EUROfusion

TSVV3 – Edge fluid modelling tools towards self-consistent reactor-relevant simulations

P. Tamain
for the TSVV3 team

EUROfusion Science Meeting on
Status of TSVV projects | 11/09/2023

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Acknowledgements

H. BUFFERAND, V. QUADRI, N. RIVALS, P. TAMAIN
CEA, IRFM, Saint-Paul-lez-Durance, France

G. BRETHES, M. CAPASSO, J. FAUSTY, G. GIORGIANI, A. MEDVEDEVA, M. SCOTTO
Aix-Marseille Univ, CNRS, Centrale Marseille, M2P2, Marseille, France

S. CARLI, R. COOSEMANS, W. DEKEYSER, O. RENDERS, S. VAN DEN KERKHOF
KU Leuven, Department of Mechanical Engineering, Leuven, Belgium

A.J. COELHO, A. COROADO, D. MANCINI, P. RICCI, L. STENGER
Ecole Polytechnique Fédérale de Lausanne (EPFL), Swiss Plasma Center (SPC), Lausanne, Switzerland

K. EDER, A. STEGMEIR, W. ZHOLOBENKO
Max-Planck-Institut für Plasmaphysik, Garching, Germany

Y. MARANDET, M. RAGHUNATHAN
Aix-Marseille Univ, CNRS, PIIM, Marseille, France

A.H. NIELSEN, A.S. POULSEN, M. WIESENBERGER
Technical University of Denmark (DTU), Department of Physics, Lyngby, Denmark

D. TSKHAKAYA
Institute of Plasma Physics of the CAS, Prague, Czech Republic

J. PARKER
UKAEA, Abingdon, United Kingdom

ACH EPFL: E. Bourne, G. Fourestey, M. Peybernes, N. Varini
ACH Poznan: D. Yadikin

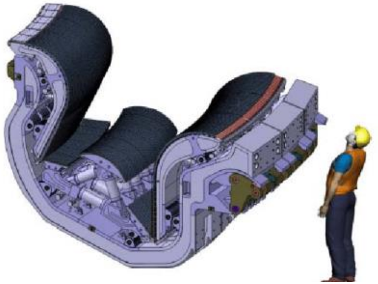
Current contributors
Contributors not funded by project
Contributors who left the project

Pushing European edge modelling tools to the next level

- TSVV3 letter of mission as part of WPAC / E-TASC:

  *"Design of **next generation European Edge and Boundary Codes for reactor relevant devices** with **various magnetic configurations** (including coupling to **turbulence** codes and pedestal-SOL interface)"*

- ITER and DEMO push the **power exhaust challenge** further
  - Access to **new physics regimes**
  - Small operational space **margins** => **reliability** of predictions critical



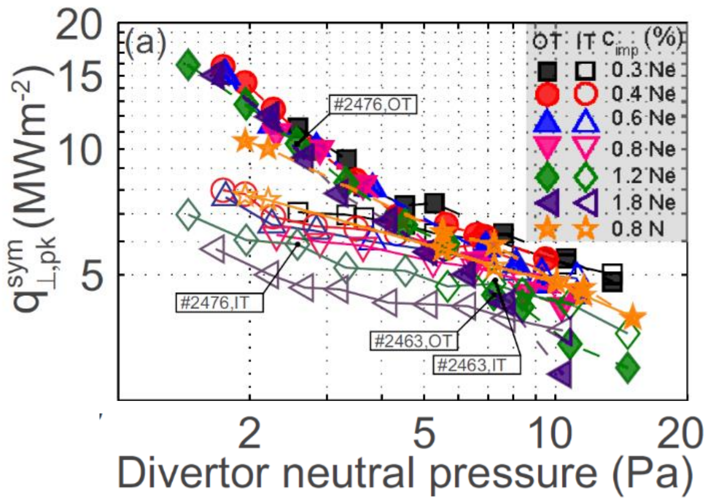
		AUG	JET	ITER (Q=10)	DEMO
	R_{geo} (m)	1.65	2.9	6.2	**8.8**
	B_T (T)	2.5	2.6	5.3	**5.8**
	I_P (MA)	1.2	2.5	15	**20.3**
	n_{GW} (10^{20}m^{-3})	1.4	1.0	1.2	**0.8**
	P_{heat} (MW)	26	25	150	**300**
	$f_{rad,core}$	0.25	0.4	0.33	**0.5**
	P_{sep} (MW)	20	16	100	**150**
	$P_{sep}/P_{L\text{-}H}$	4.5	1.8	1.4	**1.1**
	P_{sep}/R (MW/m)	12	5.2	17	**17**
$q_{\|\|} \propto$	**$P_{sep}B_0/R$ (MW·T/m)**	30	13	88	**99**
$c_z \propto$	**P_{sep}/B_p (MW/T)**	58	39	96	**138**

[Reimerdes, 4th IAEA DEMO Prog. Workshop]

Mean-field codes as the main workhorse

- For 3 decades **relied on mean-field codes**, e.g. SOLPS-ITER, SOLEDGE-EIRENE
  - ✓ Best **compromise fidelity / cost**
  - ✓ Only codes able to model **divertor regimes up to detachment**

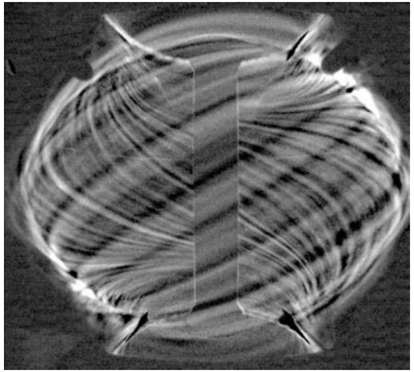
[R. Pitts, NME 2019]



- Self-consistent modelling of:
  - Neutrals recycling (PWI)
  - Plasma-neutrals interactions
  - Intrinsic and seeded impurities
  - Accurate plasma and divertor geometry

Predictive capability requires turbulence

- **Turbulence ubiquitous** in the edge plasma of tokamaks *[S. Zweben, PPCF 2007]*
  - Sets (together with // transport) SOL decay lengths
  - Even its absence *[R.J. Goldston, NF 2012]* has to be self-consistently modelled!

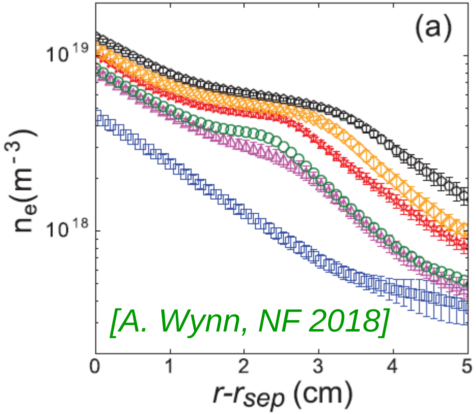


[B. Dudson, PPCF 2008]

- Mean-field approach: **gradient-diffusion** assumption

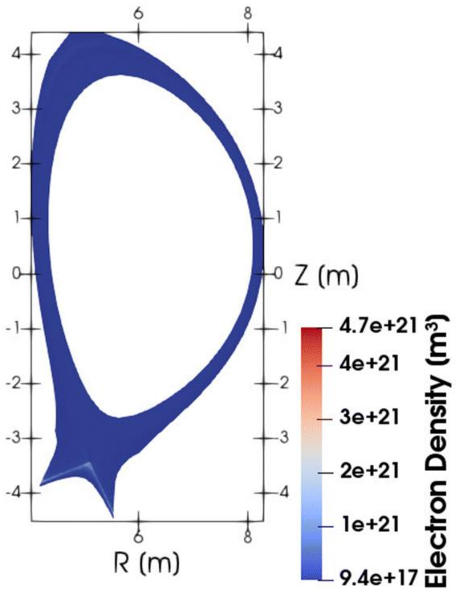
$$\vec{\Gamma}_N^{\text{turb}} \equiv -\boldsymbol{D_N}\vec{\nabla}N$$

- $\boldsymbol{D_N}$ **fixed by hand** to match λ_{SOL} scalings or expectations
  - **As predictive as scaling laws**
  - No multi-machine scaling law for **high-recycling** regimes
  - Experimental indications of **changes in turbulent transport with divertor regime**



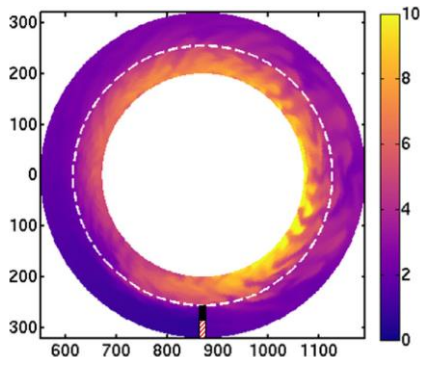
[A. Wynn, NF 2018]

Bridging the gap between turbulence and divertor physics



[D. Penko, JFE 2020]

	Mean-field (SOLPS, EMC3, SOLEDGE3X…)	3D turbulence
Self-consistent cross-field transp.		✓
Neutrals	✓ (kinetic)	
Impurities	✓	
Plasma geometry	✓	✓ (relatively recent)
Wall geometry	✓ (in general not up to the wall)	
3D equilibrium (RMPs, stellar.)	~ (only EMC3)	
Accept. runtime	~	



[P. Tamain, NME 2017]

Project strategy

- Initial assessment:
  1. No pre-identified technical solution for many issues
  2. “Easier” to incorporate missing physics in turbulence codes than to add turbulence physics into existing mean-field codes

- Strategy:
  1. **Capitalize on existing turbulence codes** to implement different solutions to add progressively and exploit **new physics capabilities**
  2. Support upstream activity on **improvement of models**

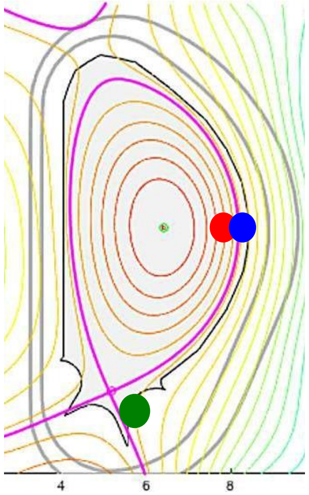
✓ **Rapid delivery of new capabilities to the community**
✓ **Risk mitigation when no ideal solution pre-identified**
✓ **Sharing of good practises**
✓ **Spin-offs to mean-field codes**

Extending models validity

- Reactor conditions = **extreme range of collisionality**

Pedestal	Upstream SOL	Target plates
$n_e \sim 10^{20}\ m^{-3}$	$n_e \sim 3.10^{19}\ m^{-3}$	$n_e \sim 10^{21}\ m^{-3}$
$T_e \sim 10keV$	$T_e \sim 500eV$	$T_e \sim 3eV$

6 orders of magnitude in ν_e!



- Standard **drift-fluid / collisional closure / Bohm BC approach questionable**

- Derivation of new models or implementation of novel approaches, e.g:
  - Revised **sheath BC for highly collisional** conditions *[D. Tskhakaya, in prep.]*
  - **Landau non-local closure** implemented in GRILLIX *[C. Pitzal, submitted to PoP]*
  - Multi-temperature **generalization of Zhdanov closure** *[M. Raghunathan, PPCF 2022]*

Gyro-fluid including collisions

- Design of **gyro-fluid model including collision and reaction terms**
  - Based on **systematic method to transpose fluid-drift equation into gyro-fluid**
  - => gyro-fluid model compatible with **neutrals and multi-species physics**
  - Implementation in **FELTOR** quasi-completed, with applications to WPTE

[M. Wiesenberger, J. Phys.: Conf. Series 2022]

$$\frac{\partial}{\partial t}N + \nabla\cdot \boldsymbol{J}_N = \Lambda_N$$

$$\frac{\partial}{\partial t}P_\perp + \nabla\cdot \boldsymbol{J}_{P_\perp} = \boldsymbol{J}_{P_\perp}\cdot\nabla\ln B + \Lambda_{P_\perp}$$

$$\frac{\partial}{\partial t}\left(mNU_\parallel\right) + qN\frac{\partial}{\partial t}A_\parallel + \nabla\cdot \boldsymbol{J}_{mNU} = F_{mNU,\nabla B} + F_{mNU,E} + \Lambda_{mNU}$$

$$\frac{\partial}{\partial t}E_\parallel + qNU_\parallel\frac{\partial A_\parallel}{\partial t} + \nabla\cdot \boldsymbol{J}_{E_\parallel} = F_{E_\parallel,\nabla B} + F_{E_\parallel,E} + \Lambda_{E_\parallel}$$

$$-\mu_0\Delta_\perp A_\parallel = \sum_s qNU_\parallel \qquad \sum_s\left[q\Gamma_1^\dagger N + \nabla\cdot\left(\sqrt{\Gamma_0}^\dagger\frac{mN}{B^2}\sqrt{\Gamma_0}\nabla_\perp\phi\right)\right] = 0$$

$$\Lambda_N = s_n - \Delta_\perp\left(\frac{ms_{p_\perp}}{2qB^2}\right) - \nabla\cdot\left(\frac{ms_n\nabla_\perp\phi}{B^2}\right) \qquad \Lambda_{NU_\parallel} = s_{nu_\parallel}$$

$$\Lambda_{P_\perp} = s_{p_\perp} - \Delta_\perp\left(\frac{ms_{r_\perp}}{2qB^2}\right) - \nabla\cdot\left(\frac{ms_{p_\perp}\nabla_\perp\phi}{B^2}\right) \qquad \Lambda_{E_\parallel} = s_{e_\parallel}$$

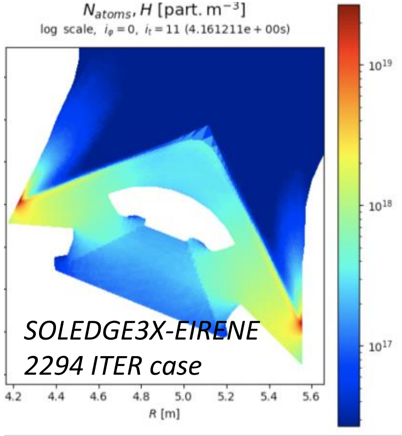
$$s_{n,i,cx} := 0 \qquad s_{mnu_\parallel,i,cx} := (m_iu_{n,\parallel} - m_iu_{i,\parallel})n_in_nK_{cx}$$

