Overview on modelling of edge-SOL transport

first principles

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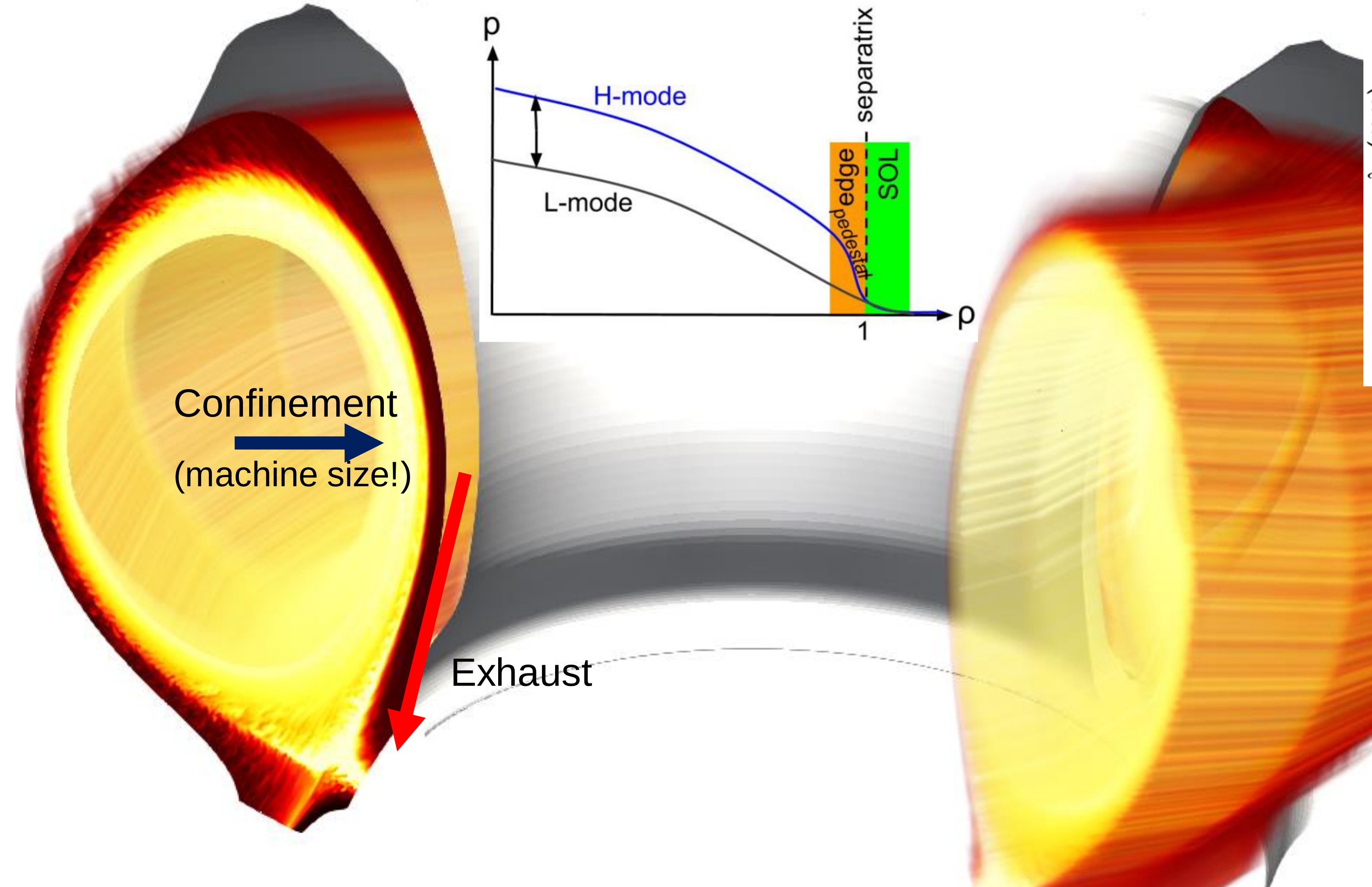
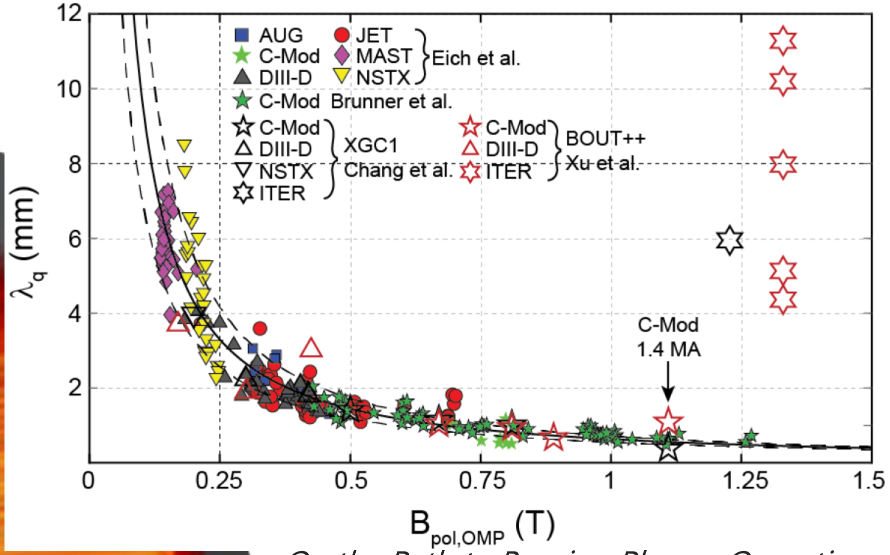
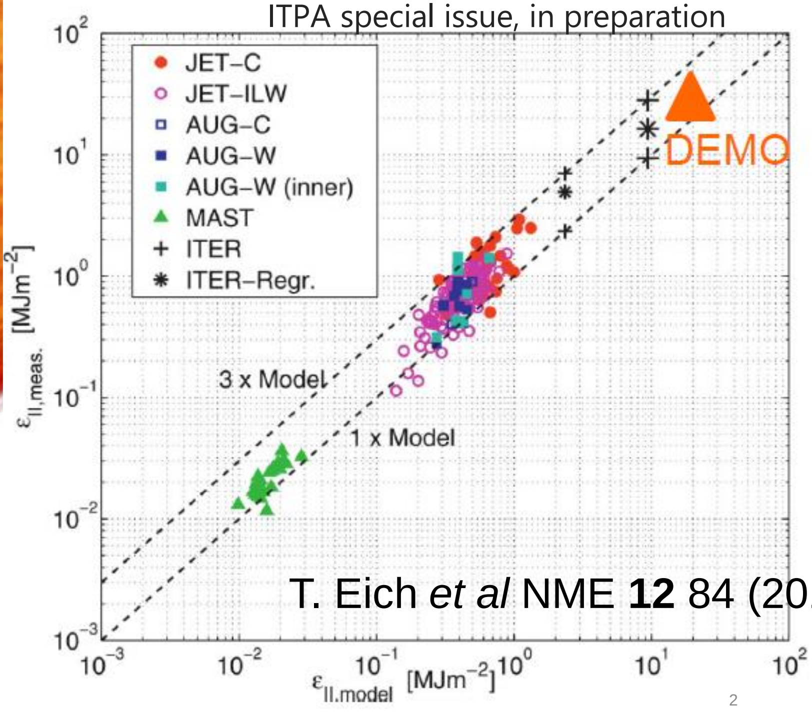
Turbulence in the tokamak edge & SOL is linked and sets the global confinement and exhaust capability



W. Zholobenko *et al* NME **34** 101351 (2023)



On the Path to Burning Plasma Operation,
ITPA special issue, in preparation



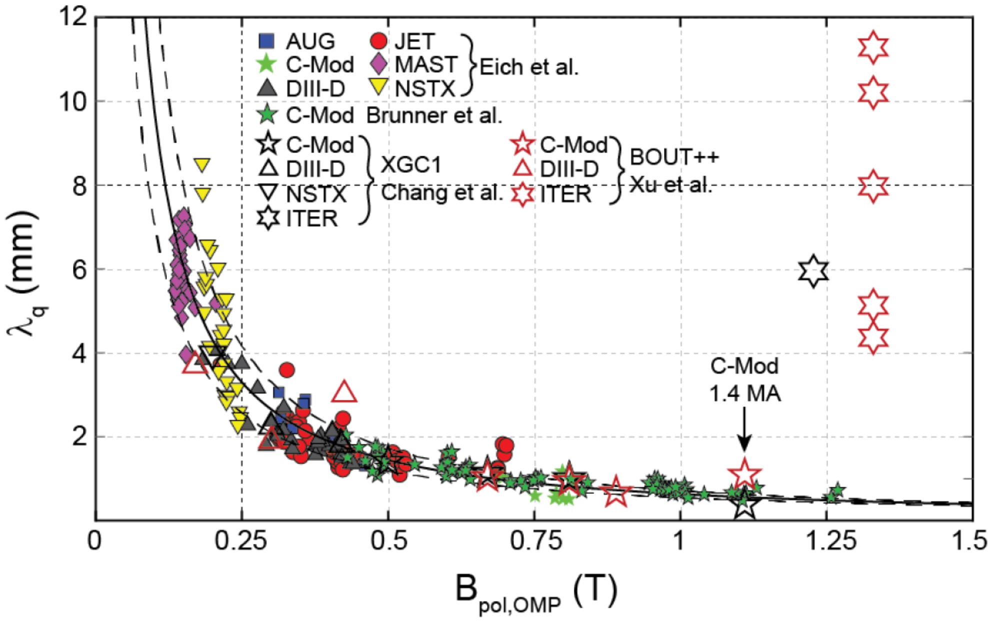
T. Eich *et al* NME **12** 84 (2017)

Overview

1. Motivation
2. Tutorial: key SOL quantities and how to study them
3. The challenges
4. Progress review: advances in modelling tools and capabilities
5. Conclusions

Will the ITER divertor melt or not?

H-mode, inter-ELM near SOL heat flux channel width.
Courtesy to *“On the Path to Burning Plasma Operation”,* ITPA (Div-SOL) special issue in Nucl. Fusion, in preparation (2023).



→ Operation in detached conditions is mandatory

- Radiation fractions of 90% are realistic, but a SOL width below 1 mm is problematic
- The uncertainty in the ITER SOL width is very large

ITER heating $P \approx 100$ MW

Divertor wetter area $A \approx 2 \cdot 2\pi R \cdot \lambda_q \div \sin(\alpha) \times f_{expansion}$

$$\approx 720\ \mathrm{m} \cdot \lambda_q$$

Heat load $q = \frac{P}{A}$ =14-280 MW/m^2 $>$ 10 MW/m^2 material limit!

What is the SOL width?

Classical textbook picture from Ulrich Stroth, Plasmaphysik, 2018; Peter C Stangeby, The Plasma Boundary of Magnetic Fusion Devices, 2000:

$$n(r) = n_{sep} e^{-\frac{r}{\lambda_n}}$$

$$\mathcal{G}_\perp = -D_r \left.\frac{\mathrm{d}n}{\mathrm{d}r}\right|_0 \quad L_c = \frac{L_c D_r n_{sep}}{\lambda_n} \qquad 2L_c \approx 2\pi R_0 \sqrt{\frac{1+\kappa_\epsilon^2}{2}} q_s$$

$$\mathcal{G}_\parallel = \int_0^\infty 0{,}5 n(r) c_s \mathrm{d}r \approx 0{,}5 \bar{c}_s n_{sep} \lambda_n$$

$$\mathcal{G}_\perp = \mathcal{G}_\parallel \quad \Longrightarrow \quad \lambda_n \approx \sqrt{\frac{L_c D_r}{0{,}5 \bar{c}_s}}$$

Scales like ~R_0, but Eich scaling is ~*1*/B_{pol}

Such 2-point models can be easily coupled to core transport frameworks (IMEP etc.)

Instead, R.J. Goldston proposed in Nucl. Fusion 52 (2012) 013009 the heuristic drift-based model:

$$\lambda_n = v_{\mathrm{dia}} \tau_\parallel = \frac{2T_{\mathrm{sep}}}{eBR} \frac{2L_\parallel}{c_s} = \frac{4a}{eB_{\mathrm{p}}R} \sqrt{\frac{m_{\mathrm{p}} T_{\mathrm{sep}}}{2}} = \frac{2a}{R} \rho_{\mathrm{p}}$$

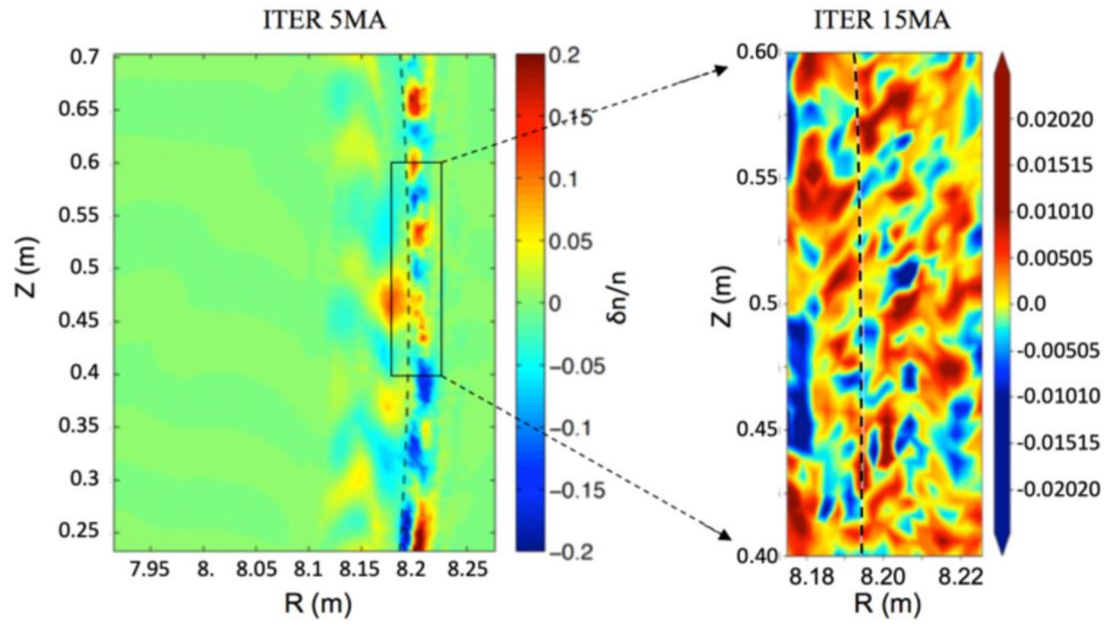
This is much more in line with the Eich scaling!

