MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

Overview over the edge fluid turbulence code GRILLIX

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EUROfusion

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BOUT++ $\leftrightarrow$ GRILLIX

GRILLIX … :

... is a 3D fluid code for plasma edge/SOL turbulence in complex (diverted) geometries

… addresses problems related with edge confinement and heat exhaust

	BOUT++	GRILLIX
Model	reduced fluid models (generic)	full-f drift reduced Braginskii
Discretisation	finite differences	finite differences
‘Coordinates’	globally field aligned (curvilinear)	FCI (locally field aligned)
Language	C++ (MPI)	Fortran (MPI + OpenMP) $\longrightarrow$ C++ for GPU
Community	global, code publicly available	~ 10 persons located mainly at IPP Garching, code available on request

Drift reduced Braginskii model

Basic assumptions:

$\lambda_{mfp,\|} \ll R_0$

$\omega \ll \Omega_i$

$\beta \ll 1$

$k_{\|} \ll k_{\perp}$

plasma density
$$\frac{\partial}{\partial t} n + \nabla \cdot (n \mathbf{v}_e) = 0 + k_{iz} n N$$

quasineutrality / vorticity
$$\nabla \cdot \mathbf{j} = \nabla \cdot (en\mathbf{v}_i - en\mathbf{v}_e) = 0$$

Drift reduction:
$$\mathbf{v}_{e\perp} = \mathbf{v}_E + \mathbf{v}_*^e \qquad \mathbf{v}_E = (\mathbf{B} \times \nabla\varphi)/B^2$$
$$\mathbf{v}_{i\perp} = \mathbf{v}_E + \mathbf{v}_*^i + \mathbf{u}_{pol}, \qquad \mathbf{v}_*^{e,i} = \mp(\mathbf{B} \times \nabla p_{e,i})/enB^2$$
$$\mathbf{u}_{pol} = \frac{m_i}{eB^2} \mathbf{B} \times \left(\frac{\partial}{\partial t} + \mathbf{v}_E \cdot \nabla \right) (\mathbf{v}_E + \mathbf{v}_*^i)$$

electromagnetic parallel dynamics
$$\mathbf{E} = -\nabla\varphi - \partial_t A_\| \mathbf{b}, \qquad \mathbf{B} = \mathbf{B_0} + \nabla \times A_\| \mathbf{b}, \qquad B \approx B_0$$

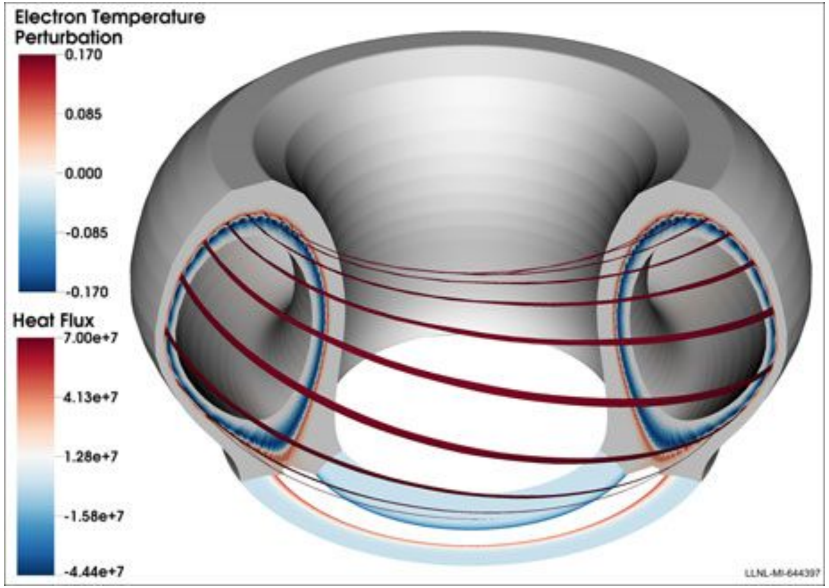
electron heat
$$\left[\frac{\partial}{\partial t} + \mathbf{v}_e \cdot \nabla\right] T_e + \frac{2}{3} T_e \nabla \cdot \mathbf{v}_e = -\frac{2}{3n} \nabla \cdot \mathbf{q}_e + \frac{2}{3n} Q_e \quad + S_{T_e}$$

ion heat
$$\left[\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla\right] T_i + \frac{2}{3} T_i \nabla \cdot \mathbf{v}_i = -\frac{2}{3n} \nabla \cdot \mathbf{q}_i - \frac{2}{3n} P_i : \mathbf{v}_i$$

diffusive neutrals
$$\frac{\partial}{\partial t} N = \nabla \cdot \frac{1}{n k_{cx}} \nabla N T_i - k_{iz} n N, \qquad N \text{ fixed at the divertor}$$