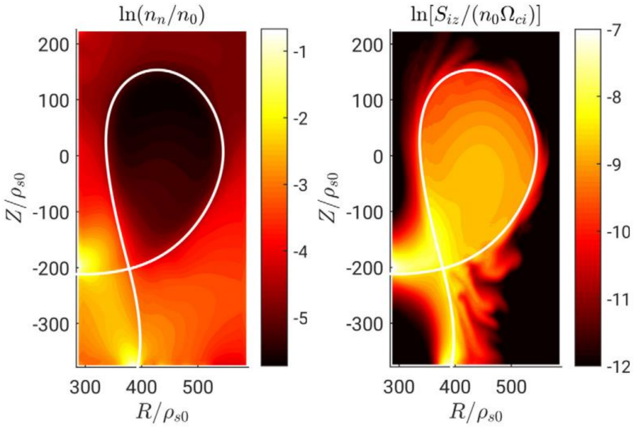
$$s_{p_\perp,i,cx} := \left(\frac{1}{2}m_iu_{n,\perp}^2 + T_{n,\perp} - t_{i,\perp}\right)n_in_nK_{cx}$$

$$s_{E_\parallel,i,cx} := \left(\frac{1}{2}m_iu_{n,\parallel}^2 + \frac{1}{2}T_n - \frac{1}{2}m_iu_{i,\parallel}^2 - \frac{1}{2}t_{i,\parallel}\right)n_in_nK_{cx}$$

3 paths for neutrals implementation (1)

1. Coupling to **EIRENE** kinetic neutrals code (SOLEDGE3X)
   - Applied to mean-field ITER simulations => major reworking of coupling scheme to ensure robustness *[N. Rivals, NME 2022]*
   - Extension to **3D achieved** but memory limits for 3D turbulence!
   - Several options to break bottleneck (new EIRENE version, different meshes…)

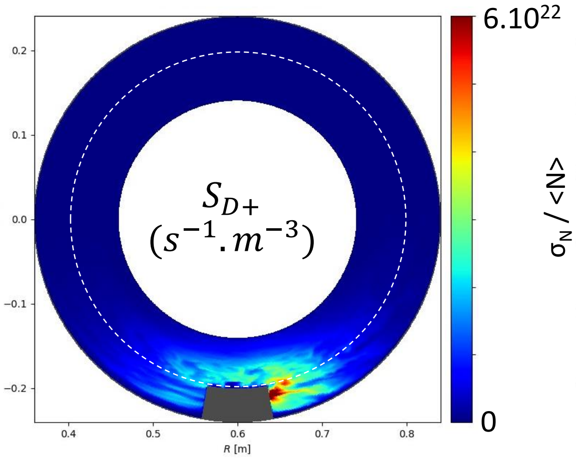


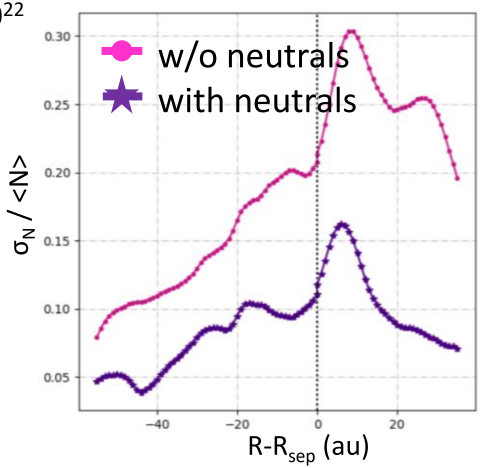


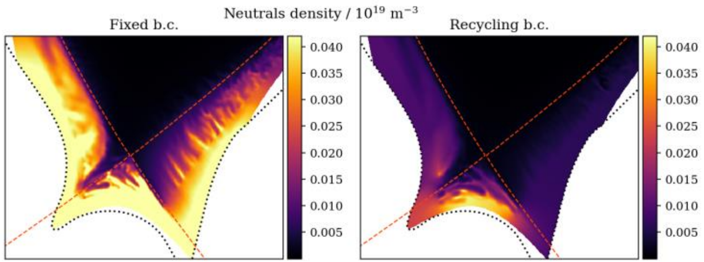
2. Embedded kinetic neutrals solver based on **method of characteristics** (GBS) *[M. Giacomin, JCP 2022]*
   - method of characteristics No Monte-Carlo noise
   - ? **numerical cost** for large simulations requires investigation (large implicit system to invert)

3 paths for neutrals implementation (2)

3. Embedded **fluid neutrals** model (GRILLIX, SOLEDGE3X, FELTOR, SOLEDGE-HDG)
   - CX-dominated model from *[N. Horsten, NF 2017]*
   - Now with recycling BC in GRILLIX => no free parameter and better match to exp.
   - Self-consistent neutrals recycling impacts profiles and turbulence properties *[V. Quadri, PET 2023]*



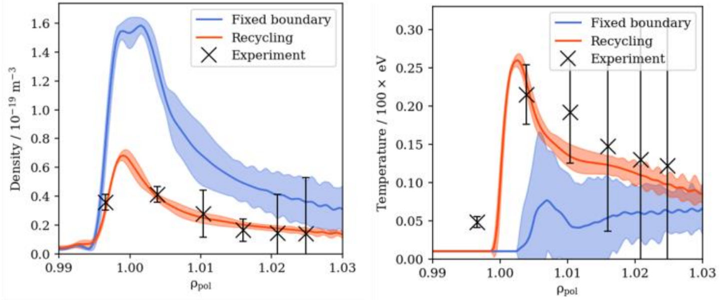




OLD: *Fixed ad-hoc value for neutral density at divertor*

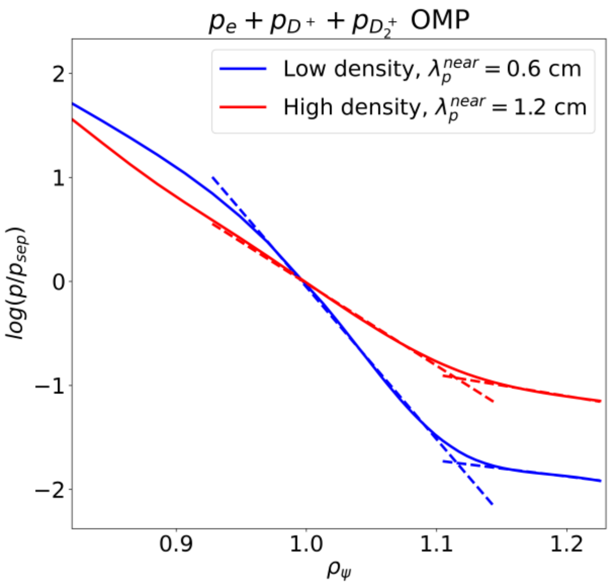
NEW: *Neutral inflow = plasma outflow*

[courtesy K. Eder]

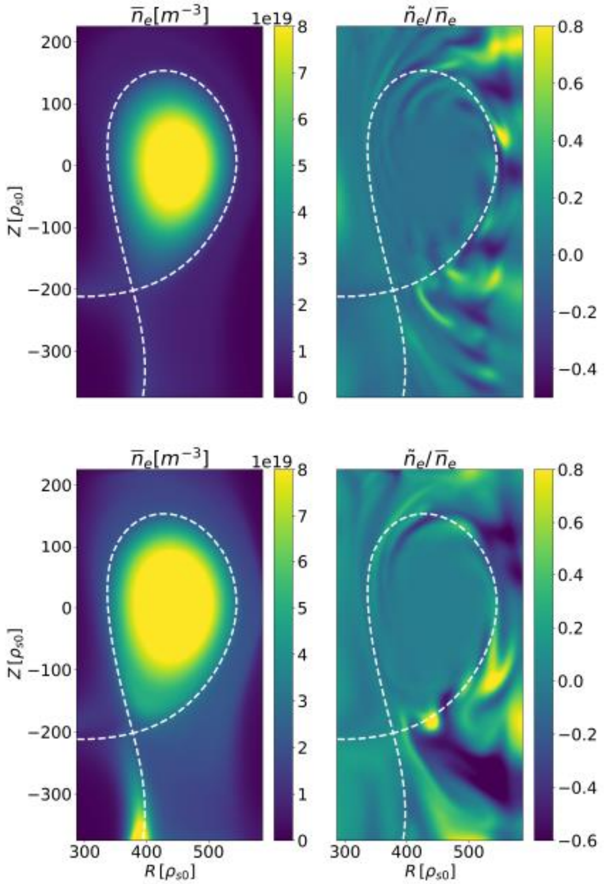


Edge turbulence in detached regime

- First-ever **3D simulation of edge turbulence in detached conditions** (GBS)
  - **Faster / bigger blobs** at high throughput
  - **Flattening** of near SOL profiles



[D. Mancini, NF submitted]

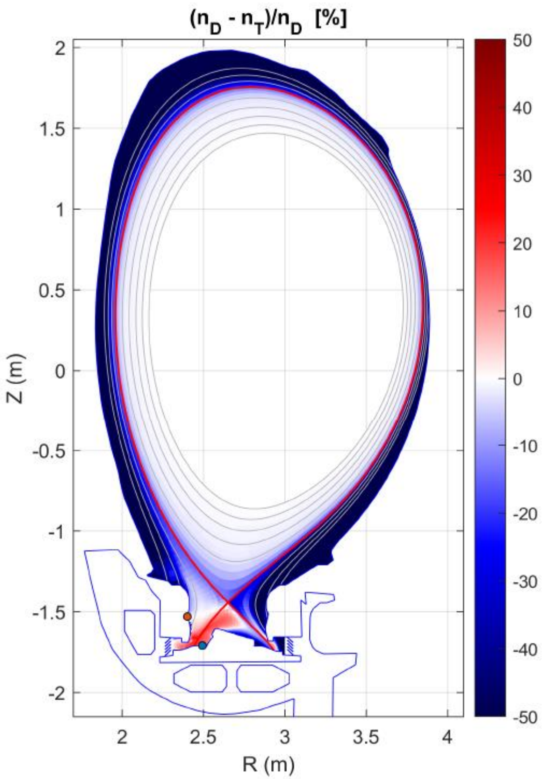


Zhdanov closure for multispecies plasmas

- **Limits of Braginskii** closure: close to unit mass and density ratios
  - Not applicable to D-T plasmas among others

- **Zhdanov closure implemented in SOLEDGE3X** and applied to **JET D-T-Ne** discharges
  - D/T far from uniform with possible implications for exhaust

- Extension to **3D turbulence** on-going
  - Approx. in model to be investigated
  - Objective: first self-consistent simulation of **turbulent transport of impurities** (incl. W) by beginning of 2024

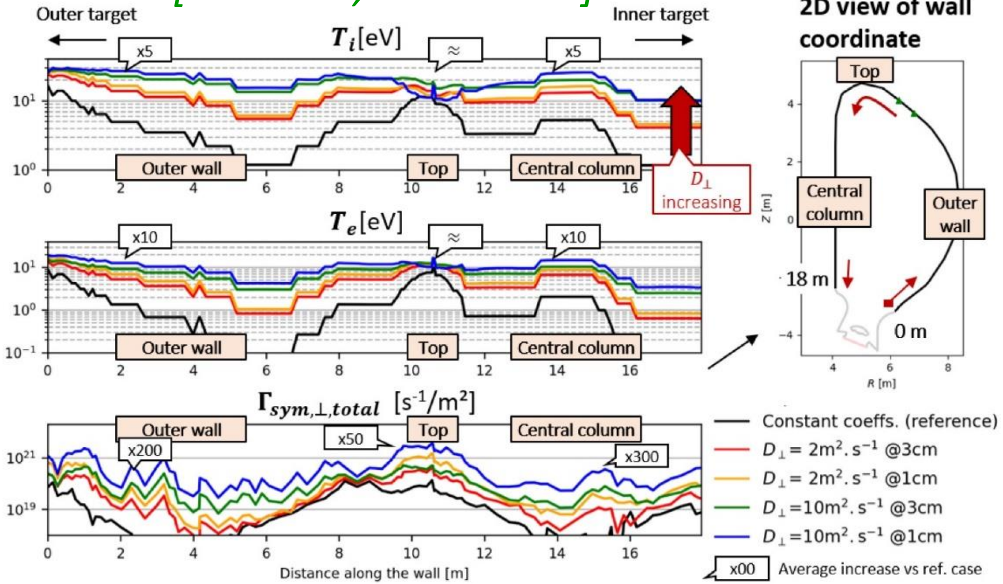


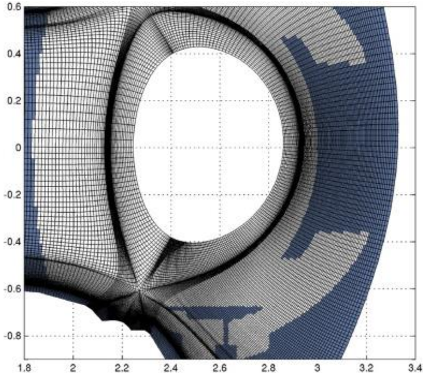
[H. Bufferand, PPCF 2022]

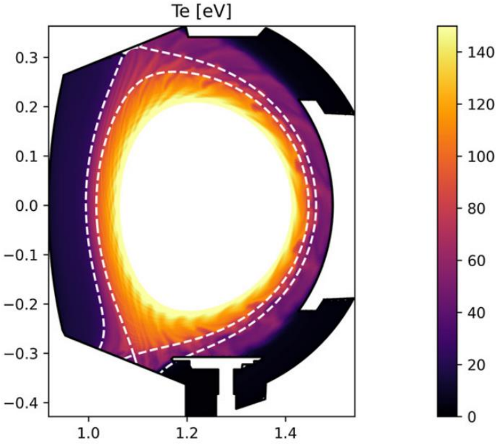
Simulations up to the first wall in real geometry (1)

