# The M3D-C<sup>1</sup> User's Guide

 $-$  VERSION 0.1  $-$ 

PPPL M3DC1 Team RPI SCOREC

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# <span id="page-6-0"></span>1 Obtaining M3D-C1

# <span id="page-6-1"></span>1.1 License Agreement

M3D-C1 is a code developed with funding from the US Department of Energy, and is intended for open scientific research. If you intend to run M3D-C1, please complete the following steps:

- 1. Sign the license agreement [https://m3dc1.pppl.gov/M3D-C1\\_License.pdf](https://m3dc1.pppl.gov/M3D-C1_License.pdf) and return to [nferraro@pppl.gov.](mailto:nferraro@pppl.gov)
- 2. Request access to the code using the form <https://pppl.tiny.us/code-release-form>. This step will involve review by PPPL to clear any potential export control issues.

Please be aware that permission to run M3D-C1 does not carry an implicit agreement to provide technical support for compiling, running, modifying, or interpreting output of, M3D-C1.

# <span id="page-6-2"></span>1.2 Preinstalled M3D-C1 Executables

For the general user, we recommend using precompiled executables and associated modules for release versions, where available. Installations are presently available on a number of systems, including:

```
GA Iris:
   module use /fusion/projects/codes/m3dc1/modules
   module load m3dc1/1.14
NERSC Perlmutter:
   module use /global/cfs/projectdirs/mp288/C1/modules/perlmutter
   module load m3dc1/1.14-cpu
PPPL Cluster:
   module use /p/m3dc1/modules
   module load m3dc1/1.14
PU Stellar:
   module use /projects/M3DC1/modules
   module load m3dc1/1.14
```
These modules will modify the user's enviroment variables appropriately to access the M3D-C1 executables, python libraries, and IDL routines.

#### <span id="page-6-3"></span>1.3 Accessing the M3D-C1 Source Code

If you choose to build the code yourself, either to use an unreleased version or to do code development yourself, you will need access to the M3D-C1 code repository. The M3D-C1 source code is located in the Github repository: PrincetonUniversity/M3DC1. To get access to this repository, please complete the license form and software access request form as described in section [1.1.](#page-6-1)

## <span id="page-7-0"></span>1.4 Makefiles and Dependencies

Some of the build scripts depend on the following environment variables to be set, to specify the location of the M3D-C1 source code and the directory in which to install any compiled executables:

- M3DC1 DIR should be set to the directory containing the M3D-C1 source code. For example: setenv M3DC1 DIR \$HOME/src/M3DC1
- M3DC1 INSTALL DIR should be set to the directory in which M3D-C1 will be installed. For example: setenv M3DC1 INSTALL DIR \$HOME/M3DC1

It is recommended to set these values in your login script.

Makefiles for a number of systems are included in the repository, with filenames \$M3DC1\_DIR/unstructured/\*.mk. For most of these systems, environment modules are also included in the repository. These modules will load the appropriate software modules for building on that particular system, and can be loaded using:

NERSC Perlmutter: module use \$M3DC1 DIR/modules/perlmutter module load m3dc1/devel PPPL Cluster: module use \$M3DC1 DIR/modules/pppl module load m3dc1/devel-centos7 PU Stellar: module use \$M3DC1 DIR/modules/stellar

module load m3dc1/devel

It is recommended to place the appropriate module use statement in your login script. The makefile should have the name  $\{\text{M3DC1}\_\text{ARCH}\}$ .mk. If  $\text{M3DC1}\_\text{ARCH}$  is not defined, it will default to  $$HOST, stripped of any trailing numbers identifying a node index on multinode systems (*e.g.* if$ \$HOST==''sunfire06'' then \$M3DC1 ARCH will default to "sunfire").

If you are building M3D-C1 on a system for which no makefile or development module is provided, please refer to the existing makefiles and modules as examples. In general, M3D-C1 requires the following dependencies:

- Compilers for  $C, C++,$  and Fortran;
- MPI
- HDF5 compiled with support for Fortran and MPI
- netcdf
- GSL
- FFTW
- PETSc compiled with support for Fortran, complex-valued functions, MUMPS and/or SuperLU dist
- PUMI meshing libraries

#### <span id="page-8-0"></span>1.5 Building

Once the appropriate makefile has been defined, the M3D-C1 executables can be built by entering \$M3DC1 DIR/unstructured and running

make all

This will run the following commands:



#### <span id="page-8-1"></span>1.6 Regression Tests

The M3D-C1 source code includes a suite of regression tests that should be run before commiting any new code to the repository. To run these tests:

#### cd \$M3DC1 DIR/unstructured/regtest ./run <arch> <test>

where  $\langle \text{arch} \rangle$  and  $\langle \text{test} \rangle$  are optional arguments specifying the specific batch script to run, and the specific regression test to run, respectively. By default,  $\text{Sarch}=\text{SMSDC1}$  ARCH.

If <test> is not specified, then all the regression tests will be run, using the batch scripts \$M3DC1 DIR/unstructured/regtest/\*/base/batchjob.<arch>.

The run script will create new directories in which to run these regression tests, named \$M3DC1 DIR/unstructured/regtest/\*/\${M3DC1 VERSION} <arch>/.

If <test> is specified, then only \$M3DC1\_ARCH/unstructured/regtest/<test>/base/batchjob.<arch> will be run (again, in a new directory named as described above). If  $\texttt{test}$  is specified, then  $\texttt{sarch}$ must also be specified.

To check the results of the regression tests

./check <arch>

# <span id="page-10-0"></span>2 GITHUB

Retrieve the current version of M3D-C1 from the GIT repository. For the first time, to check out the sources, do:

Initial access is with the *clone* command. This copies the source code from the master file into a working directory on your machine. You only do this once on each computer you work on.

module load git

git clone https://github.com/PrincetonUniversity/M3DC1

Subsequent GIT commands used to commit:

- $add/commit/push$ : You add files to a list of files to update, *commit* the chanes to your branch, and then push the changes to the master branch.
- git commit  $-m$  "message describing changes" (adding  $-a$  commits all changes)
- $\bullet$  diff lists the changes you made from the last commit, even if you haven't pushed your commits to github. To see how your files differ from what's on github, you can do:

git fetch origin master git diff origin/master

- *status* compares your branch with the master branch
- *pull origin master* updates your local branch to the current master branch
- stash takes uncommitted changes, saves them for later use, and reverts files in working directory

stash list stash drop stash apply stash pop (apply and drop)

- *stash pop* removes changes from your stash and reapplies them to working copy
- *stash apply* keeps changes in stash, but reapplies them to working copy
- reset -hard discards any changes to local branch since last commit
- *branch* tells you what branch you are in
- log (–oneline) (-after 2023-01-31) lists all the commits for the checked-out branch after that date
- *checkout hashtag* replaces your version with the version that has hastag "hashtag" (need only first 7 characters)

# <span id="page-11-0"></span>2.1 Branches in GIT

To make a new branch called fp-phase2:

- *git checkout master* switch to the master branch
- *qit pull* make sure the master branch is up to date
- git checkout -b fp\_phase  $2$  The  $=$ b creates a new branch. This will be identical tomaster to start.
- git push  $-set-upstream$  origin fp phase g push this new branch to the remote so others can access it

# <span id="page-11-1"></span>2.2 Committing changes

For example, to commit changes to newpar.f90

- *git pull* Always do thi before you start committing
- git add newpar.f90 This stages the current changes in newpar.f90 for commit. You could then make more change before committing, but you would have to add again to get those into the commit. Or, you could add -a to the following to commit all changes.
- git commit -m "Changed newpar.f90" Commit changes to your local branch.
- git push Push commits to the remote repo.  $-$ set-upstream only needs to be done the first time.

## <span id="page-11-2"></span>2.3 Merging branches

To merge changes on master into fp phase2

- *git checkout master* switch to the master branch
- *qit pull* get the latest commits on the master branch
- git checkout fp\_phase2 switch back to fp\_phase2
- *git pull* to get the latest commits to fp phase2
- git merge master merge any new commits into fp phase 2. This makes a commit. You may need to resolve conflicts.
- git push Push the merged commit to remote repo

Inverting fb<sub>-phase2</sub> and master here would merge the development branch into master locally, then the push wouuld send the merge tothe remote master

# <span id="page-12-0"></span>3 Mesh Generation and Management

Given a mesh, all the mesh support needed to run M3D- $C<sup>1</sup>$  is provided by PUMI (Parallel Unstructured Mesh Infrastructure) developed at RPI Scientific Computation Research Center (SCOREC). The PUMI is used to manage the mesh information as it is processed within the M3D- $C<sup>1</sup>$  code. PUMI is a freely available open source software. For more information on how to get and install, visit [http://www.scorec.rpi.edu/pumi.](http://www.scorec.rpi.edu/pumi)

The generation of M3D- $C<sup>1</sup>$  meshes for Tokamak geometries using the M3D- $C<sup>1</sup>$  mesh generation program involves both PUMI and Simmetrix mesh generation software. Simmetrix is commercial software which provides a set of tools and libraries for engineering simulation. As Simmetrix runs only with a valid license, any M3D-C<sup>1</sup> user who wants to install his/her own version of the M3D-C<sup>1</sup> mesh generation program should contact Simmetrix to purchase its license. For more information on Simmetrix, visit [http://simmetrix.com.](http://simmetrix.com) M3D-1<sup>1</sup> users with accounts on PPPL Portal or Princeton Stellar are allowed to run M3D- $C<sup>1</sup>$  mesh mesh generation programs on those systems.

Note that Simmetrix software is not required to run a M3D-C<sup>1</sup> simulation. Running a M3D-C<sup>1</sup> simulation using a mesh generated by a different mesh generator requires the development of a tool that creates PUMI readable model and mesh files with  $M3D-C<sup>1</sup>$  related control information required as the M3D-C<sup>1</sup> input. For more information, contact RPI SCOREC [\(shephard@rpi.edu\)](mailto:shephard@rpi.edu).

With respect to the mesh support, there are a number of files involved with housing the geometry and mesh information. First, the model file extensions are the following

- .smd: Simmetrix-readable binary format model file The model generated with Simmetrix is saved in this format.
- .dmg: PUMI-readable binary format model file The model generated from PUMI mesh
- $\bullet\,$ .txt: M3D-C<sup>1</sup>-readable ascii format model file The model is generated from mesh generation tool (See Section [3.1\)](#page-13-0)

Second, the mesh file extensions are the following.

- .sms: Simmetrix-readable binary format mesh file
	- The mesh generated with Simmetrix is saved in this format.
	- If a mesh is serial (1-part), the mesh file doesn't have a number before the extension
	- If a mesh is distributed (P-part,  $P>1$ ), the mesh file has a number before the extension to represent the global part ID.
- .smb: PUMI-readable binary format mesh file
	- This format is used in M3D-C<sup>1</sup> to import/export a mesh
	- No matter if a mesh is serial (1-part) or distributed (P-part, P>1), the mesh file has a number before the extension to represent the global part ID.

• .vtu/pvtu: binary format mesh file for visualization with Paraview. For more information, visit [http://paraview.org.](http://paraview.org)

An overview of the Model/Mesh requirements for the M3D- $C<sup>1</sup>$  mesh generation process are as follows:

- The model and mesh shall be generated as described in Section [3.1.](#page-13-0)
- The mesh file must be PUMI-readable .smb file. Note that a mesh file name contains a number before the extension (.smb) to denote a global part ID.
- The model and mesh file must be present in the work directory
- The name of model and mesh file must be specified in C1input file in the work directory
	- $-$  mesh\_model  $=$  model\_file
	- $-$  mesh filename  $=$  mesh file.smb (NOTE: do not specify a number before the file extension)
- In a 2D run with P processes, there should be P mesh files with part ID from 0 to P-1
- In a 3D run with  $P \times N$  processes where 2D mesh is distributed to P parts,
	- there should be P mesh files with part ID from 0 to P-1
	- in C1input file, specify nplanes to N (e.g. nplanes=8), where nplanes describes how many 2D mesh copies to be loaded
	- the M3D-C<sup>1</sup> code should be compiled with options "3D=1, MAX\_PTS=60".

