Self-consistent integration of plasma transport and divertor physics in the SOLEDGE3X-EIRENE code: status, results and prospects

4th IAEA Technical Meeting on Divertor Concepts, Vienna, 7-10 November 2022

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- ❑ Introduction: towards predictive edge modelling tools
- ❑ The SOLEDGE3X code for self-consistent edge physics
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  - Turbulence in realistic plasma geometry
  - Multi-component plasmas beyond the Braginskii closure
  - Self-consistent neutrals recycling
  - The challenge of realistic wall geometry
  - The path to reactor scale simulations
- ❑ Conclusion

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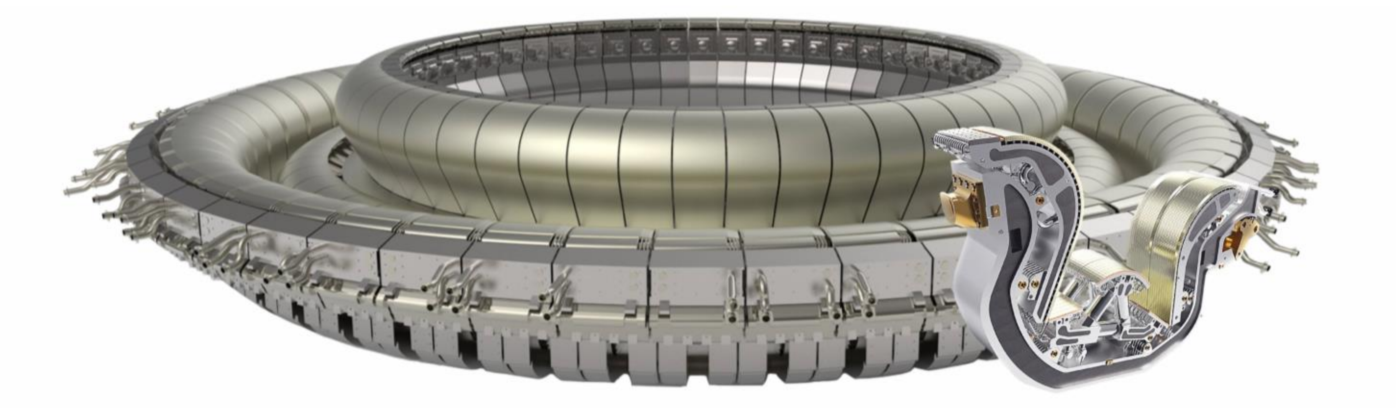
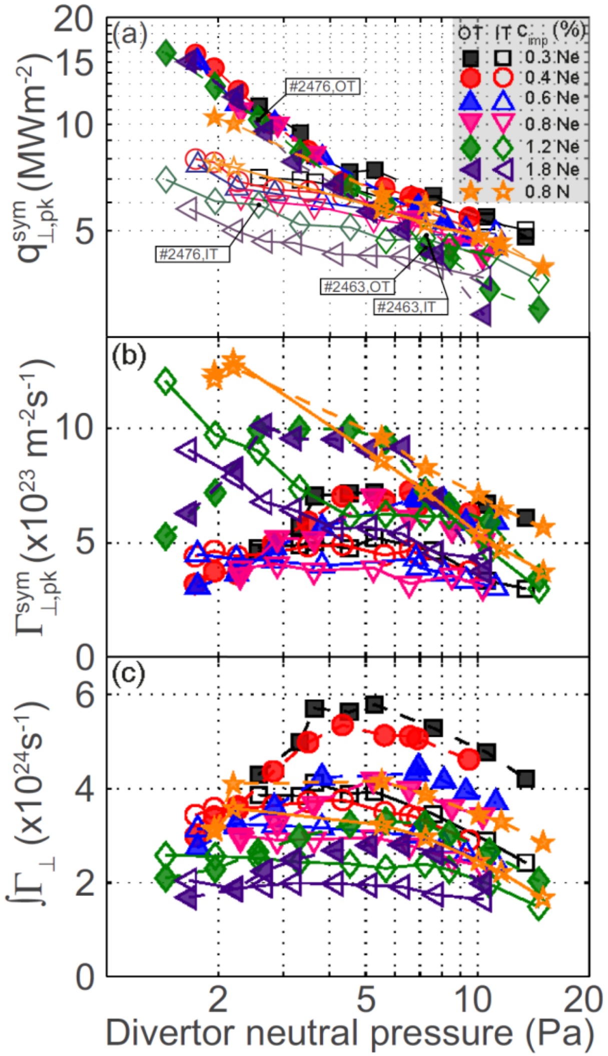
Mean-field codes are still the work-horse of exhaust modelling

- Key **exhaust** questions addressed by edge plasma modelling:
  - Evaluate **heat and particle fluxes** at the targets / wall / pumps
  - Define **operational scenarios** to fulfil engineering constraints
  - **Design** machine and systems to access these regimes

- For 2 decades **relied on mean-field codes**, e.g. SOLPS-ITER
  - ✓ Best **compromise fidelity / cost**
  - ✓ Only codes able to model **divertor regimes up to detachment**

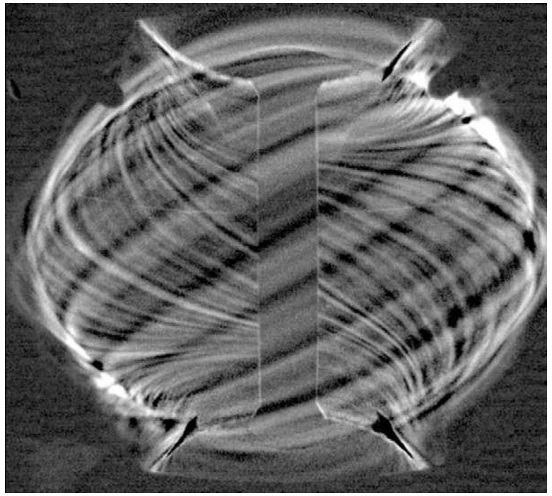




[R. Pitts, NME 2019]

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!