- Immersed boundary conditions allow **full wall flexibility in SOLEDGE3X**
  - Application to ITER first wall fluxes (mean-field)
  - Generalization to turbulence cases straightforward

[N. Rivals, NME 2022]







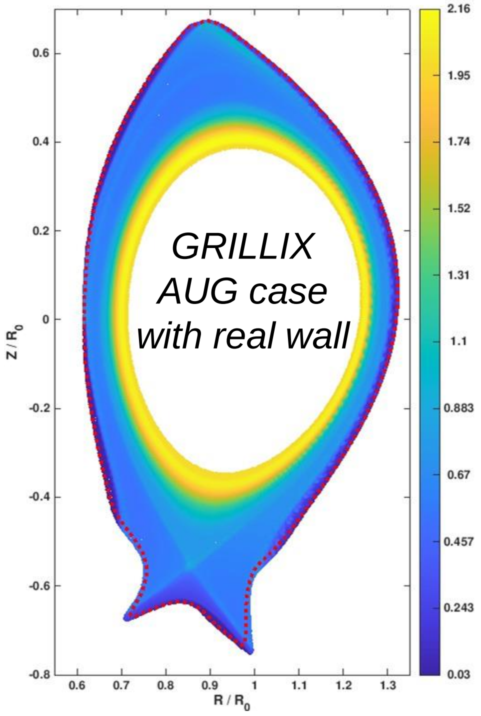
[H.Bufferand, NF 2021]

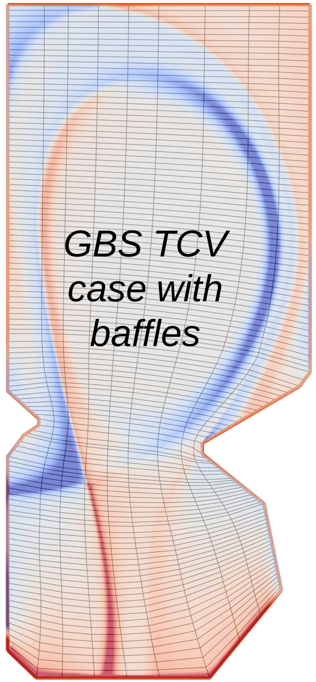
Simulations up to the first wall in real geometry (2)

- **Other options explored by other codes** due to different numerical discretization choices:
  - Immersed boundary conditions with **penalization in GRILLIX**

$$\frac{\partial f}{\partial t} = \cdots + \frac{\chi}{\epsilon}\left(f_B - f\right)$$

  - **Curvilinear grids in GBS**
  - Finite element (**HDG**) approach in EBC / SOLEDGE-HDG *[M. Scotto d'Abusco, NF 2022]*

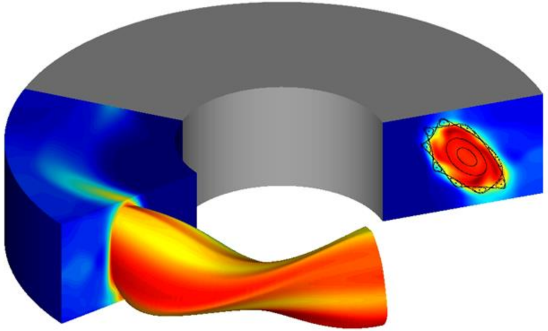




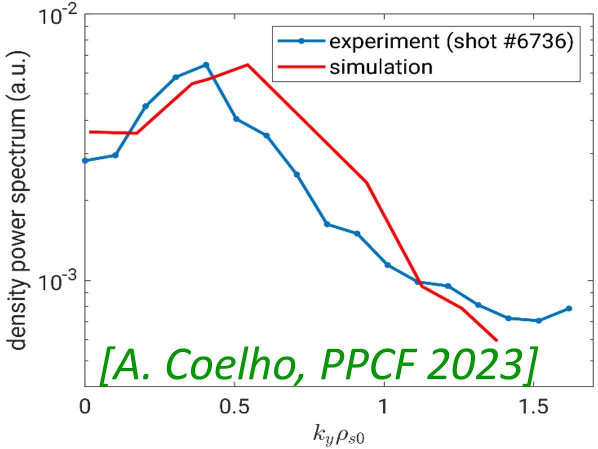
Grid: Courtesy of Jochen Hinz, MNS, EPFL

Turbulence in 3D magnetic configurations

- 3D turbulence codes adapted for **3D magnetic equilibria, including stellarators**
  - Validation against TJ-K experiment with GBS
    - ⇒ Turbulence dominated by low-m quasi-coherent mode
  - Proof of principle simulation in W7-AS geometry achieved with GRILLIX



[A. Coelho, NF 2022]

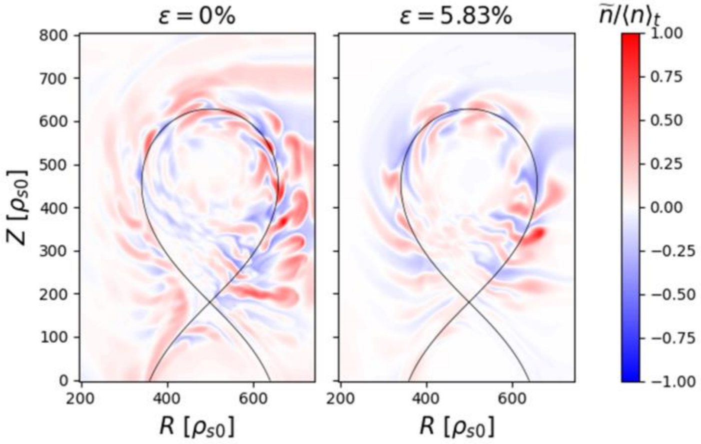


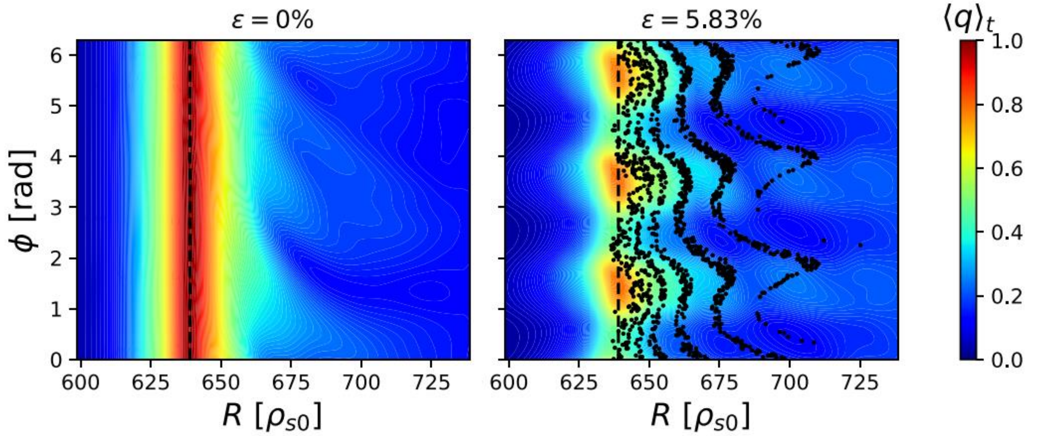
[courtesy GRILLIX team]

Impact of RMPs on heat exhaust

- **3D turbulence simulations with RMPs** in TCV geometry performed with GBS
- Key take-aways:
  - RMPs **impacts turbulence properties but level of turb. transport remains similar**
  - 2D heat flux pattern in divertor smoothened by turbulence
  - q_{peak} reduction from 2D mean field simulations recovered

[T. Boinnard, NF 2023]



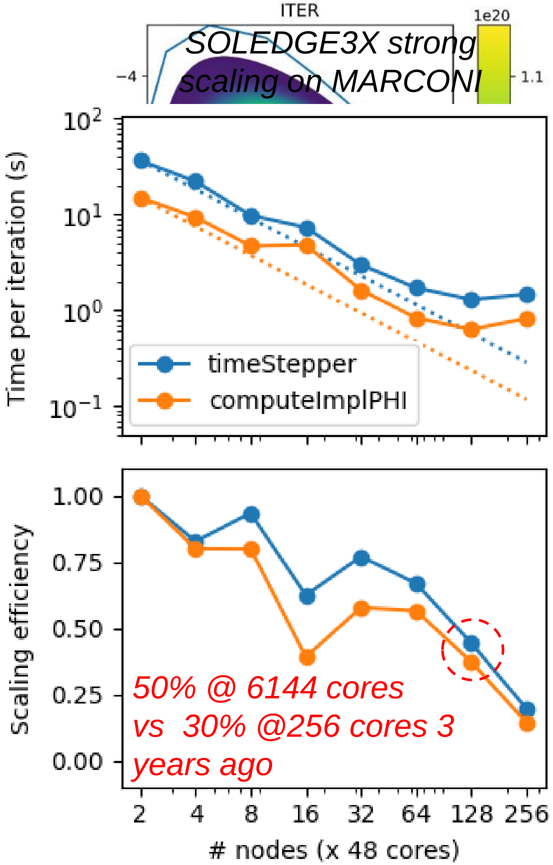


Upscaling towards ITER scale

- Work conducted in collaboration with **ACH EPFL**

- Strong **synergies** between codes on linear solvers and GPU-ization
  - Shared knowledge on optimization of iterative solvers
  - All codes 50% to 80% ported on GPU (Leonardo)

- Current status:
  - All codes capable of running **real scale simulation for medium size machine** (TCV, AUG, ~WEST) on current HPC
  - **ITER scale simulation** to be tested by the end of the year, already demonstrated by GRILLIX

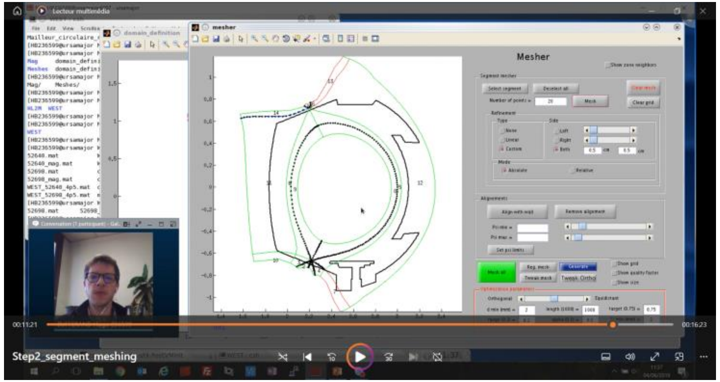


Making tools accessible

- Strong effort in project to make numerical tools accessible to the community
  - **Codes accessible** (or soon to be) either through Gateway repository or web-page
    - EBC: https://gitlab.eufus.psnc.pl/tsvv3/ebc
    - GBS: https://gitlab.eufus.psnc.pl/gbs/gbs-mirror
    - SOLEDGE3X: https://gitlab.eufus.psnc.pl/tsvv3/soledge3x (and https://www.soledge3x.com)
    - FELTOR: https://github.com/feltor-dev/feltor
    - GRILLIX: up-coming soon (licence under discussion)

- Documentation and **video tutorials prepared** for all codes (soon available)

- On-going **IMASification of IO** to allow easy set-up and post-treatment with experiments
  - Synergies based on HESEL and SOLEDGE3X experience *[ACH IPPLM]*



Video tutorial for SOLEDGE3X mesh generator

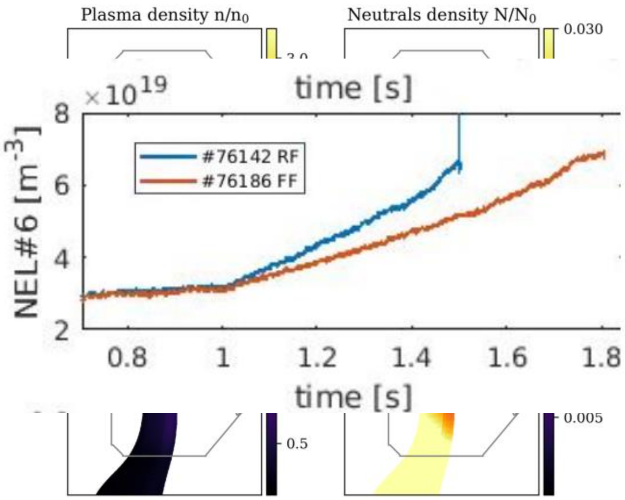
Ease comparison with experiments

- Progress on **synthetic diagnostics**
  - Standard for embedded **Langmuir probes** synthetic diagnostics defined and being implemented
  - Coupling to standard libraries (e.g. **CHERAB**) through IMAS

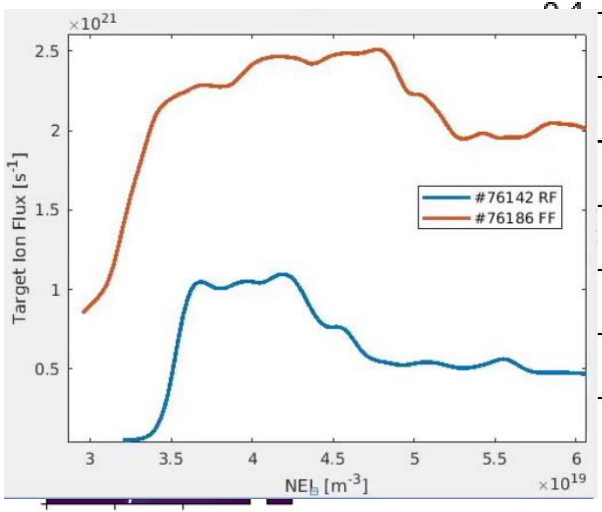
[I. Kudashev, Appl. Sci. 2022]