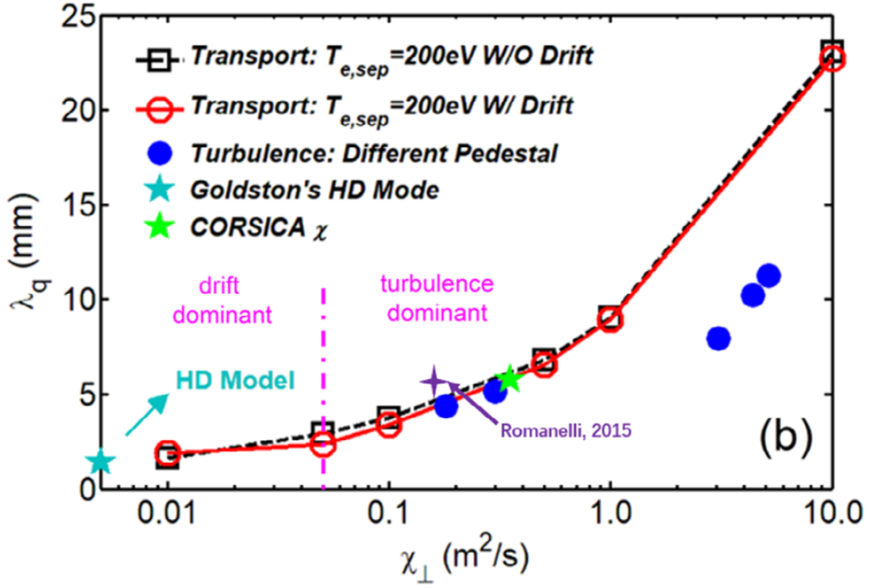
But: only valid in standard ELMy attached H-modes on current machines! Heuristic model!

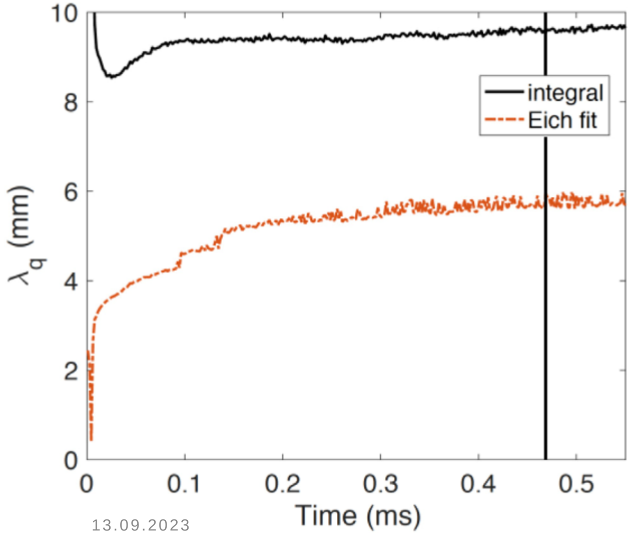
Explanation and caveats for the results from XGC1 and BOUT++

XGC1: C. S. Chang *et al* PoP **28** 022501 (2021)

BOUT++: X.Q. Xu *et al* Nucl. Fusion **59** 126039 (2019)







Global GK turbulence: TEMs, drift-waves, E_r shear, etc.

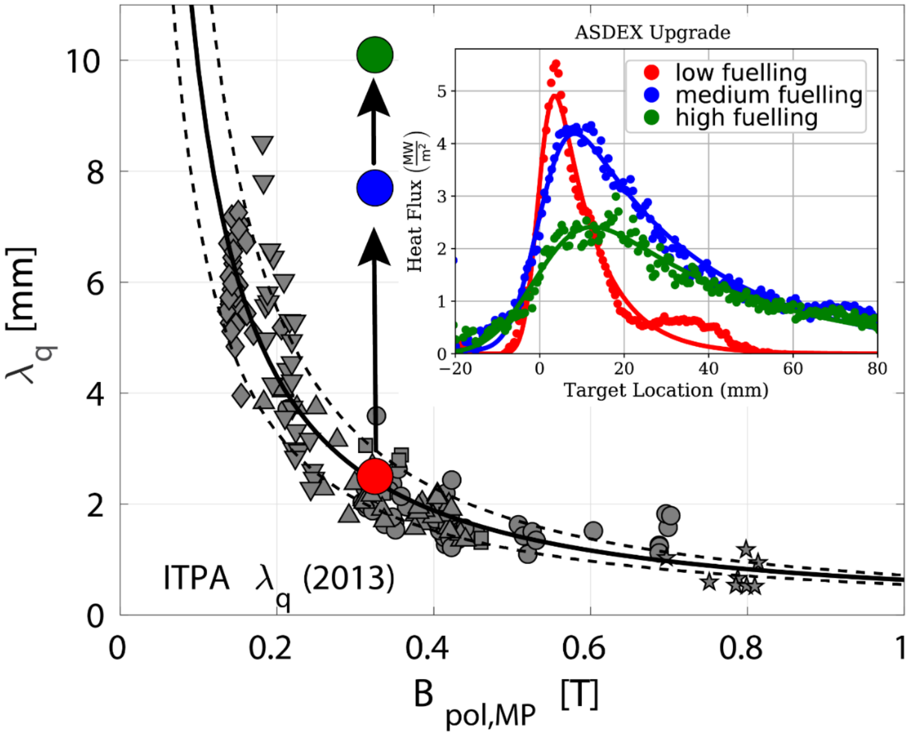
XGC1 simulations are very expensive and run only for < 1 ms. Requires high confidence in the initial background profiles!

Transport + Local MHD turbulence: peeling-ballooning modes, drift-waves

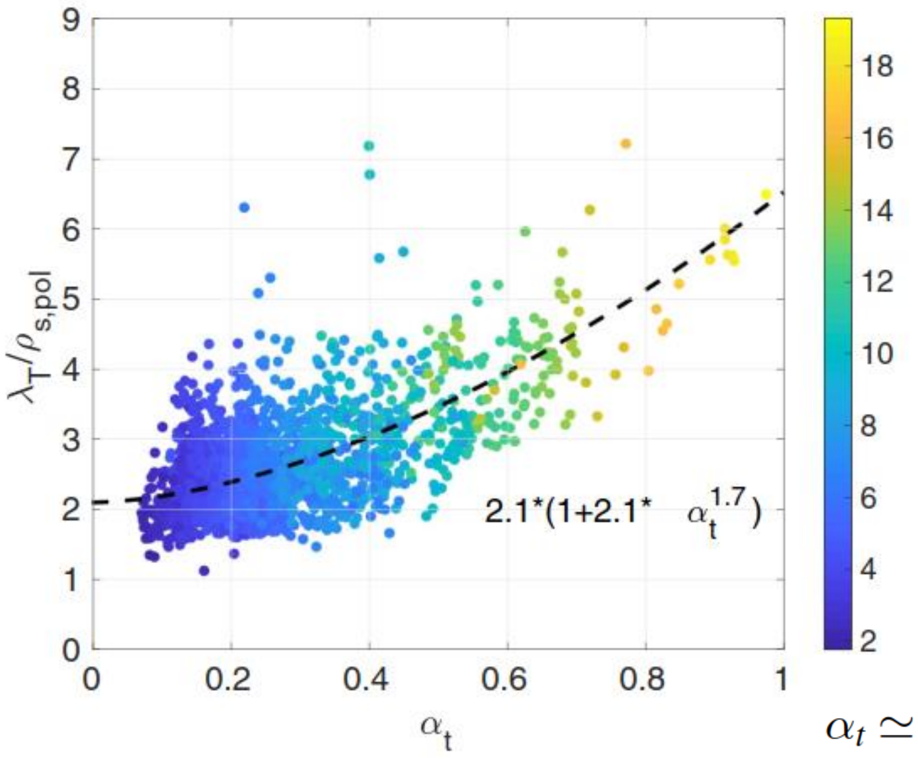
Delta-*f* (fluid) turbulence simulations with BOUT++ are not exactly valid in the SOL! But perhaps it works for the near-SOL.

More hope: effect of SOL collisionality

M. Faitsch *et al* NME **26** 100890 (2021)



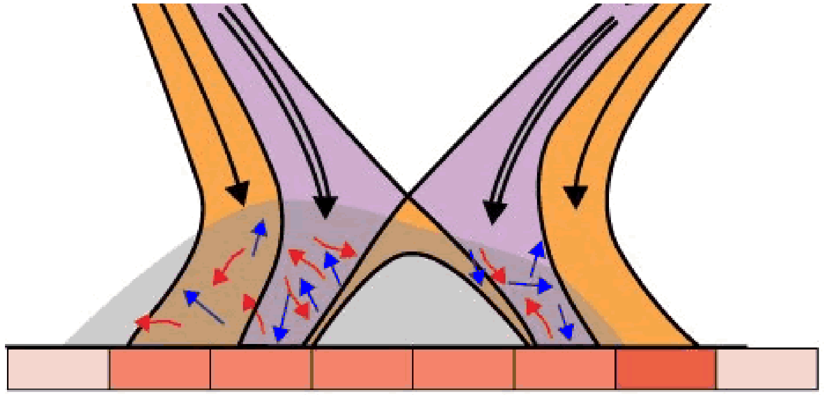
T. Eich et al 2020 Nucl. Fusion 60 056016 ν_e^*

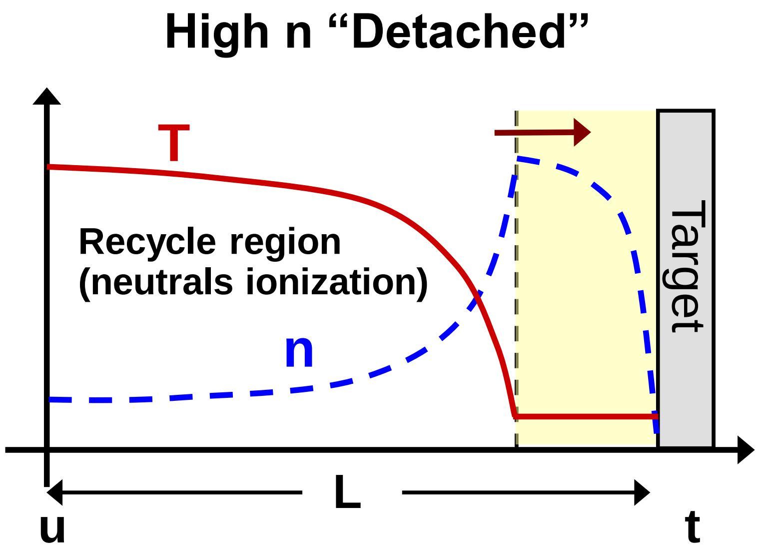


$$\alpha_t \simeq \frac{1}{100} \cdot \hat{q}_{cyl}\,\nu_e^*$$

- The SOL width seems to increase significantly with SOL collisionality. (It is also always larger in L-mode!)
- Collisionality can be detrimental for confinement.
- But high SOL ν_e^* is anyways likely due to the need for detachment!
- High confinement, no ELM regimes with high ν_e^* have been found, such as QCE and XPR.

A reactor must have a detached divertor!

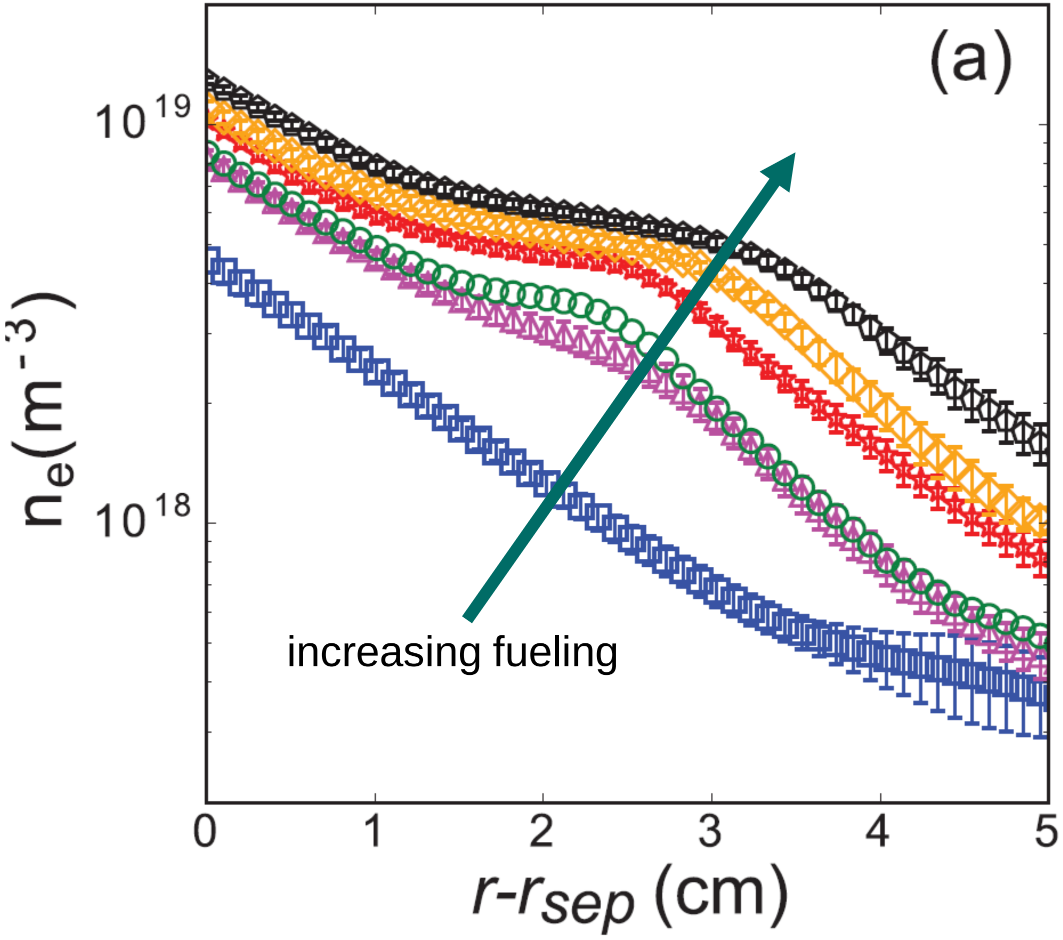




- Attached divertor experiments are typically in (high-)recycling conditions: $T_\mathrm{t} \ll T_\mathrm{u}$, but $p_\mathrm{t} \approx p_\mathrm{u}$
- Each particle hitting the divertor deposites 13.6 eV recombination energy
  - ⇒ Need to reduce p_t and particle fluxes to walls
  - ⇒ Let plasma **volumetrically** recombine, **detach** from the targets
  - ⇒ Volume recombination sets in automatically at high n / low T, but due to density limit, cooling by impurities helps a lot
- There is „partial“ detachment (only high $q_\parallel$ flux tubes) and „full“ detachment
- 2-point SOL models become obscure in detached conditions…