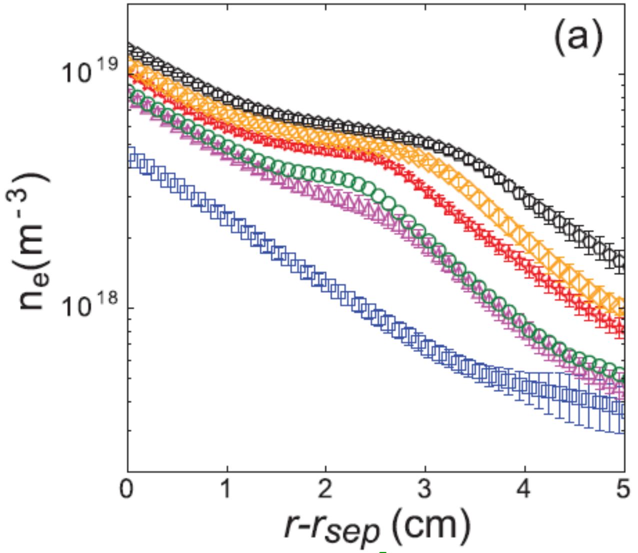


[B. Dudson, PPCF 2008]

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

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

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



[A. Wynn, NF 2018]

Milestones to predictive exhaust modelling

	mean-field (SOLPS, EMC3…)	3D turbulence
Self-consistent cross-field transport		✓
Neutrals	kinetic	
Impurities	✓	
Plasma geometry	✓	✓ (relatively recent)
Wall geometry	✓ (in general not up to the wall)	
Acceptable runtime	~	

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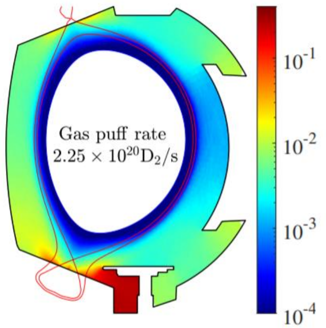
SOLEDGE3X code for self-consistent edge physics

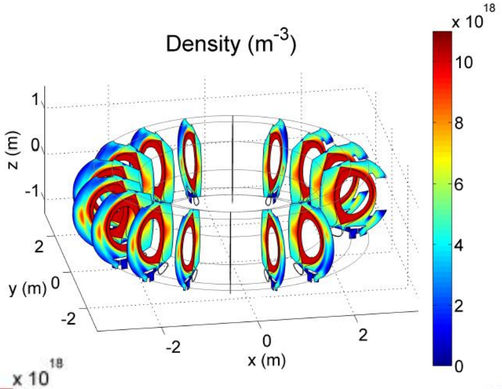
- Starting observation: **fluid plasma model in 2D mean-field code with drifts is not different from 3D turbulence codes** = drift fluid with collisional closure

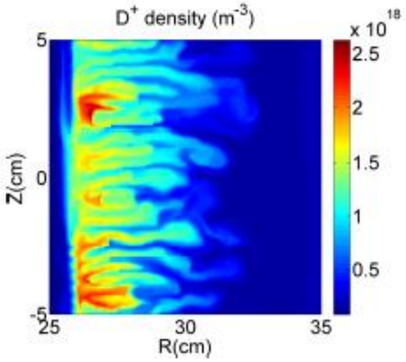
- Strategy: code that can **run in 2D or 3D as well as in mean-field or turbulence mode = SOLEDGE3X**
  - in practice: same equations, only input parameters change

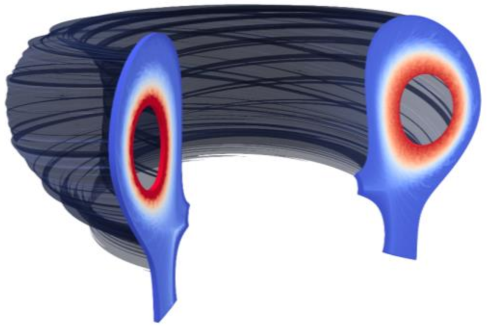
	Mean-field	Turbulence
2D	✓	✓
3D	✓	✓



(a) $n_{neu}[10^{19}m^{-3}]$







- Benefits:
  - Use **2D mean-field mode as test bench** to gather experience on neutrals / impurities… => generalize to 3D turbulence
  - Facilitate **transfer from one model to the other** (e.g, restart 3D from 2D, use transport coefficients from 3D in 2D)

