Tokamak edge simulations

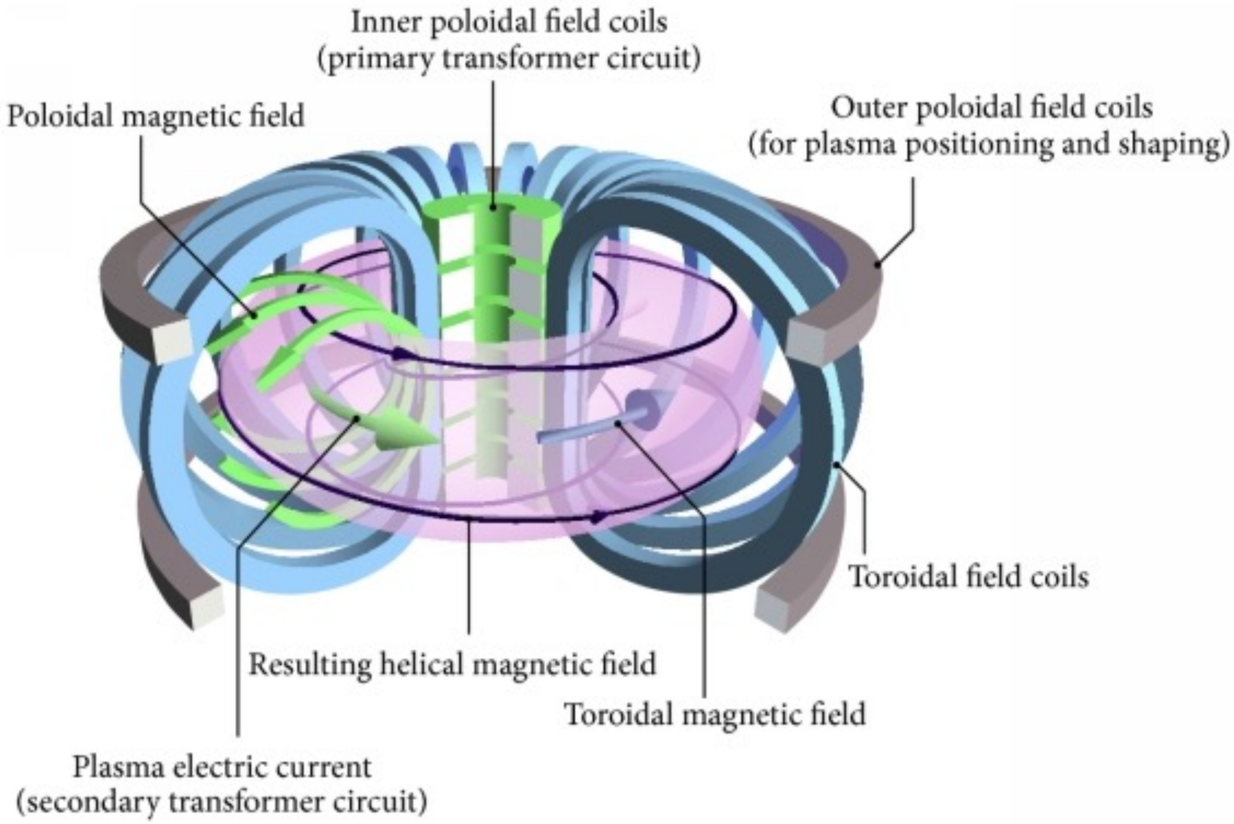
Ben Dudson, Ben Zhu
Lawrence Livermore National Laboratory