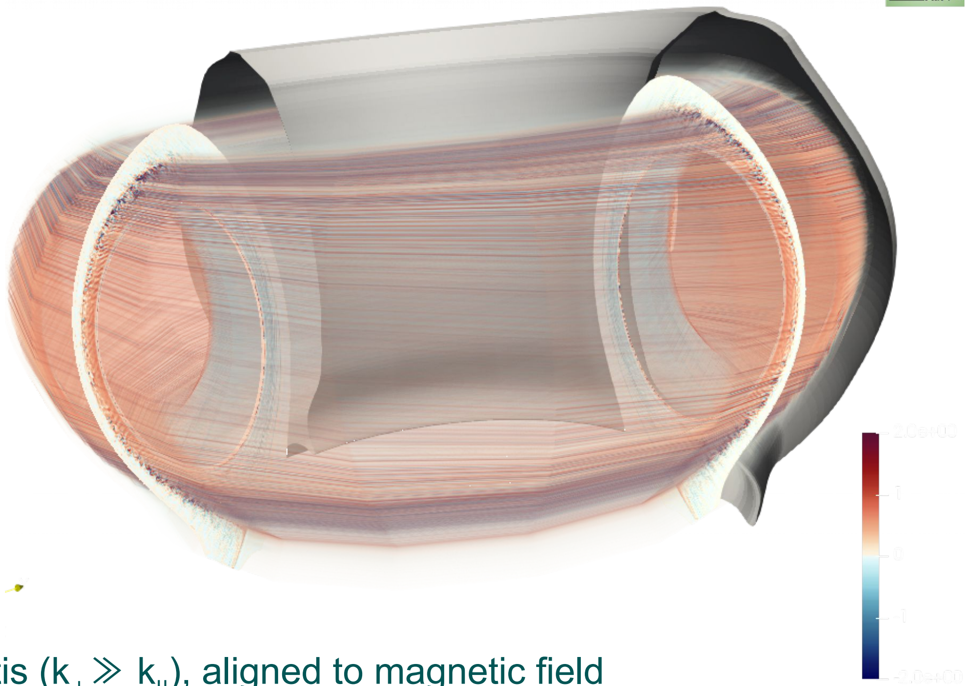
Field aligned turbulence

BOUT++



https://bout.llnl.gov/

GRILLIX



- **High anisotropy:** structures are spaghettis ($k_\perp \gg k_{||}$), aligned to magnetic field
- **Complex geometry:** divertor, X-point, advanced diverter configurations, stellarators

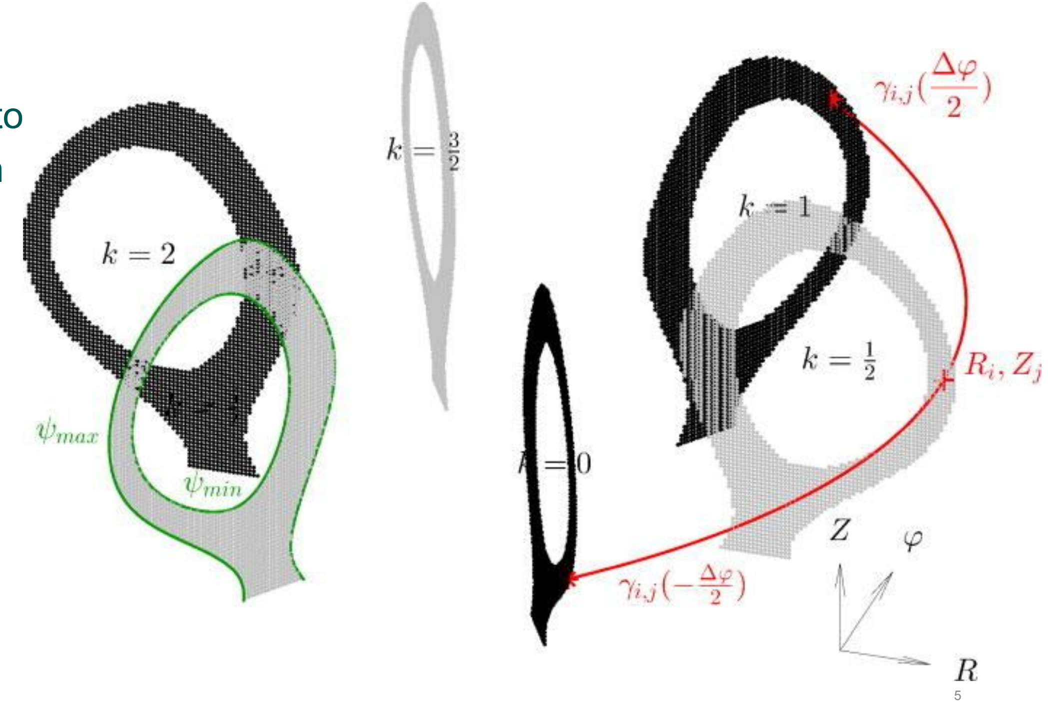
Flux-Coordinate Independent approach (FCI)

Basic concept:

- Set of few Cartesian planes
- Perpendicular operators ($\nabla_\perp$) straight forward
- Parallel operators ($\nabla_{||}$) via field line tracing to neighbouring planes and interpolation within planes

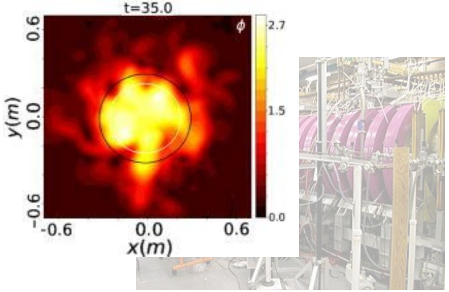
Advanced features in GRILLIX:

- Flux box volume integration
- Toroidally staggered → mimetic finite differences
- Immersed boundary method