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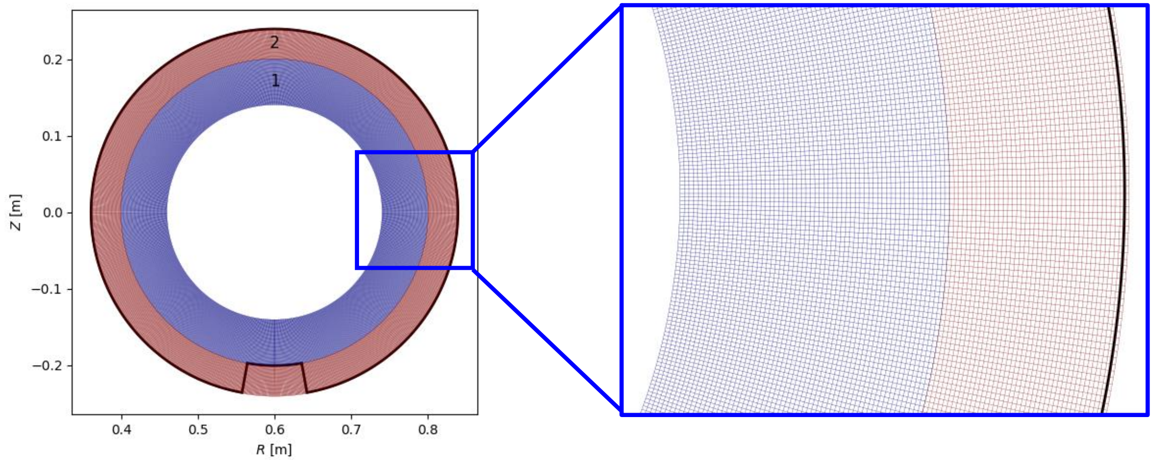
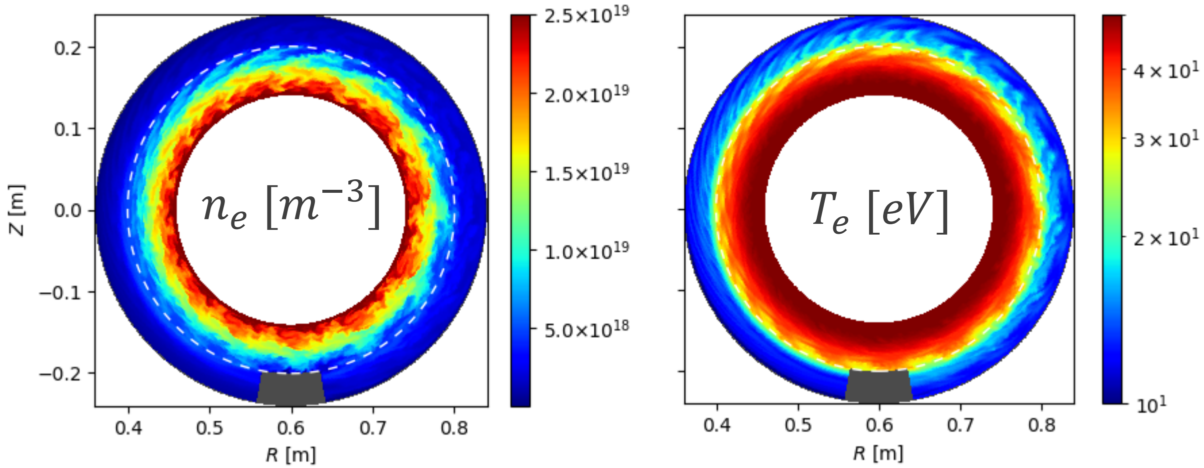
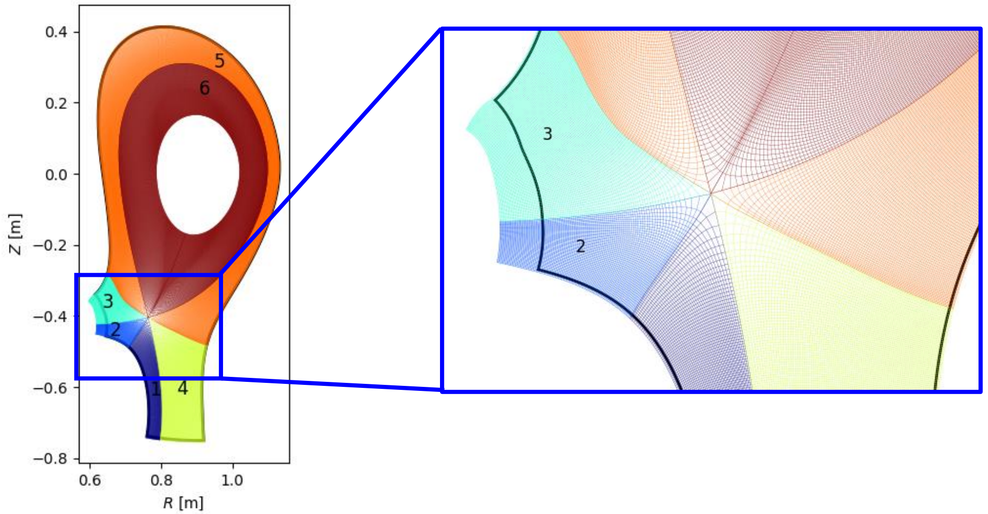
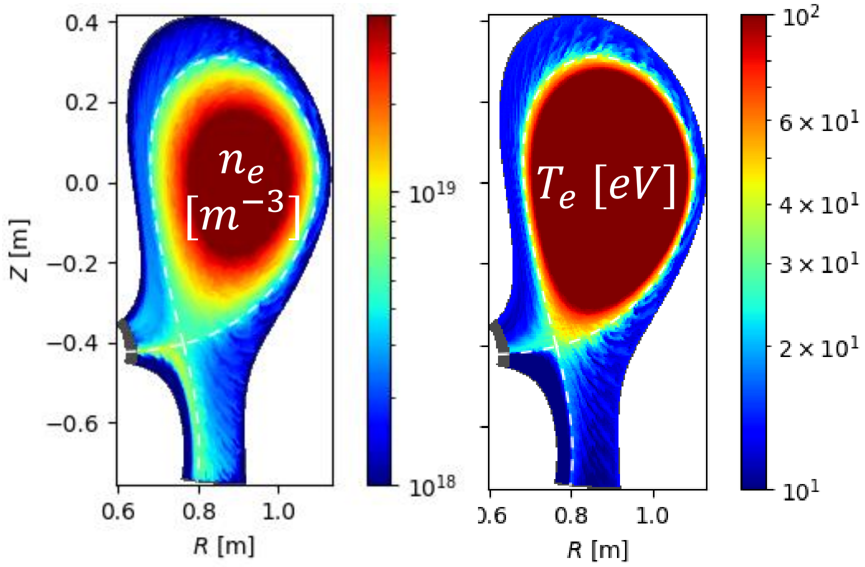
Realistic plasma geometry routinely available

- SOLEDGE3X *(like other turbulence codes)* runs **routinely in realistic axisymmetric magnetic geometries**
  - Numerical discretization inspired from 2D codes: **piece-wise structured mesh**









Turbulence in diverted geometry – lessons learnt

- 3D turbulence simulations in **realistic X-point geometry** studied in the last 6 years by a variety of turbulence codes

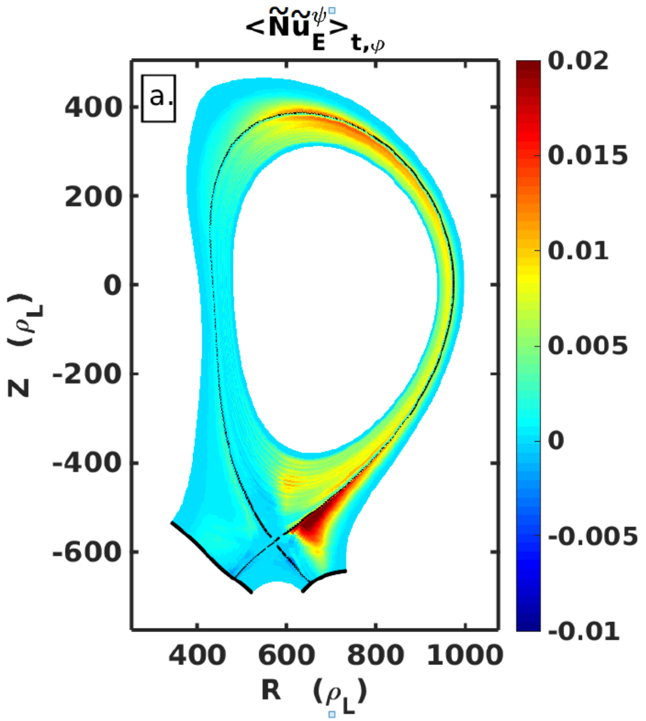
[Galassi, NF 2017; Galassi, Fluids 2019; Gallo, PPCF 2017; Nespoli, NF 2019; Nespoli, NF 2020; Zholobenko, NF 2021; Oliveira, NF 2022]

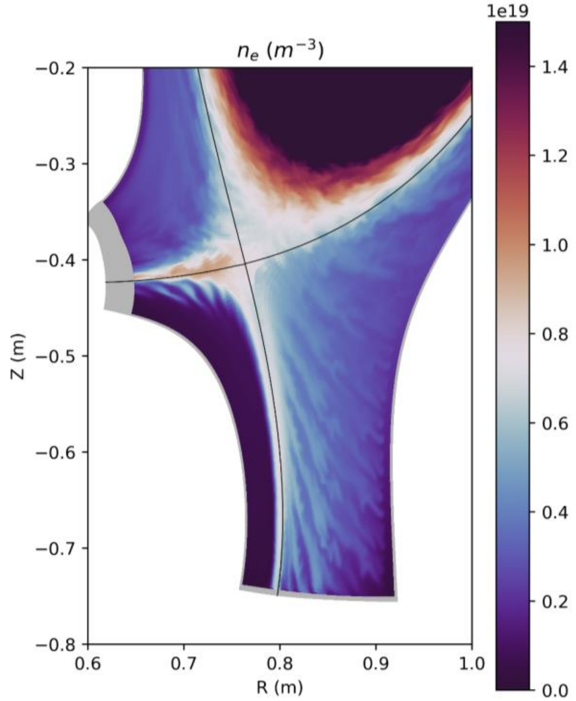
- Take-away messages concerning SOL transport:
  1. Transport is ballooned and scales with **flux expansion**

$$D_\perp \propto f_x^{1-2} \times f_{balloon.}$$

  2. Complex **ExB advection cell around X-point** drives significant transport

  3. significant **turbulence in divertor** dependent on divertor topology => λ_q and S impacted