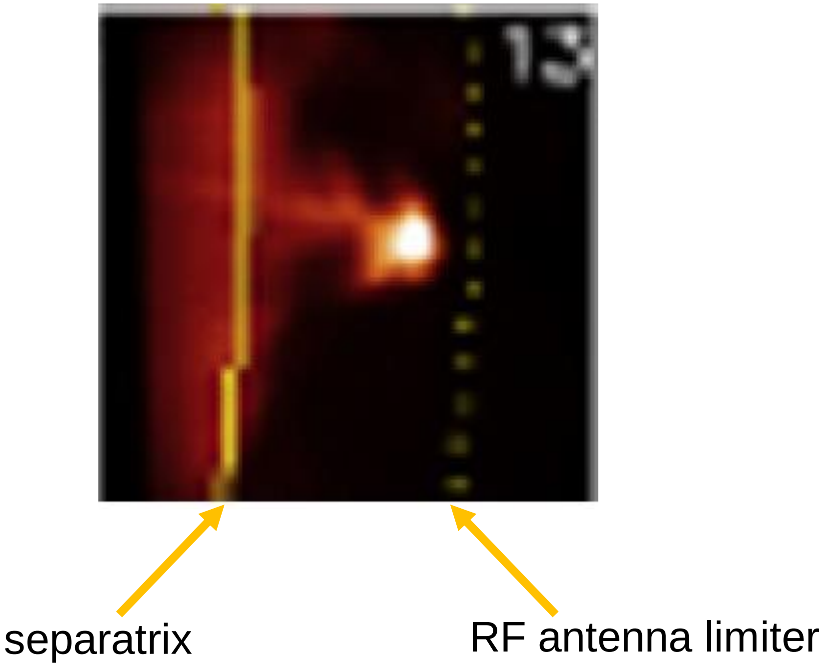
Far-SOL turbulence: blob filaments, density shoulder, wall erosion

See D. A. D'Ippolito et al., Phys. Plasmas 18, 060501 (2011) for a review.



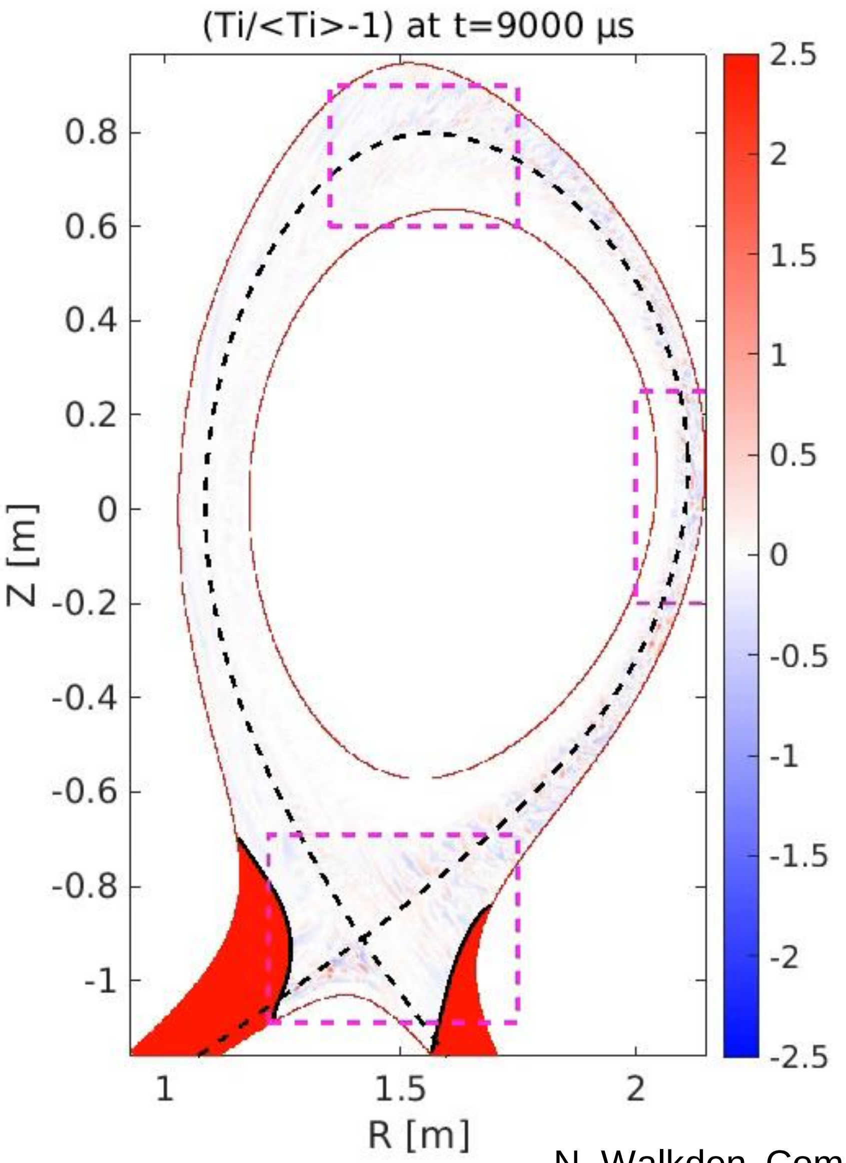
A. Wynn *et al* 2018 Nucl. Fusion **58** 056001

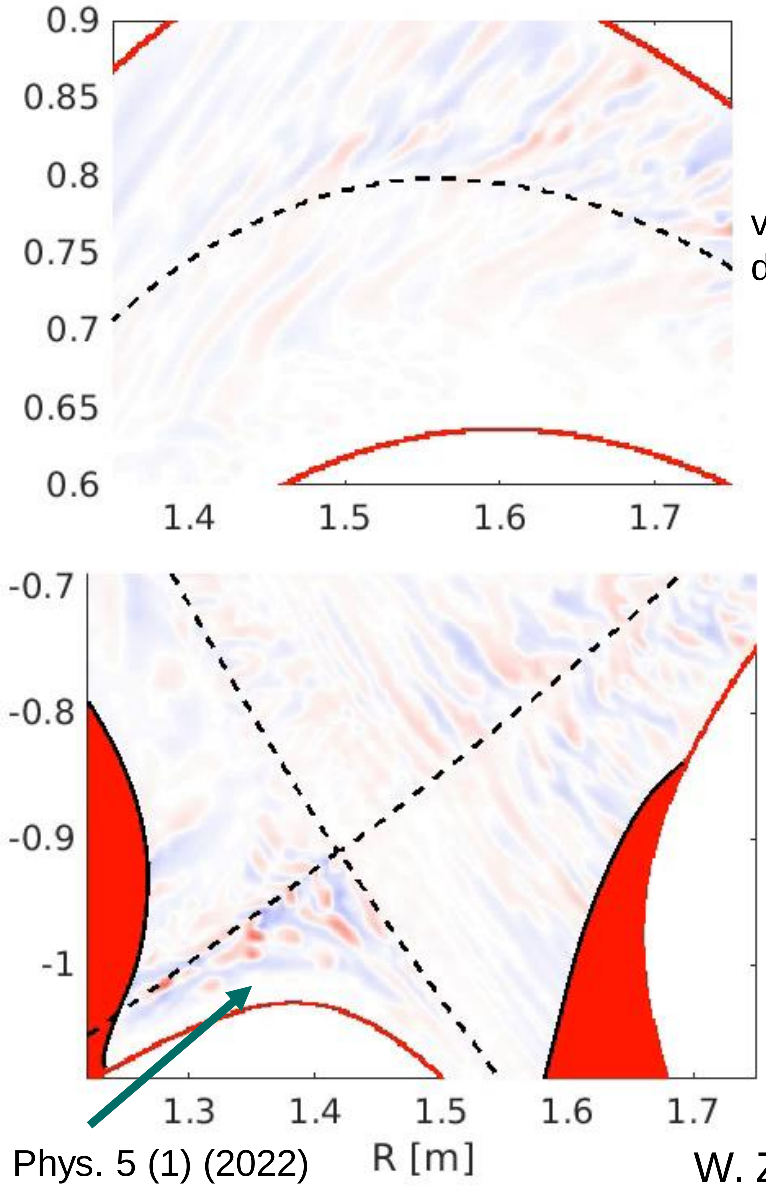
- High density plasmas also have larger λ_n
- High density (and T) at the main wall fosters its erosion!
- The broadening is attributed to blob-filaments



R. J. Maqueda *et al.* Jour. Nucl. Mat. 415 (2011) S459–S462

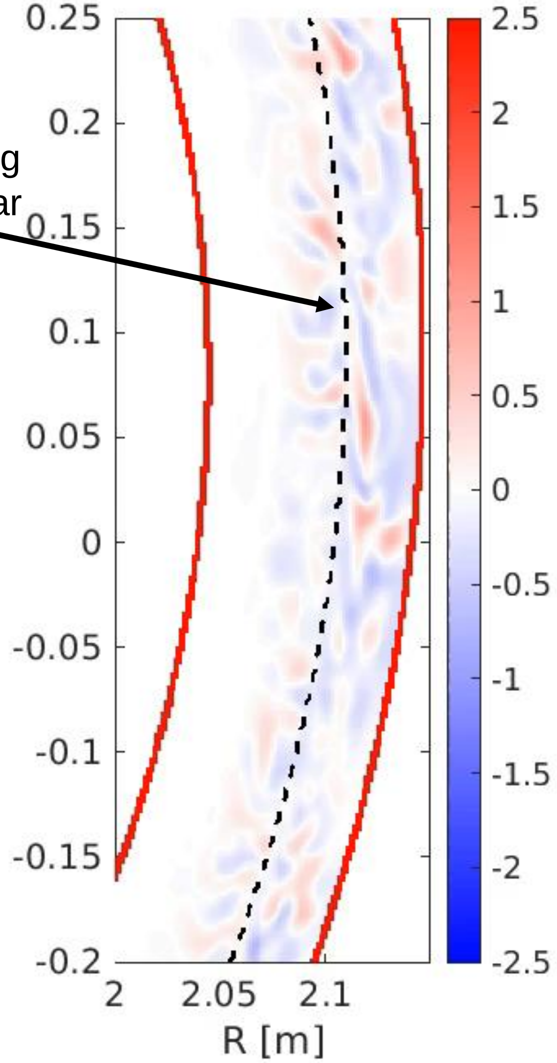
Edge-SOL turbulence: blob filaments (especially in T_i!)





