BOUT++ for divertor modelling in W7-X

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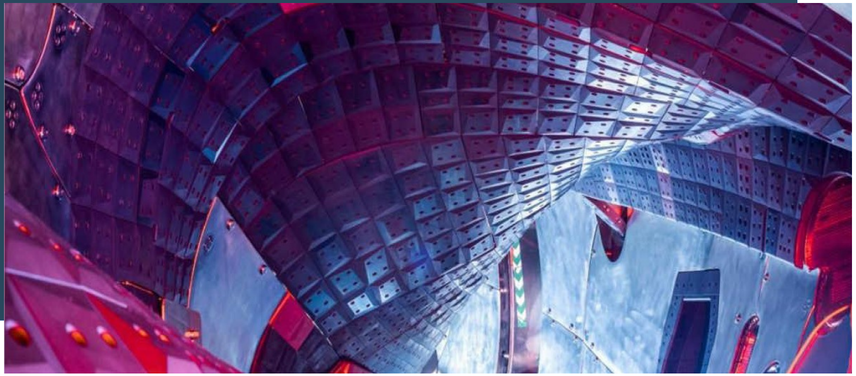

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BOUT++

BOUT++ is an open source framework for fluid (turbulence) simulations

- **finite difference / finite volume**

Physics models have straightforward syntax:

- **ddt(var) = Grad_par(var);**

Most user-interfacing is done through simple input files at run-time:

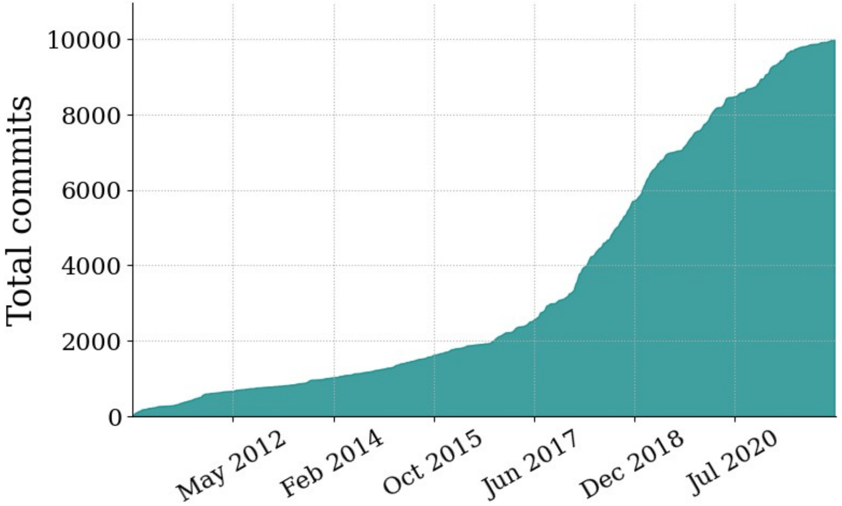
evolve_var = True
sheath_bndry = True

[var]

function = sin(X)

bndry_all = dirichlet(0.0)

source = gauss(x,0.21)



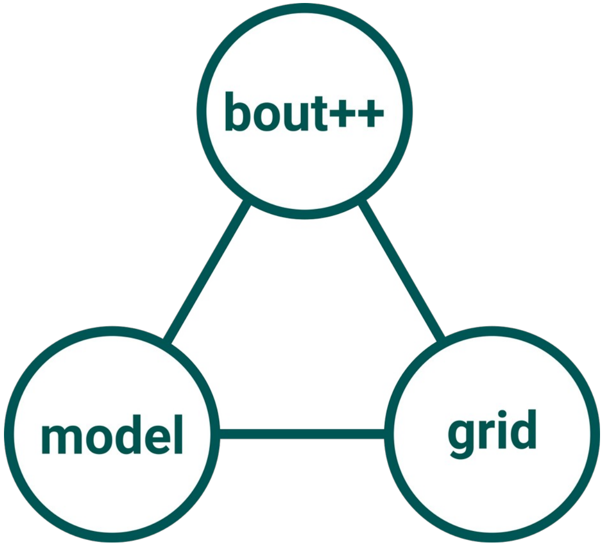
BOUT++ soups have three ingredients

BOUT++ is a framework, not a set model

Models are developed which use the methods within BOUT++

As such, new developments are either:

- **Improving BOUT++ internal methods**
- **Developing a new model**
- **Creating grids for required geometry**



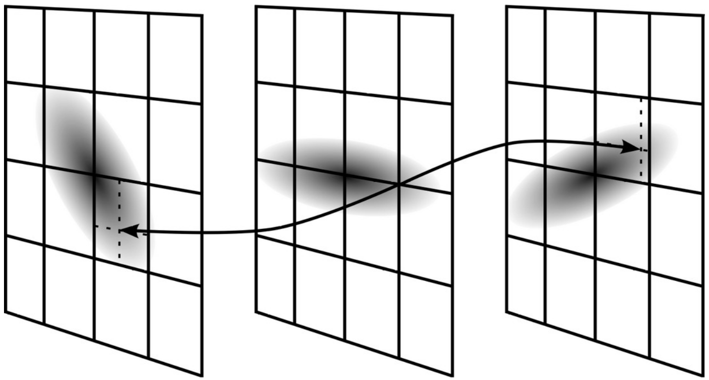
Stellarator stimulations in BOUT++ require lateral thinking

Conventionally, BOUT++ assumes a field-aligned, axisymmetric coordinate system

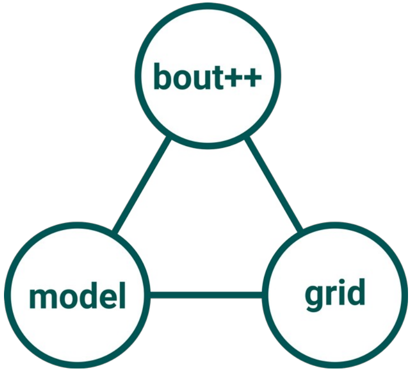
- **radial, toroidal, and ||**
  - This is complicated in the stellarator SOL
- **axisymmetric assumption must be removed**

Instead, use a method which is not aligned to the field

- **Flux Coordinate Independent (FCI) method for parallel derivates**
- **Requires changing all three BOUT++ "ingredients"**



A schematic of the FCI method



FCI models for W7-X

Some models are already available for W7-X using the FCI method

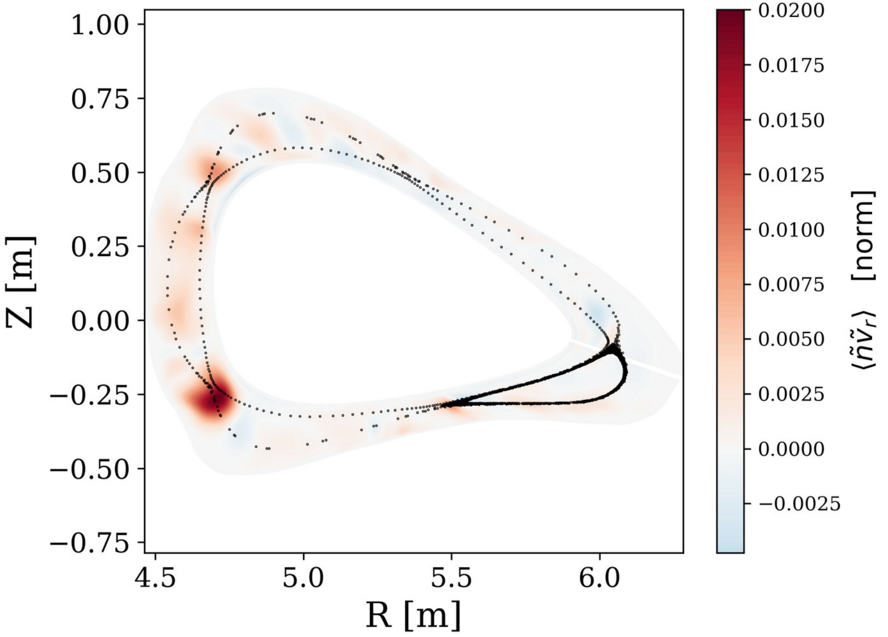
- **Heat Diffusion**
- **EMC3-lite**
- **isothermal turbulence (Hermes-i)**