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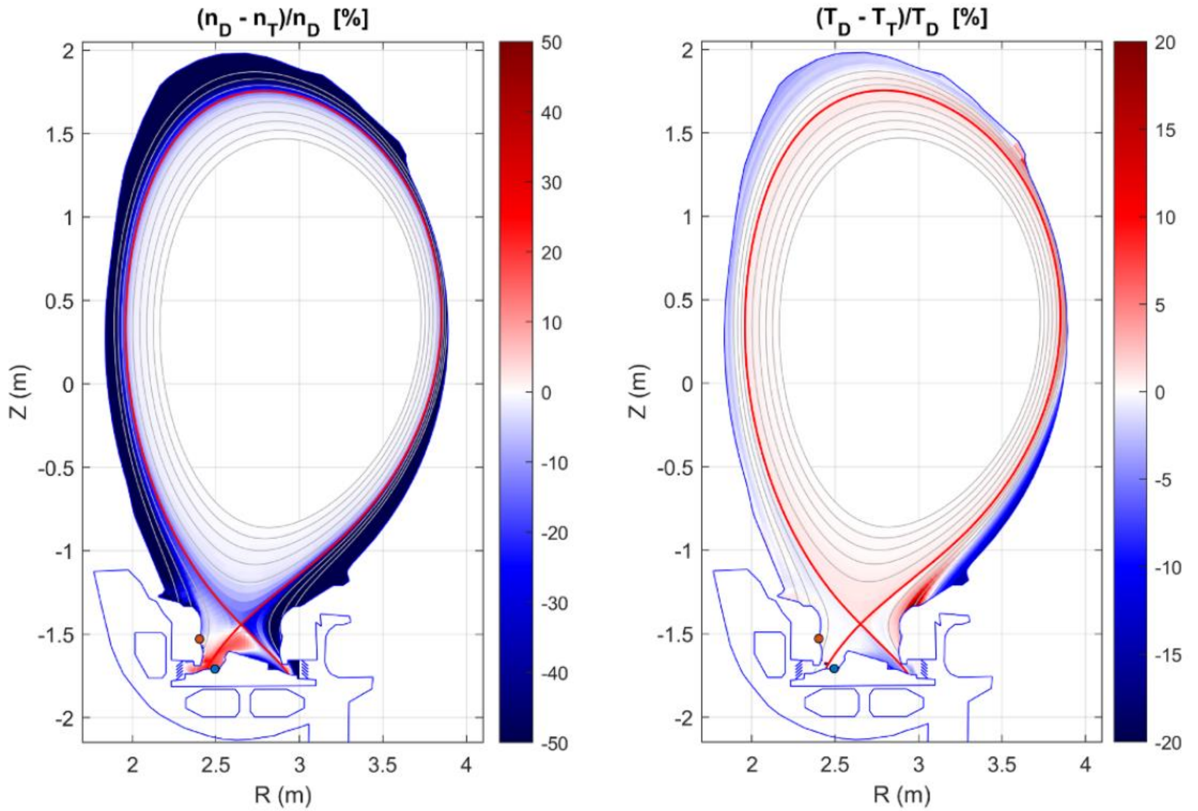
Beyond Braginskii: Zhdanov closure with multi-ion temperature

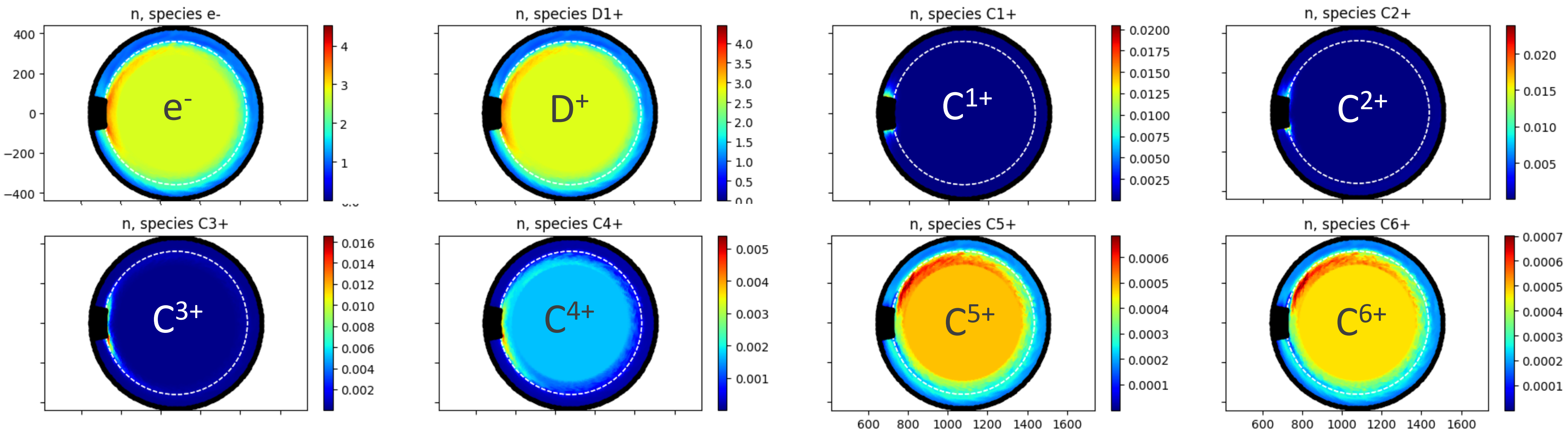
- **Limit of Braginskii** closure: not valid for close to unit mass and density ratios
  - Not applicable to D-T plasmas among others
- **Zhdanov closure implemented in SOLEDGE3X**
  - Code can run with **arbitrary number of ion species**
  - Separate energy balance (**different T_i**) for each ion species
- Applied to **JET D-T-Ne** discharges in mean-field mode
  - **D/T far from uniform** with possible implications for exhaust
  - **Temperatures can depart significantly** in far SOL - could require extension of Zhdanov *[Raghunathan, PPCF 2022]*



[Y. Marandet, this conference]
[H. Bufferand, PPCF 2022]