The rest of this section is organized as follows: Section [3.1](#page-13-0) describes a mesh generation program m3dc1 meshgen. Section [3.2](#page-19-0) describes a mesh generation program m3dc1 mfmgen. Section [3.3](#page-26-1) describes a mesh generation program polar meshgen. Section [3.5](#page-29-0) presents a mesh partitioning program "split smb" and "collapse" which changes the number of parts of the mesh. For how to visualize a mesh with Paraview, see Appendix [B.](#page-84-0)

# <span id="page-13-0"></span>3.1 m3dc1 meshgen

m3dc1 meshgen requires an ascii input file of arbitrary name that contains the following parameters.

- modelType: 0, 1, 2, 3, or 4
	- Type 0: a parameterized vacuum region defined by five doubles for analytic expression. For five doubles  $X_0$ ,  $X_1$ ,  $X_2$ ,  $Z_0$ ,  $Z_1$ , vacuum boundary is defined by

$$
X = X_0 + X_1 \cos(\theta + X_2 \ast \sin(\theta))
$$
\n<sup>(1)</sup>

$$
Z = Z_0 + Z_1 \sin(\theta) \tag{2}
$$

- Type 1: a vacuum region defined by piece-wise linear points
- Type 2: a vacuum region defined by piece-wise polynomials
- Type 3: spline-fitted 3-region model (plasma, wall and vacuum)
- Type 4: spline-fitted 3-region model (plasma, wall, and vacuum) with inner & outer boundary points to set resistive wall
- reorder: if 1, reorder PUMI mesh based on adjacency (default: 0) and generate vtk folders for mesh visualization. The mesh before and after reodering is saved in original-mesh.vtk and reordered-mesh.vtk, respectively. Note that the element order of Simmetrix mesh is not affected.
- inFile: (modelType 0) not required (modelType 1 and 2) geometry file describing the vacuum (modelType 3 and 4) geometry file describing the inner plasma wall
- bdryFile: (modelType 0-3) not required (modelType 4) geometry file describing the outer plasma wall
- outflie: output file name to save model and mesh
- mesh Size: relative mesh size for each region (default 0.05) for modelType 3, set three doubles for plasma, resistive, vacuum, respectively
- useVacuumParams: for modelType 0 or 3, if 1, use parameterized vacuum wall (default  $0$ )
- vacuumParams: five doubles to describe parameterized vacuum wall. Required if useVacuumParams=1.
- adjustVacuumParams: for modelType 0 or 3, if 1, multiply coordinates and parametric values of nodes on vacuum wall by vacuumFactor. Valid only if useVacuumParams=1 (default 0)
- vacuumFactor: for modelType 0 or 3, an optional double value used to multiply coordinates and parametric values of nodes on vacuum wall when adjustVacuumParams=1. Valid only if adjustVacuumParams=1 (default 2×PI)
- numVacuumPts: optional  $\#$  interpolation points on parameterized vacuum wall. Valid only if useVacuumParams=1 (default 20)
- meshGradationRate: for modelType 3 or 4, optional mesh gradation rate (default: 0.3). This value should be greater than or equal to 0.3. Otherwise the mesh will be fine everywhere.
- resistive-width: for modelType 3, the width of resistive wall. If resistive-width=0, only plasma region is created (default 0.02)
- plasma-offsetX: for modelType 3, the offset in x direction to the left (default  $0.0$ )
- plasma-offsetY: for modelType 3, the offset in y direction to the bottom (default  $0.0$ )
- vacuum-width: for modelType 3 or 4, the width of vacuum region (default 2.5)
- vacuum-height: for modelType 3 or 4, the height of vacuum region (default 4.0)

Locate input parameter file and all files listed as bdryFile (if applicable) in the work folder and do m3dc1 meshgen input param file, then the following output will be generated.

- The output model in three formats
	- $M3D C^1$ -readable .txt
	- Simmetrix-readable file .smd and
	- PUMI-readable .dmg
		- $\triangleright$  For modelType 0-2, the model is saved in outFile.\*
		- $\triangleright$  For modelType 3 with resistive width R, vacuum-width W and vacuum-height H, the model is saved in outFile-R-W-H.\*.
		- $\triangleright$  For modelType 4 with vacuum-width W and vacuum-height H, the model is saved in outFile-W-H.\*.
- The output mesh in three formats
	- Simmetrix-readable.sms
	- $M3D C^1/\text{PUMI~readable}$  .smb
	- Paraview
		- $\triangleright$  For modelType 0-2 with  $\#$  mesh faces F,
			- if  $F > 1000$ , the mesh is saved in outFile-(F/1000).\*
			- if  $F < 1000$ , the mesh is saved in outFile-F.\*
		- $\triangleright$  For modelType 3 with  $\#$  mesh faces F, resistive width R, vacuum-width W, vacuumheight H,
			- if  $F > 1000$ , the mesh is saved in outFile-R-W-H-(F/1000).\*
			- if  $F < 1000$ , the mesh is saved in outFile-R-W-H-F. $*$
		- $\triangleright$  For modelType 4 with  $\#$  mesh faces F, vacuum-width W and vacuum-height H,
			- if  $F > 1000$ , the mesh is saved in outFile-W-H-(F/1000).\*
			- if  $F < 1000$ , the mesh is saved in outFile-W-H-F.\*

#### <span id="page-15-0"></span>3.1.1 Type 0 (parameterized vacuum)

The figure [1](#page-16-0) illustrates a mesh generated by the following input file.

```
modelType 0
outFile analytic
meshSize 0.04
useVacuumParams 1
vacuumParams 1.65908 0.46 0.2 -0.02504 0.8
numVacuumPts 20
adjustVacuumParams 0
vacuumFactor 6.28319
```
The figure [2](#page-16-1) illustrates a mesh generated with the same vacuum region parameters and a higher mesh size value.



<span id="page-16-0"></span>Figure 1: A mesh with vacuum region defined by five parameters for analytic expression



<span id="page-16-1"></span>Figure 2: A mesh generated with vacuum region parameters and mesh size 0.1



<span id="page-17-2"></span>Figure 3: A mesh with vacuum region defined by piece-wise polynomials

# <span id="page-17-0"></span>3.1.2 Type 2 (piece-wise polynomial vacuum)

The figure [3](#page-17-2) illustrates a mesh generated by the following input file. The vacuum region's geometry information is defined by piece-wise polynomials and stored in the file in-poly.

modelType 2 inFile in-poly outFile poly

The vacuum region's geometry information is defined by piece-wise polynomials and stored in the file in-poly and the example file can be found in

/p/tsc/m3dc1/lib/SCORECLib/rhel7/intel2019u3-openmpi4.0.3/16.0-220226/bin.

# <span id="page-17-1"></span>3.1.3 Type 3 (three-regions with inner wall points)

With the model type 3, a geometric model consists of three model faces where each represents plasma region, resistive region and vacuum region, respectively. An ascii file name which describes inner plasma wall boundary has to be provied with the parameter inFile.

The figure [4](#page-18-1) illustrates a mesh generated by the following input file. In the figure, geometric model faces are different colored.



<span id="page-18-1"></span>Figure 4: A mesh with spline-fitted 3-region model

```
modelType 3
inFile in-circle
outFile circle
meshSize 0.1 0.5 0.1
useVacuumParams 1
adjustVacuumParams 1
vacuumParams 5.0 1.5 0.0 0.0 1.5
numVacuumPts 20
meshGradationRate 0.4
resistive-width 0.4
```
The example files circle-input and in-circle can be found in

/p/tsc/m3dc1/lib/SCORECLib/rhel7/intel2019u3-openmpi4.0.3/16.0-220226/bin.

#### <span id="page-18-0"></span>3.1.4 Type 4 (three-regions with inner  $\&$  outer wall points)

With the model type 4, a geometric model consists of three model faces where each represents plasma region, resistive region and vacuum region, respectively. The parameter inFile denotes a file name that contains inner plasma wall boundary. The parameter bdryFile denotes a file name that contains resistive wall boundary.



<span id="page-19-1"></span>Figure 5: A mesh with inner & outer plama wall boundary points

The figure [5](#page-19-1) illustrates a mesh generated by the following input file. In the figure, geometric model faces are different colored.

modelType 4 inFile inner\_bdry.pts bdryFile outer\_bdry.pts outFile iter meshSize 0.7 0.5 0.7 useVacuumParams 1 adjustVacuumParams 1 vacuumParams 8.25 8.0 0.2 0.0 12.5 meshGradationRate 1

The example files bdry-input, inner\_bdry.pts and outer\_bdry.pts can be found in

/p/tsc/m3dc1/lib/SCORECLib/rhel7/intel2019u3-openmpi4.0.3/16.0-220226/bin.

# <span id="page-19-0"></span>3.2 m3dc1 mfmgen

m3dc1 mfmgen requires an ascii input file of arbitrary name that contains the following parameters. The parameters can be in any order.

- numBdry: the number of boundary files defined by peice-wise linear points given for the construction of the loops (default: 0)
	- Each boundary file corresponds to a loop in PUMI
	- For numBdry=N, N lines of bdryFile should be provided,  $N > 0$
- bdryFile: For each boundary file, the user has to provide its file name followed by the unique loop ID and desired mesh size on the loop.
	- Each boundary file corresponds to a loop in PUMI
	- The unique ID can be an arbitrary integer defined by the user
	- The unique ID is used with input parameter "faceBdry" to specify the boundaries (loops) of model face
	- For more than one boundary files (numBdry $>1$ ), the boundary files can be in any order
- useVacuum: A parameter to control the vacuum boundary
	- The first number sets the mode of vacuum boundary and can be 0, 1 or 2. If 0, no vacuum boundary will be created. If 1, vacuum boundary will be created without user defined parameters. If 2, a parameterized vacuum boundary will be created by using the parameters defined in the parameter "vacuumParams".
	- The second number is the desired unique loop ID for the vacuum loop
	- The third number defines the mesh size on the vacuum boundary
- vacuum Params: if "use Vacuum  $= 2$ ", the user has to provide five doubles to define parameterized vacuum wall
- numVacuumPts: if "useVacuum =  $2$ ",  $\#$  interpolation points on parameterized vacuum wall  $(default=20)$
- thickWall: three integers and one double to control finite thickness wall
	- $-$  The first number can either be 0 or 1. If it is set to 0, no finite thickness wall will be created. If it is set to 1, a finite thickness wall will be created
	- The second number is the loop ID that will be offset for given thickness
	- The third number is the desired unique loop ID for the new loop created from offsetting for the finite thickness wall
	- The last number is the desired wall thickness
- layeredMesh: two integers to create an extruded layeded mesh on the finite thickness wall
	- The first integer is 0, no layered mesh will be created. If 1 (default), an extruded mesh with desired number of mesh layers will be created
	- The second integer defines the number of mesh layers
- numFace: the number of geometric model faces in PUMI (default 1)
	- Each geometric face corresponds to regions (e.g. plasma, resistive, vacuum) in M3DC1
	- For numFace=N, N lines of faceBdry should be provided,  $N > 0$
- faceBdry: For each model face, the user has to provide the number of loops, loop  $ID(s)$ , and desired mesh size
	- The first number gives the total number of loops bounding the face
	- the first number is followed by the loops IDs of the bounding loops. If number of loops  $=n$ , there should be *n* loop ID
	- The last number is the desired mesh size on the geometric face
- meshGradationRate: Global mesh gradation rate for the meshing. This parameter is optional and if not specified a default mesh gradation rate  $= 0.3$  is used. This value should be greater than or equal to 0.3. Otherwise the mesh will be fine everywhere.
- outFile: output file name to save model and mesh

Locate input parameter file and all files listed as bdryFile (if applicable) in the work folder and do m3dc1 mfmgen input param file. The output files are the same as those of m3dc1 meshgen.

#### <span id="page-21-0"></span>3.2.1 Mesh with parameterized vacuum wall

This section presents a mesh created with a parameterized vacuum wall. This is equivalent to Type 0 mesh of m3dc1 meshgen.

numBdry 0 useVacuum 1 1 0.1 numFace 1 faceBdry 1 1 0.09 outFile analytic-0.09

The figure [6](#page-22-0) presents the mesh generated by the input file above with two different mesh sizes.