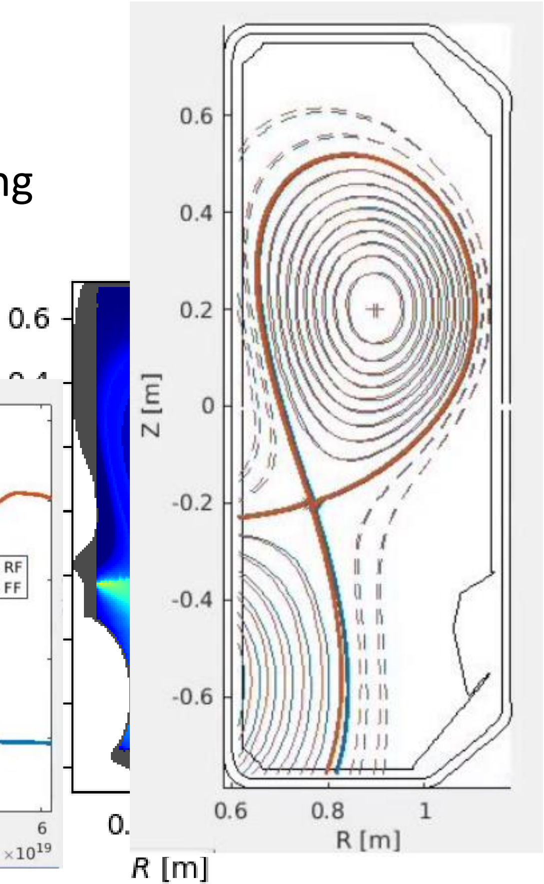
TCVX23 validation exercise

- Dedicated **TCV experiment** for turbulence through density regimes (**RT22-05**):
  - density scans in low field discharges adapted for modelling
  - max diagnostics coverage for turbulence and profiles
- Chosen as **reference case for all TSVV3** codes



GRILLIX





Proposed 2024-2025 workplan

- Progressive move of **focus towards experiments**
  - **TCVX23** as common reference case + selected applications to WPTE machines (AUG, WEST, MAST-U)

Document to be written for validation by October 2023

- Pursue development on key aspects:
  - Gyrofluid closures, sheath boundary conditions
  - Multi-species simulations in turbulent regime
  - Share kinetic neutral modules between codes
  - Code optimization for modern hardware (GPU) => ITER case as metric
  - Complete IMAS integration and couple to synthetic diagnostics

- High level physics deliverables:
  - Provide guide-line to mean-field codes for **transport coef. in high density regimes**
  - First evaluation of **turbulent transport of impurities** (light, possibly heavy)
  - Edge turbulence in **stellarators**

Deliverables 2021

Scientific deliverable	Achieved	Evidence for achievement, brief reason for partial or non-achievement
D3.1.a - Implementation and generalization of RANS transport models and related BCs in edge codes	75%	• SOLE[...] [...://drf-gitla...] • ... ersion of HDG edge ... *100% completed in 2023* *[I. Kudashev, SOFE conference, Oxford, 2023]*
D3.1.b - Implementation and generalization of RANS transport models in edge codes	100%	• SOLEDGE: results published in [Baschetti et al., Nucl. Fusion 61, 106020 (2021)] • SOLPS-ITER: improved RANS models implemented in extended grid version [commit # 7f1acf986d6352f743dfa2dfc1972b04e89c5ac4 on ITER main git repository].
D4.1 - Flash report on performance evaluation and gains	100%	• Report available on project's Wiki page [https://wiki.euro-fusion.org/wiki/TSVV-03#Documents_and_reports]
D5.1 - Implement fluid neutrals models derived in TSVV5 in existing turbulence codes (SOLEDGE3X, EBC, FELTOR)	80%	• SOLEDGE3X: crude neutrals model available since tagged version v0.9 [https://drf-gitlab.cea.fr/s3xe/soledge3x]. Results published in [Bufferand et al., Nucl. Fusion 61, 116052 (2021)] • EBC: fluid neutral model implemented in a test version of the HDG edge plasma solver. Results have been published in [Scotto et al., Nucl. Fus. accepted]. • FELTOR: delayed partly. Expected in early spring of 2022. • GRILLIX (not in initial work-plan): first results with simple fluid neutrals published in [Zholobenko et al., Nucl. F. 61, 116015 (2021)].
D9.1 - Create publicly accessible git repositories for all contributing codes and setup continuous integration environment	100%	• All codes available on publicly accessible repositories or repositories accessible on request: https://github.com/feltor-dev/feltor, http://gbs.epfl.ch, https://gitlab.mpcdf.mpg.de/phoenix/grillix_refactor, https://drf-gitlab.cea.fr/s3xe/soledge3x • All repositories ready to be transfered to Gateway once ready • Automatic tests implementation completed for GRILLIX, FELTOR and EBC (from compilation to integration tests); pipelines built for GBS and SOLEDGE3X, implementation of tests on-going

Deliverables 2022 (1)

Scientific deliverable	Achieved	Evidence for achievement, brief reason for partial or non-achievement
D1.1 - Collisional closure for full-F gyro-fluid models	100%	Paper submitted to Journal of Physics : Conference Series / 12.9.22 Theory of fusion plasmas joint Varenna – Lausanne international workshop, Varenna, Italy *[Wiesenberger, pinboard ID 33034]*
D1.3 - Neutral-interaction in full-F gyro-fluid models	100%	Paper submitted to Journal of Physics : Conference Series / 12.9.22 Theory of fusion plasmas joint Varenna – Lausanne international workshop, Varenna, Italy *[Wiesenberger, pinboard ID 33034]*
D3.2 - Selection/creation database of turbulent simulations for the design of reduced turbulence models	100%	Database of SOLEDGE3X and GRILLIX simulations made available to KUL team. Data Stored on Marconi cluster (e.g, /marconi_scratch/userexternal/vquadri0/LIMITER-3D-DRIFTS-* directories)
D4.1 - Report on performance evaluation and gain in each supported code	100%	This report and ACH EPFL report
D5.2 - Develop, implement and evaluate efficient coupling scheme with EIRENE	100%	Results presented in several conferences: *[Tamain, pinboard ID 33669]* *[Rivals, pinboard ID 32660, 32853, 33670, 33671]*
D5.3 - Extension and evaluation of the method of characteristics to treat kinetic neutrals physics in diverted geometry	100%	Results published in: 10.1088/1741-4326/ac30c9
D6.1 - Numerical implementation in the FELTOR code of drift-fluid and gyro-fluid two-ion species model in 3D including collisions	25%	Priority given to model development (D1.1 & D1.3) and to solving initial numerical stability issues. Model now derived and stability issue solved by new FCI scheme (see Task 7 report). Implementation started.

Deliverables 2022 (2)

Scientific deliverable	Achieved	Evidence for achievement, brief reason for partial or non-achievement
D6.2 - Multispecies version of GBS for electrons, D+, and D2+ with the method of characteristics.	100%	Results published in: 10.1088/1741-4326/ac47b8
D8.1 - Implement IMAS compatibility in all the codes contributing to the project	70%	Complete for SOLEDGE3X and FELTOR in existing IDSs: see git repositories (cf D9.1). On-going work in GRILLIX. Specification for extension of existing IDSs agreed upon (https://wiki.euro-fusion.org/wiki/TSVV-03). Work started for implementation of new IDSs in IMAS (e.g., https://jira.iter.org/browse/IMAS-4440).
D8.2 - Develop routines for synthetic Langmuir probes diagnostics	100%	Standard IO agreed upon (https://wiki.euro-fusion.org/wiki/TSVV-03). Implemented in FELTOR, GRILLIX and SOLEDGE3X (see Gitlab repositories). Can be requested on the fly in GBS with minor work.
D9.1 - Create publicly accessible git repositories for all contributing codes and setup continuous integration environment (from 2021)	100%	FELTOR: https://gitlab.eufus.psnc.pl/g2mwiese/feltor GBS: https://gitlab.eufus.psnc.pl/gbs/gbs-mirror SOLEDGE3X: https://gitlab.eufus.psnc.pl/tsvv3/soledge3x GRILLIX: GRILLIX waiting for legal issues to be sorted to make code open source (beyond the deliverable). In the meantime, hosted at MPCDF Gitlab server and available on request (Andreas.Stegmeir@ipp.mpg.de).
D9.2 - Provide standard documentation for each contributing code	100%	Codes' git pages (Cf D9.1).

Deliverables 2023 (1)

Scientific deliverable	Status	Comment
D1.2 - Application of gyro-fluid model with collisional closure to TCV experiment modelling (report or presentation or paper)	30%	Model implemented in FELTOR. Simulation currently being set-up.
D1.4 - Multi-species full-F gyro-fluid models with extended drift-kinetic ordering	50%	Partly achieved through Varenna paper (10.1088/1742-6596/2397/1/012015). More investigation needed.
D2.1 - Develop an updated model of the multi-ion, multidimensional sheath with finite collisionality	75%	Paper being written for collisional MS sheath model. Simulations on-going for multi-dimensional sheath.
D2.3 - Implementation and test of recommandations in edge fluid codes	75%	Variations of boundary conditions tested in GBS for COMPASS. SOLEDGE3X currently implementing new boundary conditions.
D3.1 - EBC/SOLEDGE3X/SOLPS-ITER codes including calibrated two-equation model	50%	k-epsilon model implemented in SOLEDGE3X and SOLEDGE-HDG
D3.2 - Analysis of dominant anomalous transport mechanisms in slab, limiter and divertor configurations; generalization of corresponding RANS closure models	50%	Calibration of model still on-going based on database of 3D simul. Setup of TCVX23 simulation for comparison with 3D turbulent simulations on-going.
D4.2 - Evaluation of performances of key parts of codes according to agreed performance indicator	70%	Solver performances compared on common grounds. GPUization on-going after common analysis of best-practise.
D4.3 - Application of codes (GBS, SOLEDGE3X, GRILLIX) to ITER-size case with neutrals dynamics	50%	Done for GRILLIX and HDG code. Scheduled for SOLEDGE3X and GBS.
D5.4 - Provide first analysis of impact of density regimes on turbulent transport, comparing simple fluid model and kinetic model	100%	GBS paper on turbulence in detached conditions (pinboard ID: 35096). PET contribution of V. Quadri (pinboard ID: 35107).

Deliverables 2023 (2)

Scientific deliverable	Status	Comment
D6.3 - Analysis of differences between the two above approaches on D-T case and quantification of differences to single-ion-species models	75%	First D-T simulations with Zhdanov performed with SOLEDGE3X in mean-field mode. Extension to turbulence requires numerical scheme changes.
D7.1 - Progress in the development of a numerical method for wall-conforming domain in GBS	100%	Implementation and verification of curvilinear grid completed. Now running first application test with TCV baffle configuration.
D7.2 - Develop discretization method to treat plasma boundary conditions in arbitrary wall geometry in the frame of an FCI parallel discretization	100%	Paper published on penalization method in GRILLIX (10.1016/j.cpc.2023.108801). Implementation and verification completed with first tests in AUG geometry.
D7.3 - Develop and implement full 3D finite-element approach (DG/HDG) for prototype code developed in pilot phase	50%	Implementation in SOLEDGE-HDG completed but important numerical difficulties related to matrix conditionning under invest.
D7.4 - Develop discretisation schemes for 3D geometries	100%	Completed. 2 GBS papers on stellarators + 1 on RMPs. Test simulation in W7-AS geometry in GRILLIX.
D8.3 - Development of spectroscopic synthetic diagnostics: Li-BES, He-BES and Passive spectroscopy	50%	Usage of imaging and spectoscopic synthetic diagnostics demonstrated in SOLEDGE-HDG (10.3390/app12199807). Application to other codes pending on IMASification progress.

- **Vast majority on-track** with slight delay due to start of TCVX23 validation exercise (not planned but deemed as priority for rapid feedback to WPTE following Thrust discussions)
- Main difficulties concentrated on 2 (sub-)tasks (RANS models and HDG dev.) due to **manpower (recruitment) difficulties**

Publications record

	Posters	Orals	Papers	PhD thesis
2021	4	8	16	0
2022	5	12	11	2
2023	1	12	6	1
TOTAL	**10**	**32**	**33**	**3**

** Approximative years (from pinboard entry)*

- Selected recent submissions:
  - A. Stegmeir et al., “Analysis of aligned and non-aligned discretisation schemes for reactor-scale tokamak edge turbulence simulations, CPC 2022 (ID: 32187)
  - D. Mancini et al., “Self-consistent multi-component simulation of plasma turbulence and neutrals in detached conditions”, submitted to NF (ID: 35096)
  - P. Tamain et al., “European edge fluid modelling tools for self-consistent reactor relevant conditions”, IAEA FEC 29 (ID: 34296)

Geometry milestone

Neutrals milestone

Project overview

Conclusion

- **Theoretical developments**: gyro-fluid models incl. collisions, collisional sheath boundary conditions, RANS reduced turbulence models…
  - Progressive implementation in numerical tools

- **New physics capabilities** available in edge turbulence codes: **neutrals**, **impurities**, realistic **wall geometry**, **3D magnetic geometries**
  - Relevant regimes for reactors accessible, improve comparison with experiments

- **Spin-offs to mean-field** codes, e.g RANS models in SOLPS or Zhdanov closure

- Numerical **optimization towards ITER scale** with ACHs
  - **MST cases with realistic parameters**, first attempts at ITER scale scheduled

- Effort to **ease users experience and confrontation to experiments**: IMAS, synthetic diagnostics, tutorials…

- **Workplan 2024-2025** defined: focus progressively moving to confrontation to experiments

Additional slides

Project structure

TSVV1
TSVV4

Improve models

- Task 1: gyrofluid models
- Task 2: sheath BCs
- Task 3: reduced turbulence models

TSVV2
TSVV5
TSVV6

Improve codes capabilities

ACHs

- Task 4: codes optimization
- Task 5: neutrals physics
- Task 6: multi-species plasmas
- Task 7: complex geometry