Available in 3D turbulence cases within some approximation

- **Proof of principle simulation** performed with D+C (fluid neutrals) and self-consistent sputtering



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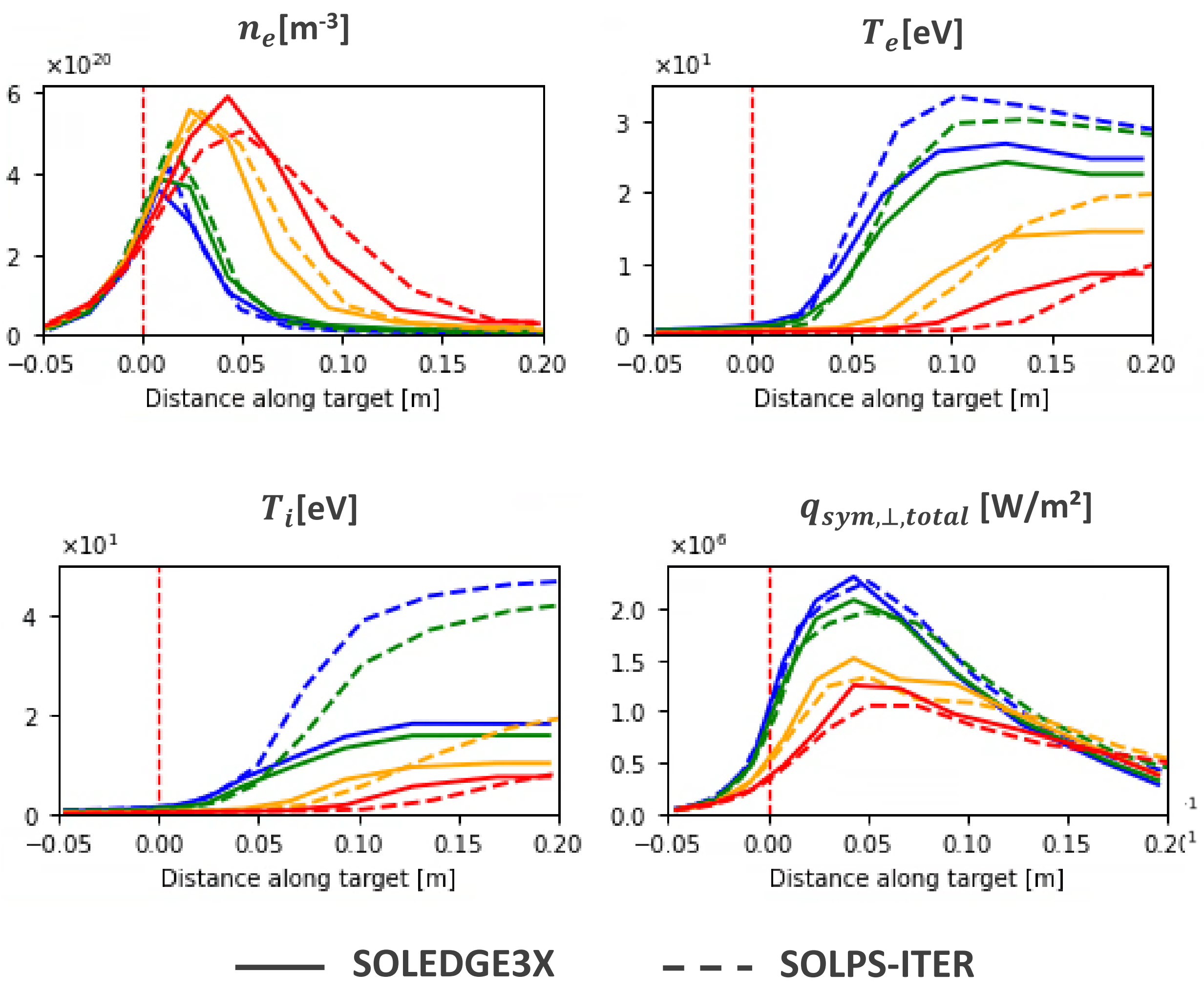
SOLEDGE3X coupled to kinetic neutrals model via EIRENE

- **SOLEDGE3X coupled to EIRENE**
  - Access to **up-to-date kinetic A&M models** (necessary for detachment)
- Applied in 2D mean-field mode to **density regimes in ITER PFPO-1 and PFPO-2 cases**

[N. Rivals, CPP 2022; N. Rivals, NME 2022; N. Rivals, this conference]

  - Successful benchmark with SOLPS-ITER database => **sane implementation**
- Lessons learnt:
  - ITER cases demanding for **code robustness** => specific numerical methods
  - EIRENE >95% of computing time => advanced coupling scheme and/or **faster kinetic neutrals solver** needed! (GPU?)

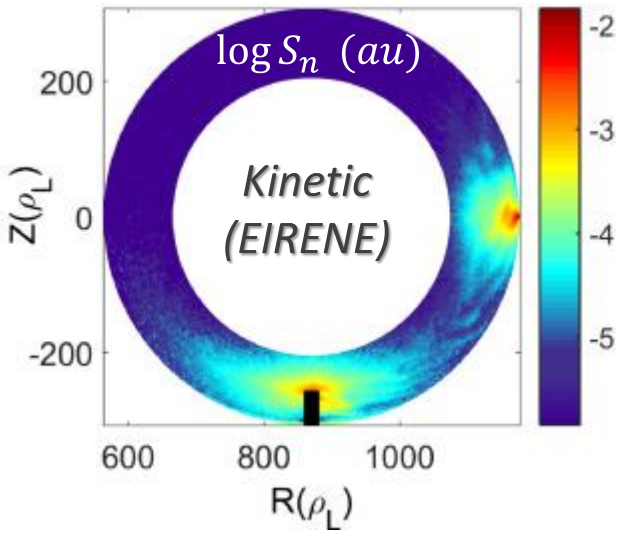


(color = through-put scan)

Generalization to 3D poses technical challenges

- Coupling to **EIRENE readily available in 3D** but blocking **technical limitations for large cases**
  - **Memory limit** due to pure MPI parallelization
  - E.g., Marconi = 48 cpu / node => >5TB of memory required per node (196 GB available) to use all cpus in full-scale TCV case

[D.M. Fan, NME 2019]