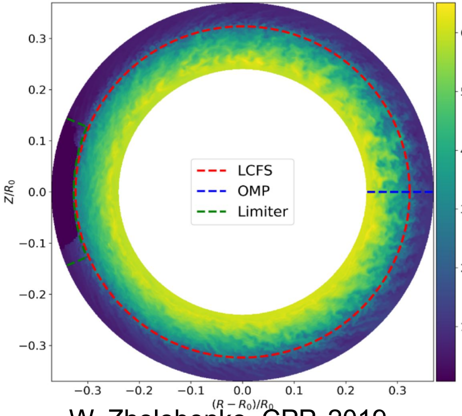
Geometric flexibility

Linear



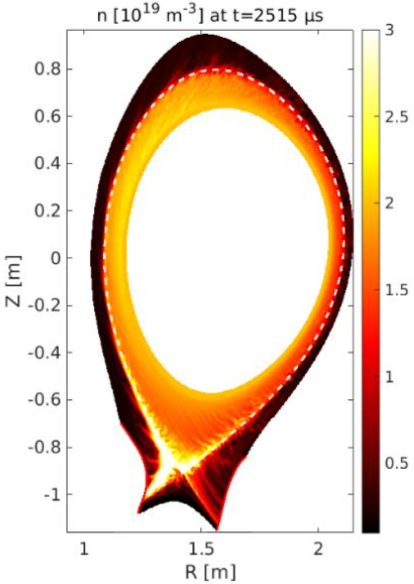
A. Ross, PoP 26, 2019

Limiter



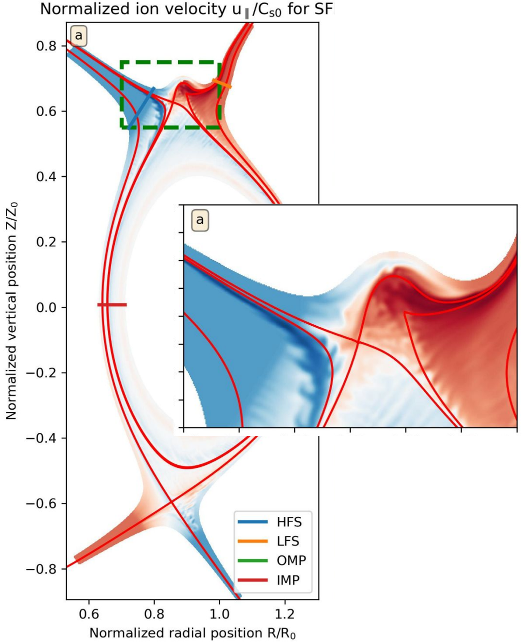
W. Zholobenko, CPP, 2019

Single null



W. Zholobenko, NF 61, 2021

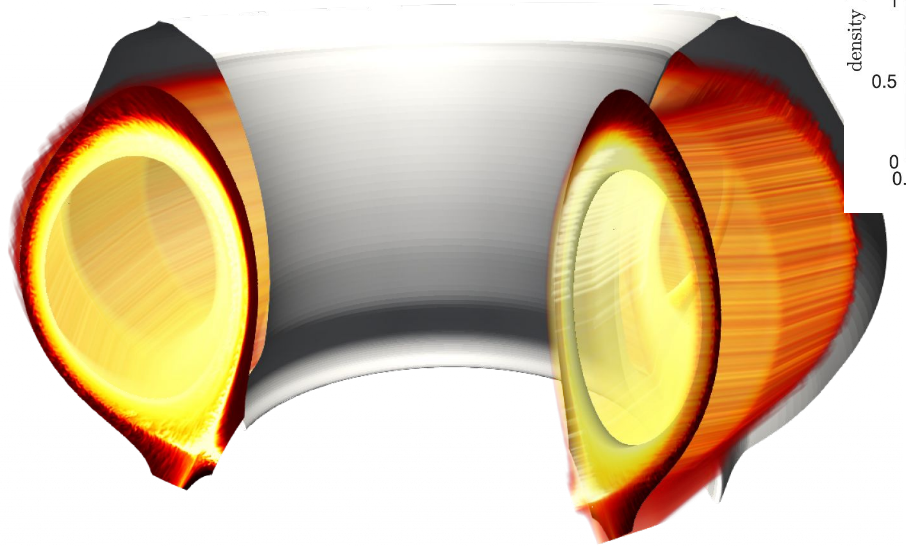
Advanced divertor concepts

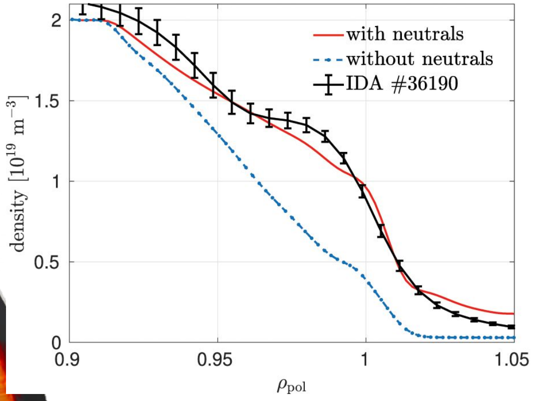


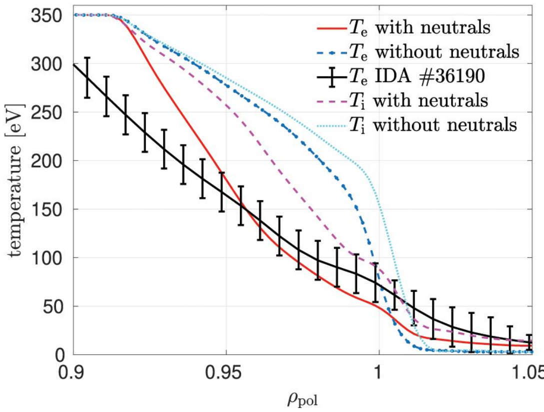
J.-W. Lin, Master thesis, TUM, 2022

Validations: AUG

ASDEX Upgrade L-mode simulation in realistic geometry and at realistic parameters







- Neutral gas density at divertor tunable
- Good match with experimental profiles with N_{div} = 5 10^{17} m^{-3}
- P_{exp}=750kW ~ P_{sim}=530kW