N. Walkden, Commun. Phys. 5 (1) (2022)

vortex breaking due to E_r shear



W. Zholobenko *et al* NME **34** 101351 (2023)

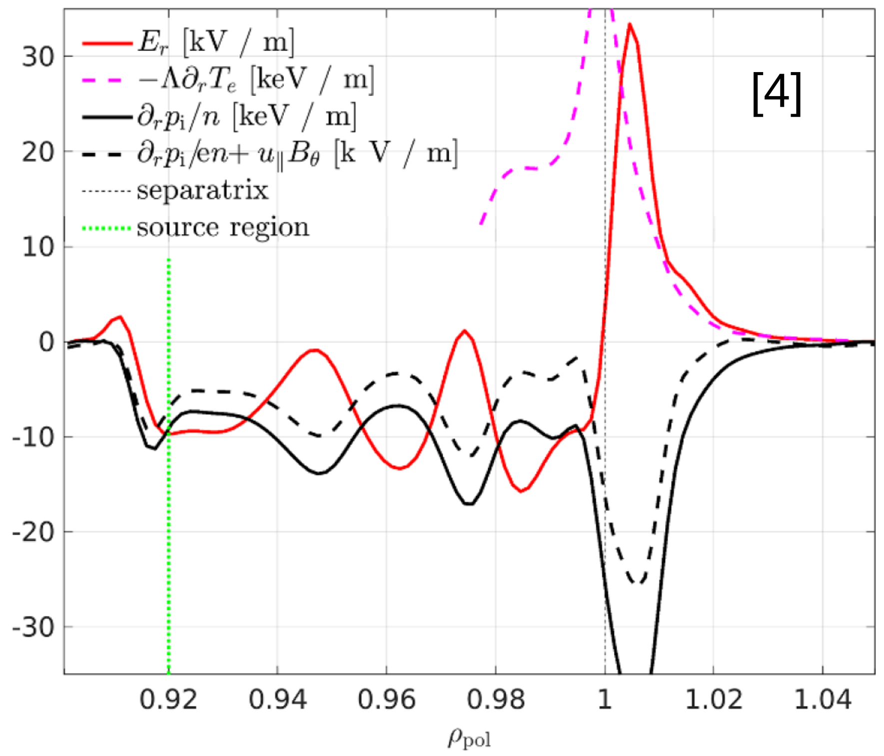
Sheared flow (incl. E_r) generation and turbulence suppression

- $\gamma_{E\times B} \approx \frac{1}{B}\partial_r E_r > \gamma_{\mathrm{turb}} \Rightarrow$ turbulence suppression (much more complex in detail!)
- Turbulence suppression by sheared ($E \times B$) flows, with relevance to the L-H transition, has been acknowledged early [1,2].
- Also in the SOL, the flow shear is important for turbulence control [3].
- Flow formation is an active research topic. It involves mean field (neoclassical) as well as turbulent (zonal) parts in the confined region [4-6]. In the SOL, parallel and sheath currents play a key role [5,7].
- Global fluid [4] as well as gyrokinetic [6] simulations predict a staircase structure.
- The mesoscale character of zonal flows, $\lambda_{\mathrm{ZF},r} \sim \sqrt{a\rho_{\mathrm{i}}}$ [8], often requires a global treatment.

$$m_{\mathrm{i}} n \left(\frac{\partial}{\partial t} + \mathbf{v}_{\mathrm{i}} \cdot \boldsymbol{\nabla} \right) \mathbf{v}_{\mathrm{i}} = -\boldsymbol{\nabla} p_{\mathrm{i}} - \boldsymbol{\nabla} \cdot \boldsymbol{\Pi}_{\mathrm{i}} + Zen(\mathbf{E} + \mathbf{v}_{\mathrm{i}} \times \mathbf{B}) - \boldsymbol{R}_{\mathrm{i}}$$

On closed flux surfaces:

$$\langle E_r \rangle \approx \frac{\partial_r \bar{p}_{\mathrm{i}}}{Ze\bar{n}} + \bar{v}_{\mathrm{tor}} B_{\mathrm{pol}} - \bar{v}_{\mathrm{pol}} B_{\mathrm{tor}} + \frac{m_{\mathrm{i}}}{Ze} \langle \mathbf{v}_{\mathrm{i}} \cdot \boldsymbol{\nabla} \mathbf{v}_{\mathrm{i}} \rangle \cdot \mathbf{e}_r$$ [4,5]



[1] H. Biglari *et al*. Phys. Plasmas 2 1-4 (1990)
[2] N. Bonanomi *et al.* Phys. Plasmas **28**, 052504 (2021)
[3] Xu Chu *et al.* Nucl. Fusion **62** 066021 (2022)
[4] W. Zholobenko *et al.* Plasma Phys. Control. Fusion **63** 034001 (2021)
[5] W. Zholobenko *et al.* NME **34** 101351 (2023)
[6] G. Dif-Pradalier *et al.* Phys. Rev. Lett. **114** 085004 (2015)
[7] D. Brida *et al.* NME **33** 101262 (2022)
[8] A. Fujisawa Nucl. Fusion **49** 013001 (2009)

Consequences of blobby transport

- SOL turbulent transport is dominated by turbulence spreading and blobs, seeded in the plasma edge [1,2,3]. **SOL turbulence is thus inseparable from the edge.**

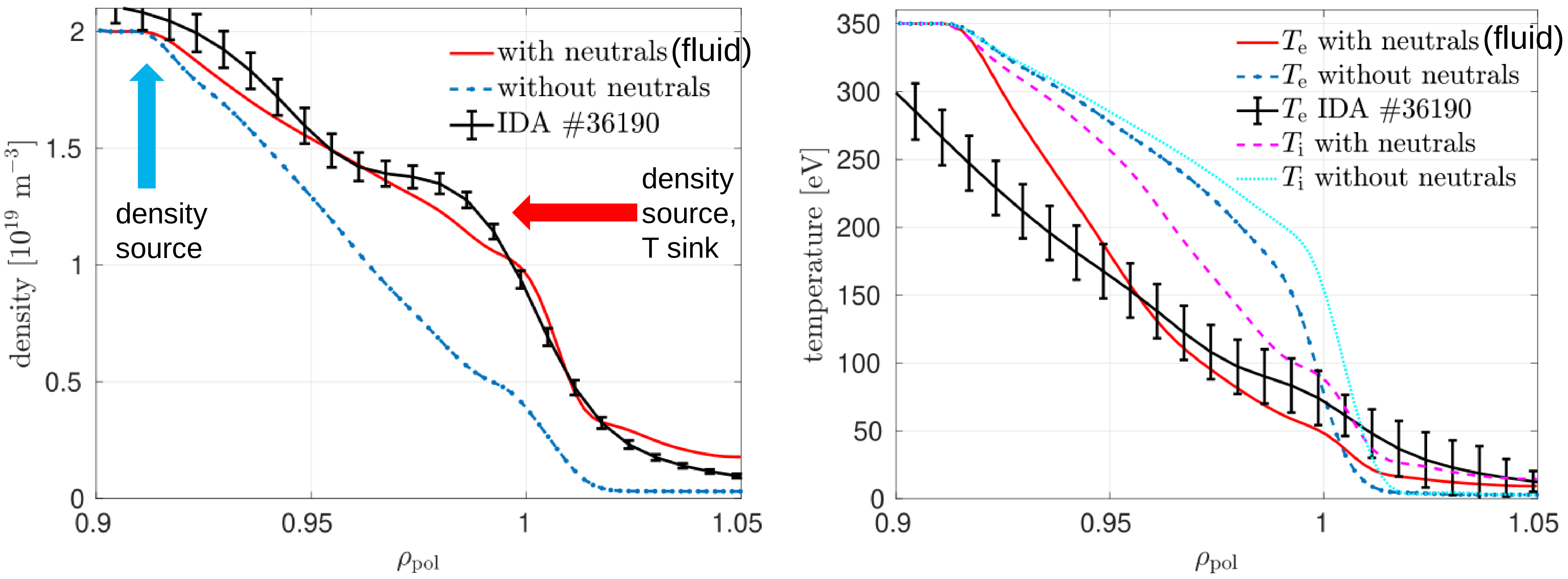
- SOL fluctuation amplitudes are $\gtrsim$100% [1-4]. There are poloidal background gradients and **strong flows**. The geometry varies strongly. Therefore, **local studies are inapplicable.**

- Divertor conditions influence not just the SOL, but also the pedestal, particularly in detached conditions [1,3,5,6].

[1] *"On the Path to Burning Plasma Operation",* ITPA (Div-SOL) special issue in Nucl. Fusion, in preparation (2023)
[2] D. A. D'Ippolito *et al.* Phys. Plasmas **18** 060501 (2011)
[3] W. Zholobenko *et al.* NME **34** 101351 (2023)
[4] S. J. Zweben *et al.* Plasma Phys. Control. Fusion **49** (7) (2007)
[5] M. G. Dunne *et al.* Plasma Phys. Control. Fusion **59** 014017(2017)
[6] M. Bernert *et al.* Nucl. Fusion **61** 024001 (2021)

The role of neutral gas in global edge-SOL turbulence simulation

Outboard mid-plane profiles in AUG #36190 attached L-mode and in GRILLIX



W. Zholobenko *et al* 2021 *Nucl. Fusion* **61** 116015

- **Neutral gas increases SOL plasma density and reduces $T_{e,i}$, thereby increasing the collisionality.**
- **Much stronger impact can be expected at high neutrals density in detached conditions!**
  (See e.g. Yanzeng Zhang, Sergei I. Krasheninnikov et al 2020 Nucl. Fusion 60 106023)

Requirements for edge-SOL turbulence simulation

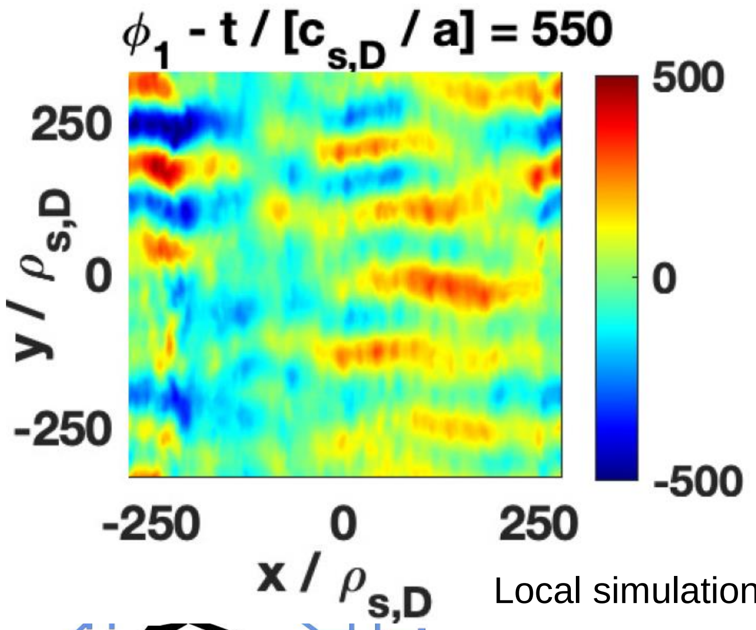
1. The model must be "full-*f*", evolving turbulence and background simultaneously.
2. The simulations must include the pedestal dynamics.
3. Density, $T_{\mathbf{e,i}}$ and ν_e^* vary by 3 orders of magnitude between pedestal top and divertor. The geometry varies strongly. SOL turbulence is non-local. The "full-*f*" model thus must be <u>global</u>.
4. The plasma background must be maintained by sources. A major source is neutral gas recycling.
5. A global model will automatically include both neoclassical and zonal flows.
6. The divertor is strongly beneficial for impurity handing, confinement and exhaust. Therefore, simulations must be performed in diverted geometry. Doing this efficiently is not trivial due to problems with field alignment!
7. A reactor will have to operate in high confinement, detached conditions, ideally without ELMs.

⇒The above challenges lead many groups to take different design decisions for their codes!

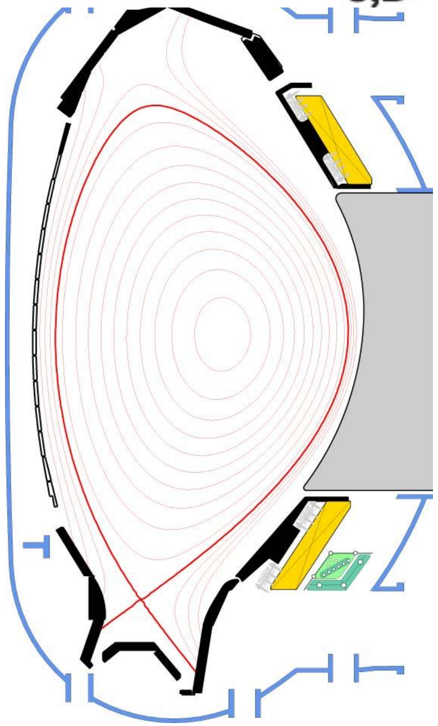
Computational challenges of global simulations

- Local flux-tube simulations have the same domain for any machine, from TCV to DEMO: 50ρ_i x 50ρ_i x 32$N_z \approx 10^5$ points.
- Parameters like T_0 are fixed, therefore less nonlinearity and fixed v-space resolution, e.g. 32 x 16 = 512
- Global simulations need to resolve a (poloidal) domain on the **machine scale** ***R***. For TCV, that is >10^6 points, and for ITER $> 10^9$, if field aligned!
- X-point flux expansion adds a ton of volume, and complicates field-alignment
- $T_\mathrm{e,i}$ changes by 3-4 orders of magnitude between pedestal top and divertor. This is extremely tough for properly resolving the velocity space!
- Not only edge-SOL simulations must be global, e.g. also core fast ion modes and strong zonal flows. But still less variation, and δf is a huge help!

⇒ **These problems require extreme high-performance computing!**

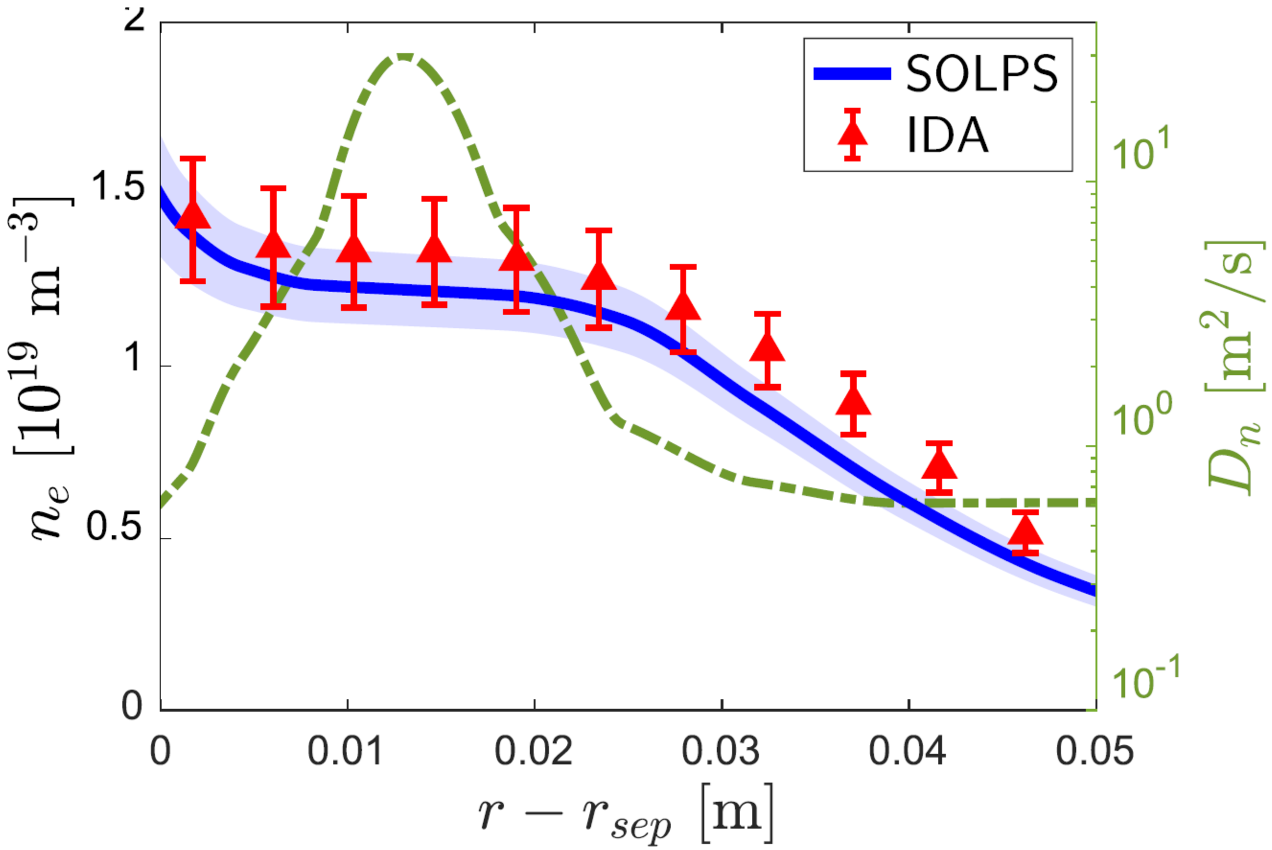


Local simulation with fast ions, $\rho_\mathrm{fast} \approx 10\rho_\mathrm{D} \Rightarrow$ must go global! A. Di Siena arXiv:2306.10780 (2023)