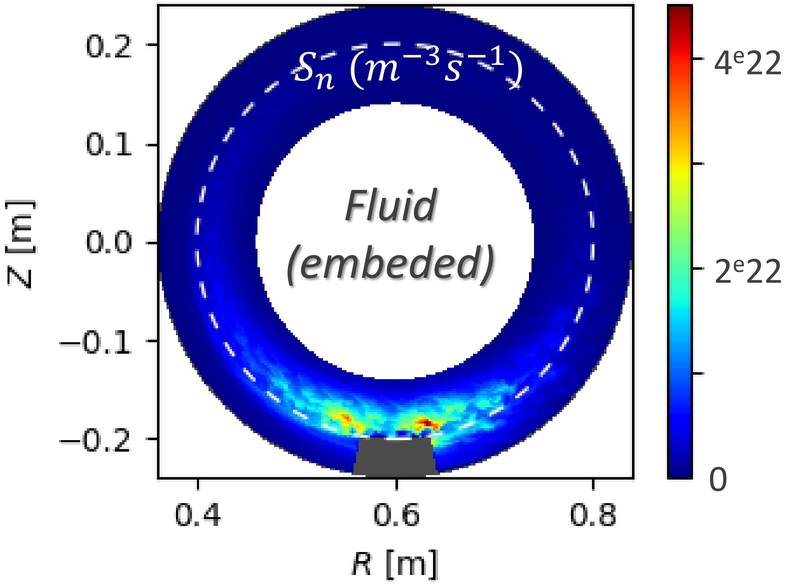


- Solutions:
  - Mid-term: **OpenMP-parallelized** version of EIRENE (TSVV5 - to be released)
  - Long-term: **domain decomposition** in EIRENE?
  - Short term: **embedded fluid neutrals model** with recycling/sputtering

$$\partial_t n_n + \vec{\nabla} \cdot \overrightarrow{\Gamma_n} = S_{n_n}$$

$$\begin{cases} \overrightarrow{\Gamma_n} = n_{n,eq} \overrightarrow{u_i} - D_p^n \vec{\nabla} p_n \\ D_p^n = \left(m \left(n_i K_{cx,m} + n_e K_i \right) \right)^{-1} \\ S_{n_n} = n_i n_e K_r - n_n n_e K_i \end{cases}$$

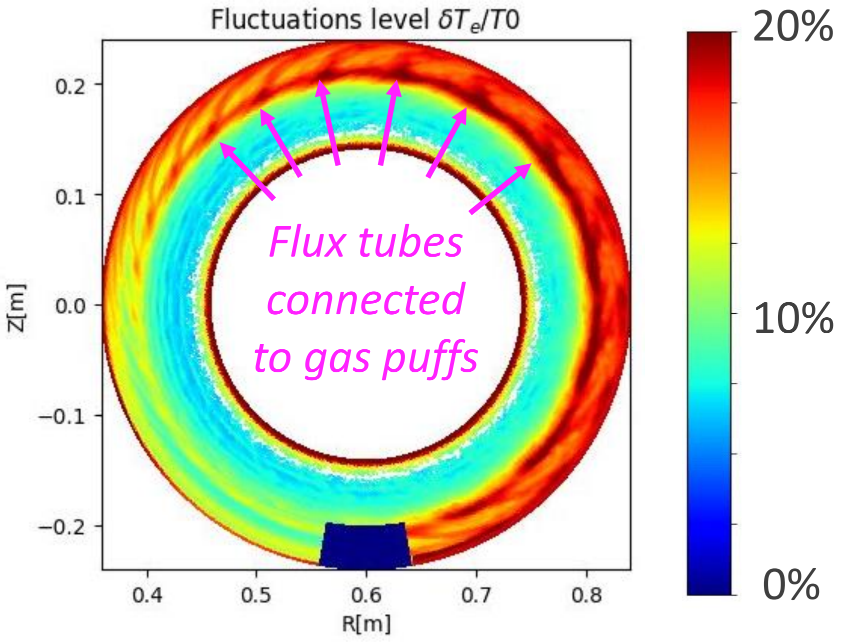
[N. Horsten, NF 2017]

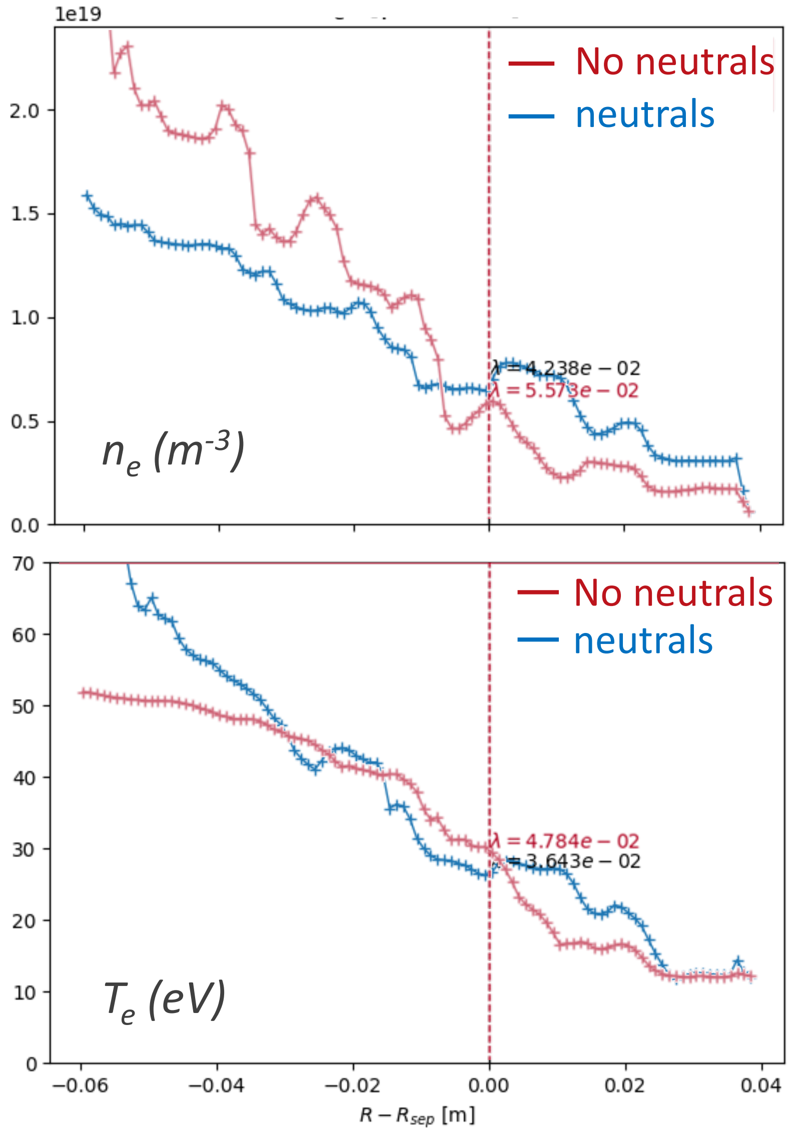


A first insight on how neutrals impact turbulent transport

- Global reorganization of turbulence to move **from convective to conductive heat transport**
  - inversion of density and temperature **profiles**, density fluctuations replaced by temperature **fluctuations**

- Turbulent **transport locally perturbed by gas puff** fuelling
  - convective cells develop around flux-tube connected to gas puff





