Mesh generation and simulation geometries

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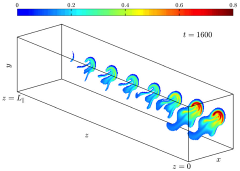
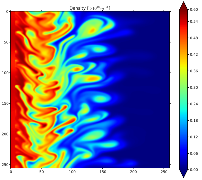
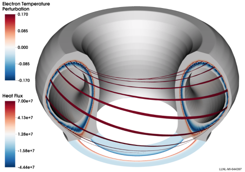
BOUT++ Workshop, LLNL

17^{th} December 2015

- Filaments / blobs
  - Transport of heat and particles in SOL
  - 2D examples run on a laptop
- Edge turbulence
  - Formation of blobs
  - Near SOL heat transport (λ_q)
- Divertor simulations
  - Spreading of particle and power fluxes to surfaces
  - Interaction with neutral gas and detachment
- Pedestal physics and ELMs
  - Gyro-fluid models to capture FLR, Landau damping, and drift resonance effects
  - L-H transition physics
  - Stability and nonlinear dynamics



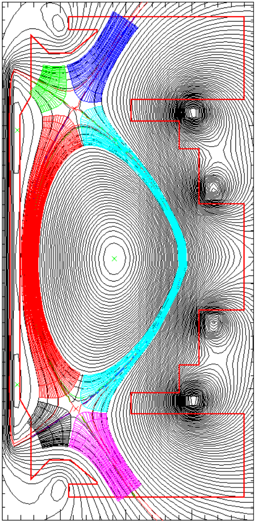




Inputs to BOUT++

See **`tools/`** sub-directory

- Analytic expressions
- Simplified grid generators e.g. flux tube (Cyclone), theta pinch, shifted circle tokamak
- TEQ (DSKGATO), ELITE formats
- EFIT equilibria (g-file)
- VMEC ... coming soon!



Hypnotoad grid generator

Coordinates

- Up to 3 dimensions (x, y, z)
- Grid spacing $\mathtt{dx}(x, y)$, $\mathtt{dy}(x, y)$, $\mathtt{dz}$

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- Up to 3 dimensions (x, y, z)
- Grid spacing $\mathtt{dx}(x, y)$, $\mathtt{dy}(x, y)$, $\mathtt{dz}$
- By convention y is the parallel direction
  - Some operators don't care:

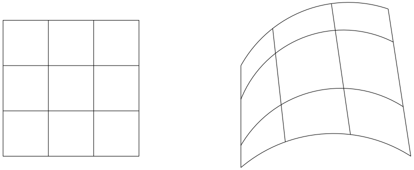
$$\underline{v} = \nabla f \qquad f = \nabla \cdot \underline{v} \qquad \underline{u} = \nabla \times \underline{v}$$

  - Some operators assume $\mathbf{B} = \nabla z \times \nabla x = \frac{1}{J}\mathbf{e}_y$

$$f = [\phi, g] \qquad f = \nabla_{||} g = \nabla \cdot (\mathbf{b} g) \qquad f = \partial_{||} g = \mathbf{b} \cdot \nabla g$$

Coordinates

- Up to 3 dimensions (x, y, z)
- Grid spacing $\mathtt{dx}(x, y)$, $\mathtt{dy}(x, y)$, $\mathtt{dz}$
- By convention y is the parallel direction
- Mapping between curved grid and logical rectangle determines metric tensor



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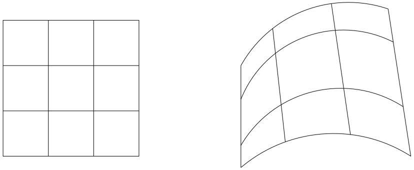


- Metric tensors are functions of x and y
  $\rightarrow$ In the "standard" tokamak geometry z is a symmetry angle (toroidal angle)
- The grid is always periodic in z (for now)

The easiest way to specify a mesh is in the input file (BOUT.inp)

```
[mesh]
nx = 260  # Note 4 guard cells in X
ny = 1
nz = 256
```

This will produce a mesh with:

- Uniform grid spacing `dx` = `dy` = `dz` = 1
- Cartesian identity matrix as metric tensor

