen**".   (update 7/11/22 now available and in new documentation)**

JSOLVER to M3D-C1

inequ → JSOLVER

fixed

read_jsolver

POLAR

convert_polar

mesh.smb

split_smb

parts.smb → M3D-C1

profiles-p
profiles-g

M3D-C1

Iread_jsolver=1
Inumgs = 0

Iread_jsolver=0
Inumgs = 1

analytic-input

m3dc1_meshgen

mesh.smb

split_smb

parts.smb

Fails

Works!

PPPL Theory Seminar 6/23/22

- Rahul Gaur: Linear stability of ultra-high-beta equilibria

- Did anyone attend this?   (I was on vacation)

- Exact global equilibria with $\beta \sim 1$
  - $n = \infty$ analysis only.   Can M3D-C1 be applied to this?

Papers in Preparation

- Chen Zhao, C. Liu, et al, "Simulation of DIII-D disruption with pellet injection and runaway electron beam"
  - *New Version circulated 7/10/22 --- Jardin to proof*

Upgrade to impurity radiation Routines

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

Any Response?

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?
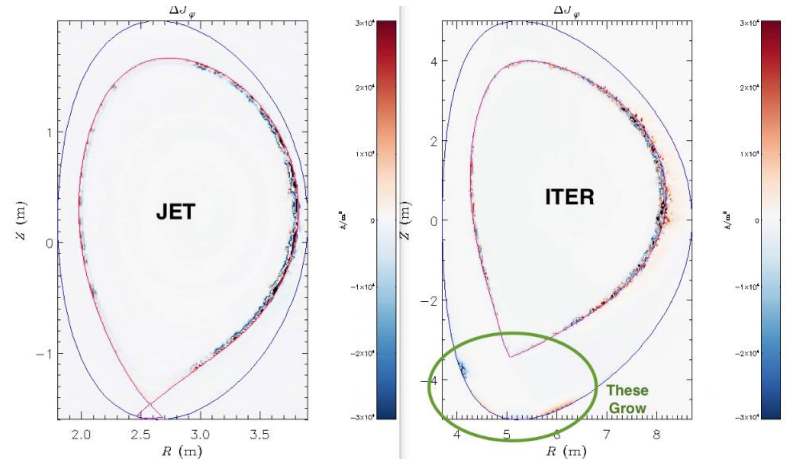
That's All I have

Anything Else ?

Next Meeting July 25