Current work horse: mean-field transport codes

- SOL turbulence simulations are challenging
- Divertor design so far is done with mean-field transport codes like SOLPS, SOLEDGE3X, UEDGE, EMC3, etc..
- A “transport code” assumes a certain level of radial transport, expressed by anomalous diffusivities.
- In the SOL, parallel transport plays a key role (2D problem), as well as neutral gas, impurities and walls
- In these matters, transport codes are very advanced. They are very useful in identifying actuators for experimentalists, such as neutral gas puffing and impurity seeding rates, the impact of divertor geometry on neutral gas transport, role of wall materials, etc.
- A key uncertainty remains, the turbulent transport, particularly in high density regimes.

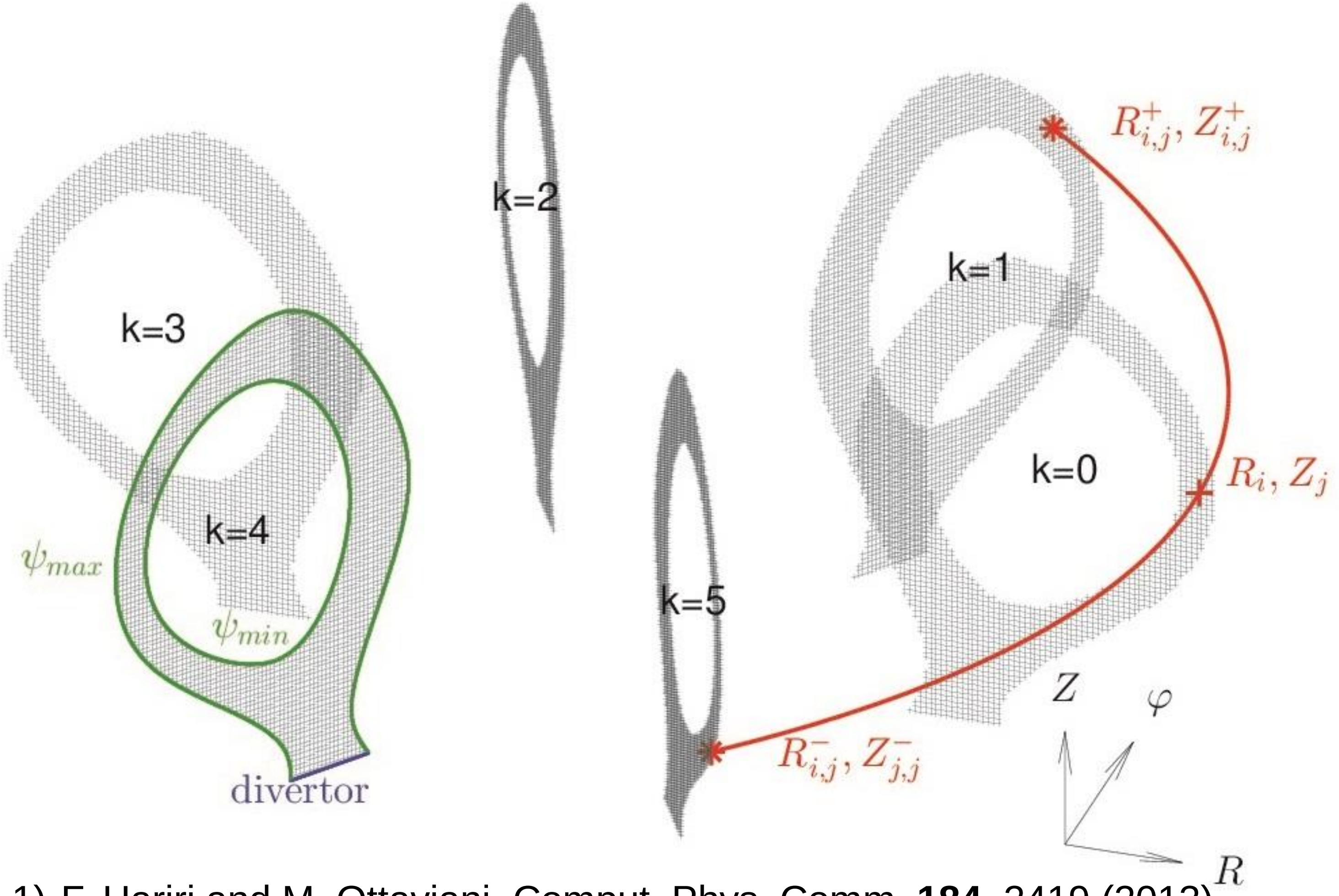


A Zito *et al* 2021 Plasma Phys. Control. Fusion 63 075003

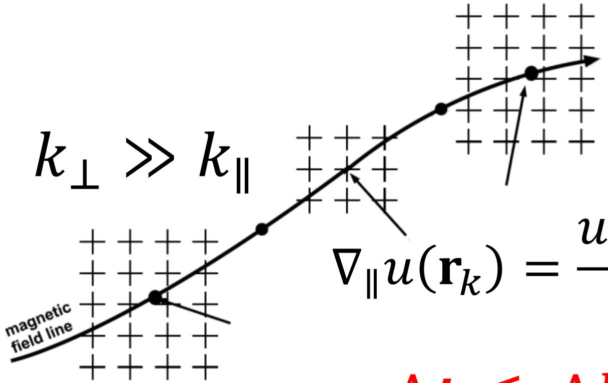
Parallelised progress in global edge-SOL turbulence simulations (divide & conquer): examples of achievements by different groups

GRILLIX (MP IPP, Germany)

Flux-coordinate independent (FCI), locally field-aligned approach allows efficient turbulence simulations in arbitrary geometry.

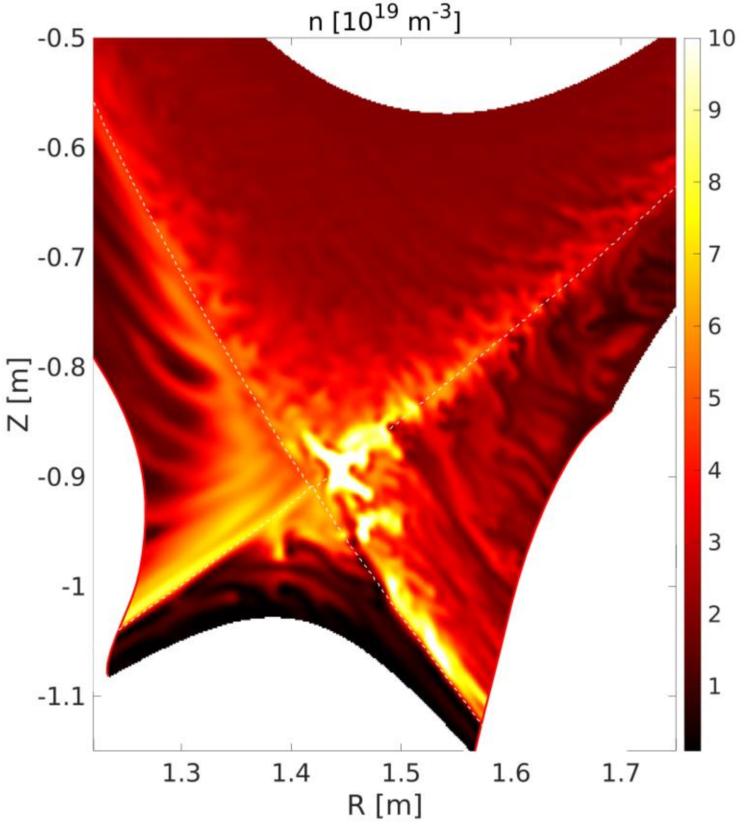


$$k_\perp \gg k_\parallel$$



$$\nabla_\parallel u(\mathbf{r}_k) = \frac{u(\mathbf{r}_{k+1}) - u(\mathbf{r}_{k-1})}{2\Delta l}$$

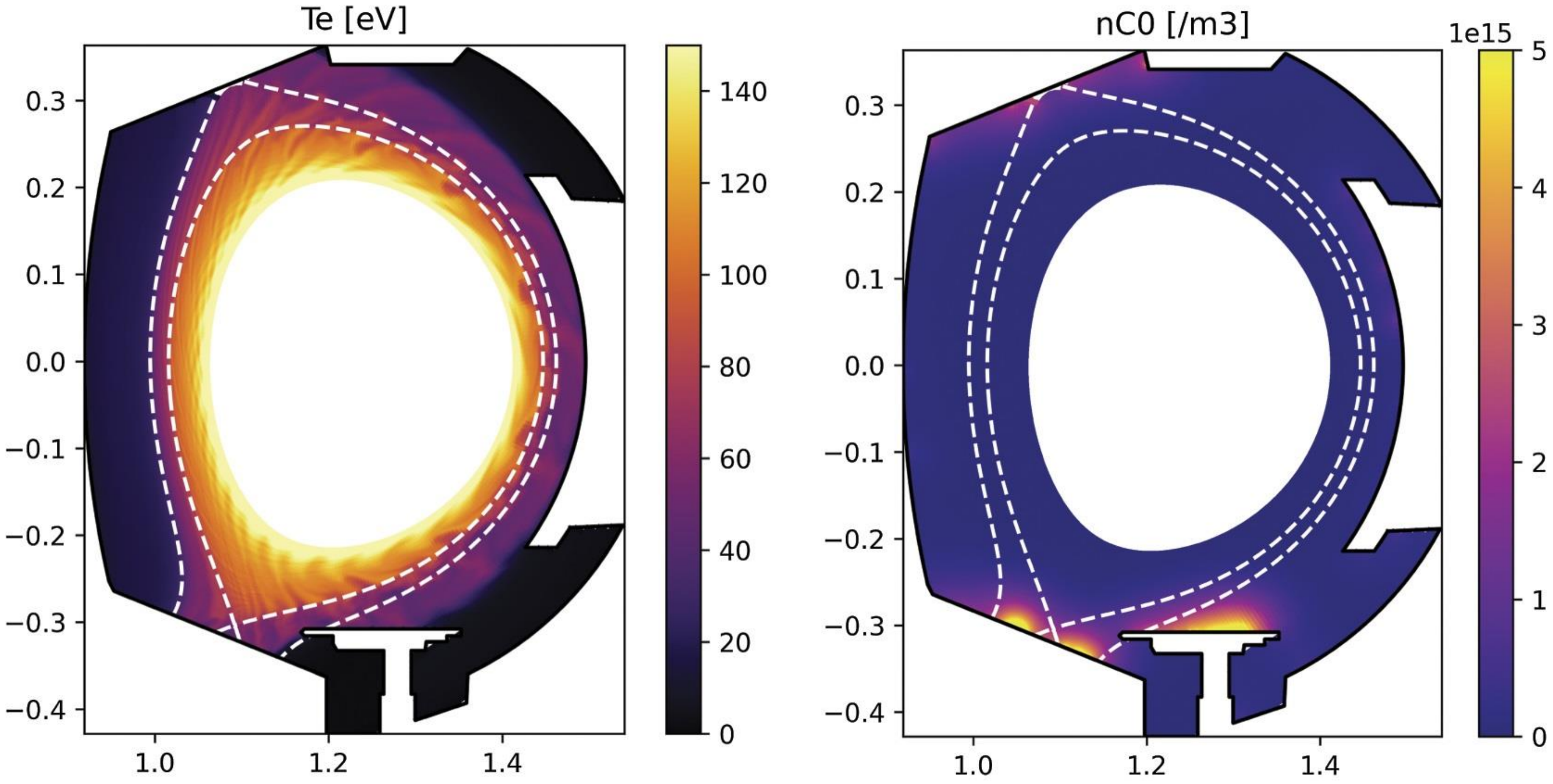
$$\boldsymbol{\Delta t \lesssim \Delta l / v_A}$$



1) F. Hariri and M. Ottaviani, Comput. Phys. Comm. **184**, 2419 (2013)
2) A. Stegmeir *et al*., Comput. Phys. Comm. **198**, 139 (2016)
3) A. Stegmeir *et al*., Phys. Plasmas **26**, 052517 (2019)

SOLEDGE3X (former TOKAM3X, CEA, France)

- Transport, turbulence and intermediate models in one code: simulate both turbulence (ms) and confinement (s) time scales
- Multi-species (Zhdanov) fluid model: can simulate D+T+He plasma with impurities like C and W
- Coupled to kinetic neutrals code EIRENE (although tough to run turbulence simulations with)



3D turbulence simulation of WEST including recycling and carbon sputtering. Left: electron temperature. Right: carbon neutral density.