#### <span id="page-21-1"></span>3.2.2 Mesh with single boundary file

```
numBdry 1
bdryFile loop1.dat 3 0.1
numFace 1
faceBdry 1 3 0.2
outFile input1
```
The figure [7](#page-22-1) presents the mesh generated by the input file above.



<span id="page-22-0"></span>Figure 6: Mesh with a parameterized vacuum region and different mesh size for model face (left) 0.2 (right) 0.09



<span id="page-22-1"></span>Figure 7: Mesh with single boundary file and no vacuum wall



<span id="page-23-1"></span>Figure 8: Mesh with two boundary files and a parameterized vacuum region

#### <span id="page-23-0"></span>3.2.3 Mesh with two boundary files and a parameterized vacuum wall

This section presents a mesh created with two boundary files and a parameterized vacuum wall. This is equivalent to Type 4 mesh of m3dc1 meshgen.

numBdry 2 bddyFile loop1.pts 1 0.5 bdryFile loop2.pts 2 0.5 useVacuum 2 3 0.5 vacuumParams 8.25 8.0 0.2 0.0 12.5 numFace 3 faceBdry 1 1 0.7 faceBdry 2 1 2 0.5 faceBdry 2 2 3 0.7 meshGradationRate 1 outFile iter

The figure [8](#page-23-1) presents the mesh generated by the input file above. As you can see, the mesh in Figure [8](#page-23-1) and [5](#page-19-1) are almost identical.





### <span id="page-24-2"></span><span id="page-24-0"></span>3.2.4 Mesh with three boundary files

```
numBdry 3
bdryFile loop1.dat 3 0.1
bdryFile loop2.dat 10 0.05
bdryFile loop3.dat 11 0.09
numFace 3
faceBdry 1 3 0.2
faceBdry 2 3 10 0.1
faceBdry 2 10 11 0.09
outFile input3
```
The figure [9](#page-24-2) presents the mesh generated by the input file above.

#### <span id="page-24-1"></span>3.2.5 Mesh with seven boundary files and a vacuum wall

numBdry 7 bdryFile loop1.dat 3 0.2 bdryFile loop2.dat 10 0.3 bdryFile loop3.dat 11 0.4



<span id="page-25-0"></span>Figure 10: Mesh with seven boundary files and a parameterized vacuum wall

bdryFile loop4.dat 21 0.4 bdryFile loop5.dat 25 0.4 bdryFile loop6.dat 17 0.2 bdryFile loop7.dat 19 0.1 useVacuum 1 9 0.1 vacuumParams 1.8 1.5 0.4 0.0 2.5 numFace 8 faceBdry 1 3 0.2 faceBdry 1 10 0.3 faceBdry 1 11 0.1 faceBdry 2 21 25 0.2 faceBdry 2 25 17 0.09 faceBdry 2 17 19 0.1 faceBdry 2 19 9 0.1 faceBdry 4 3 10 11 21 0.11 outFile input7

The figure [10](#page-25-0) presents the mesh generated by the input file above.

#### <span id="page-26-0"></span>3.2.6 Mesh with finite thickness wall and layers

Add text here

#### <span id="page-26-1"></span>3.3 polar meshgen

polar meshgen requires an ascii file of arbitrary name that contains input parameters as the following:

- inFile: input file name containing equilibrium generation by jsolver
- outFile: output file name to save model and mesh
- meshSize: relative mesh size for each region (default 0.05)
- reorder: if 1, reorder PUMI mesh based on adjacency (default: 0) and generate vtk folders for mesh visualization. The mesh before and after reodering is saved in original-mesh.vtk and reordered-mesh.vtk, respectively. Note that the element order of Simmetrix mesh is not affected.

The following presents an example input file "polar\_input".



Figure 11: Add Caption Here



Figure 12: Add Caption Here

inFile POLAR outFile polar meshSize 0.04

To run polar meshgen, place polar input and POLAR in your work folder and do "polar meshgen polar input". The program will read POLAR and generate various model and mesh files starting with "polar". For instance, polar-2K0.smb, pol-2K.sms, pol-2K.vtk, polar.dmg, polar.smd, polar.txt. If the resulting mesh is too fine, increase the value of meshSize. If the resulting mesh is too coarse, decrease the value of meshSize. If meshSize is not specified in the input file, the default value is 0.05.

The program read jsolver generates equilibrium and stores in the file POLAR. Given the input file POLAR, m3dc1 meshgen generates the following files:

- model.dmg: PUMI-readable model file
- model.txt: M3DC1-readable model file
- mesh0.smb: PUMI/M3DC1-readable mesh file
- mesh.vtk: Paraview data files
- norm curv: ascii file containing nodes' normal/curvature information

# <span id="page-28-0"></span>3.4 Mesh Control with SimModeler

SimModeler is a graphical user interface to the Simmetrix geometry and mesh generation software. In cases where the currently available capabilities of m3dc1 meshgen do not provide a satisfactory mesh, SimModeler can be used to apply alternative mesh control information to the Tokamak cross section geometry to generate different meshes. The information below indicates the application of a subset of the mesh controls that can be applied. For additional information of the full range of SimModeler mesh control options see: \*\*\*\*\*\*\*\*\*\* FILL IN POINTER TO SIMMETRIX DOC-UMENTATION \*\*\*\*\* (Contributed by D. Pfefferle on 4/27/16) On PPPL Portal, load a module simmodeler and run it.

- 1. From the menu "File→Open Model", load a model file (.smd) generated by m3dc1 meshgen
- 2. In the upper panel, in the views section, click on Front to view the model, then go to Meshing tab
- 3. Select outer region, click + in Mesh Attributes and select Mesh Size $\rightarrow$ relative. Enter a value (typically 0.1)
- 4. Select wall region, click + in Mesh Attributes and select Mesh Size $\rightarrow$ relative. Enter a value (typically 0.02)
- 5. Select inner region, click + in Mesh Attributes and select Mesh Size→relative. Enter a value (typically 0.04). Here, one can already generate the mesh by clicking on Generate Mesh and verify if the mesh sizes are suitable
- 6. Select both inner and wall regions (holding shift key), click + in Mesh Attributes and select Mesh Size→relative. Enter a function, e.g.  $0.01\times$ abs(\$y+1.5)^2+0.004 to specify an anisotropic mesh density on top of previous settings There are many available parameters for fine-tuning the mesh density. For example, Mesh Curvature Refinement with parameter packs more elements near the edges of the resistive wall.
- 7. Generate Mesh and Show Mesh to view result in new windows
- 8. If the result is satisfactory, from the menu File→Save Mesh, give it a meaningful name with the extension .sms. The original model file .smd has been automatically saved by the program with your mesh modifications.
- 9. Close simmodeler then it will release a license. Until you quit Simmodeler, no one cannot run neither m3dc1 meshgen nor simmodeler.
- 10. Copy the .txt, .smd and .sms files to the simulation directory and run the following splitting routine to obtain PUMI-readable .smb mesh files.

/p/tsc/C1/m3dc1-sunfire.r6-1.5/bin/part mesh.sh model file.smd mesh file.sms X, where X is the number of parts you need in the .smb mesh.

11. Modify the C1input file accordingly

mesh\_filename = 'part.smb' mesh model = 'filename.txt'

#### <span id="page-29-0"></span>3.5 Mesh Partitioning

#### <span id="page-29-1"></span>3.5.1 Splitting

The program split smb increases the number of parts in a mesh from P to N  $(P\le N)$ . In each machine, the program split\_smb is availble in \$SCOREC\_UTIL\_DIR provided in hostname.mk file.

In order to split P-part mesh to N parts  $(N>P)$ , run "mpirun -np N ./split\_smb input-mesh(.smb) output-mesh(.smb) X"

- the file extension of input-mesh should be .smb
- the file extension of output-mesh should be .smb
- N is the number of parts in the output mesh
- For a P-part input mesh, X must be N/P
- For both input and output mesh, do not specify a number before the file extension
- split\_smb will insert a number in the output mesh file. The number represents a global part ID.

• Make sure that the output mesh doesn't have any empty part. Otherwise, the program crashes with the following error message: APF warning: 1 empty parts split\_smb:  $\ldots$ /mds/mds.c:614: check\_ent: Assertion 'e >= 0' failed

Examples on portal:

- 1. To split a serial (1-part) mesh to 6 parts, run "mpirun -np 6 ./split\_smb struct-curveDomain.smb part.smb 6"
	- Input mesh: struct-curveDomain0.smb
	- Output mesh: part0.smb, part1.smb, part2.smb, part3.smb, part4.smb, part5.smb
- 2. To split a 2-part mesh to 6 parts, run "mpirun -np 6 ./split smb struct-curveDomain.smb part.smb 3"
	- Input mesh: struct-curveDomain0.smb, struct-curveDomain1.smb
	- Output mesh: part0.smb, part1.smb, part2.smb, part3.smb, part4.smb, part5.smb

See readme.split\_smb for detailed instructions and trouble shooting tips.

#### <span id="page-30-0"></span>3.5.2 Mesh Merging

The program collapse decreases the number of parts in a mesh from  $N$  to  $P(P\le N)$ . In each machine, the program collapse is availble in \$SCOREC UTIL DIR provided in hostname.mk file.

In order to merge N-part .smb mesh to P parts (P>0), run "mpirun -np N ./collapse input-mesh(.smb) output-mesh(.smb) X"

- the file extension of input-mesh should be .smb
- the file extension of output-mesh should be .smb
- N is the number of parts in the input mesh
- For a P-part output mesh, X must be N/P
- For both input and output mesh, do not specify a number before the file extension
- collapse will insert a number in the output mesh file. The number represents a global part ID.

Example on portal:

In order to merge 4-part mesh into a serial (1-part) mesh, run "mpirun -np 4 ./collapse part.smb serial.smb 4"

• Input mesh: part0.smb, part1.smb, part2.smb, part3.smb

• Output mesh: serial0.smb

See readme.collapse for detailed instructions and trouble shooting tips.

# <span id="page-31-0"></span>3.6 Miscellaneous

## <span id="page-31-1"></span>3.6.1 Verification

The program check smb investigates an input mesh and prints any invalid aspects of the mesh. It prints out the mesh size (the number of global, local, and owned entities per dimension) at the end.

In order to run, do "mpirun -np N ./check smb input-mesh(.smb)".

<span id="page-32-0"></span>4 Mesh Adaptation by Error Estimator

# <span id="page-33-0"></span>5 PETSc Option

# <span id="page-33-1"></span>5.1 2D

The petsc option to run 2D modes is default to superlu dist. You can add the following line on your "srun" command line to change to to mumps:

-pc\_factor\_mat\_solver\_type mumps

#### <span id="page-33-2"></span>5.2 3D

When running M3D- $C<sup>1</sup>$  in the 3D nonlinear mode, you need to include PETSc Options file. There is a number "8" in the file below. It must be equal to the number of toroidal planes. It should be changed whenever you change the number of toroidal planes in the C1input file. The recommended options bjacobi file is as follows:

```
-pc_type bjacobi
-pc_bjacobi_blocks 8
    (for 8 toroidal planes should be equal to nplanes in C1input)
-sub_pc_type lu
-sub_pc_factor_mat_solver_package superlu_dist
    (can exchange mumps for superlu_dist)
-mat_superlu_dist_rowperm NOROWPERM (only needed for superlu_dist)
-mat_mumps_icntl_14 50 (only needed for mumps)
    (50 means 50% of memory increase when needed.
    Users can make it 100 or more if encountering a runtime memory issue.)
-sub_ksp_type preonly
-ksp_type fgmres
-ksp_gmres_restart 220
-ksp_rtol 1.e-9
-ksp_max_it 10000
-on_error_abort
-hard_pc_type bjacobi
-hard_pc_bjacobi_blocks 8
    (for 8 toroidal planesshould be equal to nplanes in C1input)
-hard_sub_pc_type lu
-hard_sub_pc_factor_mat_solver_type superlu_dist
    (can change mumps for superlu_dist)
-mat_superlu_dist_rowperm NOROWPERM
    (only needed for superlu_dist)
-mat_mumps_icntl_14 50
    (only needed for mumps.)
    (50 means 50% of memory increase when needed.
```

```
Users can make it 100 or more if encountering a runtime memory issue.)
-hard_sub_ksp_type preonly
-hard_ksp_type lgmres
-hard_ksp_lgmres_argument 4
-hard_ksp_gmres_restart 220
-hard_ksp_rtol 1.e-9
-hard_ksp_max_it 10000
```
# <span id="page-34-0"></span>5.3 More

More examples are in regtest/pellet/base/ directory, such as

```
options_bjacobi.type_superludist
options_bjacobi.type_mumps
```
The following are additional optional arguments:

```
-ksp_converged_reason
-ksp_view
```
-help

-options\_table -options\_left

-trdump -malloc\_log

for diagnosing purpose.