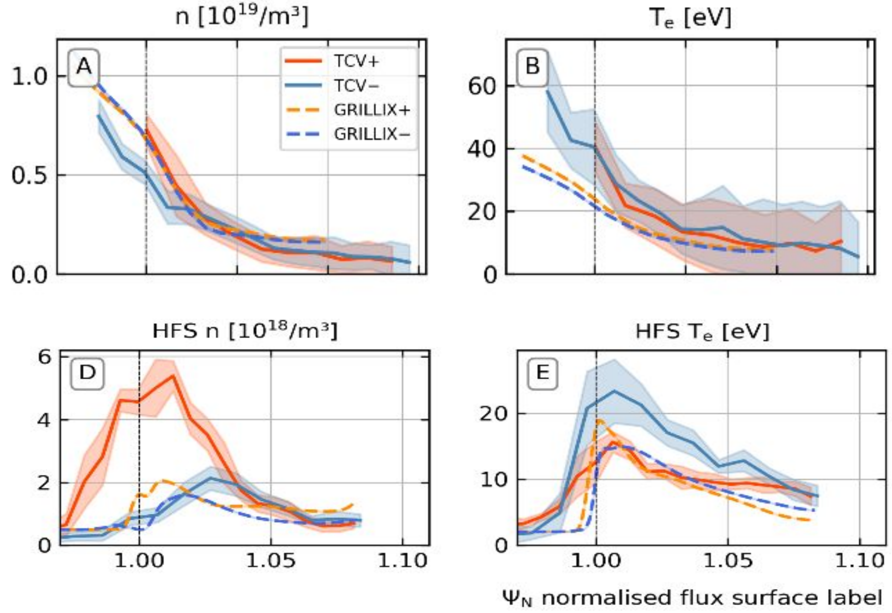
*W. Zholobenko, NF **61**:116015, 2021*

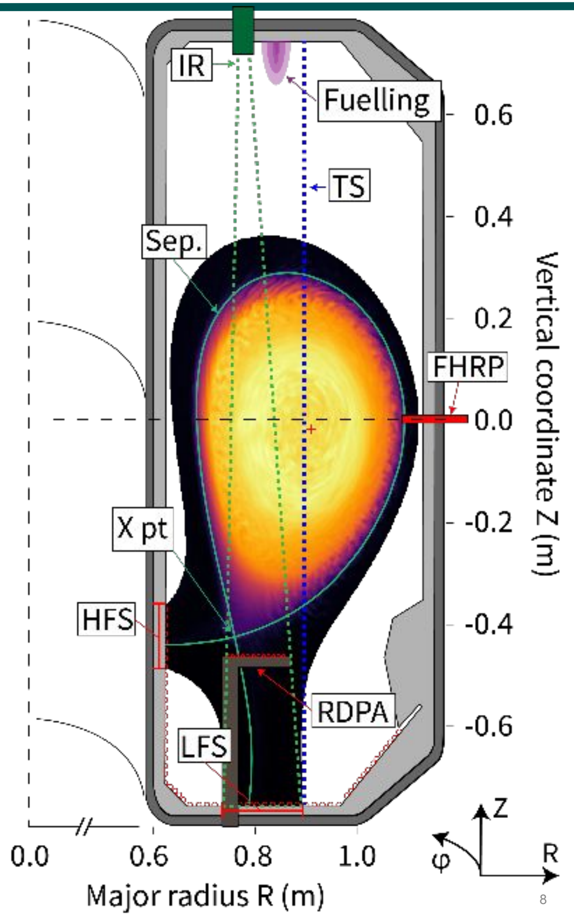
Validations: TCV-X21

- First validation of turbulence codes in diverted geometry
- Multicode validation (GBS, GRILLIX, TOKAM3X)
- Experimental and simulation data published (open access)
- Rigorous quantification of validation results