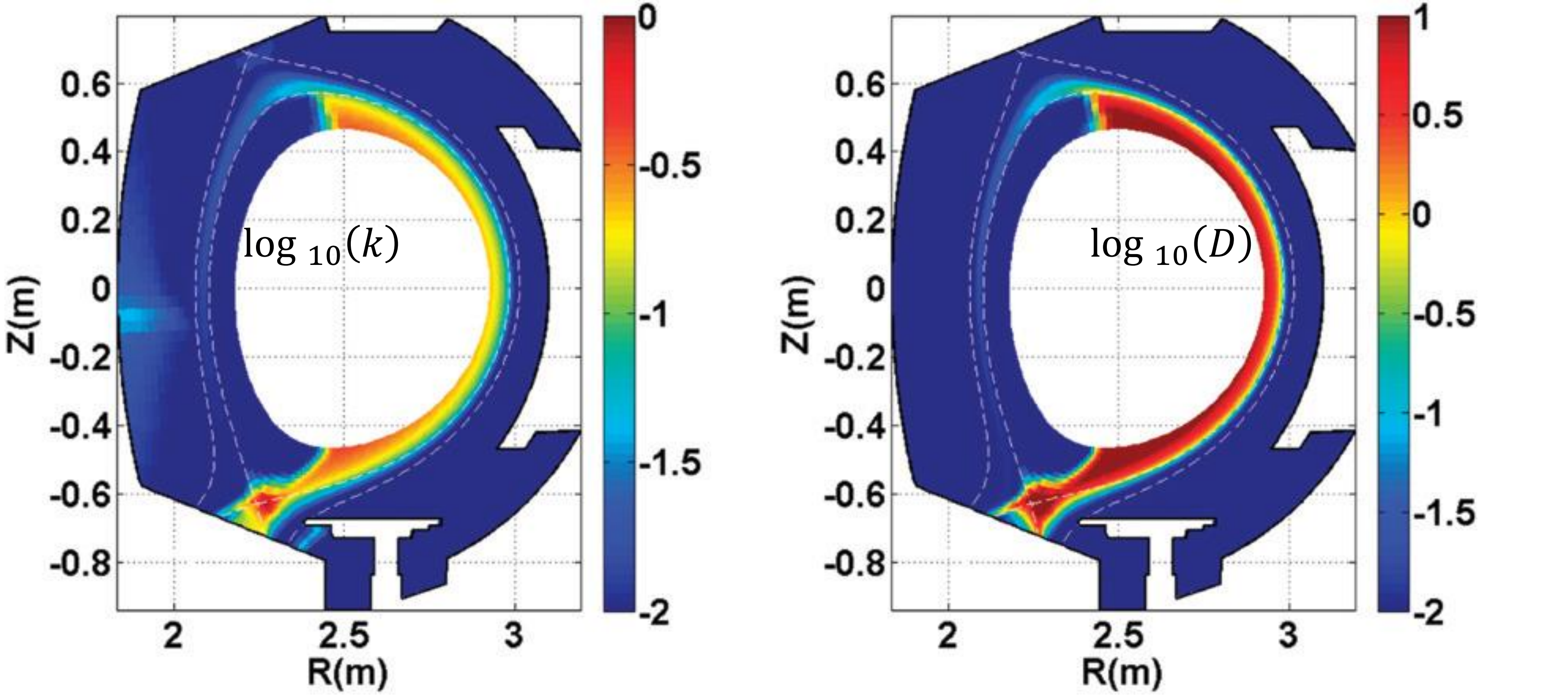
H. Bufferand *et al* 2021 Nucl. Fusion **61** 116052

Mean field codes (e.g. SOLPS) and reduced SOL turbulence models

- Meanwhile, transport codes like SOLPS remain the work horse for divertor design
- Global turbulence simulations can cover only a limited number of cases, not enough for machine optimization
- An intermediate approach might prove useful: mean-field turbulence models can be constructed, with closures approximated against direct turbulence simulations, similar to quasi-linear core turbulence models

$$\partial_t k + \nabla \cdot (k\mathbf{v}) = \gamma k - \alpha k^2 + \nabla \cdot \left(\frac{R}{c_s} k \nabla k \right)$$

S. Baschetti *et al.* Nucl. Fusion **61** 106020 (2021)
W. Dekeyser *et al.* Contrib. Plasma Phys. 2022, 62(5-6), e202100190

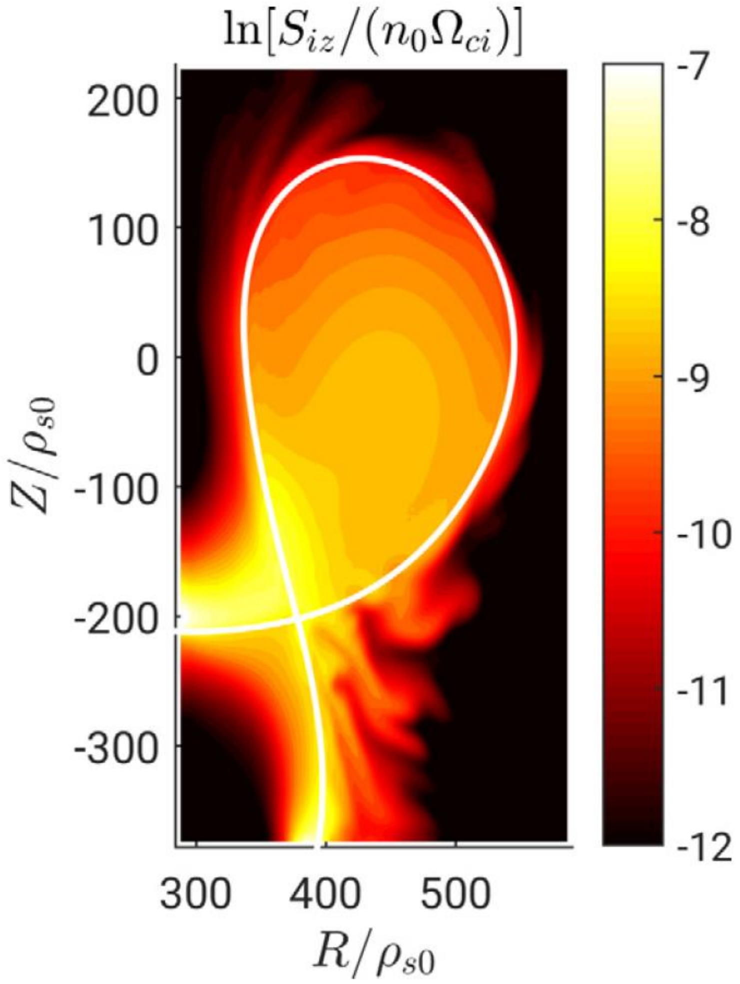


GBS (EPFL, Switzerland)

- Turbulence simulations in advanced divertors, negative triangularity, with RMPs and in stellarators
- Continuous kinetic neutral gas model: no Monte-Carlo noise
- Currently Braginskii-based, but **gyro-moment** approach is being developed
- Numerical simulations together with analytical theory, e.g.

$$n_{\mathrm{lim}} \sim A^{1/6} P_{\mathrm{SOL}}^{10/21} R_0^{1/42} B_T^{-8/21} (1+\kappa^2)^{-1/3} \frac{I_p^{22/21}}{a^{79/42}}$$

is derived in [1], an extension of the Greenwald density limit that gives a x2 higher density limit for ITER.

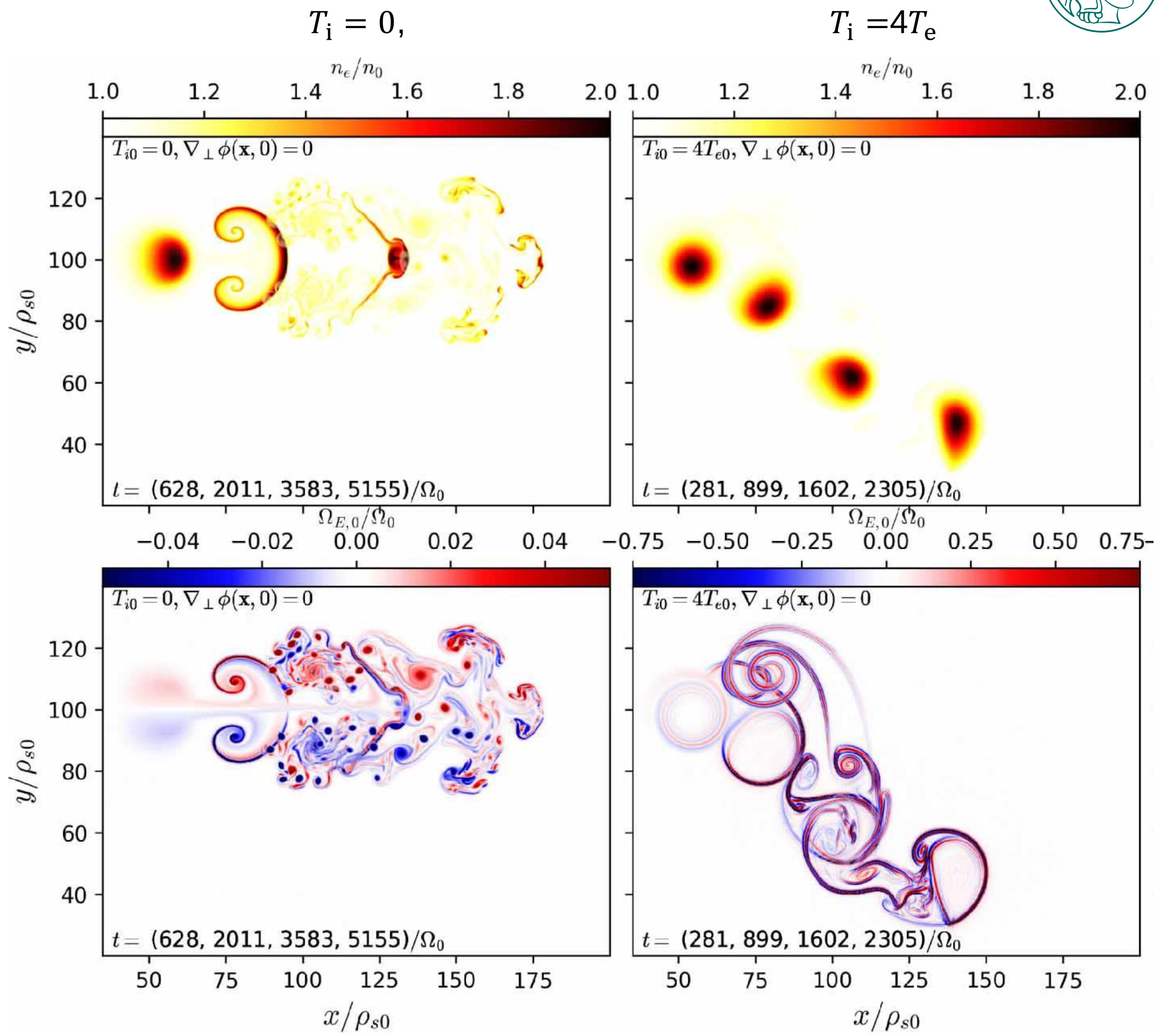


Snapshot of the ionization source in a half size TCV simulation with GBS [2]

[1] M. Giacomin, PRL 128, 185003 (2022)
[2] M. Giacomin, JCP 463 (2022) 111294

FELTOR

- Based on FCI like GRILLIX, but additionally uses Discontinuous Galerkin discretization [1]
- Gyrofluid with **arbitrary wavelength polarisation**. The only edge-SOL code avoiding the long-wavelength limit ($k_\perp \rho_\mathrm{i} < 1$).
- Modern C++ implementation, also on GPUs, **open source at https://feltor-dev.github.io/**
- Due to the complexity, so far mostly blob studies
- Incorporates HESEL with **multi-group neutrals** [2]

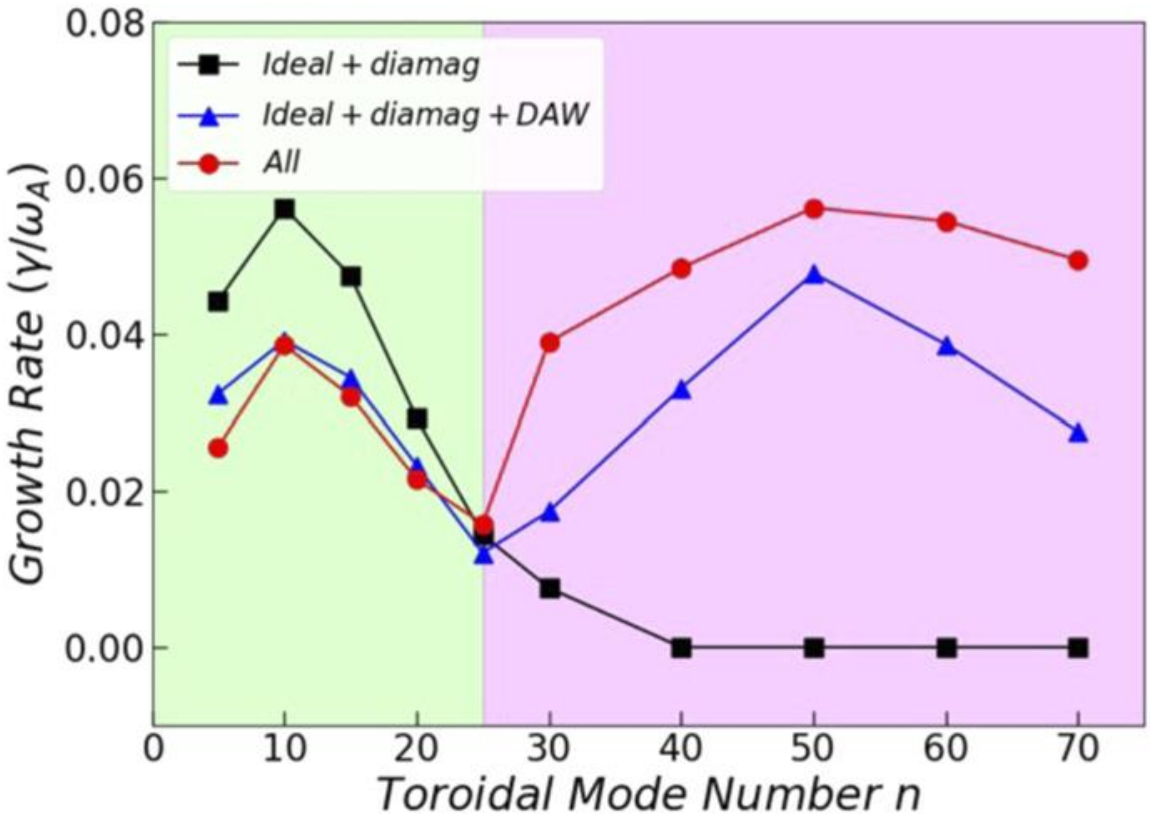


Evolution of density and vorticity for 3 different blobs.
M. Held and M. Wiesenberger 2023 Nucl. Fusion 63 026008

[1] M. Wiesen-berger & M. Held 2023, CPC 291, 108838
[2] A.S. Thrysøe et al 2018 Nucl. Fusion 58 096005

BOUT++ (University of York, UK & LLNL, USA)

- Open source, modular C++ code (https://boutproject.github.io/)
- Mainly developed in UK and US, but broadly used around the world (heavily in e.g. China and Japan)
- Active development of numerical and computational methods, and advanced models, e.g. non-Fourier Landau fluid closure [1]
- Framework with many models: 2D and 3D **transport**, local and global **turbulence** models, non-linear MHD (**ELMs**), etc.