# <span id="page-35-0"></span>6 Running Jobs

Users can find almost all of the needed example batch scripts and input files to run a job on available computing facilities from

```
unstructured/regtest/*/base/
```
directories.

#### <span id="page-35-1"></span>6.1 Running 2D or Linear Jobs

In 2D, the run can be either linear or nonlinear, depending on the C1input parameter *linear*:

 $linear = 0$  (non-linear run: must compile with the option  $RL=1$ )

 $linear = 1$  (linear run: must compile with the option COM=1)

In both cases, set

 $nplanes = 1$ 

For the linear case, use

 $ntor = nn$ 

set the toroidal mode number.

To run your job on a scratch directory, copy the following files over:

```
executable (m3dc1_2d for non-linear run or m3dc1_2d_complex for linear run)
C1input
AnalyticModel (or MultiEdgeAnalyticModel)
struct-dmg.sms
(and geqdsk if needed)
```
To run non-linear job

mpirun np 8 ./m3dc1\_2d

To run linear job

mpirun np 24 ./m3dc1\_2d\_complex -pc\_factor\_mat\_solver\_package mumps
### 6.2 Running 3D Nonlinear Jobs

For the 3D nonlinear run, set *linear*  $= 0$  and set *nplanes* equal to the number of toroidal planes in C1input file. The number of bjacobi blocks in the PETSc options file must also be equal to nplanes. The total number of processors to request must be the product of nplanes and M (the number of processors per plane, which equals the number of mesh partitions per plane).

Files required to be present to the local directory are:

executable (m3dc1 or m3dc1\_st) C1input, partnn.smb (one for each poloidal plane partition) options\_bjacobi m3dc1.xml (if using ADIOS) geqdsk (if needed)

To run linear job

mpirun np 16 ./ m3dc1 ipetsc options\_file options\_bjacobi (nplane=2, M=8)

See the previou section for the format of the PETSc option file options bjacobi. In this example job, there are  $M = 8$  mesh partition files:

part0.smb part1.smb part2.smb part3.smb part4.smb part5.smb part6.smb part7.smb

#### 6.3 Graphics Files

The graphics files are of two types. There is a single file called: C1.h5 that contains all the timedependent scalar information. This must be saved and be present in the directory of a job so that it can be added to.

In addition to this file, each plot cycle will produce a file: time\_nnn.h5, where nnn is the plot cycle number. The equilibrium is written into a file called equilibrium.h5. These must be stored in the same directory as the C1.h5 file.

#### 6.4 Restarting Jobs

By default hdf5 files are written in every time step. Therefore jobs can be restarted from the hdf5 plot file, the same one that is used by the idl routines to make plots.

By default, the hdf5 files are written in single precision. If idouble out is set to 1 in C1input file, hdf5 files are written in double precision.

#### 6.4.1 Reading restart files for 2D real, 2D complex, or 3D real runs

To start a normal simulation with the hdf5 files, set the C1input parameter irestart to 1.

However, the files C1.h5 and the final time\_nnn.h5 file must be present in the working directory. You may also restart from an intermediate time by setting irestart slice=nn where nn is the nnth plot file. If this is not set, it will restart from the final plot file.

#### 6.4.2 Reading real restart files to initialize 2D complex calculation

- Run 2D linear= $0$
- Copy 2D C1.h5 and the final time nnnn.h5 to the working directory
- Run 2D (complex) linear = 1. In the initial restart, the time and cycle number will start from t=0 and N=0 for the complex run

#### 6.4.3 Running 3D real simulation from 2D real restart files

To start a 3D simulation with 2D restart files, do the following:

- Run 2D
- Copy 2D C1.h5 and the final time\_nnn.h5 to the working directory
- In 3D work folder, set the C1 input parameter irestart = 1 Regardless of the time step when the restart files were written, the 3D simulation starts with time step 1.

#### 6.5 Monitoring Jobs

You can monitor the progress of your running job in several ways:

A. C1ke file. Each time step, one line will be added to the ASCII C1ke file in the run directory that you can open with a text editor. The first 4 fields are:

cycle time kinetic\_energy growth\_rate

B. C1.h5 file: You can monitor a time dependent run by using the idl utility described below. Especially useful is the

plot\_scalar,ke

command and also

### plot\_scalar,ke,/growth

C. You can use a text editor to monitor the log file slurm-nnnn.out file (where nnnn is the job number assigned by SLURM)

### 6.6 Exporting Node/Vector/Matrix for Standalone Study

### 6.7 Archiving Data at PPPL

### 7 Boundary Conditions

In all cases,  $f = 0$  on the boundary, and therefore also  $\hat{\mathbf{t}} \cdot \nabla f = 0$ . Some other boundary conditions that may be specified are as follows:

No normal flow (inonormalflow=1) Holds  $\hat{\mathbf{n}} \cdot \mathbf{u}$  constant.

No poloidal flow (inoslip pol=1) Holds  $\hat{\mathbf{t}} \cdot \mathbf{u}$  constant.

No toroidal flow (inoslip\_tor=1) Holds  $\hat{\varphi} \cdot u$  constant.

No normal current (Winocurrent pol inocurrent norm=1) Holds  $\hat{\mathbf{n}} \cdot \mathbf{J}$  constant.

No poloidal current (inocurrent pol=1) Holds  $\hat{\mathbf{t}} \cdot \mathbf{J}$  constant.

No toroidal current (inocurrent\_tor=1) Holds  $\hat{\varphi} \cdot \mathbf{J}$  constant.

$$
\hat{\mathbf{n}} \cdot \mathbf{u} = -R\hat{\mathbf{t}} \cdot \nabla U + \frac{1}{R^2} \hat{\mathbf{n}} \cdot \nabla \chi \tag{3}
$$

$$
\hat{\mathbf{t}} \cdot \mathbf{u} = R\hat{\mathbf{n}} \cdot \nabla U + \frac{1}{R^2} \hat{\mathbf{t}} \cdot \nabla \chi \tag{4}
$$

$$
\hat{\varphi} \cdot \mathbf{u} = R\omega \tag{5}
$$

$$
\hat{\mathbf{n}} \cdot \mathbf{B} = -\frac{1}{R} \hat{\mathbf{t}} \cdot \nabla \psi - \frac{1}{R^2} \hat{\mathbf{n}} \cdot \nabla f_{\varphi}
$$
\n(6)

$$
\hat{\mathbf{t}} \cdot \mathbf{B} = \frac{1}{R} \hat{\mathbf{n}} \cdot \nabla \psi \tag{7}
$$

$$
\hat{\varphi} \cdot \mathbf{B} = \frac{F}{R} \tag{8}
$$

$$
\hat{\mathbf{n}} \cdot \mathbf{J} = -\frac{1}{R} \hat{\mathbf{t}} \cdot \nabla F + \frac{1}{R^2} \hat{\mathbf{n}} \cdot \nabla \psi_{\varphi}
$$
\n(9)

$$
\hat{\mathbf{t}} \cdot \mathbf{J} = \frac{1}{R} \hat{\mathbf{n}} \cdot \nabla (F + f_{\varphi\varphi}) + \frac{1}{R^2} \hat{\mathbf{t}} \cdot \nabla \psi_{\varphi}
$$
(10)

$$
\hat{\varphi} \cdot \mathbf{J} = -\frac{1}{R} \Delta^* \psi \tag{11}
$$

In the above definitions,  $\hat{\mathbf{n}}$  is the unit vector normal to the boundary surface, and  $\hat{\mathbf{t}} = \hat{\varphi} \times \hat{\mathbf{n}}$ .

### 8 Discretization

#### 8.1 Finite Elements

Each field is represented as a linear combination of N basis functions  $\nu_i$  on the computational domain

$$
U = \sum_{i=1}^{N} \nu_i U_i.
$$

The finite element used in M3D- $C^1$  is the reduced quintic element [?], in which the basis functions are fifth order polynomials. At each time step, the projection of the equations onto the basis functions are computed and solved. For example, the equation

$$
\frac{\partial U}{\partial t} = F(U)
$$

becomes the system of projection equations

$$
\int dV \,\nu_i \frac{\partial U}{\partial t} = \int dV \,\nu_i F(U).
$$

These projections equations are known collectively as the weak form of the equation. Solving the equation in this manner is known as the Galerkin method. Hereafter the index  $i$  will be dropped from  $\nu_i$ .

Once the equations are cast in the weak form, integrations by parts may be carried out in order to reduce the order of the differential operators acting on the physical fields. For example,

$$
\int dV \nu \nabla^2 U = \int dV \nabla \cdot (\nu \nabla U) - \nabla \nu \cdot \nabla U
$$

$$
= \oint d\mathbf{A} \cdot \nabla U \nu - \int dV \langle \nu, \nabla U \rangle
$$

$$
= - \int dV \langle \nu, U \rangle.
$$

It is found that using integrations by parts to re-cast the equations into a form in which a roughly equal number of derivatives acts on the trial function as on the physical fields improves the numerical stability of methods for solving the equations. Thus, in the above example, the form  $-\langle \nu, U \rangle$  is preferable to  $\nu \nabla^2 U$ .

#### 8.1.1 Weak form of Physical Equations

#### Integration Identities

Rather than performing integrations by parts directly on each term in equations (??), it is simpler to begin directly from the vector form, equations (??) and use the following identities when applying the operations to extract the scalar equations:

$$
-\int dV R^2 \nu \nabla \varphi \cdot \nabla \times \mathbf{A} = -\int dV \mathbf{A} \cdot [\nabla (R^2 \nu) \times \nabla \varphi]
$$

$$
\int dV \nu \nabla \cdot \mathbf{A} = -\int dV \nabla \nu \cdot \mathbf{A}.
$$

(Note that the torodal operator,  $R^2\nu\nabla\varphi$ , is not a differential operator and therefore the integration by parts cannot be performed a priori.)

Similary, useful identities for the operators that will act on the stress tensor Π are:

$$
R^2 \nu \nabla \varphi \cdot \nabla \times (\nabla \cdot \Pi) = R^2 \partial_Z \nu \nabla \varphi \cdot \Pi \cdot \nabla \varphi - \nabla \nu \cdot \Pi \cdot \nabla Z + r \nabla \varphi \cdot [\nabla \nabla (\nu r) \dot{\times} \Pi] + \nabla \cdot \mathbf{A}_1
$$
 (12a)

$$
-R^2\nu\nabla\varphi\cdot(\nabla\cdot\Pi) = R^2\nabla\nu\cdot\Pi\cdot\nabla\varphi + \nabla\cdot\mathbf{A}_2
$$
 (12b)

<span id="page-41-0"></span>
$$
-\nu \nabla \cdot (\nabla \cdot \Pi) = -\nabla \nabla \nu : \Pi + \nabla \cdot \mathbf{A}_3 \tag{12c}
$$

where

$$
\begin{aligned}\n\mathbf{A}_1 &= -R^2 \nu \nabla \varphi \times (\nabla \cdot \Pi) - r \Pi \cdot [\nabla \varphi \times \nabla (r\nu)] + \nu \Pi \cdot \nabla Z \\
\mathbf{A}_2 &= -R^2 \nu \Pi \cdot \nabla \varphi \\
\mathbf{A}_3 &= \nabla \nu \cdot \Pi - \nu \nabla \cdot \Pi.\n\end{aligned}
$$

(These identities hold for any symmetric tensor Π.) The total divergences vanish upon integration.