Coordinate and rationalize effort

- Task 0: project coordination
- Task 10: evaluate and select approaches

Disseminate

- Task 9: make verified codes available to WPs

ACHs

WPs

Validate

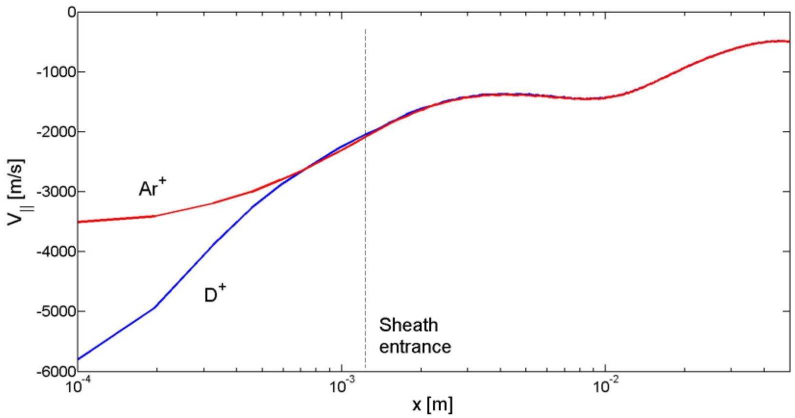
- Task 8: IMAS-ification and synthetic diagnostics
- All tasks: test new capabilities against experiments

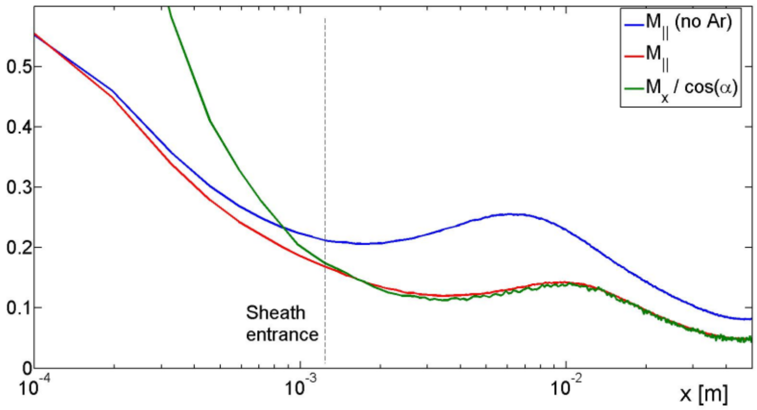
WPs

ACHs

Sheath studies in reactor-relevant conditions

- **Boundary conditions with impurities in highly collisional plasmas?**
  - Simulations with BIT1 code
- Previously: strong **effect of neutrals on boundary conditions**
  - proposed correction to standard Bohm BC => **implementation scheduled**
- New result: **minority species don't change boundary conditions**
  - **Dragged at main ion's flow velocity**
  - Perturb little main ion's flow





Revised model for BC

- Analytical model fits well PIC data:

$$M_{\parallel} = 1 + \chi - \sqrt{\chi^2 + 2\chi}$$

$$\chi = \frac{(\nu_{mt}(1-\alpha) + \nu_{ei})x_0}{2c_s \sin\theta}$$

$\alpha = V_{\parallel}^{D} / V_{\parallel}^{D+}$

Dist. of demag.: $x_0 \approx 20\rho_i$

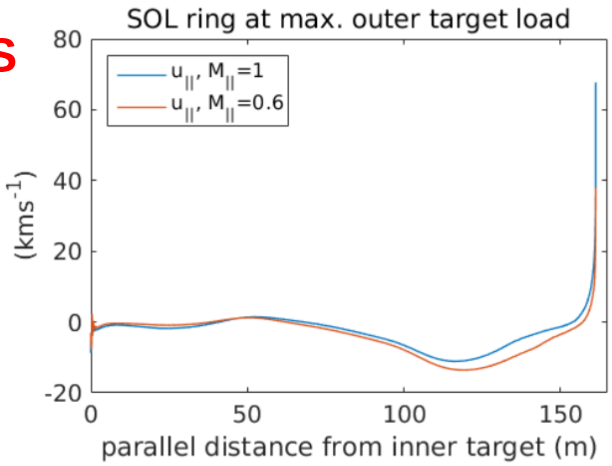
Ion-atom momentum transfer frequency

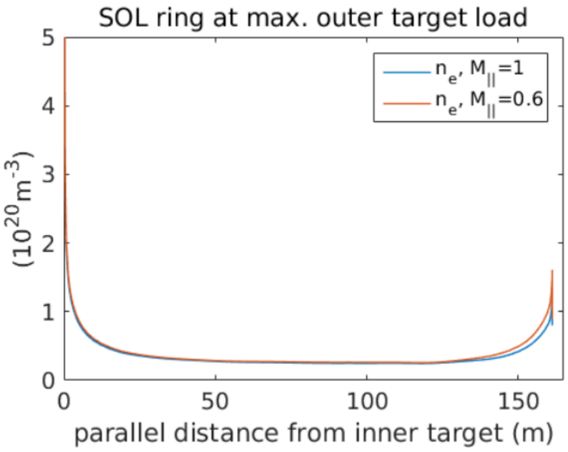
Incidence angle

[Tskhakaya, EPS 2021; D. Moulton, ISFN 09/2021]

- First **application in SOLPS** => **60% difference in target density**, likely to impact divertor regimes

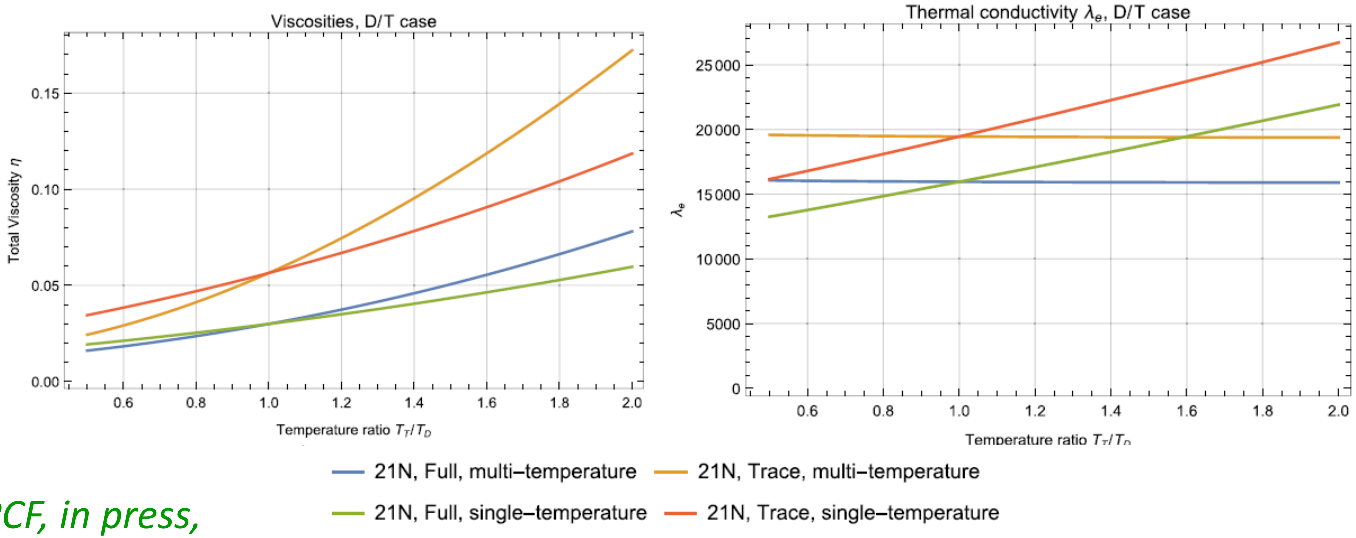
- Generalization to **multi-species plasmas** on-going





Beyond the Zhdanov closure

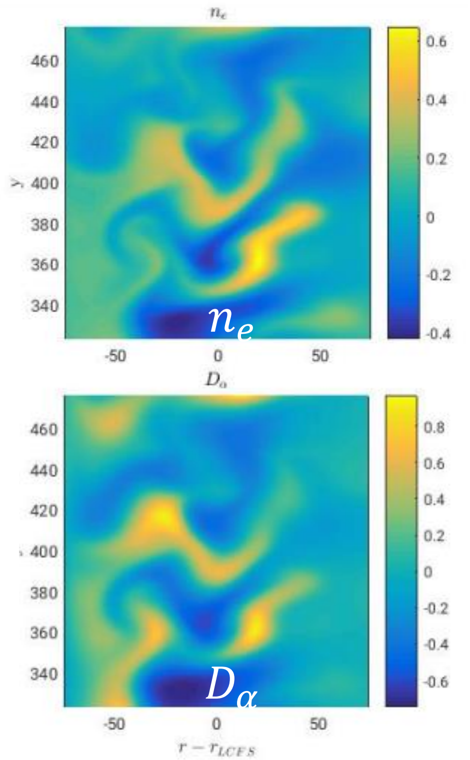
- Several limitations to Zhdanov's closure: single ion temperature, small departure from mass-average flow velocity
- On-going **theoretical developments** to go beyond these limitations
  - Practically implementable **generalization of Zhdnov's closure**
  - **On-going implementation** in FELTOR, GRILLIX and SOLEDGE3X

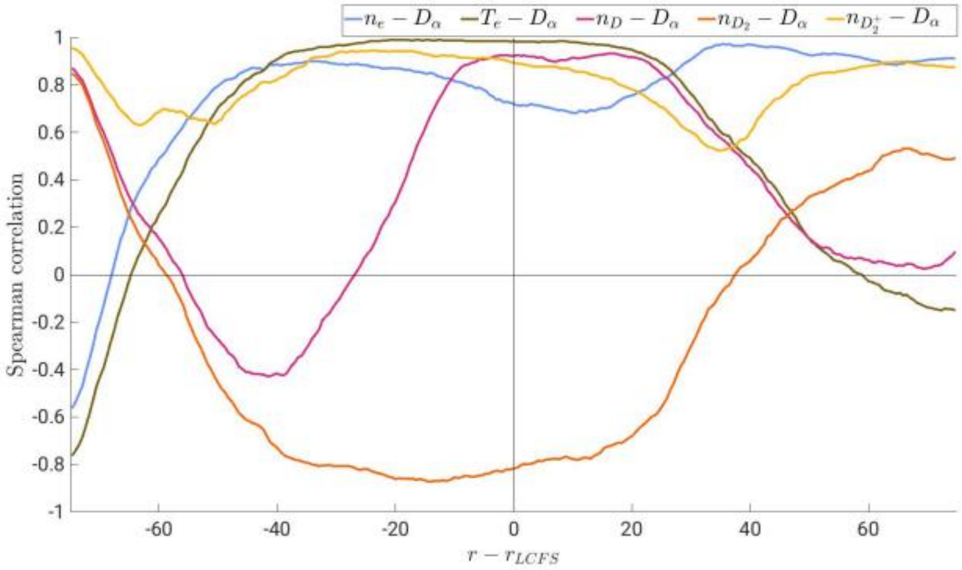


[Raghunathan, PPCF, in press, https://doi.org/10.1088/1361-6587/ac414d]

Application to Gas Puff imaging analysis

- GP imaging analyzed in **GBS simulation with kinetic neutrals**
  - Excellent correlation between n_e, T_e and D_α except in far SOL and core

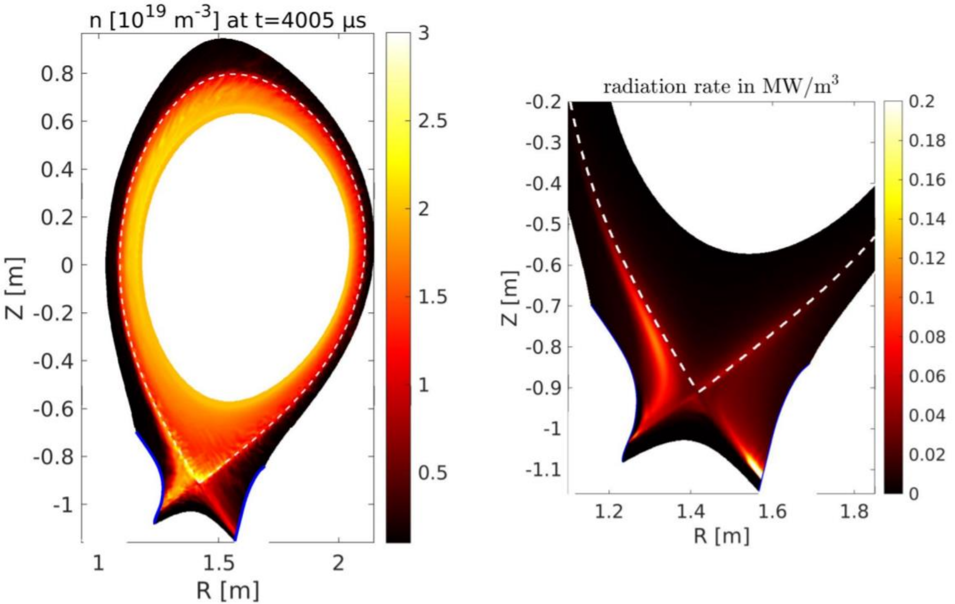




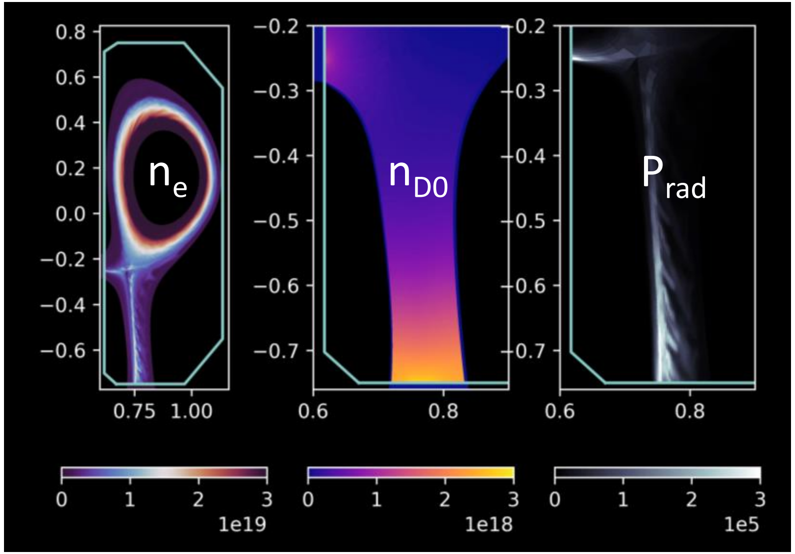
[Coroado, submitted to PoP; pinboard id: 30771]