ExcaliburML June Workshop
June 5th 2023

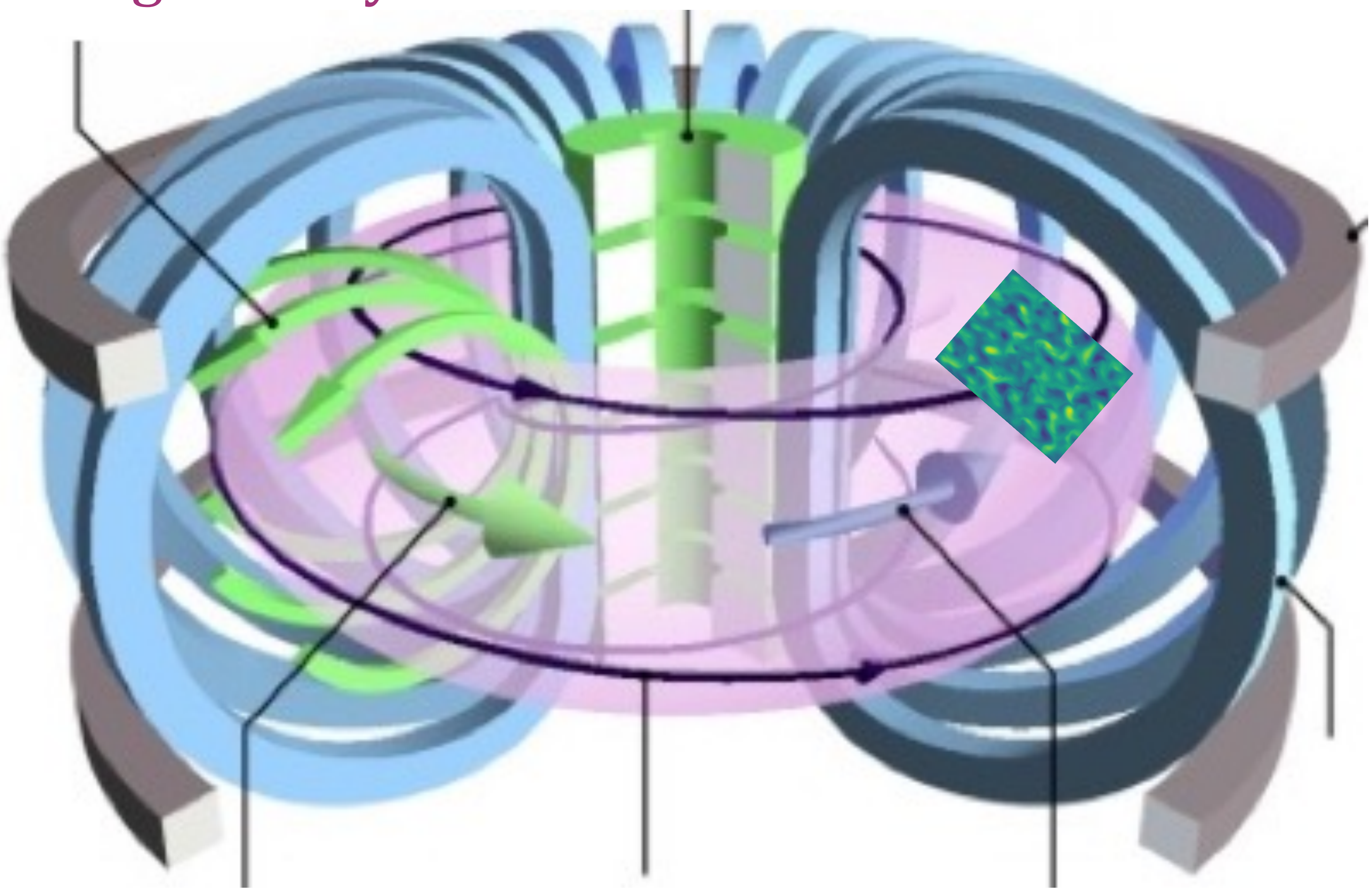
LLNL-PRES-849856

Prepared by LLNL under Contract DE-AC52-07NA27344.