#### <span id="page-41-1"></span>8.1.2 Physical Equations after Integrations by Parts

$$
\int dV N_n = \int dV \left[ N_{nU} + N_{n\chi} + N_{nD} \right] \tag{13a}
$$

$$
\int dV \left[ U_{Un} + U_{\chi n} \right] = \int dV \left[ U_{UUn} + U_{VVn} + U_{U\chi n} + U_{\chi\chi n} \right. \tag{13b}
$$
\n
$$
+ U_{\psi\psi} + U_{FF} + U_{U\mu} + U_{\chi\mu} + U_g
$$
\n
$$
+ U_{UD} + U_{\chi D} + U_{\Pi_{\parallel}} + U_{\Pi_{\chi}} \right]
$$

$$
\int dV V_{Vn} = \int dV \left[ V_{VUn} + V_{V\chi n} + V_{\psi F} + V_{V\mu} \right] + V_{VD} + V_{\Pi_{\parallel}} + V_{\Pi_{\times}} \right]
$$
\n(13c)

$$
\int dV \left[ X_{Un} + X_{\chi n} \right] = \int dV \left[ X_{UUn} + X_{VVn} + X_{U\chi n} + X_{\chi\chi n} \right. \tag{13d}
$$
\n
$$
+ X_p + X_{\psi\psi} + X_{FF} + X_{U\mu} + X_{\chi\mu} + X_g
$$
\n
$$
+ X_{UD} + X_{\chi D} + X_{\Pi_{\parallel}} + X_{\Pi_{\chi}} \right]
$$

$$
\int dV \Psi_{\psi} = \int dV \left[ \Psi_{\psi U} + \Psi_{\psi \chi} + \Psi_{\psi F n} + \Psi_{\psi \eta} \right]
$$
\n(13e)  
\n
$$
\int dV F_{\psi} = \int dV \left[ F_{\psi} + F_{\psi} + F_{\psi} + F_{\psi} + F_{\psi} \right]
$$
\n(13e)

$$
\int dV F_F = \int dV \left[ F_{FU} + F_{\psi V} + F_{F\chi} + F_{\psi n} + F_{Fn} \right]
$$
\n
$$
+ F_{pen} + F_{Fn} \tag{13f}
$$

$$
\int dV P_p = \int dV \left[ P_{pU} + P_{p\chi} + P_{p_e F n} + P_{\eta \psi} + P_{\eta F} \right]
$$
\n
$$
+ P_{\kappa} + P_{\kappa_{\parallel}} + P_{\kappa_{\times}} \right]
$$
\n(13g)

The terms in the above equations are categorized and defined in the following sections. Each term has been integrated by parts to arrive at the simplest expression having for which the order of differentiation on the trial function is roughly equal to that on the physical fields.

#### Basic Terms

The terms in this section are the basic terms in the two-fluid equations, which do not depend on any specific choice of closure.

$$
N_n(\nu, \dot{n}) = \nu \dot{n}
$$
  
\n
$$
N_{nU}(\nu, n, U) = \nu [U, n]
$$
  
\n
$$
N_{n\chi}(\nu, n, \chi) = n \langle \nu, \chi \rangle
$$
  
\n
$$
N_{nD}(\nu, n, D) = -D \langle \nu, n \rangle
$$
\n(14)

$$
U_{Un}(\nu, \dot{U}, n) = -\frac{1}{R^2} n \langle R^2 \nu, \dot{U} \rangle
$$
  
\n
$$
U_{\chi n}(\nu, \dot{\chi}, n) = -R^2 \nu [n, \dot{\chi}]
$$
  
\n
$$
U_{UUn}(\nu, U, U, n) = \frac{1}{R^2} n \Delta^* U [R^2 \nu, U] + \frac{1}{2R^2} \langle U, U \rangle [R^2 \nu, n]
$$
  
\n
$$
U_{VVn}(\nu, V, V, n) = \frac{1}{2R^2} [\nu, R^2] V V n
$$
  
\n
$$
U_{U\chi n}(\nu, U, \chi, n) = \frac{1}{R^2} n \Delta^* U \langle R^2 \nu, \chi \rangle - [U, \chi] [R^2 \nu, n]
$$
  
\n
$$
U_{\chi \chi n}(\nu, \chi, \chi, n) = \frac{1}{2} \langle \chi, \chi \rangle [R^2 \nu, n]
$$
  
\n
$$
U_{\psi\psi}(\nu, \psi, \psi) = -\frac{1}{R^2} [R^2 \nu, \psi] \Delta^* \psi
$$
  
\n
$$
U_{FF}(\nu, F, F) = -R^2 \nu F [F, \frac{1}{R^2}]
$$
  
\n
$$
U_{UD}(\nu, U, D) = \frac{1}{R^2} \langle R^2 \nu, U \rangle D
$$
  
\n
$$
U_{\chi D}(\nu, \chi, D) = -[R^2 \nu, \chi] D
$$

$$
V_{Vn}(\nu, V, n) = \nu n \dot{V}
$$
  
\n
$$
V_{VUn}(\nu, V, U, n) = \nu n [U, V]
$$
  
\n
$$
V_{V\chi n}(\nu, V, \chi, n) = -\nu n \langle \chi, V \rangle
$$
  
\n
$$
V_{\psi F}(\nu, \psi, F) = \nu [F, \psi]
$$
  
\n
$$
V_{VD}(\nu, V, D) = -\nu V D
$$
\n(16)

$$
X_{Un}(\nu, \dot{U}, n) = \nu \left[ n, \dot{U} \right]
$$
  
\n
$$
X_{\chi n}(\nu, \dot{\chi}, n) = -n \langle \nu, \dot{\chi} \rangle
$$
  
\n
$$
X_{p}(\nu, p) = \langle \nu, p \rangle
$$
  
\n
$$
X_{UUn}(\nu, U, U, n) = -\frac{1}{R^2} n \Delta^* U \langle \nu, U \rangle + \frac{1}{2} n \langle \nu, \frac{\langle U, U \rangle}{R^2} \rangle
$$
  
\n
$$
X_{VVn}(\nu, V, V, n) = \frac{1}{2} n V V \langle \frac{1}{R^2}, \nu \rangle
$$
  
\n
$$
X_{U\chi n}(\nu, U, \chi, n) = (n \nabla^2 \nu + \langle n, \nu \rangle) [U, \chi] + n \Delta^* U [\nu, \chi]
$$
  
\n
$$
X_{\chi \chi n}(\nu, \chi, \chi, n) = \frac{1}{2} n \langle \nu, \langle \chi, \chi \rangle \rangle
$$
  
\n
$$
X_{\psi\psi}(\nu, \psi, \psi) = \frac{1}{R^2} \Delta^* \psi \langle \nu, \psi \rangle
$$
  
\n
$$
X_{FF}(\nu, F, F) = \frac{1}{R^2} F \langle \nu, F \rangle
$$
  
\n
$$
X_{UD}(\nu, U, D) = [\nu, U] D
$$
  
\n
$$
X_{\chi D}(\nu, \chi, D) = \langle \nu, \chi \rangle D
$$
  
\n(17)

$$
\Psi_{\psi}(\nu, \dot{\psi}) = \nu \dot{\psi} \n\Psi_{\psi U}(\nu, \psi, U) = \nu [U, \psi] \n\Psi_{\psi \chi}(\nu, \psi, \chi) = -\nu \langle \chi, \psi \rangle \n\Psi_{\psi F n}(\nu, \psi, F, n) = d_{i} \nu \frac{1}{n} [\psi, F] \n\Psi_{\psi \eta}(\nu, \psi, \eta) = -\frac{1}{R^{2}} \langle \psi, R^{2} \nu \eta \rangle
$$
\n(18)

$$
F_F(\nu, \dot{F}) = \nu \dot{F}
$$
  
\n
$$
F_{FU}(\nu, F, U) = R^2 \nu \left[ U, \frac{F}{R^2} \right]
$$
  
\n
$$
F_{\psi V}(\nu, \psi, V) = R^2 \nu \left[ \frac{V}{R^2}, \psi \right]
$$
  
\n
$$
F_{F\chi}(\nu, F, \chi) = \frac{F}{R^2} \langle R^2 \nu, \chi \rangle
$$
  
\n
$$
F_{\psi n}(\nu, \psi, \psi, n) = d_i \frac{\Lambda^* \psi}{R^2 n} \left[ \psi, R^2 \nu \right]
$$
  
\n
$$
F_{Fn}(\nu, F, F, n) = d_i R^2 \nu F \left[ \frac{1}{R^2 n}, F \right]
$$
  
\n
$$
F_{pen}(\nu, p_e, n) = d_i R^2 \nu \left[ \frac{1}{n}, p_e \right]
$$
  
\n
$$
F_{Fn}(\nu, F, \eta) = -\frac{1}{R^2} \eta \langle R^2 \nu, F \rangle
$$
  
\n(19)

$$
P_p(\nu, \dot{p}) = \nu \dot{p}
$$
  
\n
$$
P_{pU}(\nu, p, U) = \nu [U, p]
$$
  
\n
$$
P_{p\chi}(\nu, p, \chi) = \Gamma p \langle \nu, \chi \rangle + (\Gamma - 1) \nu \langle p, \chi \rangle
$$
  
\n
$$
P_{p_e, F, n}(\nu, p_e, F, n) = d_i \left( \frac{1}{n} \nu [p_e, F] + \Gamma \nu p_e \left[ \frac{1}{n}, F \right] \right)
$$
  
\n
$$
P_{\eta, \psi}(\nu, \eta, \psi, \psi) = (\Gamma - 1) \nu \frac{(\Delta^* \psi)^2}{R^2}
$$
  
\n
$$
P_{\eta, F}(\nu, \eta, F, F) = (\Gamma - 1) \nu \frac{F^2}{R^2}
$$
\n(20)

#### Gravity

These terms are obtained assuming a gravitational force of the form given by equation (??).

$$
U_g(\nu, n) = g_r \nu [n, R] - g_Z r \nu \langle n, R \rangle
$$
  
\n
$$
X_g(\nu, n) = \frac{n}{R^2} (g_r \langle \nu, R \rangle + g_Z r [\nu, R])
$$
\n(21)

#### Heat Flux Terms

These terms are obtained assuming a heat flux density of the form described in section ??.

$$
P_{\kappa}(\nu,\kappa,T) = -(\Gamma - 1)\kappa \langle \nu, T \rangle P_{\kappa_{\parallel}}(\nu,\kappa_{\parallel},T,\psi,\psi,B^{-2}) = -(\Gamma - 1)\kappa \frac{1}{|B^2|}[\psi,\nu][\psi,T] P_{\kappa_{\times}}(\nu,\kappa_{\times},T,F,B^{-2}) = (\Gamma - 1)\kappa_{\times} \frac{F}{B}[\nu,T]
$$
\n(22)

$$
T = p/n
$$
  

$$
B^2 = \frac{1}{R^2} [ \langle \psi, \psi \rangle + F^2 ]
$$

Isotropic Viscosity

These terms result from isotropic viscosity of the form given by equation (??).

$$
U_{U\mu}(\nu, U, \mu) = \frac{1}{R^2} \left[ \left\langle \mu, R^2 \nu \right\rangle + \mu \Delta^*(R^2 \nu) \right] \Delta^* U + \nabla^2 \mu \left\langle R^2 \nu, U \right\rangle + \Delta^*(R^2 \nu) \left\langle \mu, U \right\rangle \right] U_{\chi\mu}(\nu, \chi, \mu) = -\nabla^2 (R^2 \nu) \left[ \mu, \chi \right] - \Delta^* \mu \left[ R^2 \nu, \chi \right] - \frac{1}{R^2} \Delta^*(R^2 \chi) \left[ R^2 \nu, \mu \right] V_{V\mu}(\nu, V, \mu) = \left[ \langle \nu, \mu \rangle + \frac{1}{R^2} \mu \Delta^*(R^2 \nu) \right] V X_{U\mu}(\nu, U, \mu) = \nabla^2 \nu \left[ \mu, U \right] + \nabla^2 \mu \left[ \nu, U \right] + \Delta^* U \left[ \nu, \mu \right] X_{\chi\mu}(\nu, \chi, \mu, \mu_c) = \nabla^2 \nu \left\langle \mu, \chi \right\rangle + \nabla^2 \mu \left\langle \nu, \chi \right\rangle + 2\mu_c \nabla^2 \nu \nabla^2 \chi
$$
\n
$$
(23)
$$

#### Parallel Viscosity

These terms are obtained assuming a parallel viscosity of the form given in equation (??). These equations were obtained using equations [\(12\)](#page-41-0). For compactness, derivatives are written as subscripts in the following expressions (*i.e.*  $\nu_Z = \partial_Z \nu$ ).