With others in development:

- **EMC3-like (D Bold)**
- **hot-ion turbulence (Hermes-2)**

No FCI models have neutral physics (yet).

- **Fluid neutrals included in the Hermes family, can be adapted quickly to EMC3-lite and Hermes-i**



Radial flux of the fluctuations in the W7-X SOL.

EMC3-lite in BOUT++

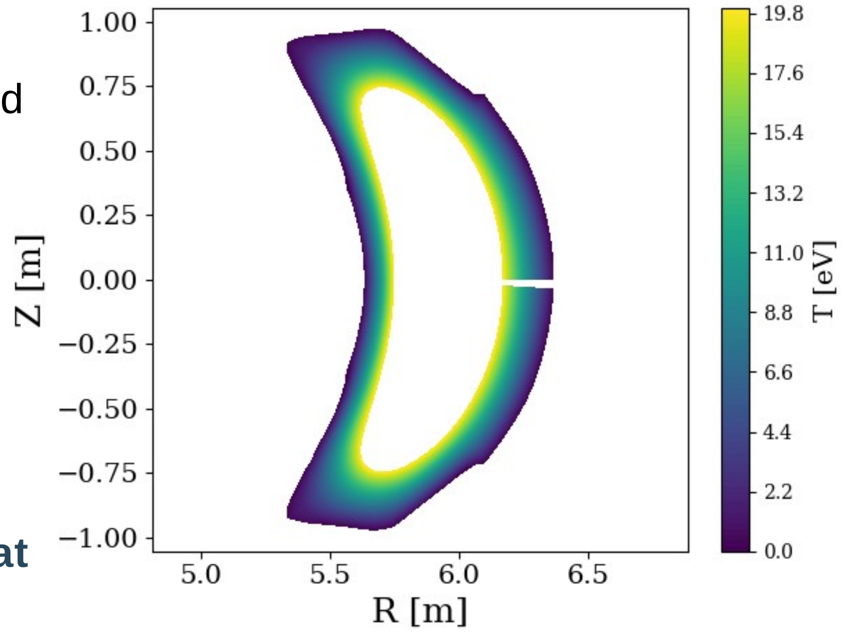
The equations for EMC3-lite have been implemented using BOUT++ FCI operators

- **available at: github.com/bshanahan/bsting-models**

Steady-state reached relatively quickly.

Pre- and post-processing work are underway.

- **Biggest limitation is grid generation and heat flux visualization**



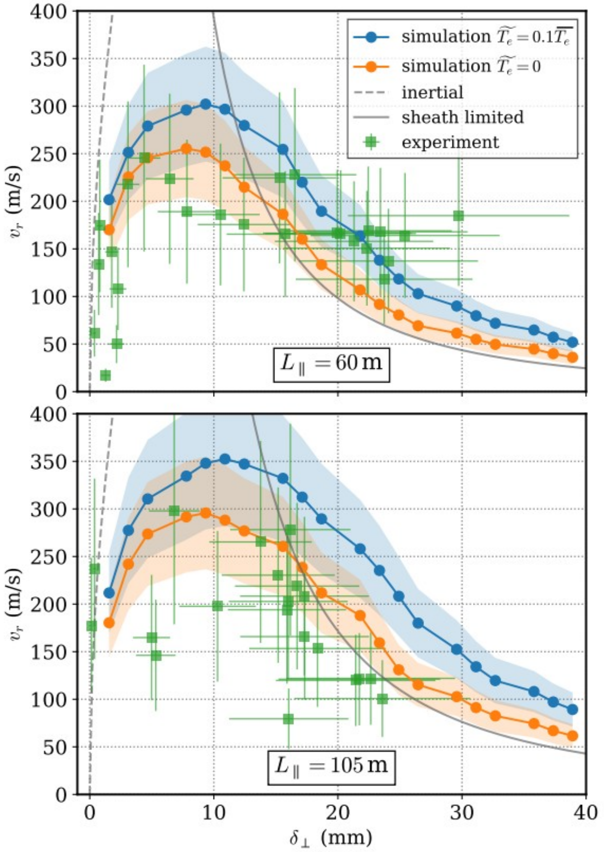
Steady-state "T" profile in BOUT++ with the EMC3-lite model