OMP

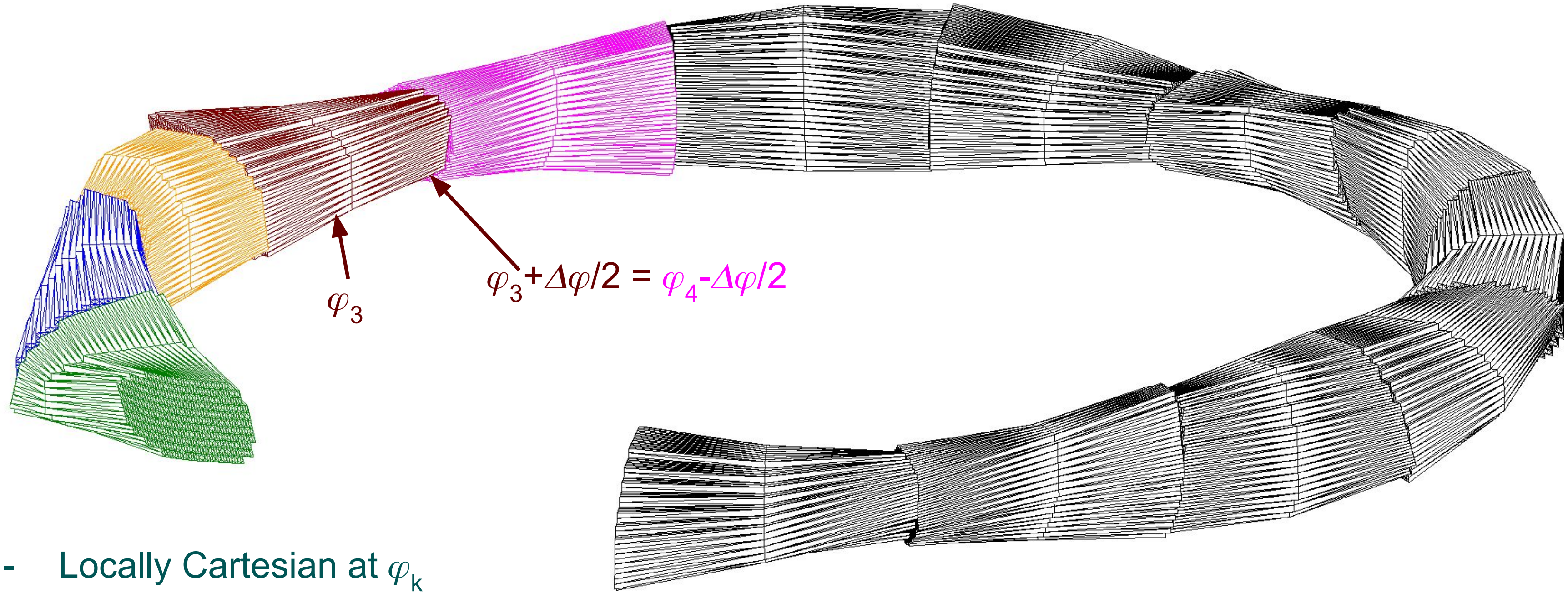
HFS Target





*D.S. Oliveira and T. Body, NF **62**:096001, 2022*

Towards stellarators

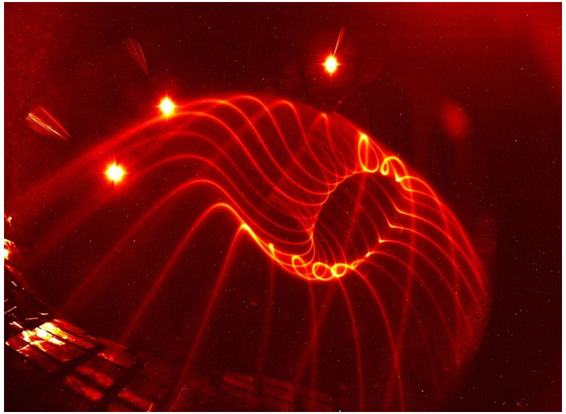


- Locally Cartesian at φ_k
- Field aligned boxes $[\varphi_k-\Delta\varphi/2 , \varphi_k+\Delta\varphi/2]$
- Non-conformal at $\varphi_k+\Delta\varphi/2$
- Actually non-straight smooth lines

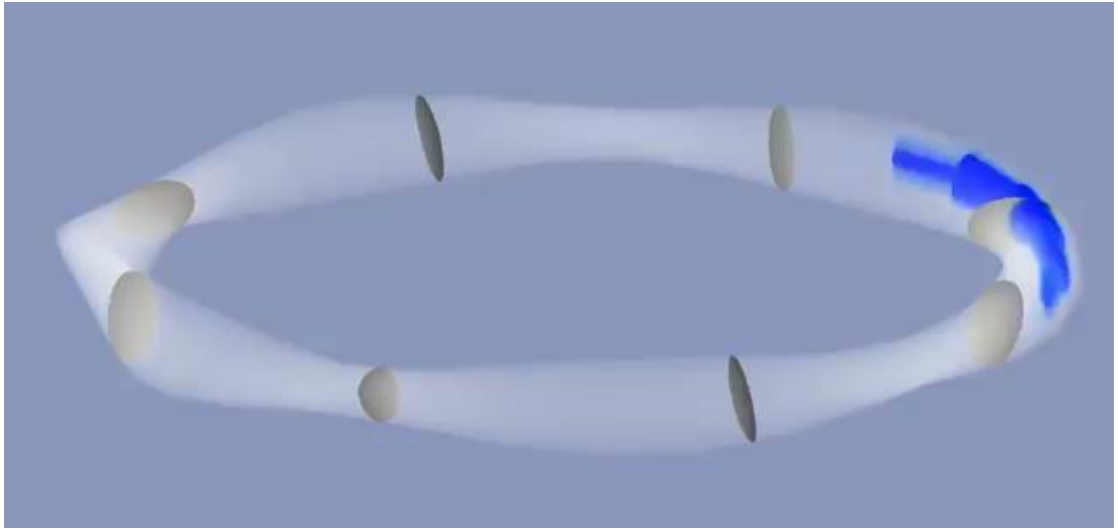
Towards stellarators

$$\partial_t u = \nabla \cdot \left[\mathbf{b}\nabla_{\parallel} u\right]$$

T. S. Pederson, Nat. Commun. 7:13493, (2016)



The field lines making up a magnetic surface are visualized in a dilute neutral gas, in this case primarily water vapour and nitrogen (pn≈10−6 mbar)[...].



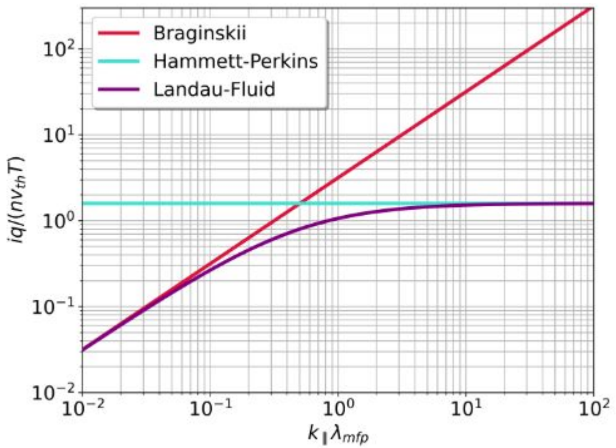
- Blob traces out magnetic field lines
- Superiority of mimetic discretisation methods holds true in 3D geometries
- Full turbulence model in GRILLIX currently adapted

Landau-Fluid closure

Heat flux most susceptible to kinetic effects

- Braginskii closure: $$q^{BG} = \chi_e \nabla_{\|} T_e, \quad \chi_e = 3.2 \frac{n T_e \tau_{ei}}{m_e}$$

- Free streaming limiter: $$q^{LIM} = \left(\frac{1}{q^{BG}} + \frac{1}{\alpha q^{FS}} \right)^{-1}$$
  - Free parameter α