Tokamak geometry

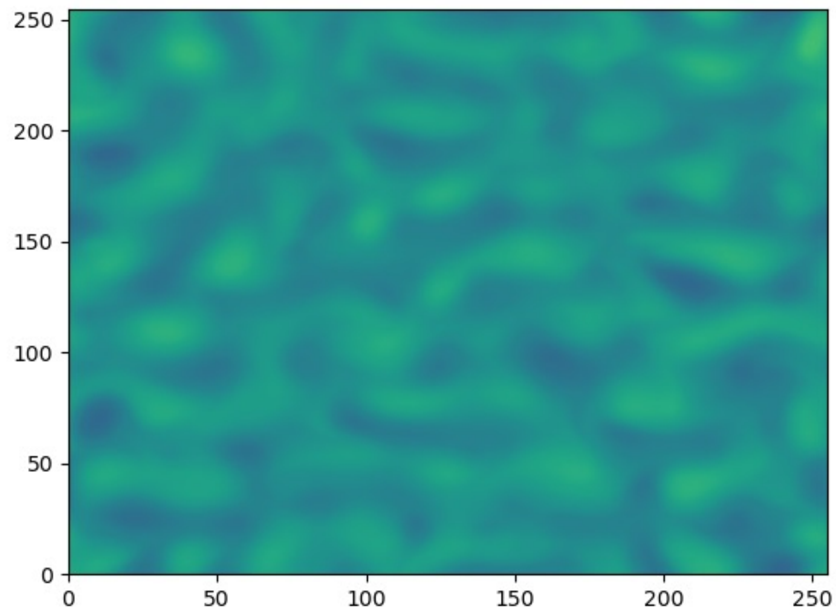


Tokamak geometry: Core flux tube



Hasegawa-Wakatani model is a common starting point

- Simplified model of magnetised plasma drift-interchange turbulence, relevant to tokamaks
- Typically solved in doubly periodic 2D domain
- Dynamics is sensitive to electron response

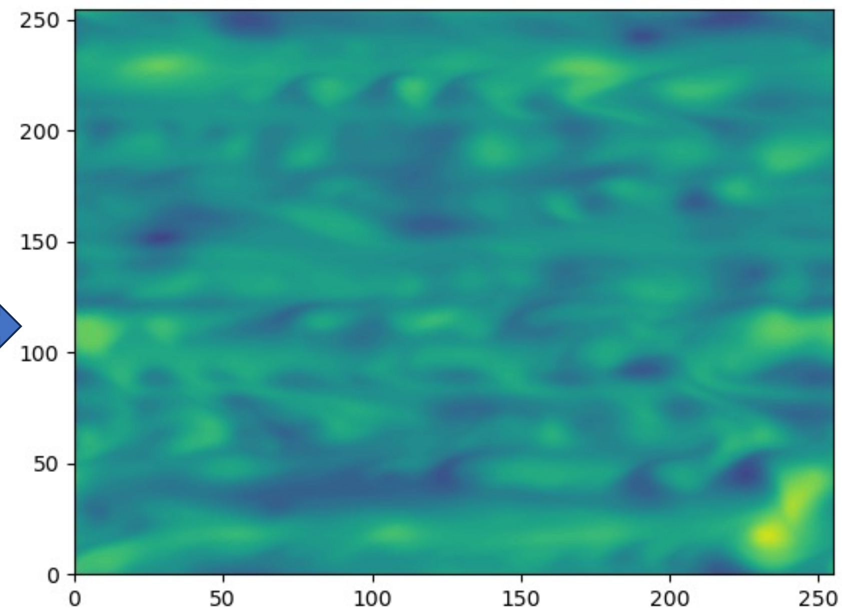


BOUT++ Hasegawa-wakatani example (modified = false)