There's another way...

We can also learn a lot from simplified geometries (1D/2D).

- **Filament behavior in stellarators**
- **Experimental comparison**

Without FCI, we have all BOUT++ models available



Comparison of 2D BOUT++ blob simulations with probe measurements in W7-X

Hermes-3

Hermes-3 is a new model using BOUT++ for edge applications **[B Dudson 2023 Submitted; https://arxiv.org/abs/2303.12131]**

- **Multifluid, 1D, 2D or 3D for transport or turbulence**
- **Arbitrary number of ion and neutral species (determined at runtime)**
- **Uses ADAS & AMJUEL, fluid neutral models**
- **"relax_potential" option for steady-state potential**

Actively developed, online manual.

No development needed for 1D/2D applications.

Even easier syntax in input files

```
[hermes]
components = d+, d, t+, t, he+, he, ne+, ne, e,
           collisions, sheath_boundary, recycling, reactions
[recycling]

species = d+, t+, he+, ne+

[reactions]
type = (
        d + e -> d+ + 2e,   # Deuterium ionisation
        t + e -> t+ + 2e,   # Tritium ionisation
        he + e -> he+ + 2e, # Helium ionisation
        he+ + e -> he,      # Helium+ recombination
        ne + e -> ne+ + 2e, # Neon ionisation
        ne+ + e -> ne,      # Neon+ recombination
       )
```

Example input from a Hermes-3 simulation with cross-field diffusion, collisions between species, sheath boundary conditions, and recycling

Hermes-3 (1D)

An example from **[Dudson et al., 2023, submitted]**

- **no-flow upstream, sheath boundary downstream**
- **Evolving all electron and ion species**
  - **Neon, Deuterium**
- **heat conduction, 100% recycling, ionization of neturals, charge exchange, feedback control of upstream density**
- **Thermal force included.**

Immediately applicable to W7-X, with the relevant parameters – no development needed.

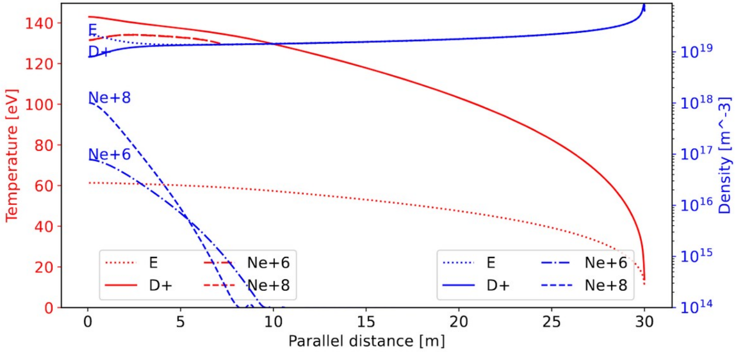


Figure 7: Steady state solution with 100% recycling, evolving all charge states of neon as separate fluids with their own densities, temperatures and flow velocities. A subset of species densities (blue lines) are shown on a logarithmic scale. Simulation inputs in `examples/1D-neon` of the Hermes-3 repository.

The stellarator two-point model in Hermes-3

Previous work by Feng et al. [1] created a stellarator-two point model.