Fluid neutrals in turbulence simulations

- Rudimentary **fluid neutrals models implemented in 3D turbulence codes** GRILLIX and SOLEDGE3X and applied to WPTE machines



GRILLIX / AUG [Zholobenko, NF 2021]

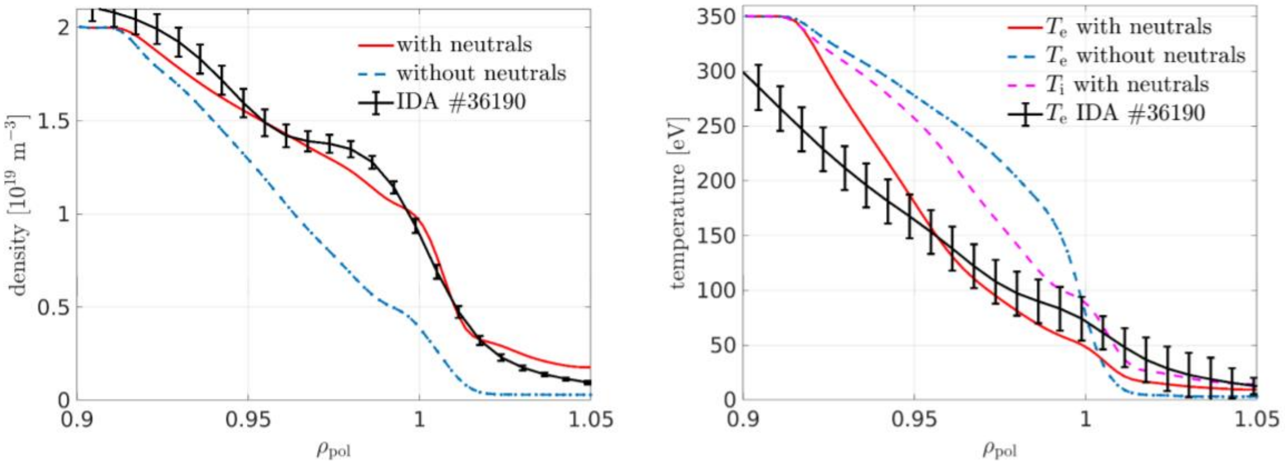


SOLEDGE3X / TCV

[Bufferand, CPP 2021; Bufferand, NF 2021]

A better match thanks to neutrals

- Even in low-density attached conditions and with coarse neutrals model, **neutrals improve comparison with experiments** *[Zholobenko, NF 2021]*

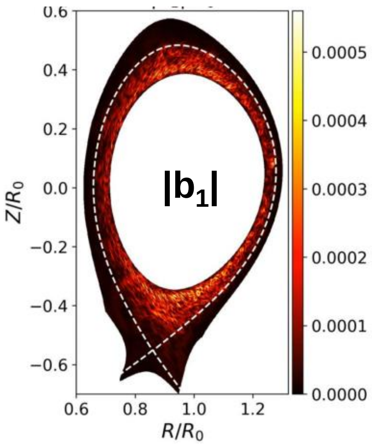


- Refined fluid neutrals model being implemented in collaboration with TSVV5 to **open high-recycling regimes**

GRILLIX: Model extensions (1)

Magnetic flutter:

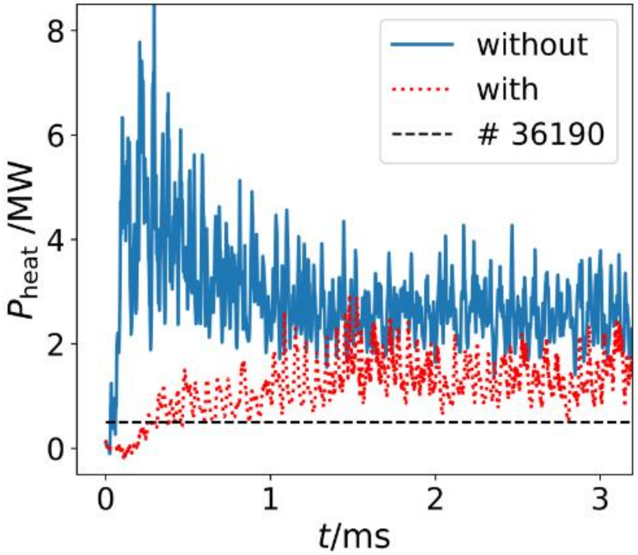
$$\mathbf{b}\cdot\nabla f = \underbrace{\mathbf{b}_0\cdot\nabla f}_{\text{FCI map}} + \underbrace{\mathbf{b}_1\cdot\nabla f}_{=[A_{\parallel 1}, f]_{R,Z}}$$



Reduction of turbulence:

- Electromagnetic transport negligible
- Electrostatic ExB transport strongly reduced even in low beta-cases (L-mode), where $|b_1| \sim 10^{-4}$.
- Flutter decreases turbulent phases in subtle way *[B.Scott 2021]*

$$\alpha_{n,\phi} = [\underbrace{2\beta\gamma\omega_R}_{\text{induction}} - \underbrace{\beta\gamma(2+0.71)\omega_* k\rho_s}_{\text{flutter}} + \underbrace{2\mu\gamma\omega_R(k\rho_s)^2}_{\text{inertia}} + \underbrace{\eta_\parallel\omega_R(k\rho_s)^2}_{\text{resistivity}}]/k_\parallel^2$$



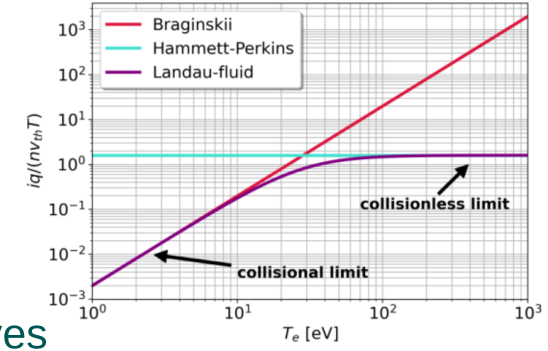
→ Magnetic flutter is of high importance, even in low-beta cases

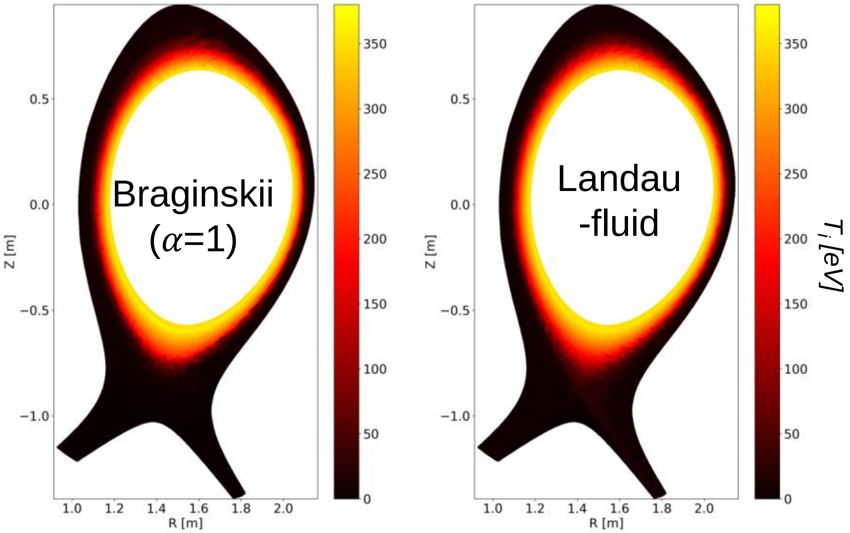
[K. Zhang et al., in preparation, NF23]

GRILLIX: Model extensions (2)

Landau-fluid closure:

- Braginskii heat flux vastly overestimated at low collisionalities
- Original Formulation in k-space: $$q^{LF}_{\parallel j,k} = -A \frac{ik_\parallel}{|k_\parallel| + \frac{\delta_j}{\lambda_{mfp}}} T_{j,k}$$
- Translation to configuration space results in set of 3D elliptic solves





Effects:

- Self-consistently **limits heat-flux**
- Introduces **non-local dynamics** that average out poloidal asymmetries
- **Higher fidelity** of model for only little increase in computational cost

[C. Pitzal et al., submitted to PoP]

Neutrals model and TCV-X23

Neutral fluid model with recycling:

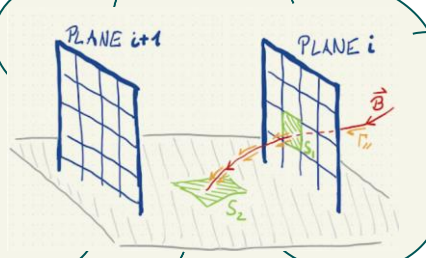
Neutrals continuity eq.: $\frac{dN}{dt} = \nabla \cdot \frac{D}{T_N}\nabla(NT_N) - S_{iz} + S_{N,rcy}$

(Diffusion by charge exchange; Ionization; Recycling source)

Plasma continuity eq.: $\frac{dn}{dt} + \nabla \cdot (\cdots) = \cdots + S_{iz}$

(Plasma density fluxes)

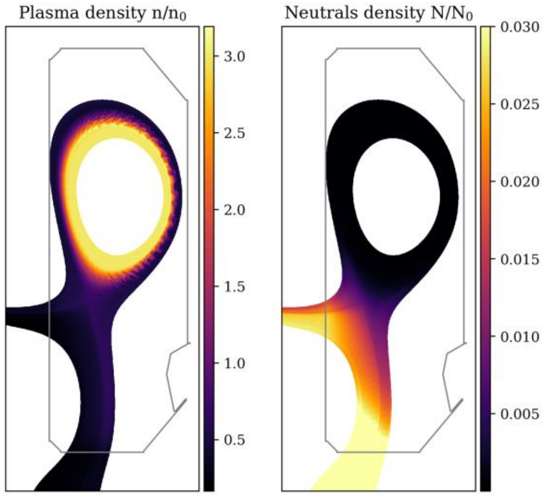
*Computation of **plasma flux** through target in **FCI** tricky*



*Then neutral recycling as **source***

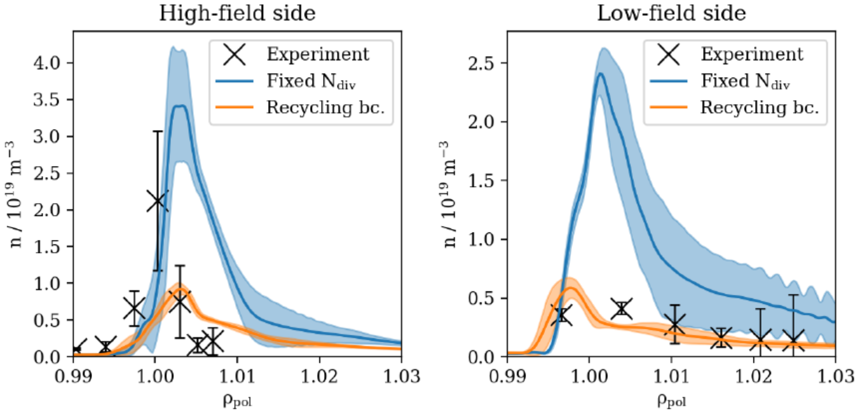
$S_{N,rcy} = R_0\,(\Gamma_{n,\parallel} + \Gamma_{n,\perp})$

Validation against TCV-X23 ongoing:



AUG validation #36190:

Fixed neutrals density at target vs. recycling boundary conditions



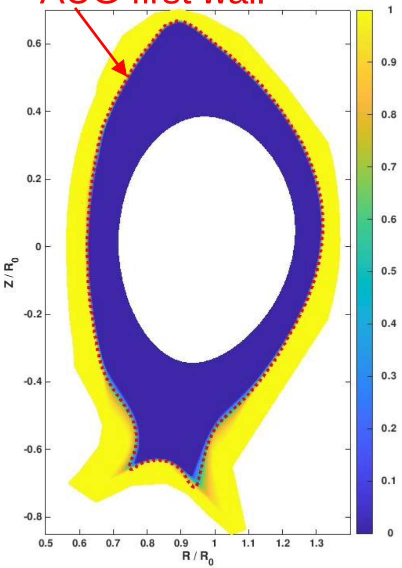
GRILLIX: Geometry extensions (1) (Work in progress)

Extension of immersed boundary method to first wall:

- Boundary conditions enforced via strong source term in extended domain

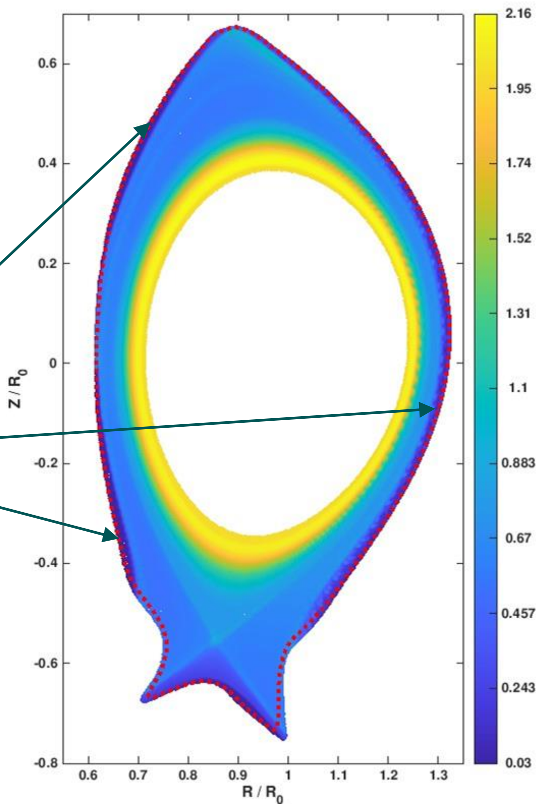
$$\frac{\partial f}{\partial t} = \cdots + \frac{\chi}{\epsilon}(f_B - f)$$