Hasegawa-Wakatani model with modifications

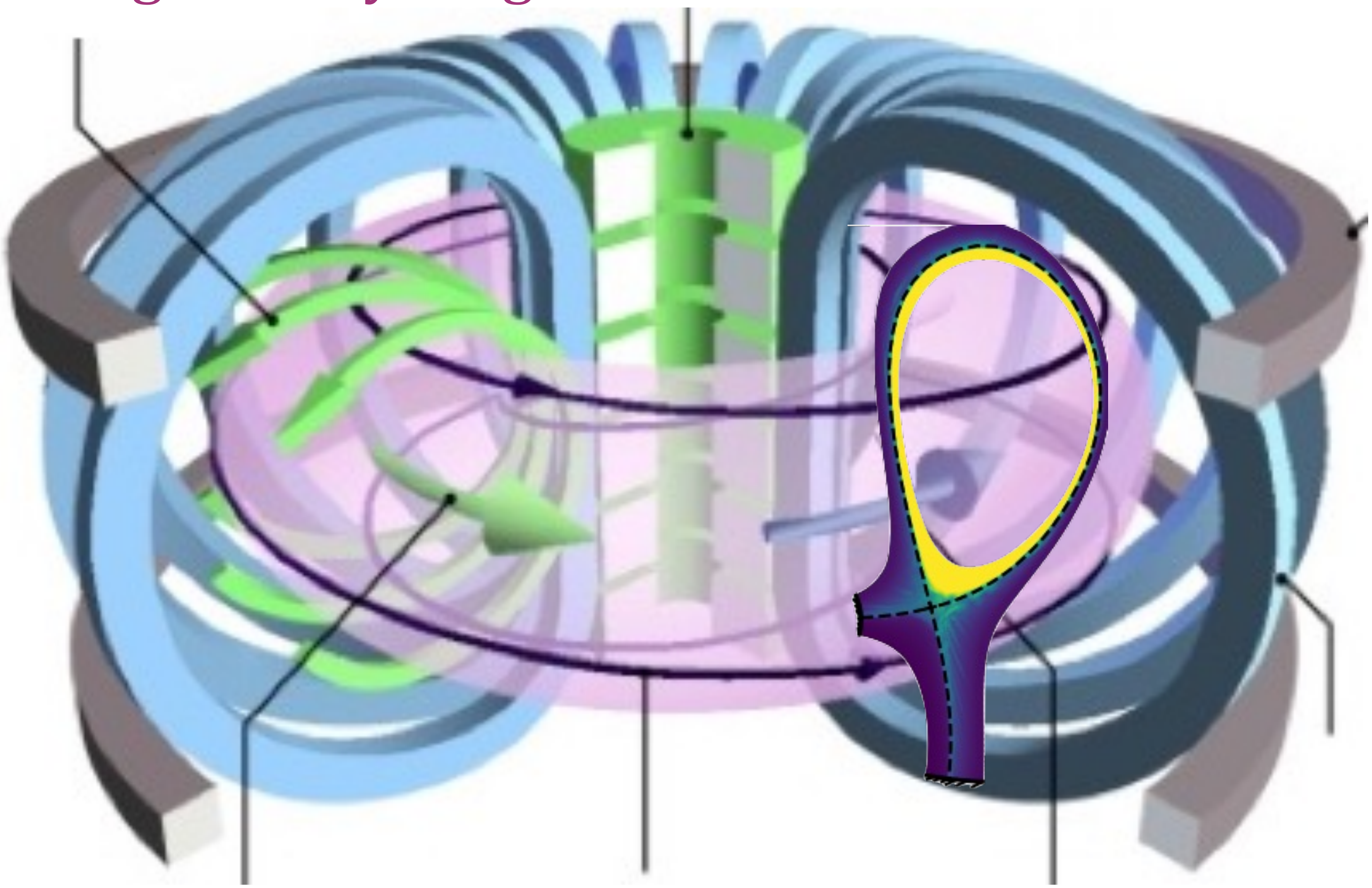
- Simplified model of magnetised plasma drift-interchange turbulence, relevant to tokamaks
- Typically solved in doubly periodic 2D domain
- Dynamics is sensitive to electron response
  - e.g. spontaneously formed "zonal" flows

Some extensions
- 3D domain with parallel currents
- Gyro-fluid and Gyro-kinetic models in flux tube geometry. No boundaries, but "twist-shift".



BOUT++ Hasegawa-wakatani example (modified = true)