Linear growth rates in a QH-mode pedestal [2]. Ideal MHD + diamagnetic drift yield **peeling modes** driven by the bootstrap current, while adding drift-Alfven wave dynamics destabilises higher n modes.

[1] Ben Zhu *et al.* CPC 267 (2021) 108079
[2] Zeyu Li *et al.* 2022 Nucl. Fusion 62 076033

JOREK: non-linear MHD and GK turbulence in one place

- Edge-SOL transport is intertwined with MHD
- JOREK is a state-of-the-art MHD code for e.g. ELMs & disruptions [2]
- Kinetic neutral gas and impurity models have been implemented [2].
- Recently extended by fluid and gyrokinetic turbulence models (ITG and TEM) [1].
- This allows to combine turbulence and MHD simulations in X-point geometry, including RMPs.

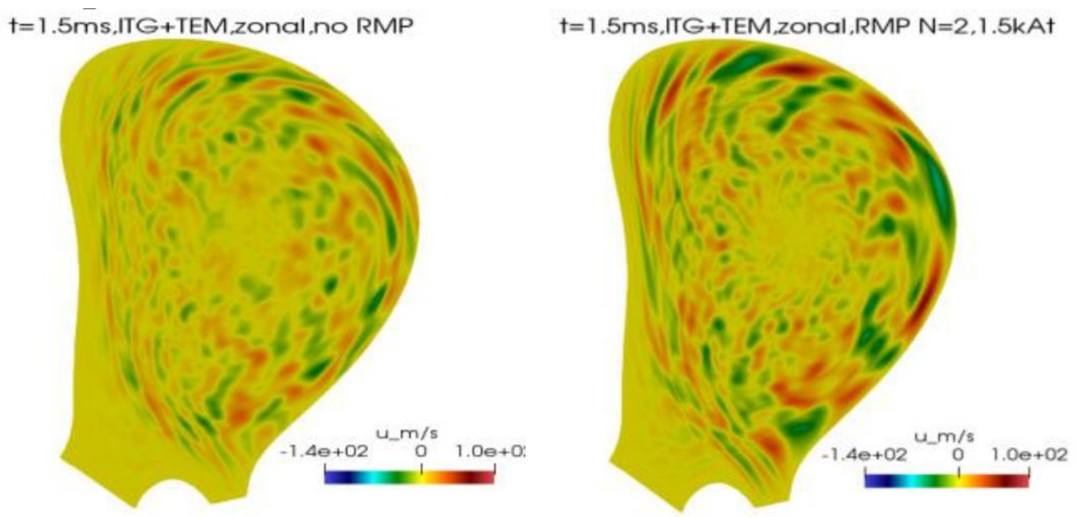
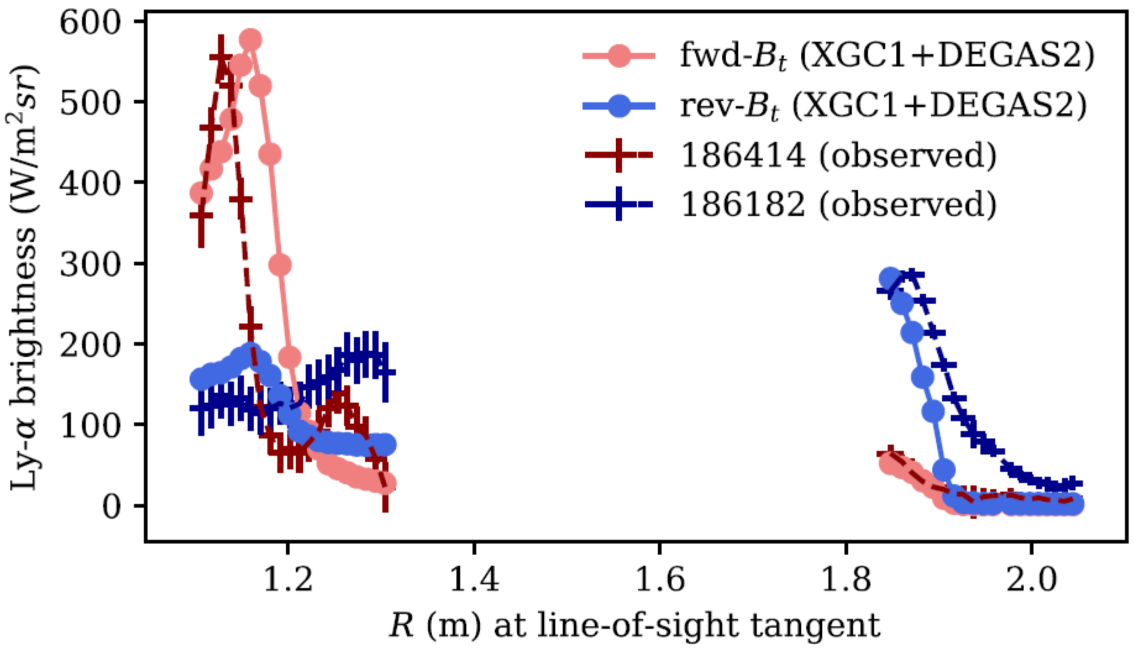


Fig.1.Electrostatic potential perturbations in L-mode discharge (COMPASS#8078) without (left) and with(right) RMP N=2, 1.5kAt. Toroidal harmonics taken into account in modelling of gyro-kinetic ITGs+TEMs: N=2:2:16.

[1] M.Bécoulet *et al.* IAEA FEC 2023
[2] M. Hoelzl *et al.* Nucl. Fusion **61** 065001 (2021)

XGC (PPPL, USA)

- Full-*f*, global, electromagnetic, PIC gyrokinetic model
- Advanced collision operators
- Extremely parallelized
- Coupled to DEGAS2 for Monte-Carlo neutrals



The Lyman-alpha brightness predicted by XGC1+DEGAS2, G. J. Wilkie *et al.* IAEA FEC 2023

GENE-X (MP IPP, Germany)

Fluid turbulence models + (fluid) neutral gas

Numerical tools for FCI (Modern 2008 Fortran)

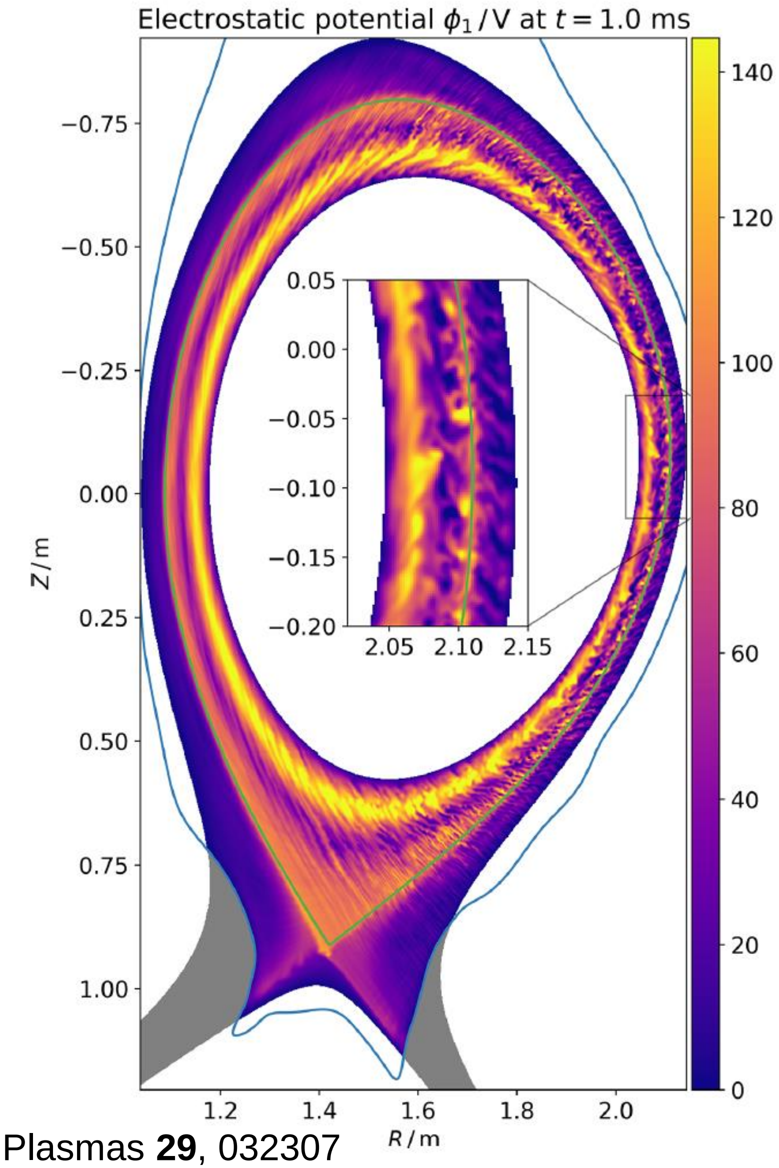
Multi-fidelity framework:

- Fluid model at high ν_e^* (divertor)
- Gyrokinetics at low ν_e^* (pedestal)
- Extend both towards arbitrary ν_e^*!

GENE-X validated against attached L-mode ASDEX [1] and TCV-X21 [2]

Continuum, full-f, electromagnetic, collisional gyrokinetic model

Velocity space discretization

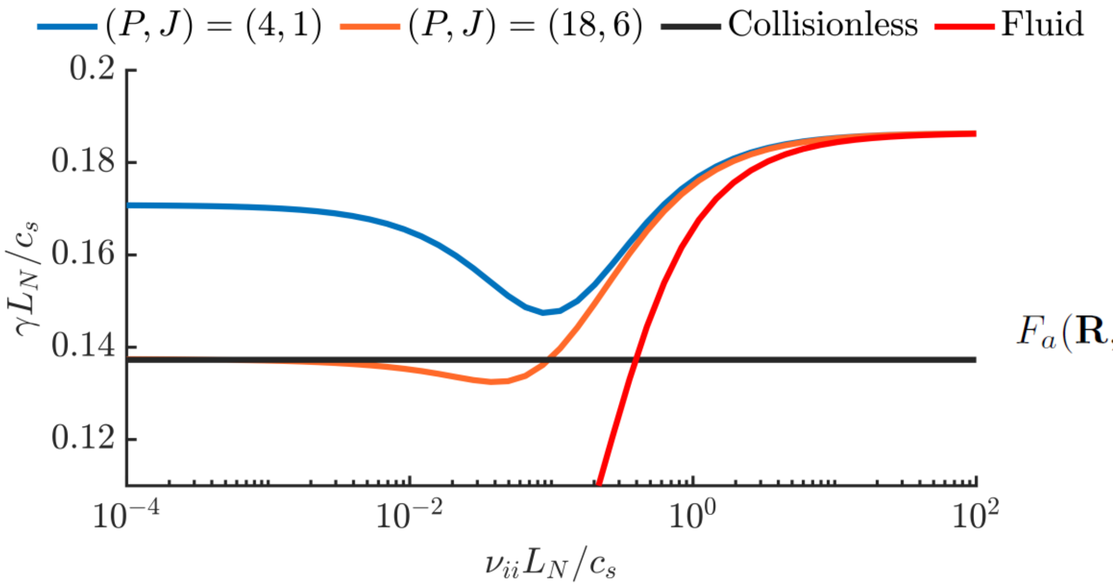


[1] Dominik Michels *et al*. 2022, Phys. Plasmas **29**, 032307
[2] Philipp Ulbl *et al*. 2023, Phys. Plasmas **30**, 052507

Fluid, gyro-fluid, gyro-kinetic – gyro-moment

For decades, people have tried to close the gap between drift-fluid and gyrokinetic models with gyrofluid models. However, these still suffer from problems with the fluid closure, and difficulties with incorporating trapped particles properly.

A possible solution is the “gyro-kinetic moments approach”. It extends the gyro-fluid method to a larger number of fluid moments. Thereby, the expansion is simply truncated at the last moment, without closure. In the limit of many moments (e.g. 100+, compared to typically 4 in gyrofluid models), the method reproduces gyrokinetics exactly.