- **Effects of cross-field transport introduced through the field line pitch – Θ − the ratio the radial distance to the parallel arc length in the SOL**
- **In tokamaks, Θ is about 2 orders of magnitude larger than in stellarators (0.1 vs. 0.001)**

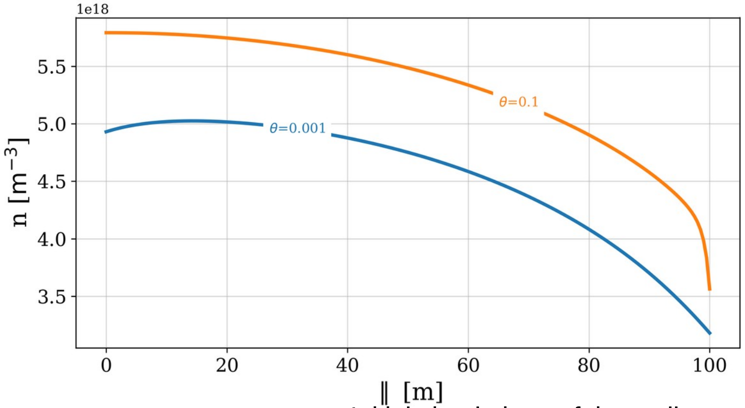
Rewriting the terms in [1] in the parallel direction.

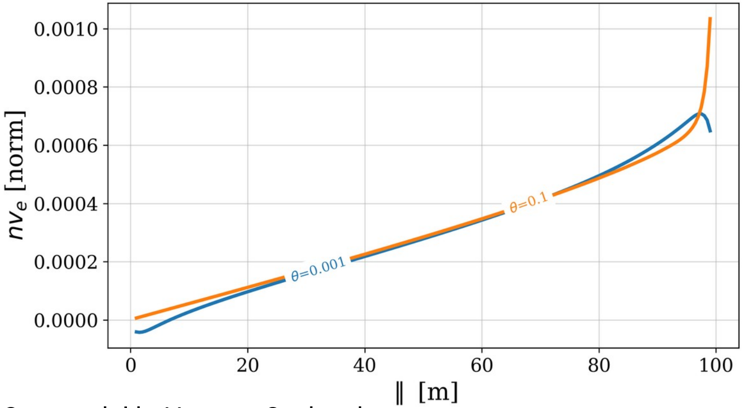
- **D, χ, and ν are prescribed coefficients**

$$\frac{\partial N}{\partial t} = \ldots + \nabla \cdot \left(\mathbf{b} \frac{D}{\Theta} \partial_{||} N \right)$$

$$\frac{\partial P}{\partial t} = \ldots + \frac{2}{3} \nabla \cdot \left(\mathbf{b} \frac{\chi}{\Theta} N \partial_{||} T \right)$$

$$\frac{\partial}{\partial t}(NV) = \ldots + \nabla \cdot \left(\mathbf{b} \frac{\nu}{\Theta} \partial_{||} NV \right)$$





Initial simulations of the stellarator 2-pt model in Hermes-3, showing the difference between tokamak and stellarator transport in the SOL.

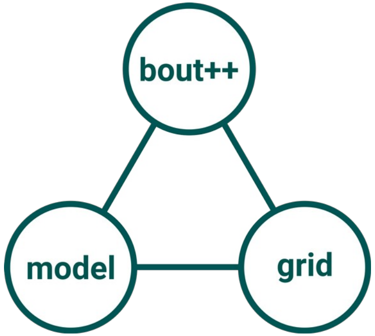
[1] Y Feng et al., *PPCF* 53 024009 (2011)

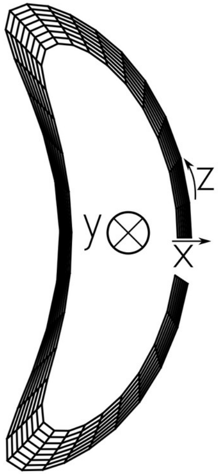
Hermes-3 for W7-X?