Tokamak geometry: Edge annulus



3D edge turbulence simulations

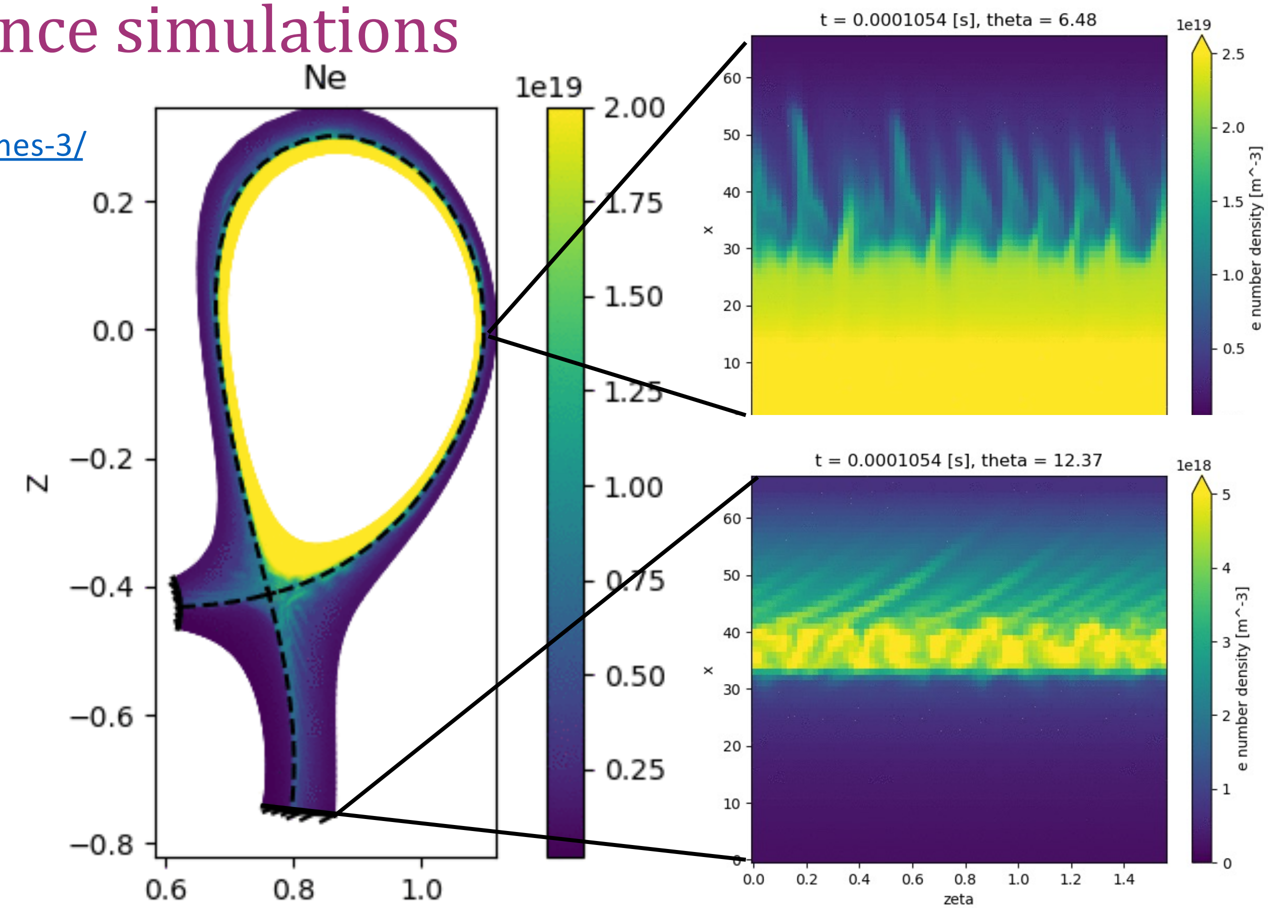
Hermes-3
https://github.com/bendudson/hermes-3/

- ✓ Full-f, flux-driven, including zonal potential evolution
- ✓ X-point geometry
- ✓ Evolving N_e, $V_{e||}$, $V_{i||}$, ω

- Resolution 64 (radial) x 32 (parallel) x 81 (toroidal)
- 0.9ms ~ 130 hours, 64 cores

Simplifications

- ➢ Electrostatic
- ➢ Boussinesq approximation
- ➢ Heavy electrons (60x)
- ➢ Single ion species (D+)
- ➢ No neutrals
- ➢ Orthogonal mesh, not aligned to divertor surface



TCV-X21: D.S. Oliveira *et al* 2022 *Nucl. Fusion* **62** 096001
DOI 10.1088/1741-4326/ac4cde

Features of tokamak edge turbulence

- Spatially inhomogeneous
  - Change in magnetic topology across separatrix
  - Turbulence in leg and core region
- Strongly impacted by boundary conditions
  - Plasma in contact with material surfaces forms ”sheath”
  - Nonlinearly couples plasma temperature, flows, currents
- Long-distance coupling
  - Dynamics determined by electromagnetic fields
  - Electrons flow rapidly along magnetic fields