AUG first wall



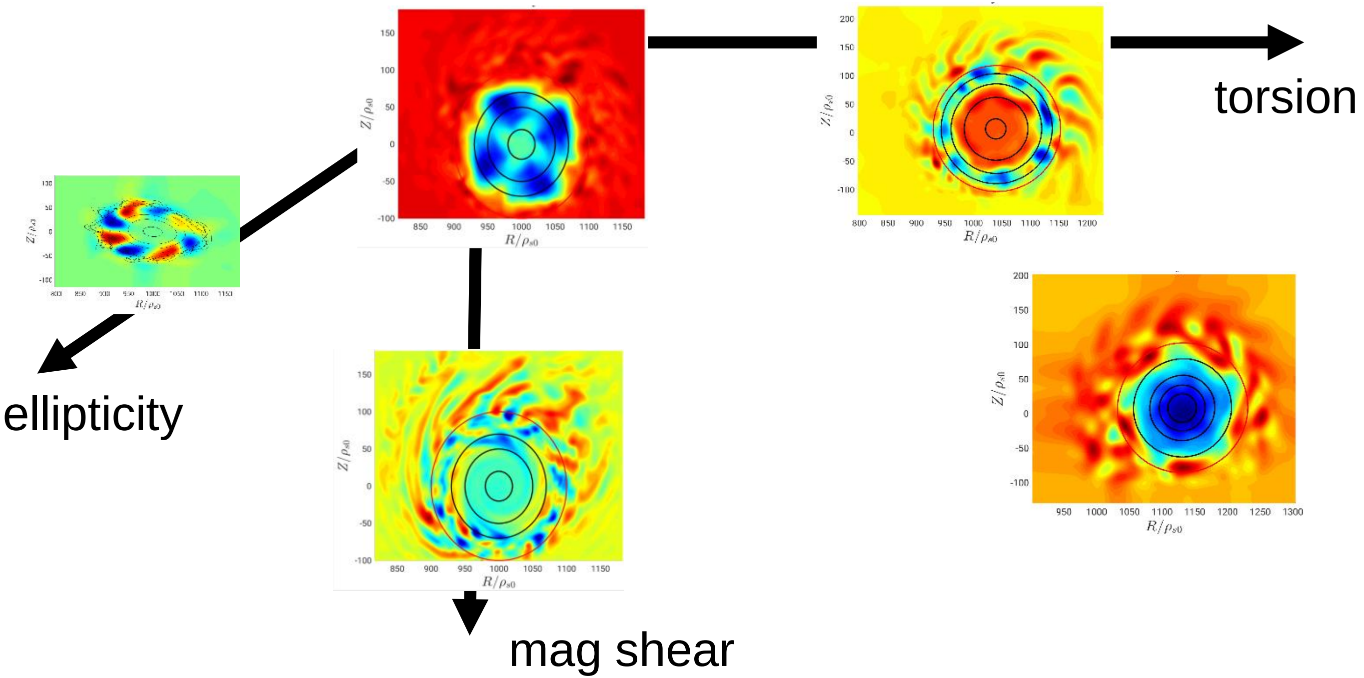
- Arbitrary wall shapes possible
- Development of **secondary scrape-off layers**
- Application to 3D geometries…

n / 1E19m^{-3}



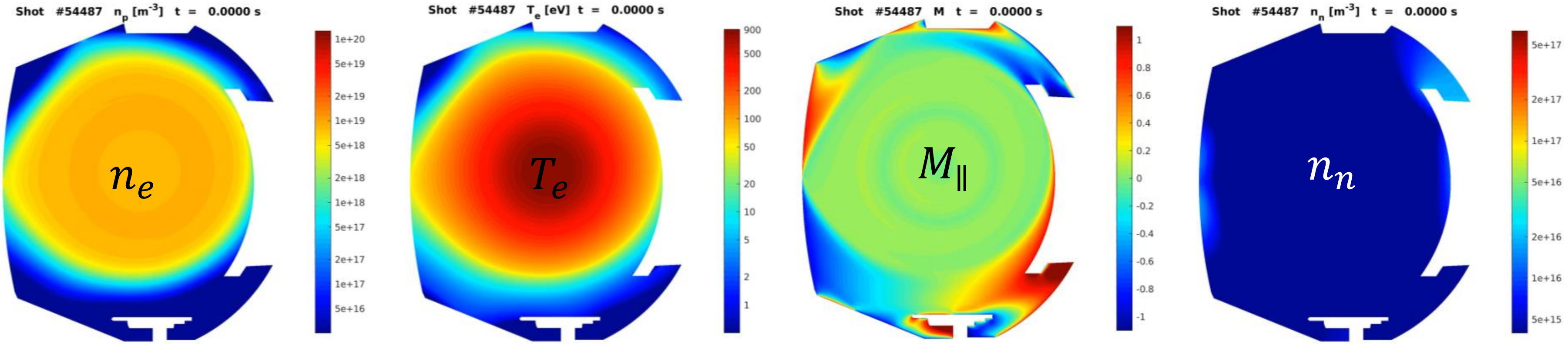
GBS - Task 7: complex geometries

- Currently exploring the stellarator phase space in terms of **magnetic shear, torsion** and **ellipticity:**



Equilibrium independent HDG boundary plasma solver

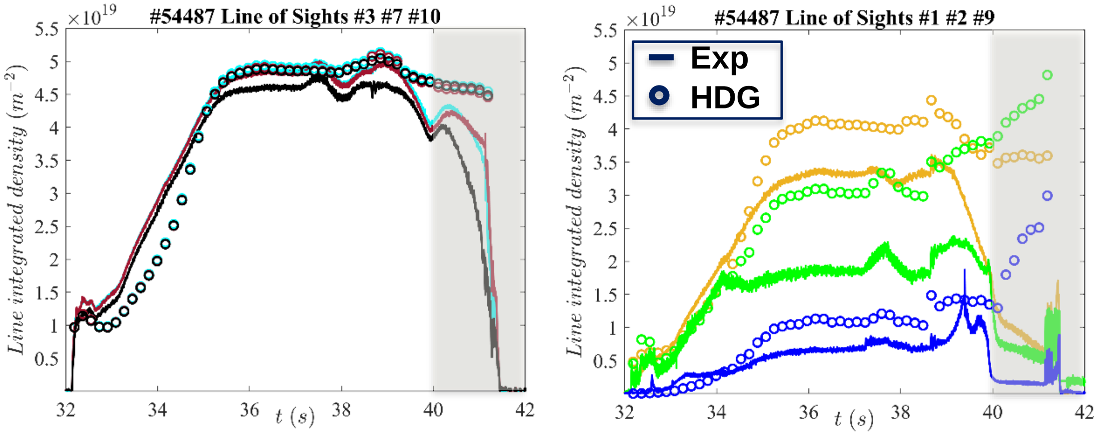
- **2D mean-field model** implemented with **fluid neutrals** in **HDG** solver
  - Allows **dynamic equilibrium** simulations **from plasma center to first-wall** in full geometry
- Application to simulation of WEST pulse from break-down to termination

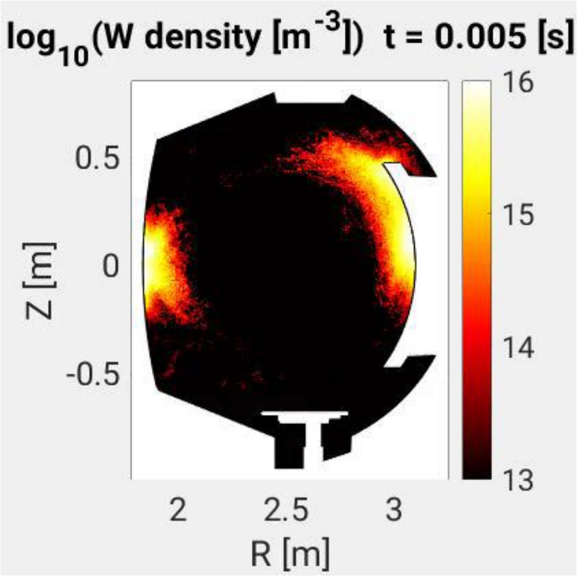


[M. Scotto d’Abusco, NF 2022]

Equilibrium independent HDG boundary plasma solver

- **2D mean-field model** implemented with **fluid neutrals** in **HDG** solver
  - Allows **dynamic equilibrium** simulations **from plasma center to first-wall** in full geometry
- Application to simulation of WEST pulse from break-down to termination
  - W content strongly driven by plasma initial phase



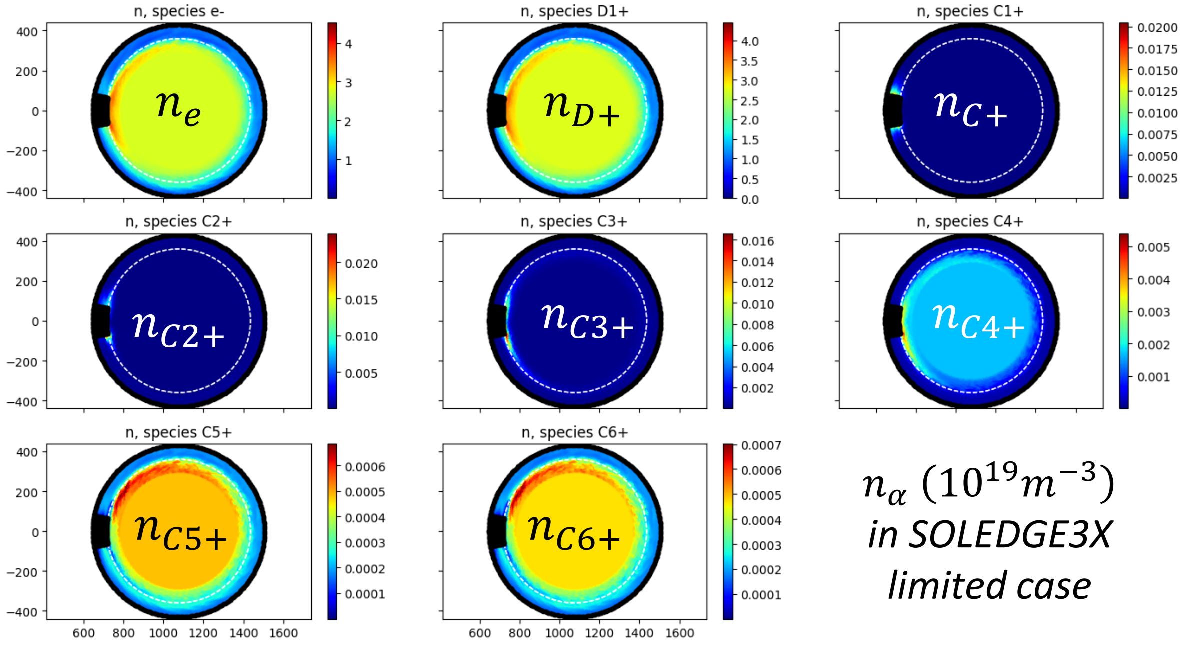


[S. Di Genova, in prep]

Physics of impurities (1/2)

- Progress along 2 axes:
  1) Test of implementation of **Zhdanov closure** in 3D fluid turbulence code
  2) Investigation of implementation of self-consistent **2D turbulence multi-fluid model**

- Zhdanov closure **implemented in SOLEDGE3X-EIRENE**
  - Requires local solve of small dense linear system
  - Costly (as much as other explicit terms) but **no major difficulty**



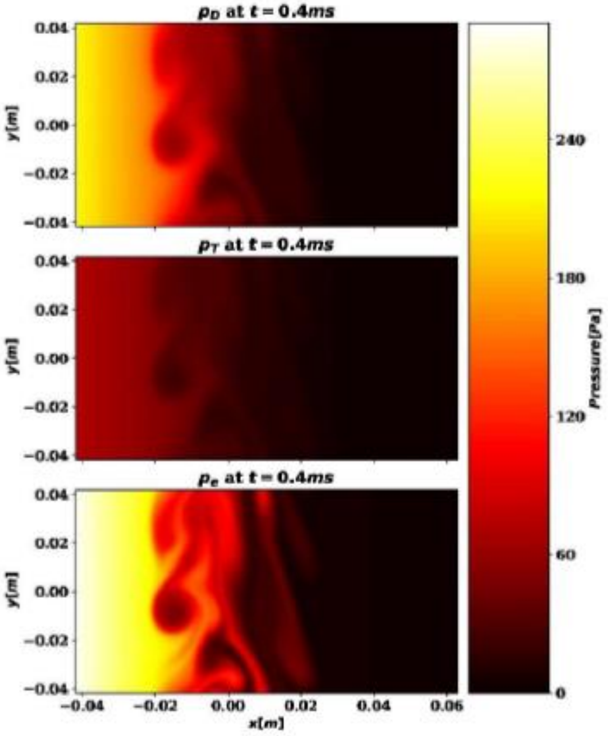
n_α $(10^{19} m^{-3})$ in SOLEDGE3X limited case

Physics of impurities (2/2)

- **Multi-species turbulent model** implemented and running in miHESEL
  - Self-consistent conservation of particle and energy balance requires inversion of **non-linear mass-matrix coupling all fields**!

$$\begin{pmatrix} -\Sigma_\alpha a_\alpha \mu_\alpha \nabla^2 & -\frac{\mu_1}{Z_1}\nabla^2 & -\frac{\mu_2}{Z_2}\nabla^2 & \cdots \\ -\frac{\mu_1}{Z_1}\nabla^2 & \frac{3}{2}\frac{1}{p_1} - \frac{\mu_1}{Z_1^2 a_1}\nabla^2 & 0 & \\ -\frac{\mu_2}{Z_2}\nabla^2 & 0 & \frac{3}{2}\frac{1}{p_2} - \frac{\mu_2}{Z_2^2 a_2}\nabla^2 & \\ \vdots & & & \ddots \end{pmatrix} \cdot \begin{pmatrix} \partial_t \phi \\ \partial_t p_1 \\ \partial_t p_2 \\ \vdots \end{pmatrix} = \cdots$$

  - Very cumbersome to code and might be a show-stopper in terms of performances
  - Need to **investigate alternative methods**



[A. Poulsen, PoP 2020]

What are reduced turbulence models?