$$
U_{\Pi_{\parallel}U}(\nu, U) = \mu_{\parallel U}D_U
$$
  
\n
$$
U_{\Pi_{\parallel}V}(\nu, V) = \mu_{\parallel V}D_U
$$
  
\n
$$
U_{\Pi_{\parallel}X}(\nu, \chi) = \mu_{\parallel \chi}D_U
$$
\n(24)

$$
V_{\Pi_{\parallel} U}(\nu, U) = \mu_{\parallel U} D_V
$$
  
\n
$$
V_{\Pi_{\parallel} V}(\nu, V) = \mu_{\parallel V} D_V
$$
  
\n
$$
V_{\Pi_{\parallel} \chi}(\nu, \chi) = \mu_{\parallel \chi} D_V
$$
\n(25)

$$
X_{\Pi_{\parallel} U}(\nu, U) = \mu_{\parallel U} D_X
$$
  
\n
$$
X_{\Pi_{\parallel} V}(\nu, V) = \mu_{\parallel V} D_X
$$
  
\n
$$
X_{\Pi_{\parallel} \chi}(\nu, \chi) = \mu_{\parallel \chi} D_X
$$
\n(26)

$$
D_U = \frac{3}{B^2} \left\{ -\frac{1}{2} R^2 \left[ \nu, \frac{\langle \psi, \psi \rangle}{R^2} \right] + \langle \psi, [\nu, \psi] \rangle - \frac{1}{R^2} F^2 \nu_Z - \frac{2}{R^2} \left[ \nu_Z (\psi_Z^2 - \psi_R^2) + 2 \nu_r \psi_r \psi_Z \right] \right\}
$$
  
\n
$$
D_V = -3 \frac{F}{B^2} [\nu, \psi]
$$
  
\n
$$
D_X = -\nabla^2 \nu \left( 1 - \frac{3}{R^2} \frac{\langle \psi, \psi \rangle}{B^2} \right) + \frac{3}{R^2 B^2} \left( \frac{1}{2} R^2 \left\langle \nu, \frac{\langle \psi, \psi \rangle}{R^2} \right\rangle - \langle \psi, \langle \nu, \psi \rangle \rangle + \frac{1}{R} F^2 \nu_r \right)
$$

$$
\mu_{\parallel_{U}} = \eta_{0} \frac{p_{i}\tau_{i}}{R^{2}B^{2}} \left( -\frac{1}{2}R^{2} \left[ U, \frac{\langle \psi, \psi \rangle}{R^{2}} \right] + \langle \psi, [U, \psi] \rangle - \frac{1}{R^{2}} F^{2} U_{Z} \right)
$$
  
\n
$$
\mu_{\parallel_{V}} = -\eta_{0} p_{i} \tau_{i} \frac{F}{B^{2}} \left[ \psi, \frac{V}{R^{2}} \right]
$$
  
\n
$$
\mu_{\parallel_{\chi}} = \eta_{0} \frac{p_{i} \tau_{i}}{R^{2}B^{2}} \left( \frac{1}{2}R^{2} \left\langle \chi, \frac{\langle \psi, \psi \rangle}{R^{2}} \right\rangle - \langle \psi, \langle \chi, \psi \rangle \rangle + \frac{1}{R} F^{2} \chi_{r} + \nabla^{2} \chi \langle \psi, \psi \rangle \right)
$$

Gyroviscosity

These terms are obtained using equations [\(12\)](#page-41-0) assuming a gyroviscosity of the form given by equation (??).

$$
U_{\Pi_X U}(\nu, U) = -\frac{p_i F}{2R^3 B^2}
$$
  
\n
$$
\times \left\{\n\begin{array}{l}\n(1 + \frac{3}{2R^2} \frac{\langle \psi, \psi \rangle}{B^2})\n\end{array}\n\left[\n-( [R^3 \nu_Z]_Z - [R^3 \nu_r]_r)\n\begin{pmatrix}\n\left(\frac{U_R}{R}\right)_Z + \left[\frac{U_Z}{R}\right]_r\n\end{pmatrix}\n\right]\n\times\n\left\{\n\begin{array}{l}\n+\frac{9}{2r^2 B^2} \\
\times \left[\n\begin{array}{l}\n(\psi_Z^2 - \psi_R^2)\left(r\nu_Z \left[\left(\frac{U_Z}{R}\right)_Z - \left(\frac{U_R}{R}\right)_r\right] - \frac{1}{R^3} U_Z \left[(R^3 \nu_Z)_Z - (R^3 \nu_r)_r\right]\n\end{array}\n\right]\n\end{array}\n\right\}
$$

$$
U_{\Pi_{\times}V}(\nu, V) = -\frac{p_i}{B^2}
$$
  
\n
$$
\times \left\{\n\begin{array}{l}\n\frac{1}{4R^2} \left(1 - \frac{3F^2}{B^2 R^2}\right) \\
\times \left(\left\langle \frac{V}{R^2}, R^4 [\psi, \nu] \right\rangle - \left\langle \psi, R^4 [\nu, \frac{V}{R^2}] \right\rangle + \frac{1}{R^2} [\nu, R^6 \left\langle \frac{V}{R^2}, \psi \right\rangle] \\
-\frac{3}{4B^2} [\psi, \frac{V}{R^2}] \\
\times \left(2 \left\langle \psi, \left\langle \psi, \nu \right\rangle \right\rangle - R^2 \left\langle \nu, \frac{\left\langle \psi, \psi \right\rangle}{R^2} \right\rangle - \Delta^* \nu \left\langle \psi, \psi \right\rangle + 6 \psi_Z [\nu, \psi]\right)\n\end{array}\n\right\} + \frac{9F^2}{2B^2 R^2} \nu_Z \left\langle \psi, \frac{V}{R^2} \right\rangle
$$

$$
U_{\Pi_{\times} \chi}(\nu, \chi) = -\frac{p_i F}{2R^3 B^2}
$$
  
\$\times \left\{ \begin{array}{l} \left[ (\chi\_{RR} - \chi\_{ZZ}) \left( [R^3 \nu\_r]\_r - [R^3 \nu\_Z]\_Z \right) + 2 \chi\_{RZ} \left( [R^3 \nu\_r]\_Z + [R^3 \nu\_Z]\_r \right) \right] \\ + \frac{3}{R^2 B^2} \left[ \begin{array}{l} \left( \Delta^\* \chi [\psi\_Z^2 - \psi\_R^2] - \chi\_{ZZ} \psi\_Z^2 + \chi\_{RR} \psi\_R^2 \right) \left( [R^3 \nu\_r]\_r - [R^3 \nu\_Z]\_Z \right) \\ + 2 \chi\_{RZ} \left( \psi\_Z^2 [R^3 \nu\_r]\_Z + \psi\_R^2 [R^3 \nu\_Z]\_r \right) \\ - 2 \psi\_r \psi\_Z \left( [\chi\_{ZZ} - \frac{1}{R} \chi\_r] \left[ R^3 \nu\_r \right]\_Z + [\chi\_{RR} - \frac{1}{R} \chi\_r] \left[ R^3 \nu\_Z \right]\_r \right) \end{array} \right\} \end{array} \right\}

$$
V_{\Pi_{\times}U}(\nu, U) = \frac{p_i}{4rB^2}
$$
  
\$\times \left\{ \begin{array}{l} \left(1 - \frac{3}{R^2} \frac{F^2}{B^2}\right) \left(\langle \psi, R[U, \nu] \rangle + \langle \nu, R[U, \psi] \rangle - \frac{1}{R^3} \left[U, R^4 \langle \nu, \psi \rangle \right] + U\_r \left[\nu, \psi\right] + \frac{2}{R} \psi\_Z \langle \nu, U \rangle \right) \\ + \frac{3}{R^3} \left[\psi, \nu\right] \left(2 \langle \psi, \langle U, \psi \rangle \rangle - \Delta^\* U \langle \psi, \psi \rangle - \frac{1}{R^2} \langle U, R^2 \langle \psi, \psi \rangle \rangle + \left[\psi, R^2\right] \left[\psi, U\right] \right) \\ - \frac{18}{R^2} \frac{F^2}{B^2} \left[U, R\right] \langle \nu, \psi \rangle \end{array} \right\} \right\} \right\} \right\} \right\} \right\} \right\} \right\} \right\} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \left[ \frac{1}{2} \frac{1}{2} \left[ \frac{1}{2} \frac{F^2}{B^2} \left[\psi, R\right] \langle \psi, \psi \rangle \right] \right\} \frac{1}{2} \frac{1}{2} \left[ \frac{1}{2} \frac{F^2}{B^2} \left[\psi, R\right] \langle \psi, \psi \rangle \right] \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi, \psi \rangle \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi, \psi \rangle \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi, \psi \rangle \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi, \psi \rangle \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi, \psi \rangle \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi, \psi \rangle \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi, \psi \rangle \frac{1}{2} \frac{1}{2} \left[ \psi, R\right] \langle \psi

$$
V_{\Pi_X V}(\nu, V) = \frac{p_i FR^2}{4B^2} \left(1 - \frac{3}{R^2} \frac{\langle \psi, \psi \rangle - F^2}{B^2}\right) \left[\nu, \frac{V}{R^2}\right]
$$

$$
V_{\Pi_{\times}\chi}(\nu,\chi) = \frac{p_i}{B^2}
$$
  
\$\times \left\{ \begin{array}{l} \left(\frac{1}{R^2} \left\langle \chi, R^2 \left\langle \nu, \psi \right\rangle \right\rangle - \left\langle \nu, \left\langle \chi, \psi \right\rangle \right\rangle - \left\langle \psi, \left\langle \nu, \chi \right\rangle \right\rangle \right) \\ + \frac{3}{2rB^2} \left[ \psi, \nu \right] \left( \left\langle \psi, R \left[ \chi, \psi \right] \right\rangle - \frac{1}{2} r \left[ \chi, \left\langle \psi, \psi \right\rangle \right] \right) \\ + \frac{3}{4R^2} \frac{F^2}{B^2} \left( \left\langle \psi, \left\langle \chi, \nu \right\rangle \right\rangle + \left\langle \nu, \left\langle \chi, \psi \right\rangle \right\rangle - \left\langle \chi, \left\langle \nu, \psi \right\rangle \right\rangle - 2\Delta^\* \chi \left\langle \nu, \psi \right\rangle \right) \end{array} \right\}\$}

$$
X_{\Pi_{\times}U}(\nu, U) = \frac{p_i F}{2R^2 B^2}
$$
  
\n
$$
\times \left\{\n\begin{array}{l}\n\langle \langle \nu, U \rangle \rangle - R^2 \left[ |\nu, U| \right] + \frac{1}{R} \left[ U_r(\nu_{ZZ} - \nu_{RR}) - 2U_Z \nu_{RZ} - \frac{1}{R} U_r \nu_r \right] \\
\left( \left[ \frac{U_Z}{R} \right]_Z - \left[ \frac{U_R}{R} \right]_r \right) (\nu_{ZZ} \psi_R^2 - \nu_{RR} \psi_Z^2 + \frac{1}{R} \nu_r [\psi_Z^2 - \psi_R^2]) \\
+ 2\nu_{RZ} \left( \left[ \frac{U_R}{R} \right]_Z \psi_R^2 + \left[ \frac{U_Z}{R} \right]_r \psi_Z^2 - \frac{1}{R^2} U_Z [\psi_Z^2 - \psi_R^2] \right) \\
- 2\psi_r \psi_Z \left( \left[ \frac{U_R}{R} \right]_Z \nu_{RR} + \left[ \frac{U_Z}{R} \right]_r \nu_{ZZ} - \frac{1}{R^2} U_Z [\nu_{ZZ} - \nu_{RR}] \\
-\frac{1}{R} \nu_r \left[ \left( \frac{U_R}{R} \right)_Z + \left( \frac{U_Z}{R} \right)_r \right]\n\end{array}\n\right\}
$$