B. J. Frei. *et al.* J. Plasma Phys. **88** 905880304 (2022): ITG growth rate with gyro-moment method with (4,1) and (18,6) moments, collisionless gyro-kinetic solution, and collisional fluid solution (Braginskii)

$$F_a(\mathbf{R},\mu,v_\parallel,t)=\sum_{p=0}^{\infty}\sum_{j=0}^{\infty}N_a^{pj}(\mathbf{R},t)\frac{H_p(v_\parallel)L_j(\mu)}{\sqrt{2^p p!}}F_{Ma}$$

$$N_a^{00}=N_a$$

$$N_a^{10}=U_{\parallel a}$$

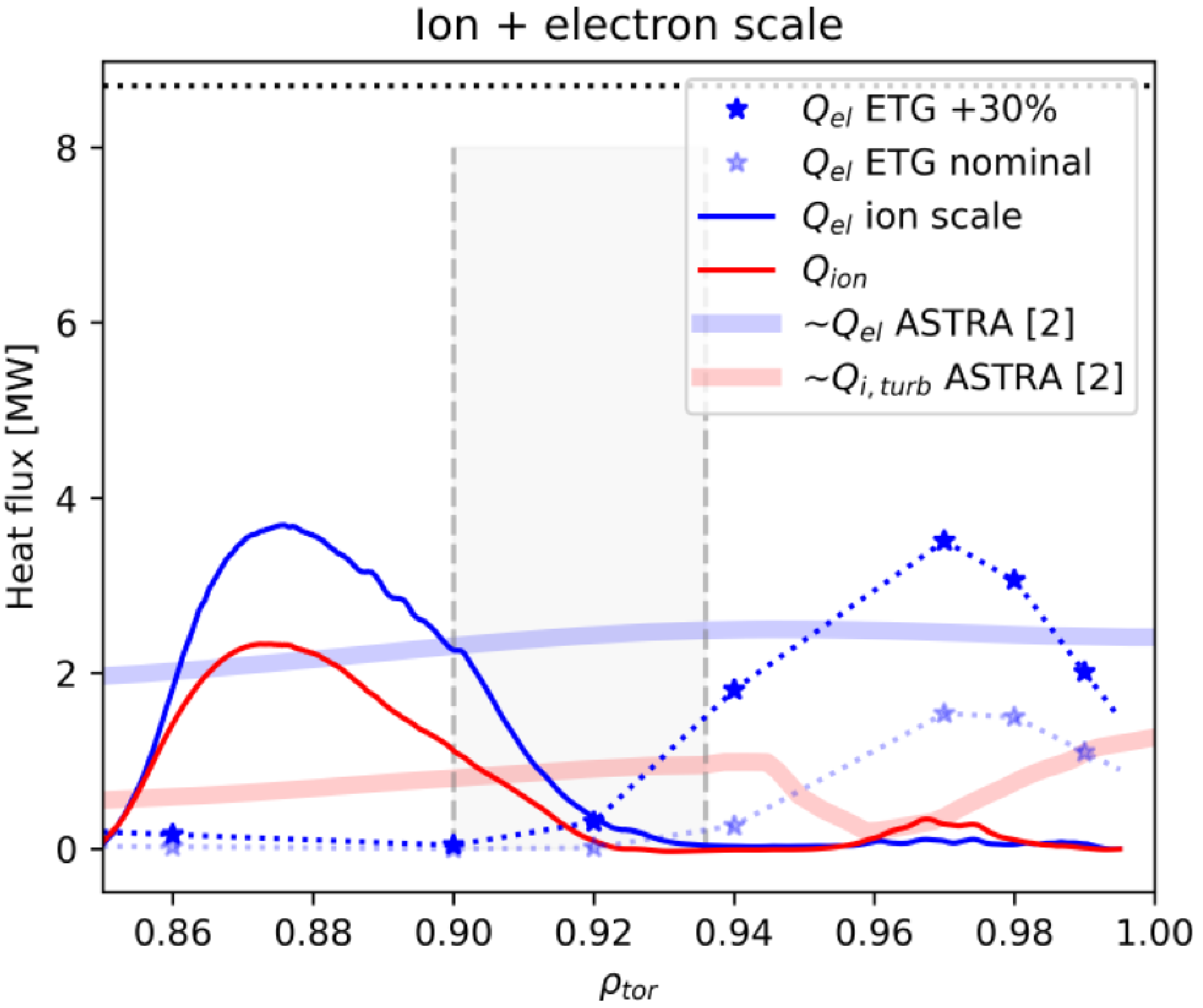
$$\frac{\partial}{\partial t}N_a^{pj}+\nabla\cdot\|\dot{\boldsymbol{R}}\|^{pj}-\frac{\sqrt{2l}}{v_{th\parallel a}}\|\dot{v}_\parallel\|^{p-1j}+\ldots=\boxed{\sum_b C_{ab}^{pj}}$$

It remains to be seen whether in practice, a good enough representation of the gyro-kinetic solution (at both high and low collisionality) can be obtained with a low enough number of moments to retain a computational advantage.

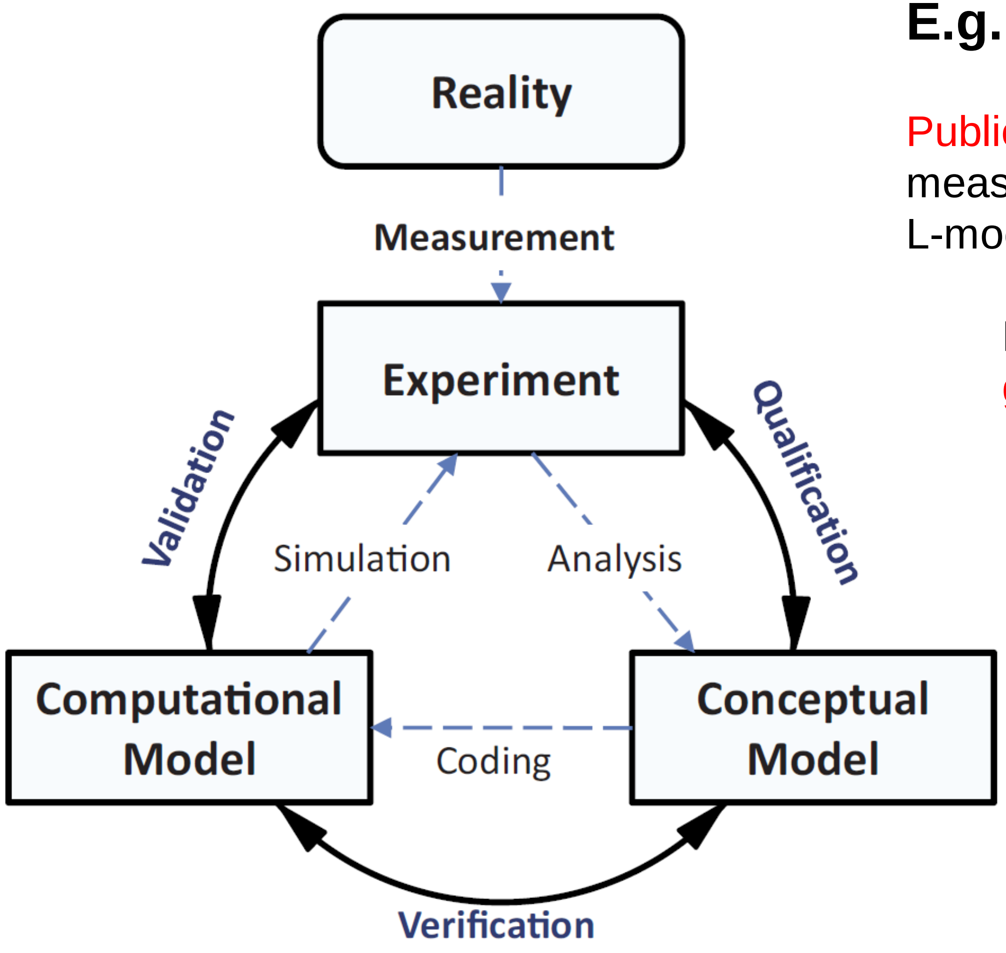
Multi-scale turbulence problem in global simulations: δf insights

L.A. Leppin *et al.* arXiv:2303.10596v1 (2023), Local and global simulations of pedestal turbulence in ASDEX Upgrade:

- At the pedestal foot, ETG turbulence drives up to 100% of the transport!
- Including ETG turbulence in global simulations is impossible: resolution has to increase by $(\rho_i/\rho_e)^2 = (m_i/m_e) \approx 4000$.
- Local simulations thus remain important.
- It might be possible and necessary to include ETG transport in global turbulence simulations.
- In the SOL, we do not know, but we can hope that ion scale turbulence prevails.



Extensive code validation efforts are required



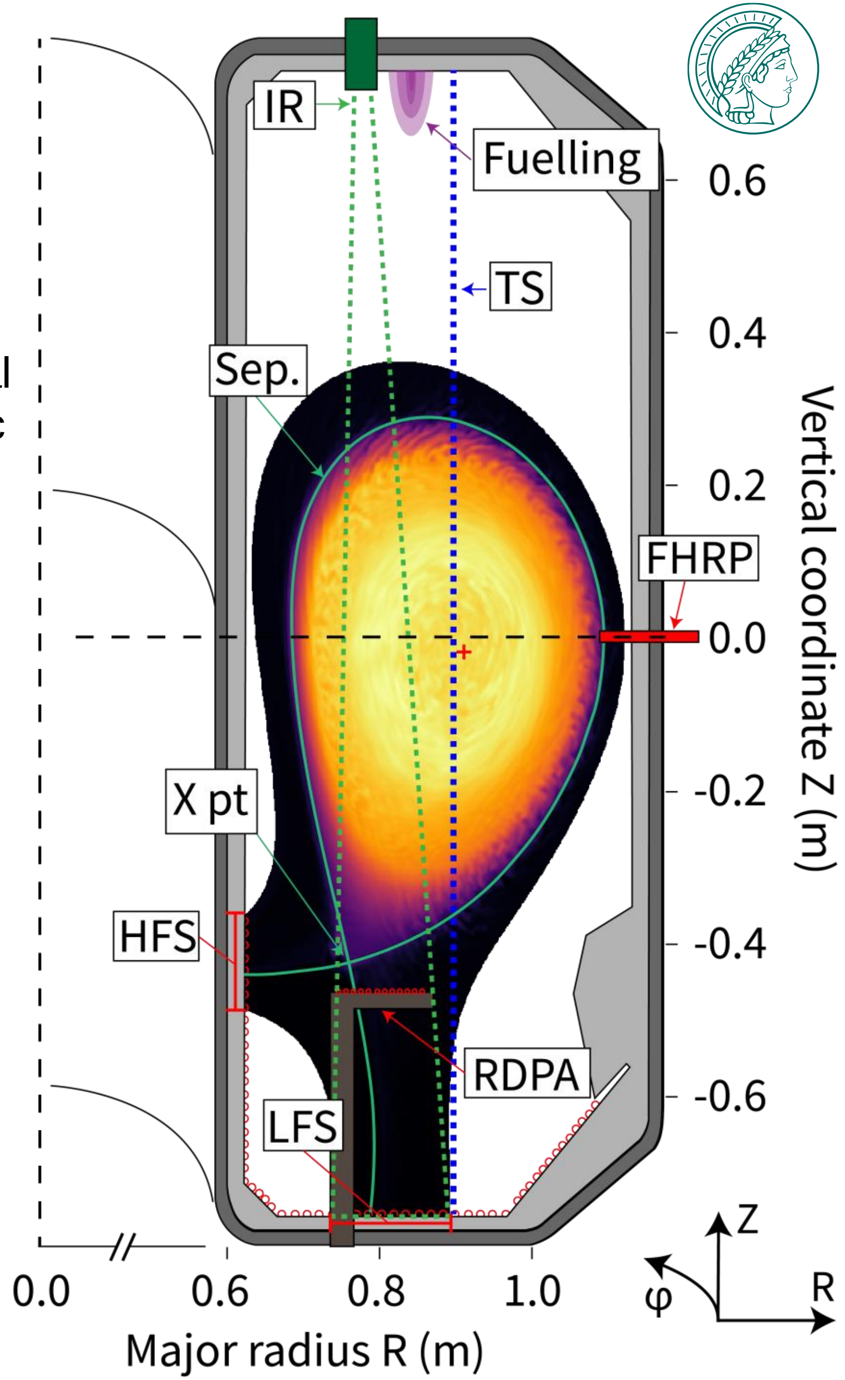
M. Greenwald, Phys. Plasmas 17, 058101 (2010)

E.g. TCV-X21

Publicly available dataset of experimental measurements from TCV diverted Ohmic L-mode discharges at reduced $\boldsymbol{B_{tor}}$

Download link:
github.com/SPCData/TCV-X21

So far, comparison between GBS, GRILLIX, TOKAM3X and GENE-X (10.5281/zenodo.7894731)



Conclusions

- Progress in edge-SOL turbulence modelling is made on various fronts, by different groups:
  - ✓ high-recycling in AUG L-mode done in GRILLIX [1], first detachment simulations with GBS (next talk) [2],
  - ✓ H-mode simulations by XGC [3] and BOUT++ [4],
  - ✓ ELMs well understood, e.g. with BOUT++ [4] and JOREK [5],
  - ✓ Advanced divertor configurations are being explored [6], …
- Now we have to **put everything together**, at reactor scale, without ELMs, and develop a deeper understanding
- Predictive capability requires extreme computational resources and complex codes
- Note: understanding of SOL turbulence in stellarators is in its infancy…
- **We all have 1 common goal: fusion energy.** Convergence of the approaches, results, and communication between people is critical – use the opportunity at this conference!
- Progress will be facilitated by coordinated validation efforts, multi-code comparisons and open science.

[1] W. Zholobenko *et al. Nucl. Fusion* **61** 116015 (2021)
[2] Davide Mancini *et al.* arXiv:2304.09687 (2023)
[3] C. S. Chang *et al.* Phys. Rev. Lett. **118**, 175001 (2017)
[4] Z. Li *et al.* 2022 Nucl. Fusion 62 076033
[4] M. Hoelzl *et al.* Nucl. Fusion **61** 065001 (2021)
[5] M. Giacomin *et al.* Nucl. Fusion **60** 024001 (2020)

Thank you for your attention!