Analytic inputs

examples/hasegawa-wakatani/data/BOUT.inp

The easiest way to specify a mesh is in the input file (BOUT.inp)

```
[mesh]
nx = 260   # Note 4 guard cells in X
ny = 1
nz = 256

dx = 0.2
dz = 0.2
```

This will produce a mesh with:

- Uniform grid spacing as specified
- Cartesian identity matrix as metric tensor

Analytic inputs

`examples/hasegawa-wakatani/data/BOUT.inp`

The easiest way to specify a mesh is in the input file (BOUT.inp)

```
[mesh]
nx = 260   # Note 4 guard cells in X
ny = 1
nz = 256

Lx = 51.2
Lz = Lx

dx = Lx / (nx - 4)
dz = Lz / nz
```

This will produce a mesh with:

- Uniform grid spacing as specified
- Cartesian identity matrix as metric tensor

Cylindrical coordinates
examples/lapd-drift/pisces

Analytic expressions can use:

- Normalised index space coordinates $0 \leq \mathtt{x} \leq 1$, $0 \leq \mathtt{y} \leq 2\pi$, and $0 \leq \mathtt{z} \leq 2\pi$,
- Constants `pi` and `e`
- Common mathematical functions like sin, cos, tanh, *erf*

```
[mesh]
...
Rmin = 5e-3    # minimum radius in meters
Rmax = 2.5e-2  # maximum radius
Rxy = Rmin + (Rmax - Rmin) * x
dr = (Rmax - Rmin) / (nx - 4)

dx = Bpxy * Rxy * dr
dy = length / ny
```

Example: 1-D modelling of divertor detachment

B.Dudson, B.Lipschultz

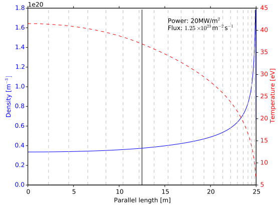
The SD1D model is being developed to study detachment dynamics and stability

- Fluid equations for plasma and neutrals
- Requires highly nonuniform grid

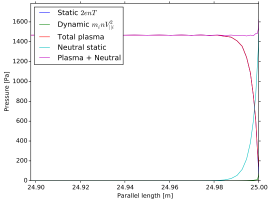
```
[mesh]

ny = 400
length = 25

dymin = 0.02
dy = (length / ny)
     * (1 + (1-dymin)*(1-y/pi))
```



1D profiles in high recycling regime



Static, dynamic and neutral pressure

Input from mesh/grid file

- Analytic meshes make convergence (MMS) testing easier
- More complicated geometries don't have "nice" analytic form
- Require grid input file for e.g. experimental profiles:

```
grid = "inputgrid.nc"
```

- See conduction example:
  - `examples/conduction/data/BOUT.inp` : Analytic input
  - `examples/conduction/fromfile/BOUT.inp` : From grid file (`conduct_grid.nc`)

Tools to generate grid files

Grid files can be generated from scratch:

- Sheared slab: `tools/slab/slab.pro`
- Cyclone flux tube: `tools/tokamak_grids/cyclone`
- Shifted circle equilibria: `tools/tokamak_grids/shifted_circle`

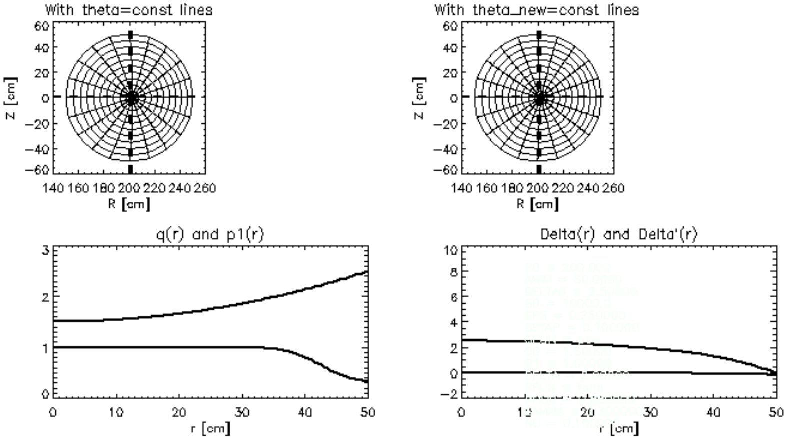
Or from existing equilibria

- DSKGATO ('t') files: `tools/tokamak_grids/gato/`
- ELITE input format: `tools/tokamak_grids/elite/`