Some SiMLInt applications

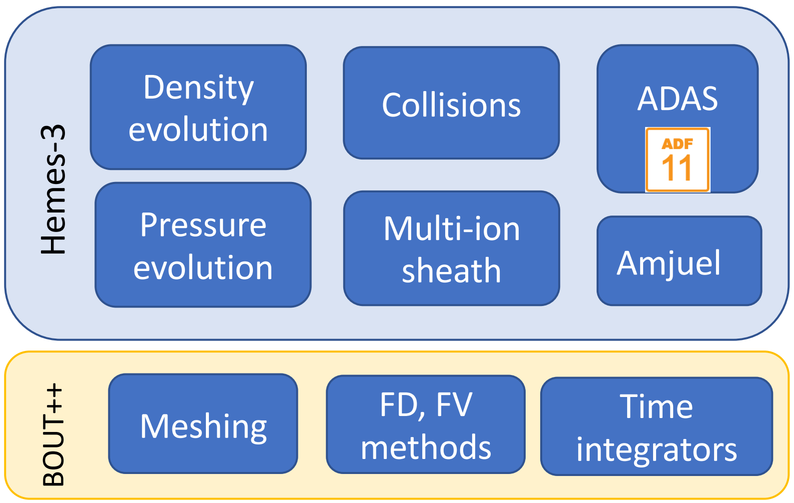
- Turbulent closures i.e. “Large Eddy Simulations”
  - Recover high-resolution result given low-resolution state
  - Model provides quantities like Reynolds stress
  - See J. Castagna (STFC), StyleGANs
- Surrogate models
  - 2D “transport” simulations include geometry but not turbulence. Typically use diffusive approximation but better models are needed. See e.g. Dekeyser, Baelmans
  - Given toroidal average density, temperatures & flows, calculate cross-field turbulent fluxes of particles, energy & momentum
- Fluid model closures
  - Compute e.g. heat flux (v^3) given density (v^0), velocity (v^1), temperature (v^2)
    - See e.g. “non-local”, ”Landau fluid” or “Hammett-Perkins” models
  - Extend accuracy towards ”kinetic” model (low collisionality)
- Solver accelerators
  - Better “predictor” as initial guess for state at next time
  - Predictor and preconditioner of electromagnetic potential

Extra slides

Hermes-3: Multi-species transport and turbulence models

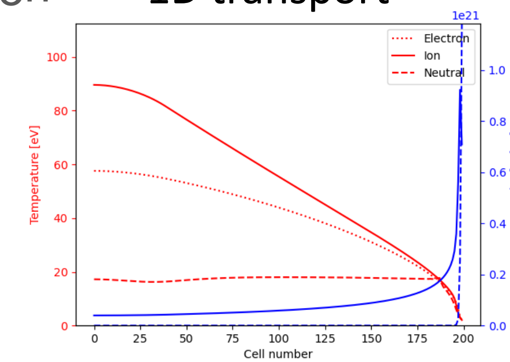
https://github.com/bendudson/hermes-3 https://hermes3.readthedocs.io

- Arbitrary number of species and ionisation states: D, T, He, Ne, …
- Full-f, flux-driven transport & turbulence

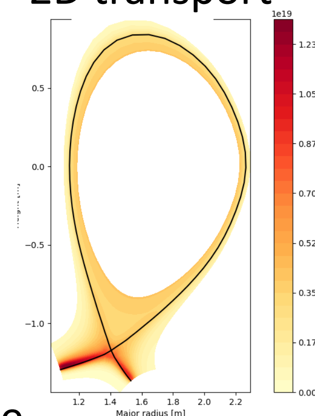


PETSc hypre sundials

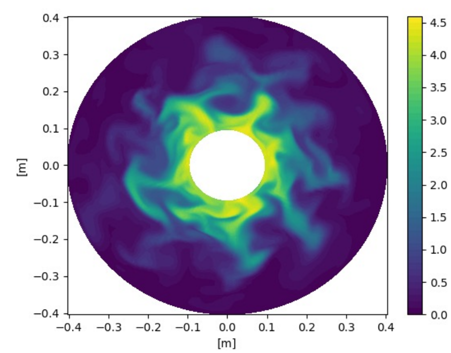
1D transport



2D transport



3D turbulence



Isothermal model

Electrons

$$\frac{\partial n_e}{\partial t} = -\nabla \cdot \left[n_e \left(\mathbf{v}_{E\times B} + \mathbf{b} v_{||e} + \underbrace{\mathbf{v}_{de}}_{\texttt{diamagnetic\_drift}} \right) \right]$$

$$\frac{\partial}{\partial t}\left(m_e n_e v_{||e} \right) = -\nabla \cdot \left[m_e n_e v_{||e} \left(\mathbf{v}_{E\times B} + \mathbf{b} v_{||e} + \underbrace{\mathbf{v}_{de}}_{\texttt{diamagnetic\_drift}} \right) \right]$$
$$- \partial_{||} p_e - e n_e E_{||} + \underbrace{m_e n_e \nu_{ei} \left(v_{||i} - v_{||e} \right)}_{\texttt{collisions}}$$