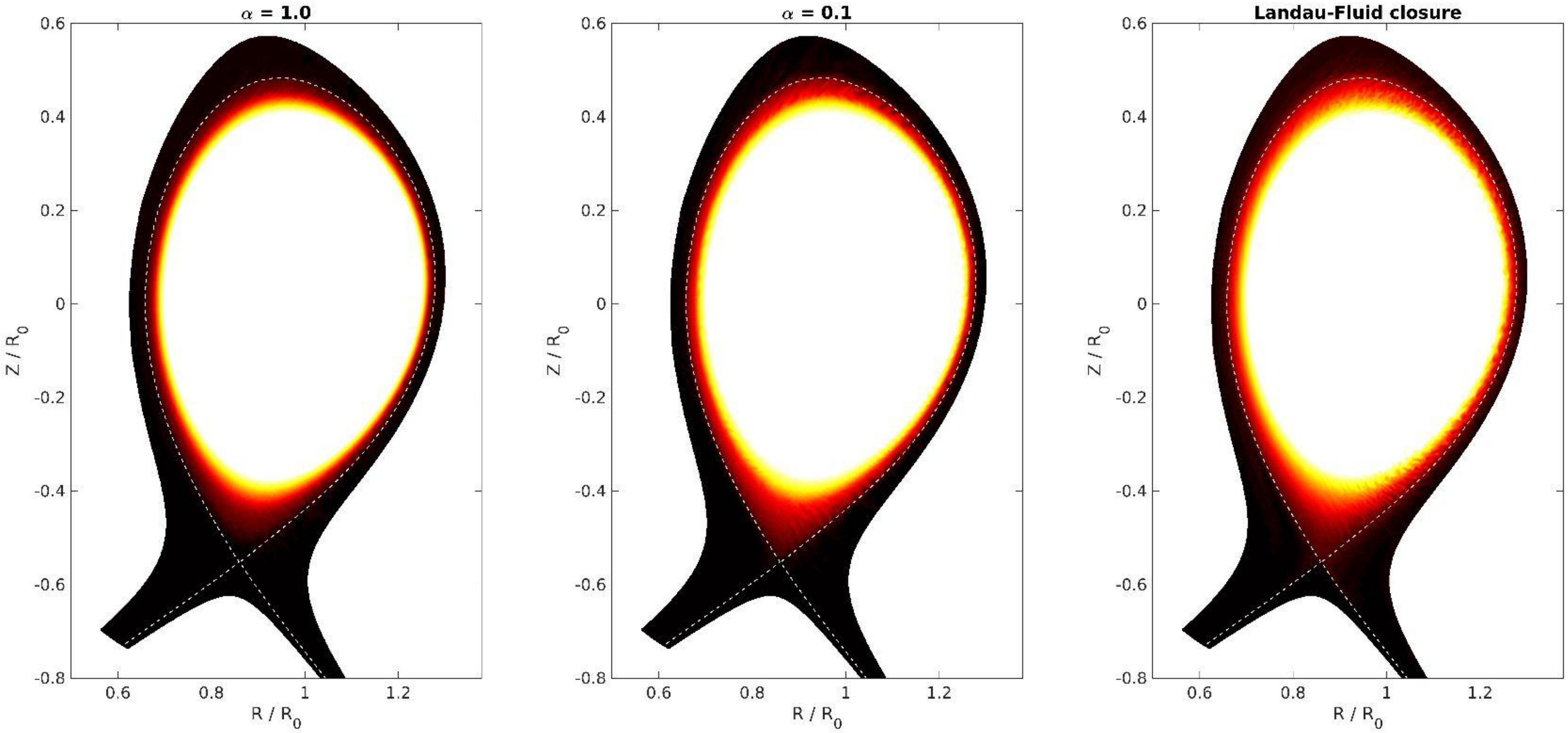
- Landau-fluid closure:
  - Self-consistent heat flux limiter
  - Non-local effects
  - Requires set of full 3D solves within FCI

$$q^{LF} = -A \frac{ik_{\|}}{|k_{\|}| + \zeta_0} T_e \approx \sum_{n=1}^{N} q_n^{LF}$$

$$\left[-\nabla_{\|}^2 + (\zeta_0 \beta_n)^2 \right] q_n^{LF} = -A \zeta_0 \alpha_n \nabla_{\|} T$$