Shifted circle equilibria

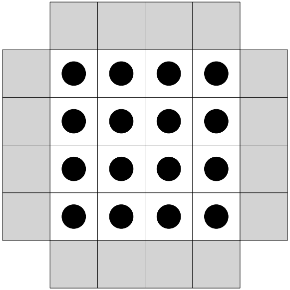
M.V.Umansky

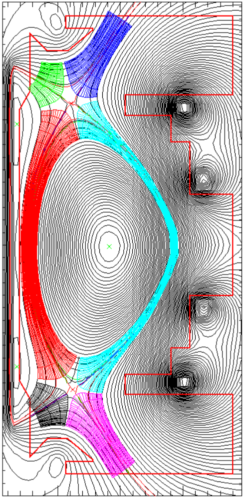
- See README in `tools/tokamak_grids/shifted_circle`
- Two steps: Generate mesh; process to create BOUT++ input



The grid used for field-aligned X-point simulations consists of several blocks

- Every processor in BOUT++ has a logically rectangular grid

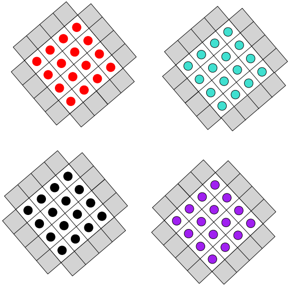


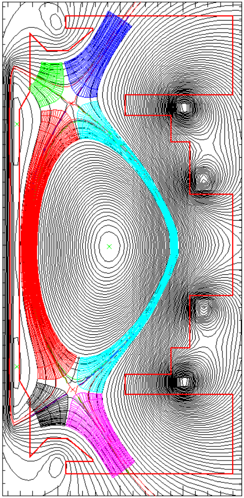


Branch cuts and communications

The grid used for field-aligned X-point simulations consists of several blocks

- Every processor in BOUT++ has a logically rectangular grid
- Connections between blocks are done by changing communications between processors





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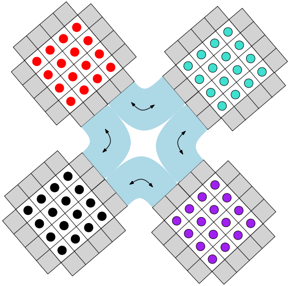
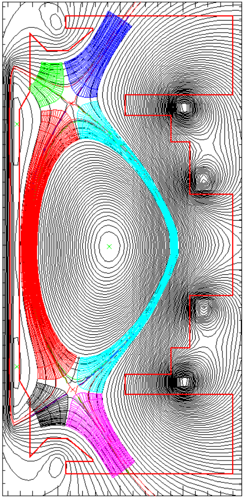
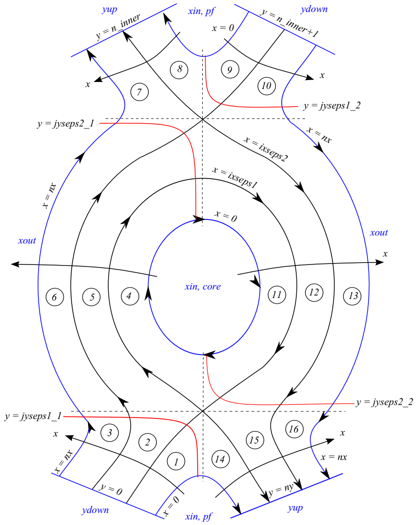




The locations of these branch cuts are controlled by quantities in the input mesh:

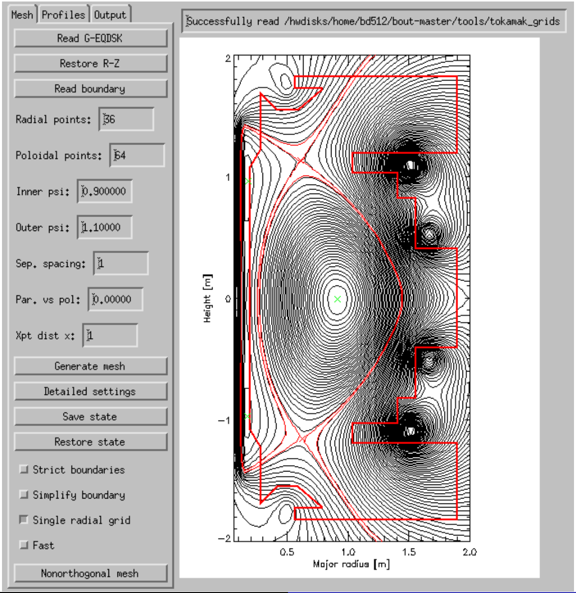
- `ixseps1`, `ixseps2` : Separatrix radial locations (number of points inside each separatrix)
- `jyseps1_1`, `jyseps2_1`, `jyseps1_2`,`jyseps2_2` : Poloidal (y) branch cut locations



Hypnotoad grid generator
tools/tokamak_grids/gridgen

- Create a field-aligned mesh from EFIT G-EQDSK files
- Largely automatic, given required ψ ranges and resolution
- Uses mainly heuristic methods
- Written in IDL
- A partial translation to Python also exists
  tools/tokamak_grids/pyGridgen (thanks to G.Breyiannis)

Hypnotoad grid generator
tools/tokamak_grids/gridgen



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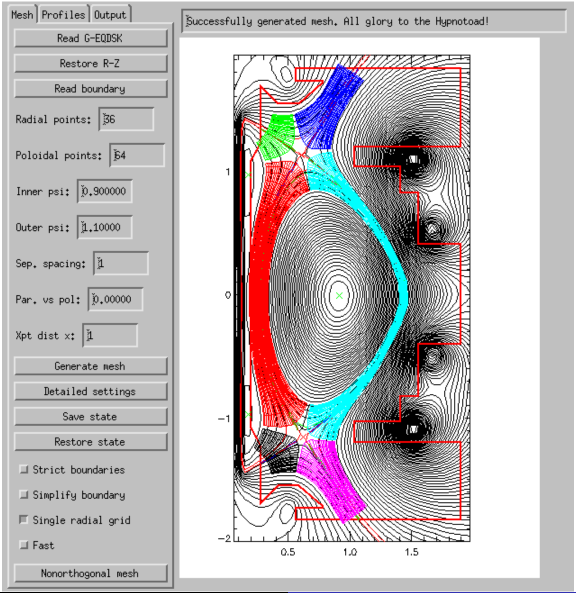

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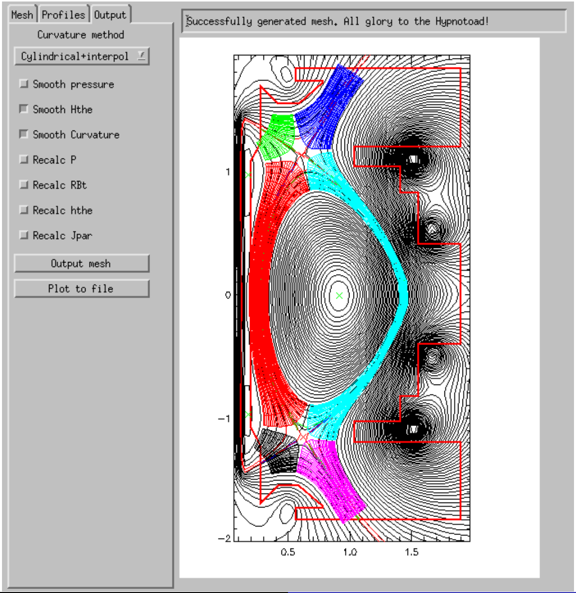

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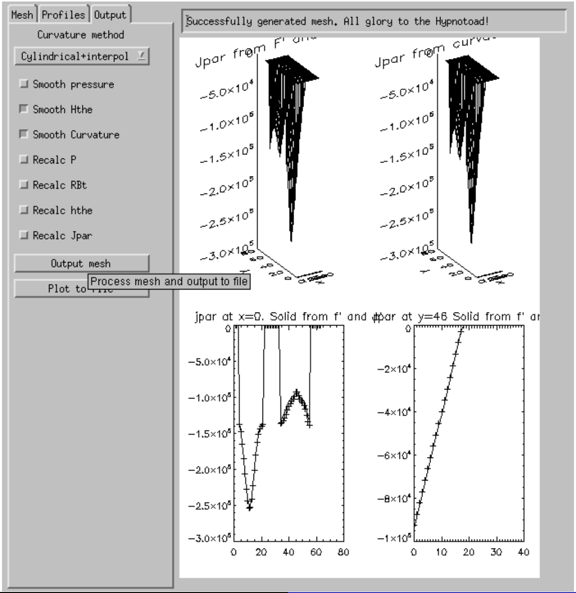