Field-aligned grids are still assumed, but perhaps we can find a W7-X field-aligned grid

Currently "tricking" Hermes-3 and BOUT++ to do a closed-field-line W7-X simulation.

- **Now we only need to change 1 "ingredient"**
- **Instead of x=∇ψ, y=||, z=φ, we use z=ϑ**
- **Initial tests seem to work**
- **No sheath/neutral physics as we are in the closed field line region**
  - Ideas for how to move to the edge
- **Transport, turbulence within closed field lines on the near-term agenda.**
  - Includes steady-state potential calculation





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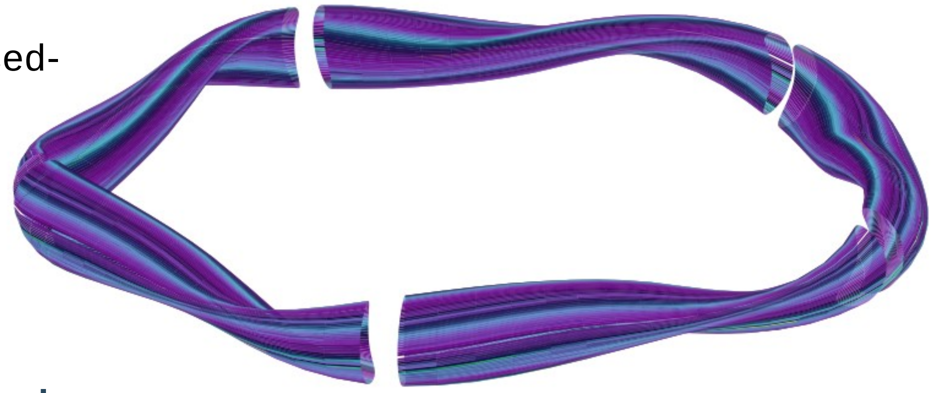


Numerical test in W7-X geometry for Hermes-3

Conclusions

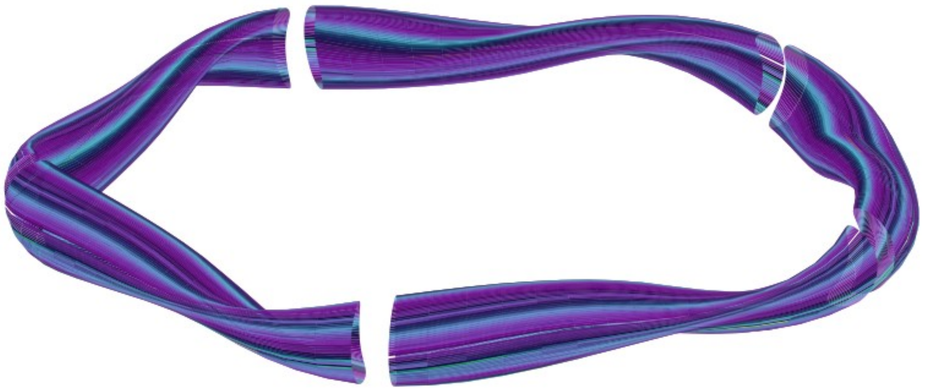
BOUT++ is a flexible tool for the edge of stellarators

The FCI approach in BOUT++ has allowed simulations out to the plasma facing components

Simplified models in BOUT++ can provide novel insights into physics of the edge

The Hermes-3 model has tremendous potential for W7-X studies

- **Multifluid simulations in 1D and 2D are available today.**
- **Extensions to W7-X geometries underway**
  - Long-term goal of reaching the outer SOL, as with FCI.



Numerical test in W7-X geometry for Hermes-3

Reaching the SOL

W7-X has a complex SOL with an island chain and chaotic fields.

- **Step 1: adapt the code to allow more than 2 X-points**
- **Step 2: Apply boundaries in an "immersed" boundary, where a function defines an arbitrary 3D boundary**
  - Done previously in B Shanahan & B Dudson, *PPCF* **58** 125003 2016