Coarse-graining $\langle \ldots \rangle$

$$\partial_t n_e + \vec{\nabla} \cdot (n_e \vec{u}) = S_n \quad \Rightarrow \quad \partial_t \bar{n}_e + \vec{\nabla} \cdot (\bar{n}_e \bar{\vec{u}}) + \vec{\nabla} \cdot \langle \tilde{n}_e \tilde{\vec{u}} \rangle = S_n$$

Mean-field + gradient-diffusion ansatz

$\langle \tilde{n}_e \tilde{\vec{u}}_\perp \rangle \equiv -D \vec{\nabla} n_e$

N_{grid} free parameters

Machine /case dependent

Cpu-time: ~10kh.cpu

Mean-field reduced turbulence model

$\langle \tilde{n}_e \tilde{\vec{u}} \rangle = ?$

Few free parameters

Universal

Cpu-time: ≳10kh.cpu

Direct numerical simulation

$\partial_t n_e + \vec{\nabla} \cdot (n_e \vec{u}) = S_n$

No free parameter

Cpu-time: ~10Mh.cpu

☹ Not predictive → ☺☺? → ☹ Costly and slow → *Fidelity / computing time*

Aim & approach: closure models for self-consistent description of anomalous transport in mean-field codes

Turbulence model / code

RANS approach from hydrodynamic turbulence

Reference data

Mean-field (averaged) plasma edge model

Model closure, parameter estimation & model validation

Split in mean + fluctuating components

'Reynolds' $x = \bar{x} + x', \ \bar{x} = \lim_{T \to \infty} \frac{1}{T} \int_0^T x dt$

'Favre' $x = \tilde{x} + x'', \ \tilde{x} = \frac{\overline{nx}}{\bar{n}}$

Time-average governing equations

e.g. $\partial_t \bar{n} + \nabla \cdot \bar{\mathbf{\Gamma}} = \bar{S}$

$\Rightarrow \partial_t \bar{n} + \nabla \cdot \left(\bar{n}\, \bar{\boldsymbol{u}} + \overline{n' \boldsymbol{u}'} \right) = \bar{S}$

Mean-field transport model consistent with turbulence model

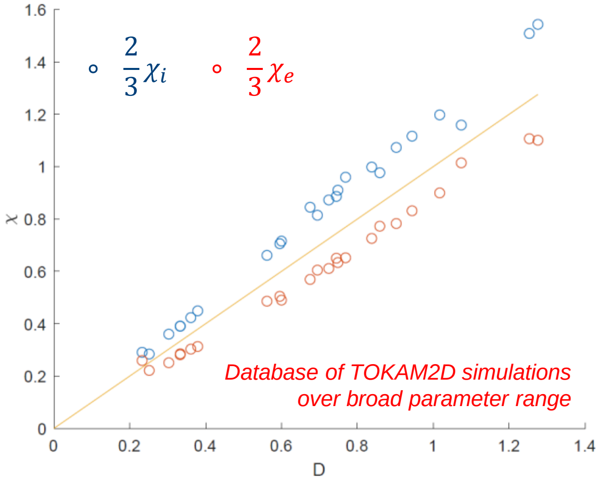
e.g. $\overline{n' \boldsymbol{u}'} = -D(\kappa_\perp) \nabla_\perp \bar{n}$

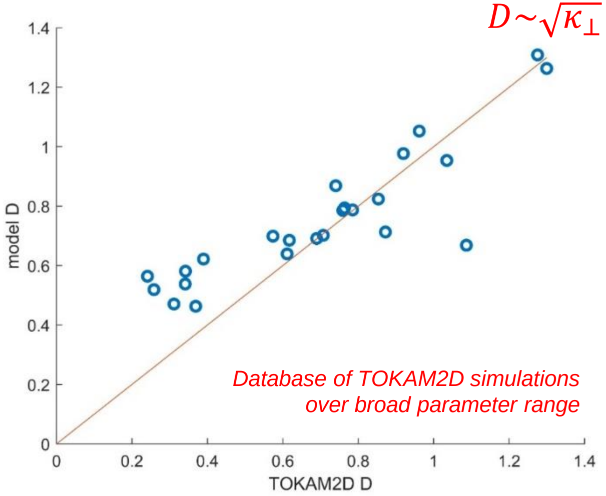
KU LEUVEN

Insights from 2D interchange simulations

[Coosemans et al., PET 2021, accepted for publication in CTPP.]

- Propose diffusive model
  - $\overline{\boldsymbol{\Gamma}}_{i,E\times B} = \overline{n_i' \boldsymbol{u}_{E\times B}'} \sim -D_{E\times B} \nabla \overline{n}_i$
  - $\overline{\boldsymbol{Q}}_{i,E\times B} = \frac{3}{2}\overline{n_i \boldsymbol{u}_{E\times B}'' T_i''} \sim -\chi_{i,E\times B}\, \overline{n}_i \nabla_\perp \tilde{T}_i$





- Link coefficients to turbulent kinetic energy:

$$D_{E\times B} = C_D \rho_L \sqrt{\frac{\kappa_\perp}{m_i}}$$

$$\chi_{i/e,E\times B} = C_{i/e} D_{E\times B} \sim \frac{3}{2} D_{E\times B}$$

Self-consistent anomalous transport model for mean-field plasma edge codes

- $\kappa_\perp$ equation for 2D electrostatic interchange turbulence

$$\frac{\partial}{\partial t}\bar{n}\kappa_\perp + \nabla \cdot \nabla \cdot \left(\bar{\boldsymbol{\Gamma}}_i \kappa_\perp + \frac{1}{2}\overline{mn\boldsymbol{V}''V_{E\times B}''^2} + \overline{\phi'\boldsymbol{J}_{||}'} \right) = \bar{S}_{IC} + \bar{S}_{||} + \bar{S}_{RS}$$

  - Analytical (!) closure for interchange source / sink
  - Fast parallel transport due to current fluctuations
- Coupled to ‘regular’ mean field equations
  - Transport coefficients now determined by local value of $\kappa_\perp$

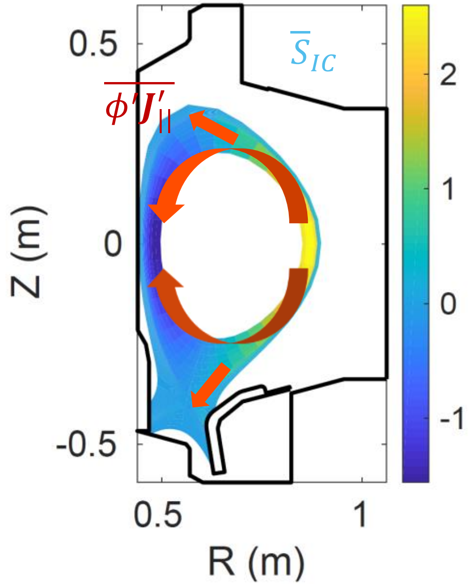
$$D_{E\times B} \sim \frac{C_D \kappa_\perp}{\sqrt{\kappa_\perp / \mathrm{m}_i}/\rho_L + C_s \left| \nabla \bar{V}_{E\times B} \right|} \qquad \chi_{E\times B} \sim D_{E\times B} \sim \eta_{E\times B}$$

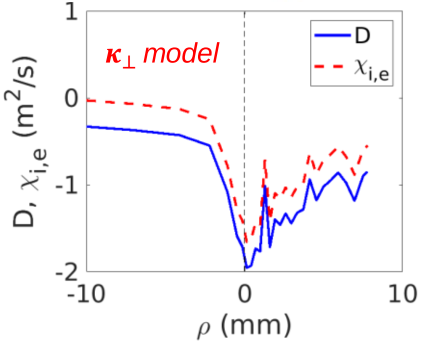
  - Global energy conservation ensured (mean-field + turbulent)
- Implemented in new ‘extended grids’ version of SOLPS-ITER

[Dekeyser et al., NME **27** (2021) 100999.]

- Validation with C-Mod data ongoing

[Dekeyser et al., PET2021, Lausanne, submitted to CTPP.]

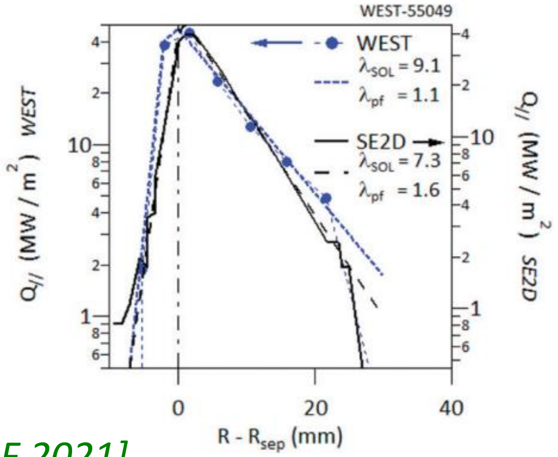




Intermediate step in hierarchy of transport models

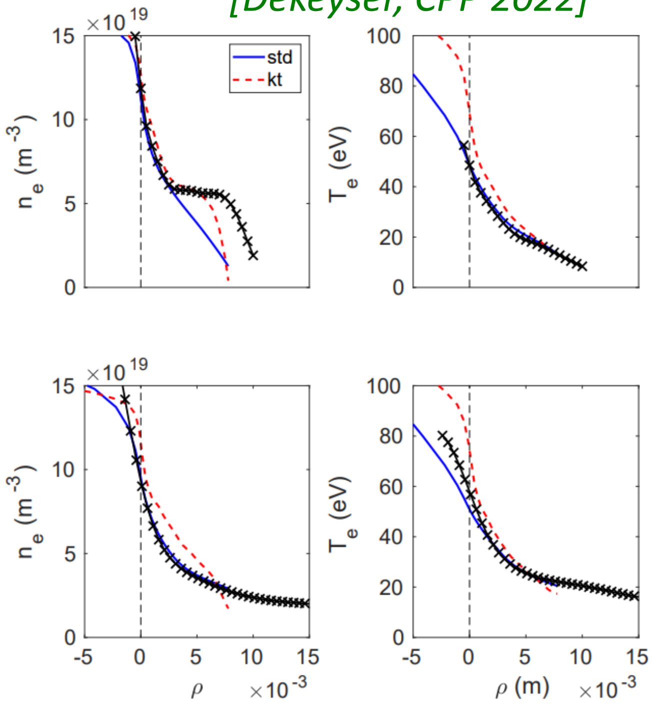
Direct Numerical Simulation of turbulence → **RANS models** → Mean-field models with gradient-diffusion ansatz

- **Reduced turbulence models** further developped and tested:
  - **Theoretical** basis + numerically based **closure**
  - **Validation** against experiments (WEST, C-mod)



[Baschetti, NF 2021]

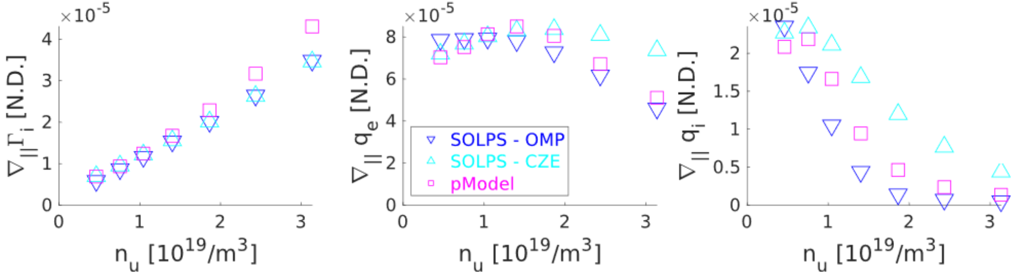
[Dekeyser, CPP 2022]



Task 3: intermediate turbulent transport description

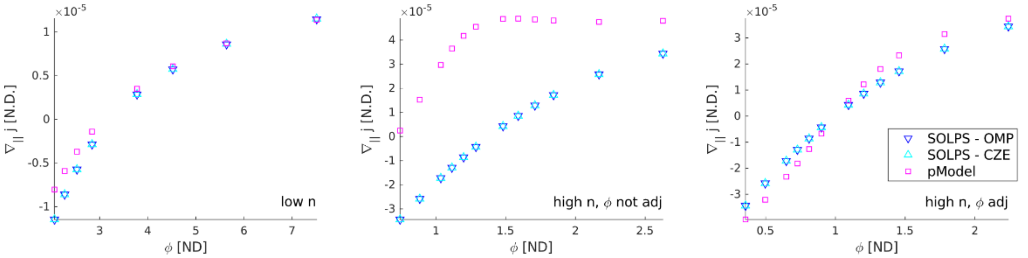
1. Development and implementation of a model for the 3rd (parallel) direction ...

- Conclusions of validation exercise:
  - Reasonably captures trends in (performed) density / power / recycling scans



‘Effective parallel sinks’ of particles & energy

  - As expected: model requires different upstream potentials for floating conditions



‘Effective parallel current sink’

Task 3: intermediate turbulent transport description

2. Development of RANS-model based on 3D simulations

Status: post processing SOLEDGE3X data in progress

- Created script to evaluate toroidally averaged values required for k_E −equation evaluation (i.e. $\langle NXY\rangle_{tor}$, $\langle XY\rangle_{tor}$, $\langle N\rangle_{tor}$) [no neutrals]
- Translation to ensemble averages in progress
- Initial assessment of RANS-related quantities: test scaling $D \sim \rho_0\sqrt{k_E}$

Preliminary results!