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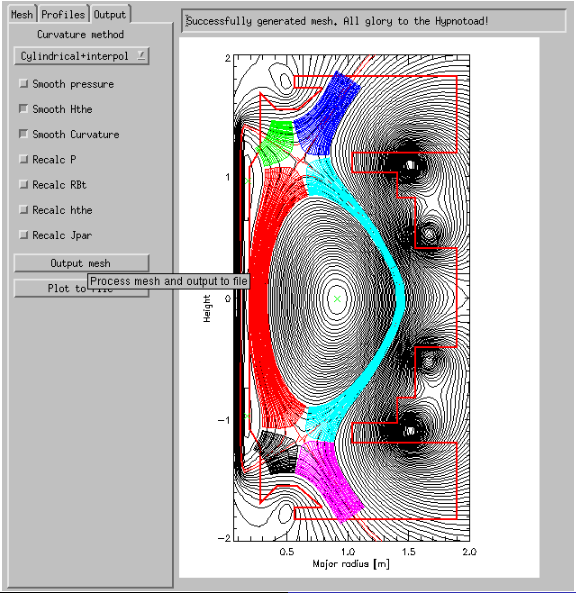
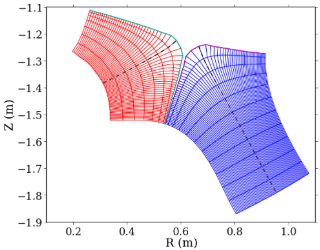


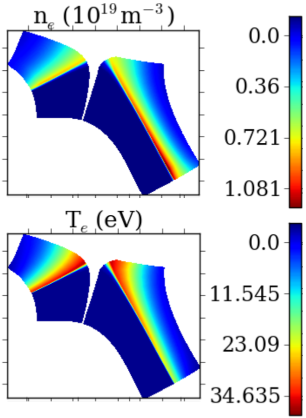
Divertor leg simulations
N.Walkden (CCFE)

- The mesh can be processed to keep only some domains
- N.Walkden studying divertor transport



N.Walkden : Collisional electron transport in MAST.

Submitted to PPCF (2015)



Divertor leg simulations
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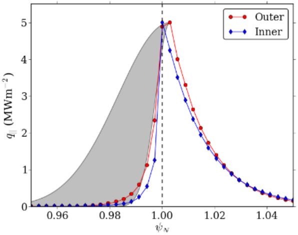
- Strong enhancement of collisional (Braginskii) transport needed to match experiment



(d) $\alpha = 400, \beta = 2000$

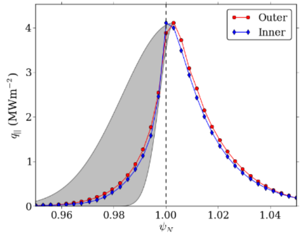
N.Walkden : Collisional electron transport in MAST.

Submitted to PPCF (2015)

- The mesh can be processed to keep only some domains
- N.Walkden studying divertor transport
- Strong enhancement of collisional (Braginskii) transport needed to match experiment
- Significant Bohm-like diffusion can reproduce reasonable profiles

N.Walkden : Collisional electron transport in MAST.

Submitted to PPCF (2015)

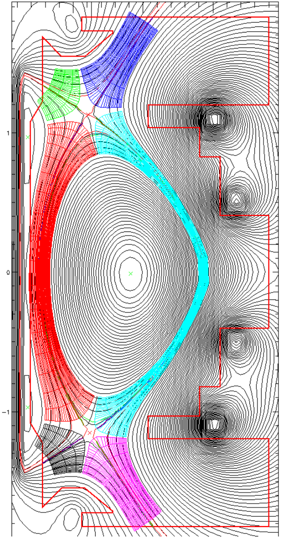


(c) $\alpha = 0.1, \beta = 0.5$

Coming soon...