$$p_e = e T_e n_e$$

Ions

$$n_i = n_e$$

$$\frac{\partial}{\partial t}\left(m_i n_i v_{||i} \right) = -\nabla \cdot \left[m_i n_i v_{||i} \left(\mathbf{v}_{E\times B} + \mathbf{b} v_{||i} + \underbrace{\mathbf{v}_{di}}_{\texttt{diamagnetic\_drift}} \right) \right]$$
$$- \partial_{||} p_i + e n_i E_{||} + \underbrace{m_e n_e \nu_{ei} \left(v_{||e} - v_{||i} \right)}_{\texttt{collisions}}$$

$$p_i = e T_i n_i$$

Drifts

$$\mathbf{v}_{de} = -T_e \nabla \times \frac{\mathbf{b}}{B}$$

$$\mathbf{v}_{E\times B} = \frac{\mathbf{b} \times \nabla \phi}{B}$$

$$\mathbf{v}_{di} = T_i \nabla \times \frac{\mathbf{b}}{B}$$

Vorticity

$$\frac{\partial \Omega}{\partial t} = -\nabla \cdot \left(\Omega \mathbf{v}_{E\times B} \right) + \nabla \cdot \left[\left(p_e + p_i \right) \nabla \times \frac{\mathbf{b}}{B} \right] + \nabla \cdot \left(n_i v_{||i} - n_e v_{||e} \right)$$

$$\nabla \cdot \left[\frac{m_i}{B^2} \left(\overline{n} \nabla_\perp \phi + \nabla_\perp p_i \right) \right] = \Omega$$

System of equations specified in input file

- Top-level components specify the species, collective effects and modifiers

```
[hermes]
components = (e, i, sound_speed, vorticity,
              sheath_boundary, collisions,
              diamagnetic_drift)
```

- Each species' equations are:

```
[e]
type = evolve_density, evolve_momentum, isothermal

[i]
type = quasineutral, evolve_momentum, isothermal
```

Electron equations

```
[e]
type = evolve_density, evolve_momentum, isothermal
AA = 60 / 1836   # Atomic mass
charge = -1
temperature = 20 # eV
```

$$\mathbf{v}_{de} = -T_e \nabla \times \frac{\mathbf{b}}{B}$$

$$\mathbf{v}_{E\times B} = \frac{\mathbf{b}\times\nabla\phi}{B}$$

$$\boxed{\frac{\partial n_e}{\partial t} = -\nabla\cdot\left[n_e\left(\mathbf{v}_{E\times B} + \mathbf{b}v_{||e} + \underbrace{\mathbf{v}_{de}}_{\texttt{diamagnetic\_drift}}\right)\right]}$$

$$\boxed{\begin{aligned}\frac{\partial}{\partial t}\left(m_e n_e v_{||e}\right) =& -\nabla\cdot\left[m_e n_e v_{||e}\left(\mathbf{v}_{E\times B} + \mathbf{b}v_{||e} + \underbrace{\mathbf{v}_{de}}_{\texttt{diamagnetic\_drift}}\right)\right] \\ & - \partial_{||}p_e - e n_e E_{||} + \underbrace{m_e n_e \nu_{ei}\left(v_{||i} - v_{||e}\right)}_{\texttt{collisions}}\end{aligned}}$$

$$\boxed{p_e = e T_e n_e}$$

Ion equations

```
[i]
type = quasineutral, evolve_momentum, isothermal
AA = 2             # Atomic mass
charge = 1
temperature = 20 # eV
```

$$\mathbf{v}_{di} = T_i \nabla \times \frac{\mathbf{b}}{B}$$

$$\boxed{n_i = n_e}$$

$$\frac{\partial}{\partial t}\left(m_i n_i v_{||i}\right) = -\nabla\cdot\left[m_i n_i v_{||i}\left(\mathbf{v}_{E\times B} + \mathbf{b}v_{||i} + \underbrace{\mathbf{v}_{di}}_{\texttt{diamagnetic\_drift}}\right)\right] - \partial_{||}p_i + e n_i E_{||} + \underbrace{m_e n_e \nu_{ei}\left(v_{||e} - v_{||i}\right)}_{\texttt{collisions}}$$