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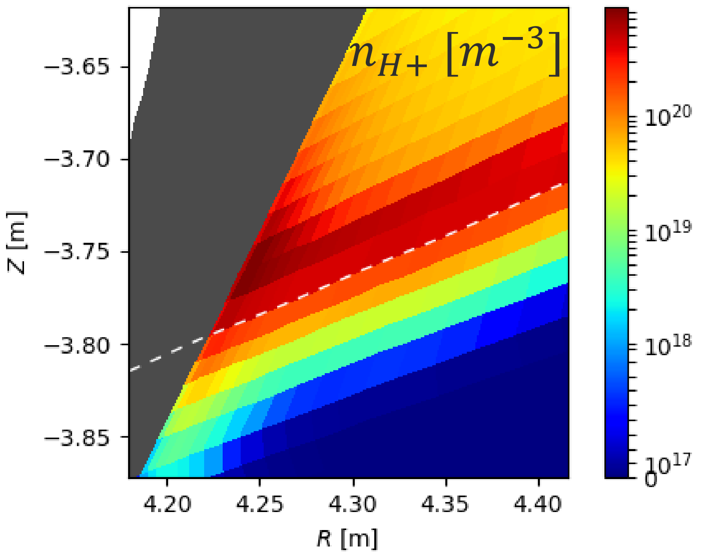
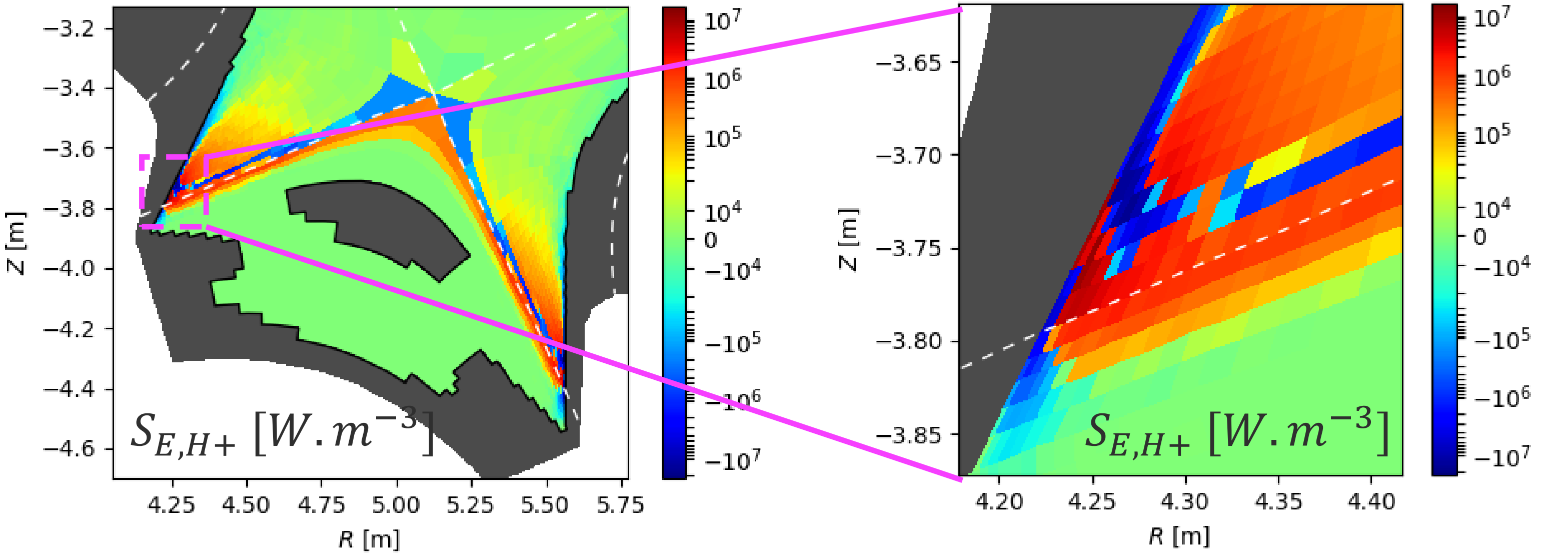
Wall conformity: a major constraint for discretization schemes

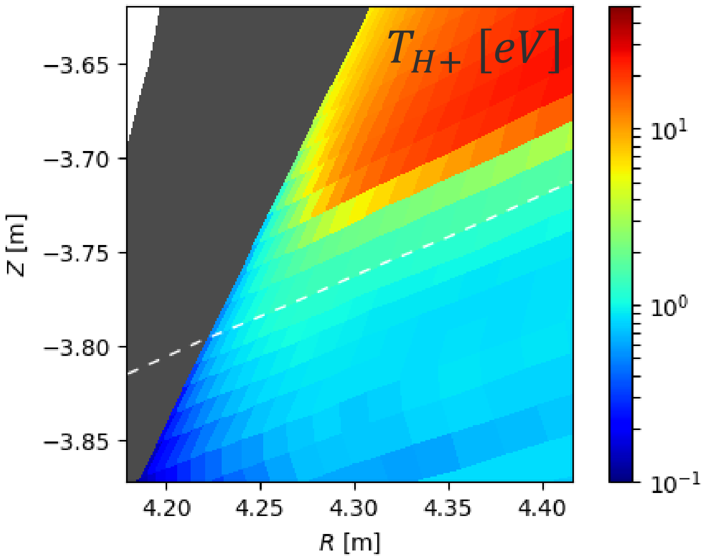
- **Wall conformity is mandatory** for modelling of high-recycling cases
  - **gradient lengths can be ≲1mm** at target plates in high density regimes
  - an approximate wall geometry can lead to wrong results *[P. Tamain, NME 2021]*

- Constraint not compatible with all discretization schemes



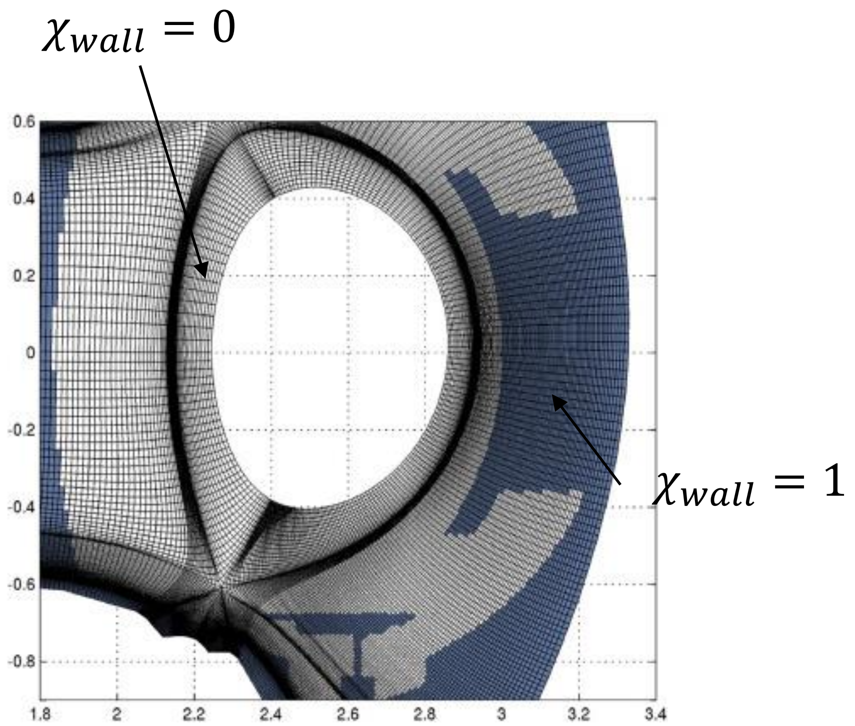
ITER PFPO1 pure H L-mode case #2299 [N. Rivals, CPP 2022]