Non-orthogonal meshes

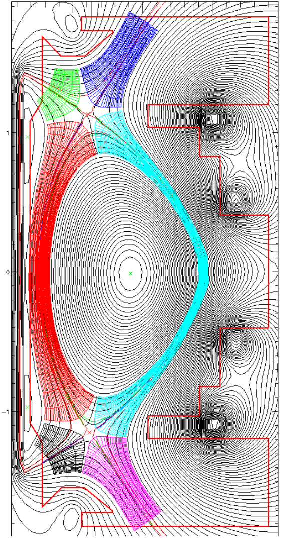
J.Leddy, B.Shanahan, N.Walkden, B.Dudson

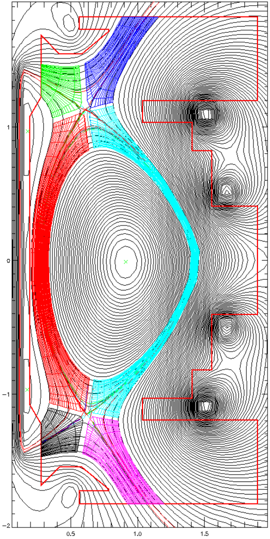


- The standard mesh and coordinate system is orthogonal in the poloidal plane
- Does not conform to divertor surfaces
- Produces large variation in cell spacing around X-point

Non-orthogonal meshes

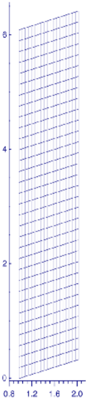
J.Leddy, B.Shanahan, N.Walkden, B.Dudson



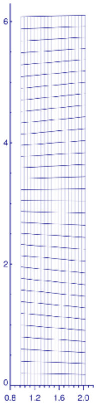


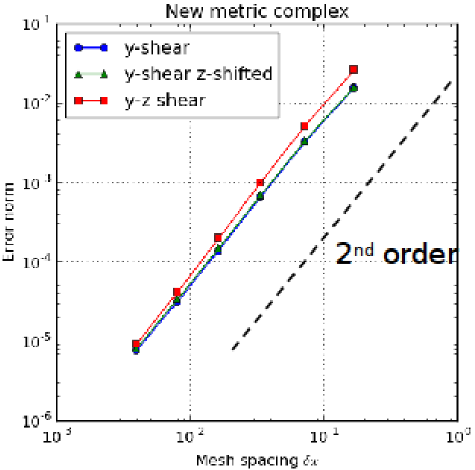
J.Leddy, B.Shanahan, N.Walkden, B.Dudson

$\eta = \text{const}$



$\eta \neq \text{const}$

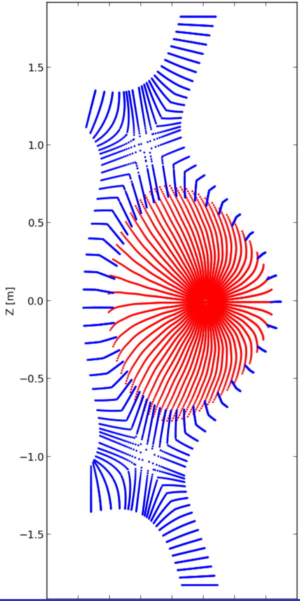




Non-orthogonal meshes: Core-edge coupling

J.Leddy, B.Dudson

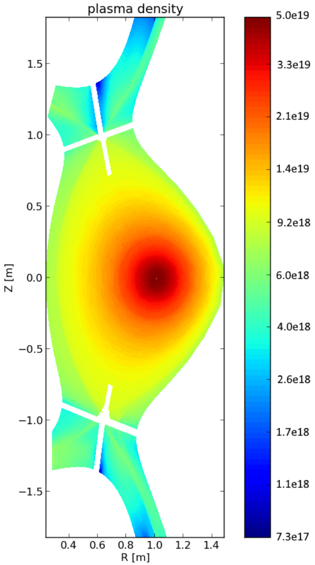
- Core-Edge coupling with BOUT++ and CENTORI
- Sharing via an overlap region ("handshake" method)