$$
X_{\Pi_{\times}V}(\nu, V) = \frac{p_i}{4B^2}
$$
  
\n
$$
\times \left\{ \begin{array}{l} \left(1 - \frac{3}{R^2} \frac{F^2}{B^2}\right) \left(\frac{1}{R^2} \left\langle \nu, R^2 \left\langle \frac{V}{R^2}, \psi \right\rangle \right\rangle - \left\langle \psi, \left\langle \frac{V}{R^2}, \nu \right\rangle \right\rangle - \left\langle \frac{V}{R^2}, \left\langle \psi, \nu \right\rangle \right\rangle \right) \\ + \frac{6}{B^2} \left[\psi, \frac{V}{R^2}\right] \left(\frac{1}{R} \left\langle \psi, R \left[\nu, \psi\right]\right\rangle - \frac{1}{2} \left[\nu, \left\langle \psi, \psi\right\rangle\right]\right) \\ - 6 \frac{F^2}{B^2} \left\langle \psi, \frac{V}{R^2} \right\rangle \left[\left(\frac{\nu_Z}{R^2}\right)_Z + \left(\frac{\nu_R}{R^2}\right)_r\right] \end{array} \right\}
$$

$$
X_{\Pi_{\times}\chi}(\nu,\chi) = -\frac{p_i F}{B^2}
$$
  
\$\times \left\{\n\begin{array}{l}\n\left(1 + \frac{3}{2R^2} \frac{\langle \psi, \psi \rangle}{B^2}\right) \left[\langle \nu, \chi \rangle\right] \\
+ \frac{3}{2B^2} \left[\n\begin{array}{l}\n\left(-\frac{1}{2} \left[\chi, \langle \psi, \psi \rangle\right] + \frac{1}{R} \langle \psi, R \left[\chi, \psi\right] \rangle\right) \left(\left[\frac{\nu\_R}{R^2}\right]\_r + \left[\frac{\nu\_Z}{R^2}\right]\_Z\right) \\
- \left(-\frac{1}{2} \left[\nu, \langle \psi, \psi \rangle\right] + \frac{1}{R} \langle \psi, R \left[\nu, \psi\right] \rangle\right) \left(\left[\frac{\chi\_R}{R^2}\right]\_r + \left[\frac{\chi\_Z}{R^2}\right]\_Z\right)\n\end{array}\n\right\}\n\right\}

#### 8.1.3 Spatial Integration

The integrals required to calculate the weak-form equations of the Galerkin method are computed numerically using a 79-point Gaussian quadrature. That is, the value of each field is calculated at 79 points for each triangular element, and a weighted sum of these values is computed to approximate the integral.

$$
\int dA \ f(x) \simeq \sum_{i=1}^{79} w_i f(x_i),
$$

where the integrand  $f(x)$  is restricted to a single element. The sampling points and weights appropriate for a equilateral triangle are taken from ref. [?].

The coordinates of the sampling points are given in the "natural coordinates"  $(\alpha, \beta, \gamma)$  in ref. [?]. These coordinates may be converted to cartesian coordinates  $(r, Z)$  for an equilateral triangle e having vertices

$$
\left\{ \left( -\frac{\sqrt{3}}{2}, -\frac{1}{2} \right), \left( \frac{\sqrt{3}}{2}, -\frac{1}{2} \right), (0, 1) \right\}
$$

using the linear transformation

$$
\phi_{n \to e}(\alpha, \beta, \gamma) = \left(\frac{\sqrt{3}}{2}(\beta - \gamma), \frac{1}{2}(3\alpha - 1)\right).
$$

The weights must be multiplied by the Jacobian of this transformation,

$$
\mathcal{J}_{\phi_{n\to e}} = \frac{3\sqrt{3}}{4}.
$$

To find the coordinates of the sampling points for a general triangle g having vertices  $\{(-b, 0), (a, 0), (0, c)\},\$ as in ref. [?], one may use the linear transformation

$$
\phi_{e \to g}(r, Z) = \left( \frac{a+b}{\sqrt{3}} x + \frac{a-b}{3} (1-y), \frac{c}{3} (2y+1) \right)
$$
  

$$
\mathcal{J}_{\phi_{e \to g}} = \frac{2c}{3\sqrt{3}} (a+b).
$$

The transformation from natural coordinates to cartesian coordinates for a triangle having vertices  $\{(-b, 0), (a, 0), (0, c)\}\;$  is therefore

$$
\phi_{n \to g}(r, Z) = \left(\frac{1}{2}(a+b)(\beta - \gamma) + \frac{1}{2}(a-b)(1-\alpha), c\alpha\right)
$$
  

$$
\mathcal{J}_{\phi_{n \to g}} = \frac{1}{2}(a+b)c.
$$

The 79-point quadrature gives the exact results for integrands which are polynomials of degree 20 (or less). In the case of quintic finite elements, this means the integration is exact for terms involving products of three fields or fewer, not including the degree-five trial function  $\nu$ . In cylindrical geometry, the presence factors of  $1/R$  will cause the quadrature not to be exact, as  $1/R$  is not in the form of a polynomial. The weights  $w_i$  must also be multiplied by  $R_i$  in cylindrical coordinates to account for the Jacobian of the transformation from cartesian to cylindrical coordinates.

#### 8.2 Time Step

#### 8.2.1 Implicit Time Advance

For the implicit time advance, equations [\(13\)](#page-41-1) are evaulated at the  $\theta$ -advanced time (e.g.  $F(\psi) \rightarrow$  $F(\psi + \theta \delta t \psi + \cdots)$ ), linearized (*i.e.*  $\mathcal{O}(\delta t^2)$  and higher are dropped), and then discretized temporally according to the chosen time integration method  $(i.e. \dot{\psi} \rightarrow (\psi^{(n+1)} - \psi^{(n)})/\delta t)$ .

$$
\begin{pmatrix}\nS_{11}^{v} & R_{11}^{v} & S_{12}^{v} & R_{12}^{v} & S_{13}^{v} & 0 & R_{14}^{v} & R_{13}^{v} \\
R_{11}^{B} & S_{11}^{B} & R_{12}^{B} & S_{12}^{B} & R_{13}^{B} & S_{13}^{B} & 0 & 0 \\
S_{21}^{v} & R_{21}^{v} & S_{22}^{v} & R_{22}^{v} & S_{23}^{v} & 0 & R_{24}^{v} & R_{23}^{v} \\
R_{21}^{B} & S_{21}^{B} & R_{22}^{B} & S_{22}^{B} & R_{23}^{B} & S_{23}^{B} & 0 & 0 \\
S_{31}^{v} & R_{31}^{v} & S_{32}^{v} & R_{32}^{v} & S_{33}^{v} & 0 & R_{34}^{v} & R_{33}^{v} \\
R_{31}^{B} & S_{31}^{v} & R_{32}^{B} & S_{32}^{v} & R_{33}^{B} & S_{33}^{v} & 0 & 0 \\
R_{31}^{v} & 0 & R_{32}^{v} & 0 & R_{33}^{v} & 0 & S^{r} & 0 \\
R_{31}^{v} & 0 & R_{32}^{v} & 0 & R_{33}^{v} & 0 & 0 & S^{r} & 0 \\
Q_{11}^{v} & D_{11}^{v} & Q_{12}^{v} & D_{12}^{v} & Q_{13}^{v} & 0 & Q_{14}^{v} & Q_{13}^{v} \\
Q_{21}^{B} & D_{21}^{B} & Q_{22}^{B} & Q_{23}^{B} & D_{13}^{B} & 0 & 0 & 0 \\
D_{21}^{v} & Q_{21}^{v} & D_{22}^{v} & Q_{22}^{v} & D_{23}^{v} & 0 & Q_{24}^{v} & Q_{23}^{v} \\
Q_{21}^{B} & D_{21}^{B} & Q_{22}^{B} & D_{22}^{B} & Q_{23}^{B} & D_{23}^{B} & 0 & 0 \\
Q_{31}^{v} & Q_{31}^{v} & Q_{32}^{v} & Q_{33}^{v} & Q_{
$$

### 8.2.2 Split Time Step Method

Time is advanced using a split time-step method in which the velocity field is advanced first, then the density and total pressure fields are advanced separately, and finally the magnetic field and electron pressure are advanced together. Though the velocity and magnetic field are advanced separately, the Alfvén and magnetosonic waves are treated implicitly by using equations  $(??-??)$ to calculate analytically the advanced-time values of the pressure and magnetic field for use in the velocity time step.

$$
\begin{pmatrix}\nS_{11}^v & S_{12}^v & S_{13}^v \\
S_{21}^v & S_{22}^v & S_{23}^v \\
S_{31}^v & S_{32}^v & S_{33}^v\n\end{pmatrix}\n\begin{pmatrix}\nU \\
V\n\end{pmatrix}^{(n+1)} \\
= \begin{pmatrix}\nD_{11}^v & D_{12}^v & D_{13}^v \\
D_{21}^v & D_{22}^v & D_{23}^v \\
D_{31}^v & D_{32}^v & D_{33}^v\n\end{pmatrix}\n\begin{pmatrix}\nU \\
V\n\end{pmatrix}^{(n)} + \begin{pmatrix}\nQ_{11}^v & Q_{12}^v & Q_{13}^v \\
Q_{21}^v & Q_{22}^v & Q_{23}^v \\
Q_{31}^v & Q_{32}^v & Q_{33}^v\n\end{pmatrix}\n\begin{pmatrix}\n\psi \\
F\n\end{pmatrix}^{(n)} \\
+ \begin{pmatrix}\nO_1^v \\
O_2^v \\
O_3^v\n\end{pmatrix}
$$
\n(28)

$$
S^{n}n^{(n+1)} = D^{n}n^{(n)} + (R_{1}^{n} R_{2}^{n} R_{3}^{n}) {U \choose V}^{(n+1)} + (Q_{1}^{n} Q_{2}^{n} Q_{3}^{n}) {U \choose V}^{(n)}
$$
\n(29)

<span id="page-49-1"></span>
$$
S^{p}p^{(n+1)} = D^{p}p^{(n)} + (R_{1}^{p} R_{2}^{p} R_{3}^{p}) {U \choose V}^{(n+1)}
$$
  
+  $(Q_{1}^{p} Q_{2}^{p} Q_{3}^{p}) {U \choose V}^{(n)}$  (30)

<span id="page-49-0"></span>
$$
\begin{pmatrix}\nS_{11}^{B} & S_{12}^{B} & S_{13}^{B} \\
S_{21}^{B} & S_{22}^{B} & S_{23}^{B} \\
S_{31}^{B} & S_{32}^{B} & S_{33}^{B}\n\end{pmatrix}\n\begin{pmatrix}\n\psi \\
F\n\end{pmatrix}^{(n+1)} \\
= \begin{pmatrix}\nD_{11}^{B} & D_{12}^{B} & D_{13}^{B} \\
D_{21}^{B} & D_{22}^{B} & D_{23}^{B} \\
D_{31}^{B} & D_{32}^{B} & D_{33}^{B}\n\end{pmatrix}\n\begin{pmatrix}\n\psi \\
F\n\end{pmatrix}^{(n)} + \begin{pmatrix}\nR_{11}^{B} & R_{12}^{B} & R_{13}^{B} \\
R_{21}^{B} & R_{22}^{B} & R_{23}^{B} \\
R_{31}^{B} & R_{32}^{B} & R_{33}^{B}\n\end{pmatrix}\n\begin{pmatrix}\nV \\
V\n\end{pmatrix}^{(n+1)} \\
+ \begin{pmatrix}\nQ_{11}^{B} & Q_{12}^{B} & Q_{13}^{B} \\
Q_{21}^{B} & Q_{22}^{B} & Q_{23}^{B}\n\end{pmatrix}\n\begin{pmatrix}\nV \\
V \\
V\n\end{pmatrix}^{(n)} + \begin{pmatrix}\nO_{1}^{B} \\
O_{2}^{B} \\
O_{3}^{B}\n\end{pmatrix}
$$
\n(31)

#### Linear Calculations

Linear calculations may be performed by calculating each matrix once, and recalculating the matrixvector products each time step with the updated vectors. This method is very efficient because the S matrices need only be inverted once, and in all subsequent time steps the only matrix operations carried out are addition and matrix-vector multiplication. Non-linear simulations require all the matrices to be recalculated each time step, and the  $S$  matrices must be inverted each time step.