J.G. Chen et al., CPC ***236****:128, 2019*

Landau-Fluid closure



C. Pitzal et al., in preparation, 2023

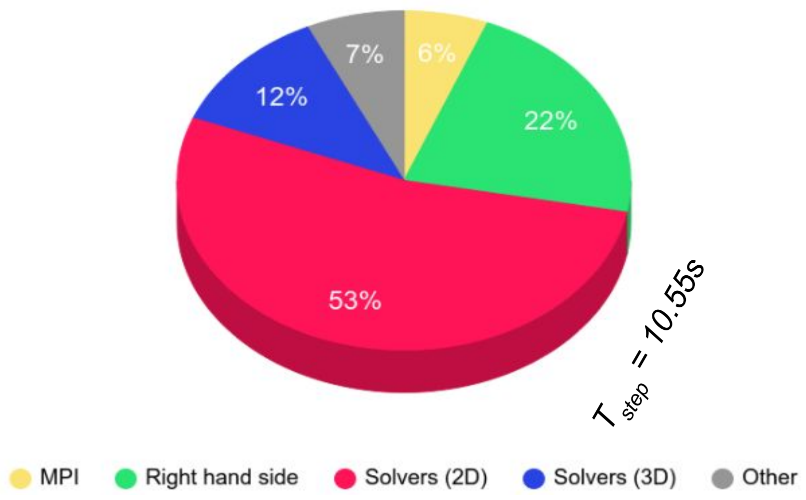
Performance

Parallelisation concept

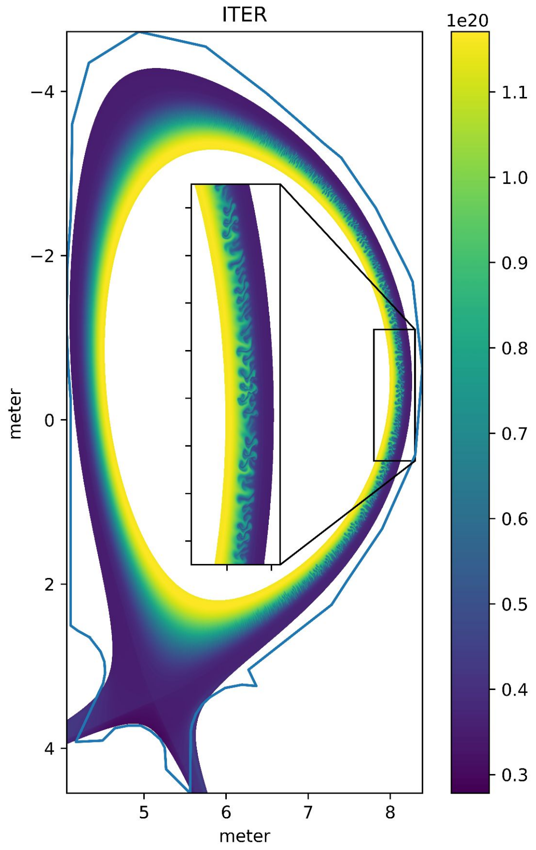
- MPI domain decomposition across planes
- OpenMP within planes

ITER Q=10 scenario

- Resolution: $3\varrho_s$ @OMP separatrix,16 plane
- Number of mesh points: 11 437 831 x 16



#OMP threads	Speedup
2	2.0
5	4.9
10	8.9
20	17.9
40	23.8



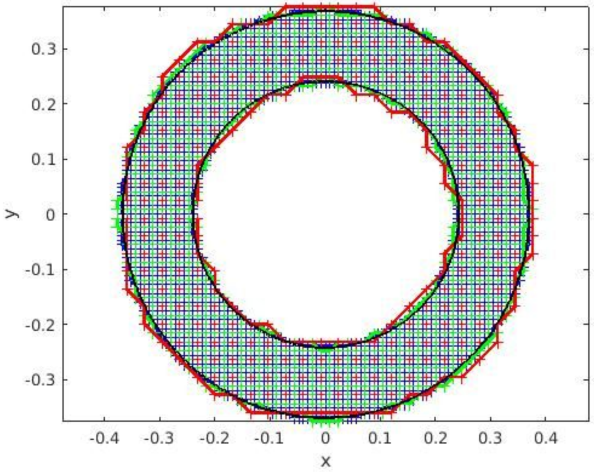
Elliptic solver

Elliptic Problem:

$$\lambda\phi - \nabla \cdot (c\nabla_\perp \phi) = b$$

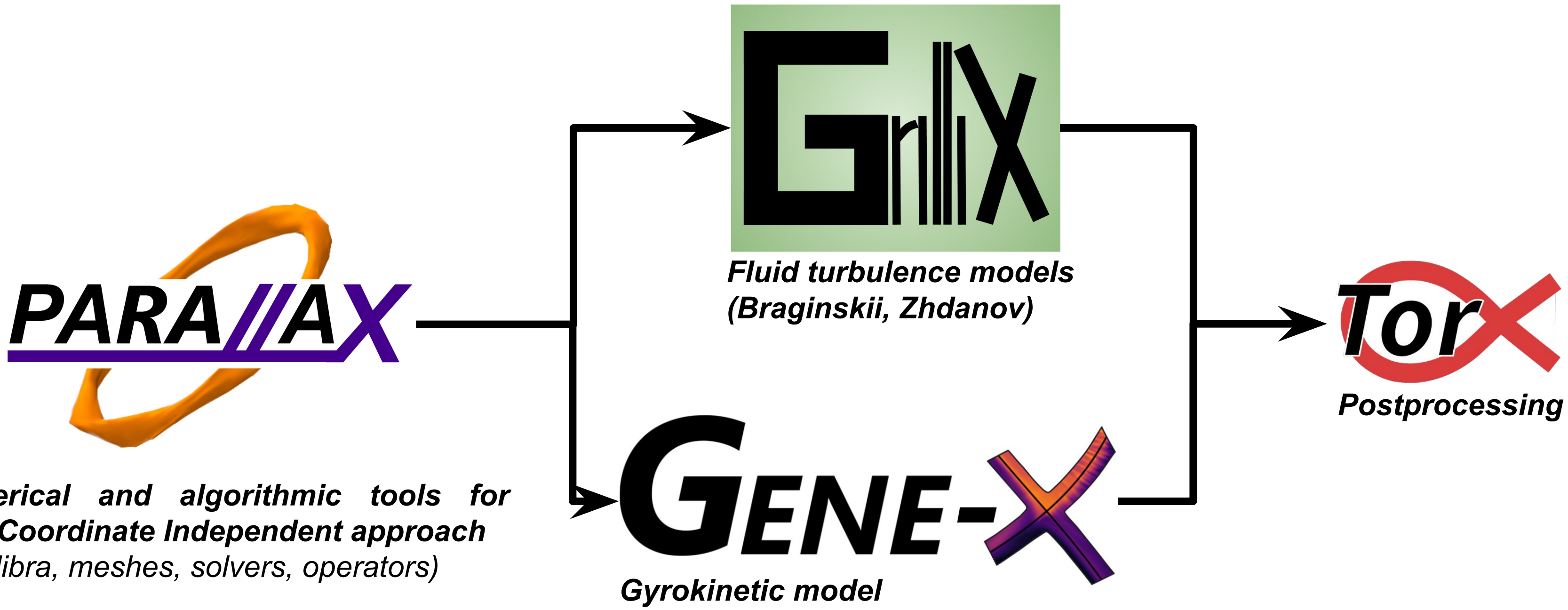
on an set of 2D poloidal planes independently (no MPI)