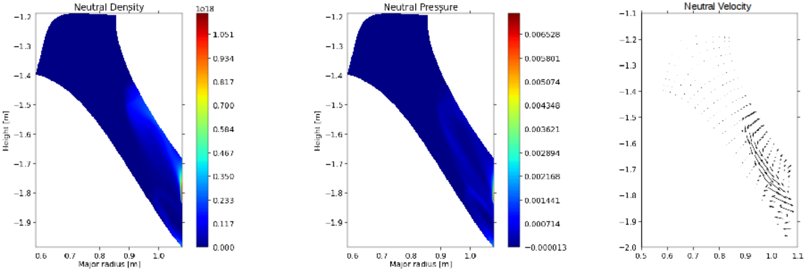
Non-orthogonal meshes: Core-edge coupling

J.Leddy, B.Dudson

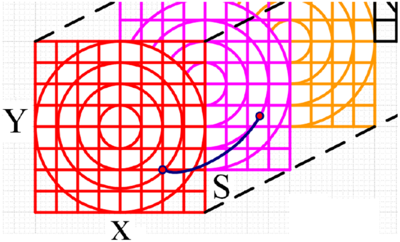
- Core-Edge coupling with BOUT++ and CENTORI
- Sharing via an overlap region ("handshake" method)
- Profiles evolve self-consistently
- Fluctuations from the core propagate to target



- Interaction of plasma with fluid neutrals (Navier Stokes), and coupling to EIRENE
- Impact of divertor angle on divertor heat loads and detachment



- An alternative approach to parallel derivatives
- Grid points are not aligned on magnetic field
- Coordinate system can be Cartesian, cylindrical. **No singularity at X-point**
- Follow field-lines to neighboring planes and interpolate
- Magnetic field needs to be locally integrable, but not globally. **No assumption of flux surfaces**

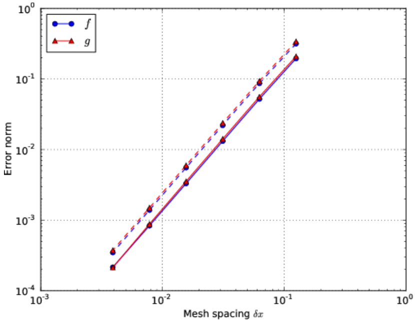


F Hariri et al, PoP 21 (8): 2419-2429 (2013)

Flux-Coordinate Independent (FCI)

P.Hill, B.Dudson, B.Shanahan

- Implemented in BOUT++
- Convergence tested using MMS



Flux-Coordinate Independent (FCI)

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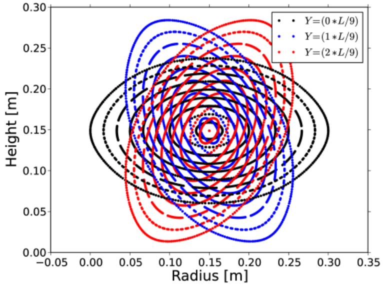
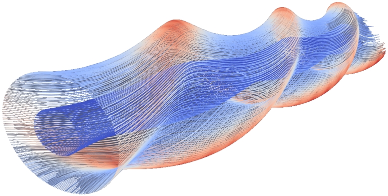
- Straight stellarator geometry
- Cartesian mesh in $x - z$, FCI in y

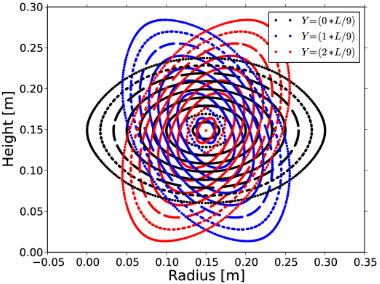


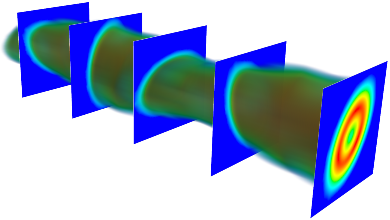


P.Hill, B.Dudson, B.Shanahan

- Implemented in BOUT++
- Convergence tested using MMS
- Straight stellarator geometry
- Cartesian mesh in $x-z$, FCI in y
- Diffusion equation to test numerical diffusion

$$\partial_t f = \nabla_{||}^2 f$$





Conclusions

- BOUT++ geometry and topology are quite flexible
- Retain some limitations from tokamak simulation origins
- Many scripts and examples to get started in a range of geometries

- Ongoing efforts to improve schemes for tokamak and more complicated geometries