#### Implementation of Electron Pressure Equation

Because it is the electron pressure which appears in the generalized Ohm's law, equation (??), if the electron pressure equation is retained, it is solved with the magnetic field as the third row in equation [\(31\)](#page-49-0) so as to keep the fast magnetosonic wave implicit. In this case, the full pressure is evolved independently in equation [\(30\)](#page-49-1). If the electron pressure equation is not included, the third row in equation [\(31\)](#page-49-0) is the total pressure equation, and the electron pressure is assumed to remain always at a specific fraction of the total pressure, which is determined by the initial conditions.

#### 8.2.3 Crank-Nicholson

The Crank-Nicholson time step is defined by the following discretization:

$$
\frac{\partial U}{\partial t} \rightarrow \frac{U^{(n+1)} - U^{(n)}}{\delta t}
$$
  

$$
U \rightarrow \theta U^{(n+1)} + (1 - \theta)U^{(n)}.
$$

By Taylor expanding about  $U$ ,

$$
U^{(n+1)} = U + \theta \,\delta t \,\dot{U} + \frac{1}{2} \theta^2 \delta t^2 \ddot{U} + \frac{1}{6} \theta^3 \delta t^3 \dddot{U} + \cdots
$$
  

$$
U^{(n)} = U + (\theta - 1) \delta t \,\dot{U} + \frac{1}{2} (\theta - 1)^2 \delta t^2 \ddot{U} + \frac{1}{6} (\theta - 1)^3 \delta t^3 \dddot{U} + \cdots
$$

the trunctation error of the time-derivative operator can be calculated directly:

$$
\Delta_{CN}(\delta t,\theta) = \frac{U^{(n+1)} - U^{(n)}}{\delta t} - \dot{U}
$$
  
= 
$$
\left(\theta - \frac{1}{2}\right) \delta t \ddot{U} + \frac{1}{2} \left(\theta^2 - \theta + \frac{1}{3}\right) \delta t^2 \ddot{U} + \cdots
$$

When  $\theta = 1/2$ , the time differencing is "time-centered" because the two points involved in the time differencing are equidistant in the logical time coordinate from the point at which the field itself is evaluated. In this case, the leading-order truncation error is  $\mathcal{O}(\delta t^2)$ :

$$
\Delta_{CN}(\delta t, \theta = 1/2) = \frac{1}{24} \delta t^2 \dddot{U} + \cdots.
$$
\n(32)

#### 8.2.4 BDF2

The BDF2 time step is defined by the following discretization:

$$
\frac{\partial U}{\partial t} \rightarrow \frac{3U^{(n+1)} - 4U^{(n)} + U^{(n-1)}}{2 \delta t}
$$
  
U \rightarrow U^{(n+1)}

Taylor expanding about U:

$$
U^{(n+1)} = U
$$
  
\n
$$
U^{(n)} = U - \delta t \dot{U} + \frac{1}{2} \delta t^2 \ddot{U} - \frac{1}{6} \delta t^3 \dddot{U} + \cdots
$$
  
\n
$$
U^{(n-1)} = U - 2 \delta t \dot{U} + 2 \delta t^2 \ddot{U} - \frac{4}{3} \delta t^3 \dddot{U} + \cdots
$$

and the truncation error is

$$
\Delta_{BDF2}(\delta t) = \frac{3U^{(n+1)} - 4U^{(n)} + U^{(n-1)}}{2\,\delta t} - \dot{U} = -\frac{1}{3}\delta t^2 \dddot{U} + \cdots. \tag{33}
$$

# 9 Input Parameters

## 9.1 Model Options





# 9.2 Initial Conditions Options









# 9.3 Grad-Shafranov Solver Options



For iread omega=0, the function  $\alpha(\psi)$  is parameterized by:

 $\tilde{\alpha} = \alpha_0 + \alpha_1 s + \alpha_2 s^2 + \alpha_3 s^3$ 

For iscale\_rot\_by\_p = 0:  $\alpha = \tilde{\alpha} \times n(\psi)/p(\psi)$  . For iscale\_rot\_by\_p = 1:  $\alpha = \tilde{\alpha}$ . For iscale\_rot\_by\_p = 2:  $\alpha = \left[ \alpha_0 + \alpha_1 e^{-\left[ (\psi - \alpha_2)/\alpha_3 \right]^2} \right] \times n(\psi)/p(\psi)$ In all cases, the angular velocity is then determined by:

$$
\omega = \left[\frac{2\alpha p(\psi)}{R_0^2 n(\psi)}\right]^{\frac{1}{2}}
$$





## 9.4 Transport Coefficients





# 9.5 Hyper-Diffusivity



### 9.6 Unit Normalizations





## 9.7 Boundary Conditions

# 9.8 Time Step



### 9.9 Mesh



### 9.10 Solver

![](_page_64_Picture_231.jpeg)

### 9.11 Mesh Adaptation (will be depricated soon)

![](_page_64_Picture_232.jpeg)

# 9.12 Numerical Options

![](_page_65_Picture_234.jpeg)

![](_page_66_Picture_144.jpeg)

# 9.13 Input Options

![](_page_67_Picture_233.jpeg)

# 9.14 Output Options

![](_page_68_Picture_148.jpeg)

![](_page_68_Picture_149.jpeg)

# 9.16 Sources/Sinks

![](_page_69_Picture_495.jpeg)

![](_page_70_Picture_485.jpeg)

![](_page_71_Picture_442.jpeg)


## 9.17 Resistive Wall





## 9.18 Miscellaneous

## 9.19 Deprecated



## 9.20 Trilinos Options



# 9.21 Simple Radiation Model



## 9.22 KPRAD Radiation Model



# 9.23 Stellarator Geometry



## A IDL Postprocessor

## A.1 Introduction

The IDL routines described here have been created for the purpose of reading, displaying, and manipulating data written by  $M3D-C<sup>1</sup>$  to an HDF5 output file. These routines are contained within files stored in the subdirectory  ${\tt trunk/unstructured/idl/}$  in the  ${\rm M3D\text{-}C^1}$  SVN repository.

Invoking IDL

First, IDL must be given access to the postprocessor routines. This may be accomplished either by copying the \*.pro files in the repository to the working directory where IDL will be run, or to set the environment variable IDL PATH to include the directory where these files are located.

The IDL module must first be loaded to run IDL on portal.pppl.gov. This is done by

module load idl

IDL may then be invoked by

idl

Once IDL is running, the postprocessor routines must be compiled. This is done by

```
.run plot_routines
.run power_spectrum
.run read_h5
```
The functions and procedures described in the following section are now ready to use.

Help In IDL

IDL has an on-line help system which may be invoked from the IDL command prompt by

?

Information about a specific intrinsic IDL routine, **stratifierally**, may be obtained by

? <routine>

Note on function/procedure descriptions Functions and procedures in IDL are differentiated by whether a value is returned (as with functions) or not (as with procedures). Both functions and procedures may take "arguments" and "keywords" as command line parameters. In the following descriptions, the arguments of the function or procedure are shown with the command, and keywords are listed separately. Optional arguments are enclosed by square brackets. Keywords are always optional. (This notation differs from that in the on-line IDL help only in that keywords are not listed with the command.) Keywords are specified on the command line by

<keywordname>=<value>

Writing

/<keywordname>

has the same effect as

<keywordname>=1

and is therefore useful for boolean options. Some common examples are given below.

#### Common Examples

To display the field "psi" at time slice 1 of file "C1.h5", sampled on a regular  $100 \times 100$  grid, with an overlay of the LCFS and the mesh,

plot\_field, 'psi', 1, filename='C1.h5', /iso, /lcfs, /mesh, points=100

To plot the time series of the kinetic energy of file "C1.h5" in domain  $0 < t < 100$ ,

plot\_scalar, 'ke', filename='C1.h5', xrange=[0,100]

To plot the flux-averaged temperature profiles of files " $1/C1.h5$ " and " $2/C1.h5$ " at time slice 1, versus the normalized poloidal flux,

plot\_flux\_average, 'T', 1, filename=['1/C1.h5', '2/C1.h5'], /norm

#### A.2 Functions/Procedures in plot\_routines.pro

### A.2.1 Procedure contour and legend

```
contour_and_legend, z [,x, y]
```
Description

This procedure draws a two-dimensional color contour plot of the data z, with horizontal and vertical coordinates  $x$  and  $y$ .  $nt$  frames are drawn.



#### Keywords



## A.3 Functions/Procedures in read h5.pro

#### A.3.1 Function read\_field

 $field = read\_field(name, r, z, t)$ 

#### Description

This function reads the raw field data associated with name in the specified output file. The data is interpolated onto a uniform retangular grid, and returned in an array.

#### Return Value

float  $[nt, points, points]$  field containing the value of the field at points  $\times$  points spatial sampling points at nt time slices.

#### Arguments



## A.3.2 Function flux\_average

 $result = \texttt{flux}$  average(field, slice)

Description

This function finds the flux-surface average of the field *field*.

## Return Value

float[bins] result contains the value of the flux-averaged field for a range of values of flux.

### Arguments



Keywords

flux average takes all of the optional arguments for read field. In addition,



 $t$  are all provided as input, the  $flux$  average will not read the flux field itself.

### A.3.3 Function read scalar

 $result = read\_field(name)$ 

#### Description

This function reads the scalar quantity associated with name in the specified output file. The data is returned as an array .

## Return Value

float $[nt]$  result contains the value of the scalar at each time step.



Keywords



### A.3.4 Procedure plot field

plot field, name, slice, r, z, t

### Arguments



#### Keywords

plot field takes all of the optional arguments for read field and contour and legend. In addition,



### A.3.5 Procedure plot\_flux\_average

plot flux average, field, slice

## Description

Plots the flux-surface average of a field as a function of poloidal flux. Data from multiple files or multiple times may be plotted at once.

#### Arguments





## A.3.6 Procedure plot\_timings

### plot\_timings

Keywords

#### Description

This function plots the relative time spent in various subroutines of M3D- $C<sup>1</sup>$ . This data is only available if  $\text{itemer} = 1$  was specified in the input file.

#### Keywords

plot flux average takes all of the optional arguments for flux average. In addition,



### A.3.7 Procedure write geqdsk

### write geqdsk

Description This procedure writes equilibrium data do disk in the geqdsk format.

Arguments

None.

Keywords



write geqdsk takes all of the optional arguments for read field and read parameter. In addition,



<span id="page-84-0"></span>Figure 13: To visualize a mesh, select .pvtu file from Open File menu

## B Mesh Visualization

Paraview is program created by Kitware, Inc. which can visualize meshes and fields on meshes. It is the program of choice for viewing meshes created by the PUMI libraries. The API  $m3dc1$ -mesh-write writes a mesh either in "smb" or "vtk".

```
// filename: output file name
// option: 0 vtk file with field; 1 smb file
m3dc1_mesh_write(char* filename, int *option)
```
If the first argument is "output"" and the second argument is 0, filename is output, it creates the files output.pvtu. Opening the output.pvtu file in Paraview will show users the mesh. Figures [13](#page-84-0) and [14](#page-85-0) illustrate "Open File" window and a mesh rendered in "Surface" mode by default.

Changing "Surface" to "Surface with Edges" will outline each visible element. Figures [15](#page-85-1) and [16](#page-86-0) illustrate how to make the decomposition visible.

Also, the mesh by default is rendered in one "Solid Color". There should be other options corresponding to the fields and numberings that were on this mesh at the time of file writing. There is an "apf part" alternative for files written by APF, which allows users to see the parallel partitioning of the mesh in color.

Mesh generation program provides "gface" alternative, which allows users to see the geometric face of the mesh in color. Figure [17](#page-86-1) depicts a Paraview window with a mesh rendered with "gface".

Figure [18](#page-87-0) illustrates the "Color Palette" tab of "Settings" menu which allows the users to change the colors of "Render View" such as edges, background, etc..



Figure 14: Initial Paraview window with a mesh

<span id="page-85-0"></span>

<span id="page-85-1"></span>Figure 15: To render mesh decomposition, choose "Surface With Edge"



Figure 16: A mesh with "Surface With Edge"

<span id="page-86-1"></span><span id="page-86-0"></span>

Figure 17: A mesh rendered with "gface"



<span id="page-87-0"></span>Figure 18: "Color Palette" tab of "Settings" menu"