$$\boxed{p_i = eT_i n_i}$$

Vorticity equation

- Current continuity gives the vorticity equation:

$$\underbrace{\frac{\partial \Omega}{\partial t} = -\nabla\cdot\left(\Omega \mathbf{v}_{E\times B}\right)}_{\text{Polarisation current}} + \underbrace{\nabla\cdot\left[\left(p_e + p_i\right)\nabla\times\frac{\mathbf{b}}{B}\right]}_{\text{Diamagnetic current}} + \underbrace{\nabla\cdot\left(n_i v_{||i} - n_e v_{||e}\right)}_{\text{Parallel current}}$$

- The vorticity is inverted to calculate the potential

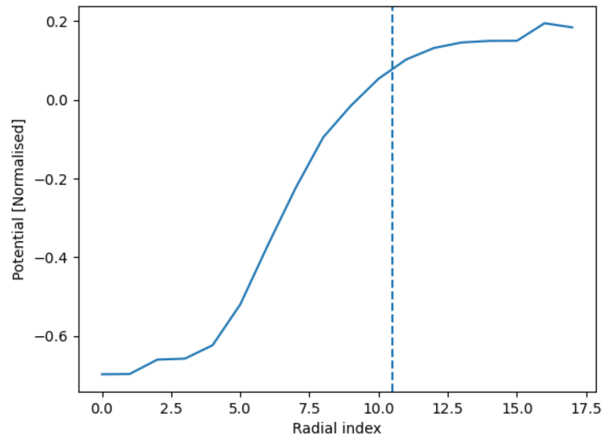
$$\nabla\cdot\left[\frac{m_i}{B^2}\left(\overline{n}\nabla_\perp\phi + \nabla_\perp p_i\right)\right] = \Omega$$

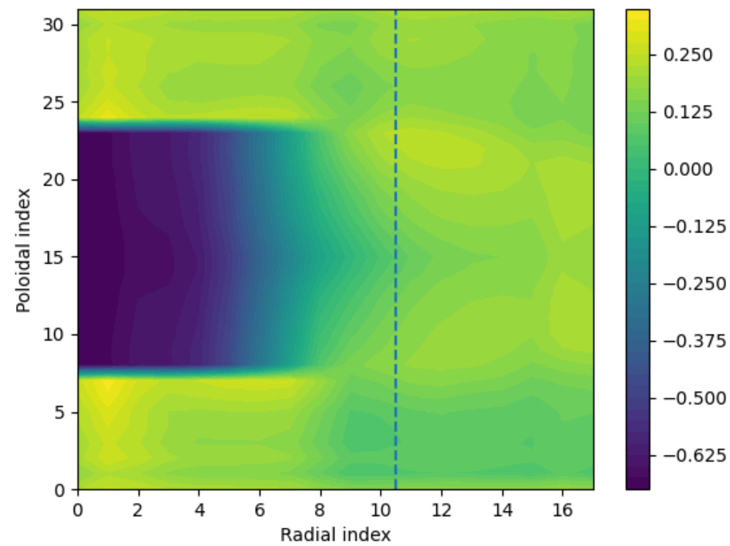
Boussinesq
approximation

Solving for potential

- Using BOUT++ standard 2D (toroidal plane, X-Z) solver
- Boundary conditions:
  - Zero-gradient radial inner and outer
  - “Free” (linear extrapolation) at targets

- Avoids ill-posed problem by using “relaxing” radial boundaries
  - Laplacian inversion fixed boundaries
  - Value at the boundary updates to relax towards zero-gradient on short timescale (1μs here)





Miscellaneous details

- Sheath boundary condition: Sound speed flow into the targets, current using Boltzmann relation for electrons: exp(-phi/Te) form
- Density fixed at inner boundary, zero-gradient at outer boundary
- Initial condition: constant radial gradient (in cell index space)
- Te = Ti = 20 eV
- “Full-f” simulation: No separation between background & fluctuation

Numerics

- Parallel dynamics stabilised using flux splitting & MC limiter
- Perpendicular advection uses MC limiter
- Hyper-diffusion of all evolving fields in Z direction (not X)
    - Using nz = power of 3 can help, but not sufficient