- for logically unstructured grid
- inhouse developed GMRES with geometric multigrid preconditioner
- Being ported to GPU (C++/Fortran interoperability)



Algorithm:	time per solve [s]
GMRES with geometric multigrid preconditioner	3.99
DIRECT (MKL)	72.80
PETSC -ksp_type gmres, -pc_type hypre	57.26

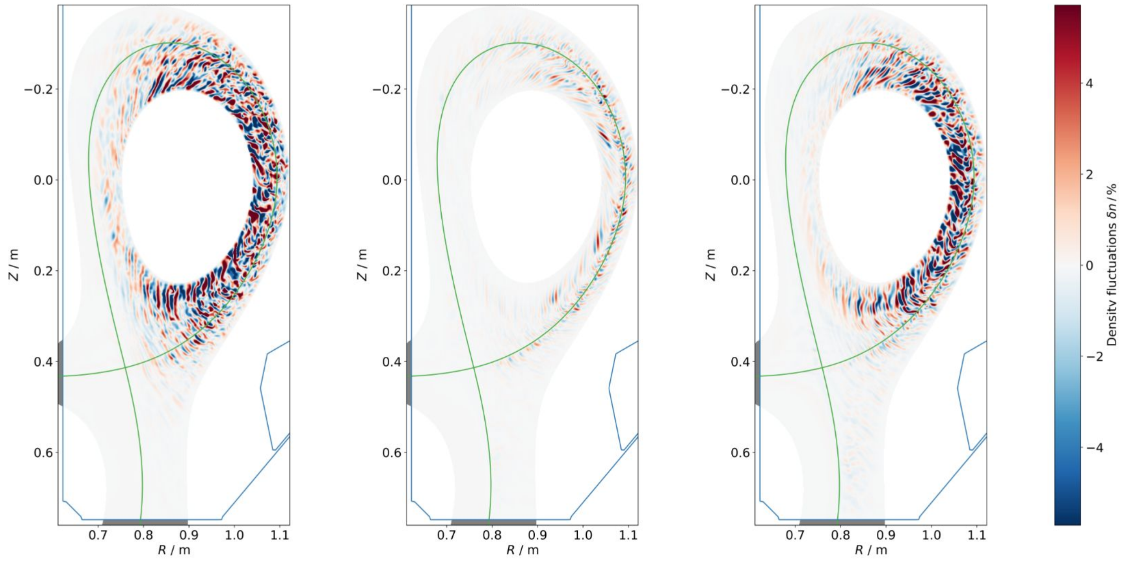
Code framework

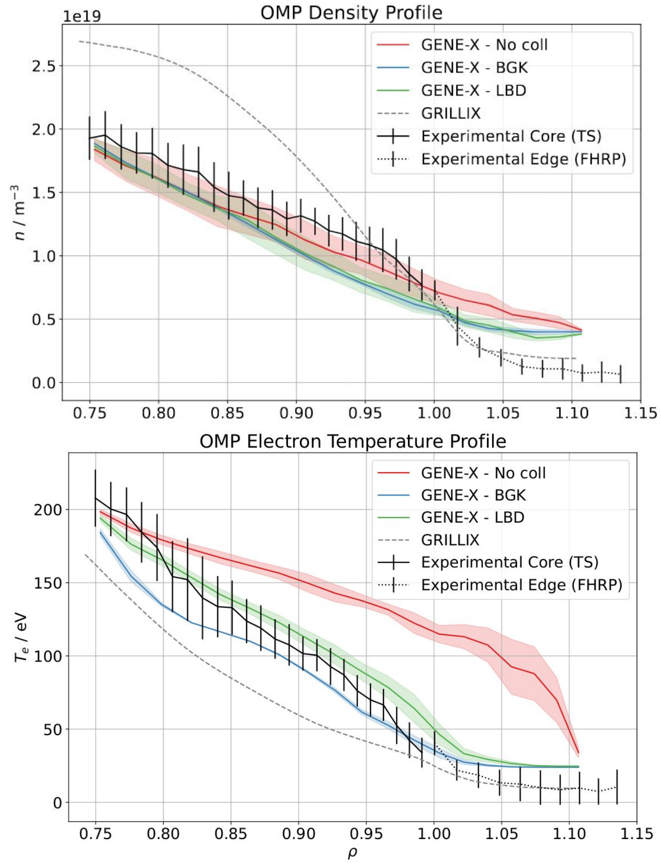


Numerical and algorithmic tools for Flux-Coordinate Independent approach
(Equilibra, meshes, solvers, operators)

GENE-X: collision models for TCV-X21

No collisions | Bhatnagar-Gross-Krook | Lenard-Bernstein/ Dougherty





Core dynamics of TCV dominated by trapped electron mode (TEM), which is not captured by fluid model

P. Ulbl et al., in preparation, 2023

Summary

GRILLIX

- has a similar scope to BOUT++
- is more targeted and specific in its model and approach
- less generic and modular with smaller community
- written in Fortran, GPU extension in C++ under development

Applications

- Variety of complex geometries
- Validations of TCV and AUG

Ongoing extensions

- Stellarator geometries
- Landau Fluid closure
- …

GENE-X

- Flux-coordinate independent approach applied to gyrokinetic model
- Shares common API PARALLAX