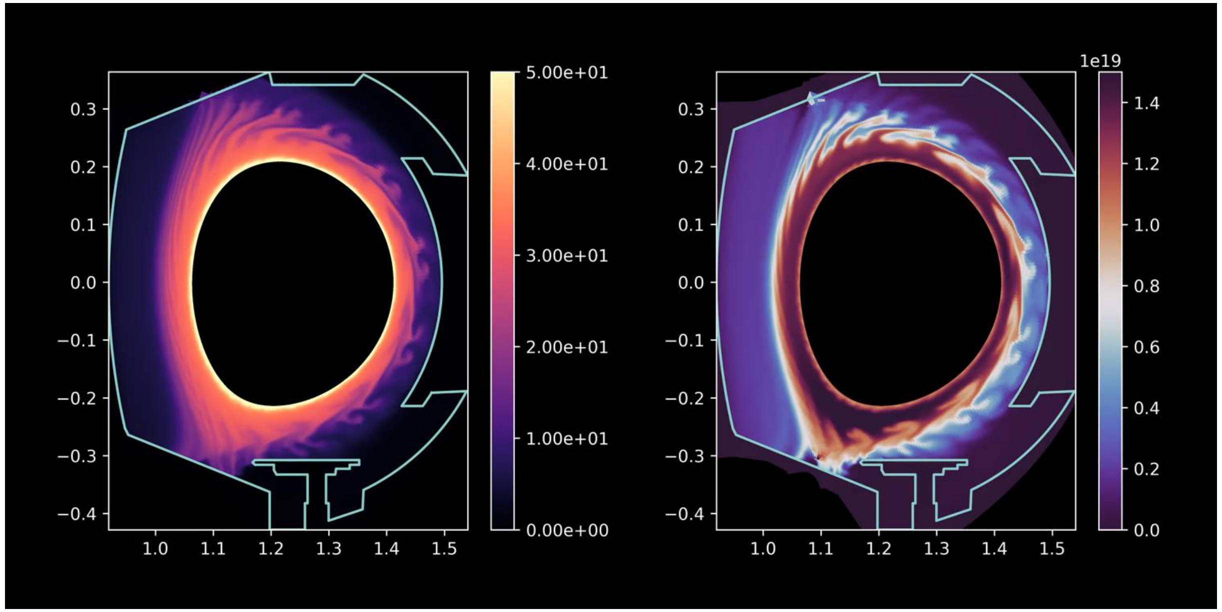




Arbitrary 3D wall geometry in SOLEDGE3X

- Solution in SOLEDGE3X: **use of mask function** inspired from penalization methods
  - Allows **arbitrary wall shape** independently of the mesh, **including 3D**

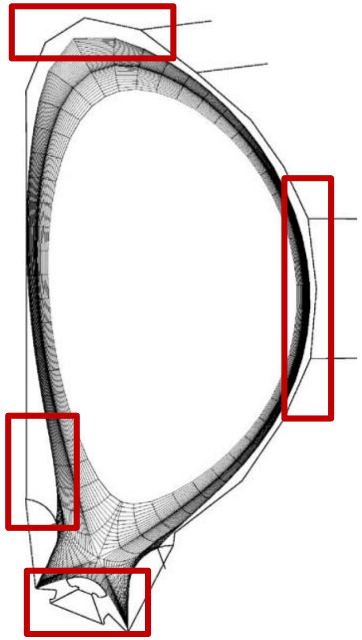




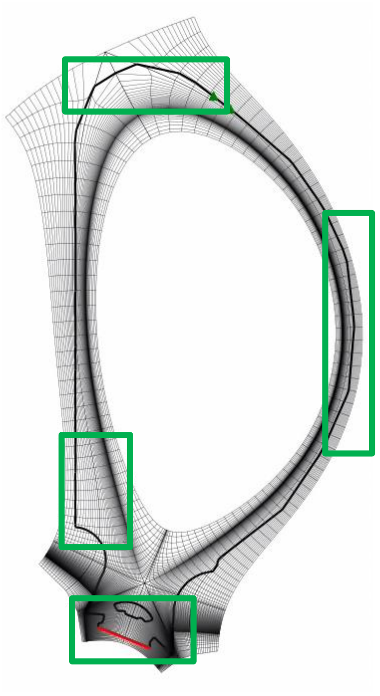
Up-to–the wall simulations

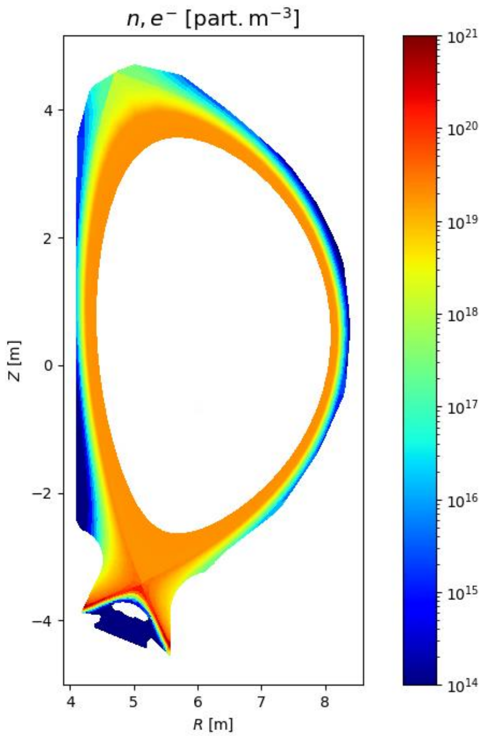
- Mask approach for wall geometry unlocks **simulations up-to-the wall**
  - necessary for evaluation of **first-wall fluxes** but also for **complex divertor geometries** (e.g., slot)
- Application to ITER PFPO cases in 2D mean-field mode with full kinetic neutrals model *[N. Rivals, NME 2022]*

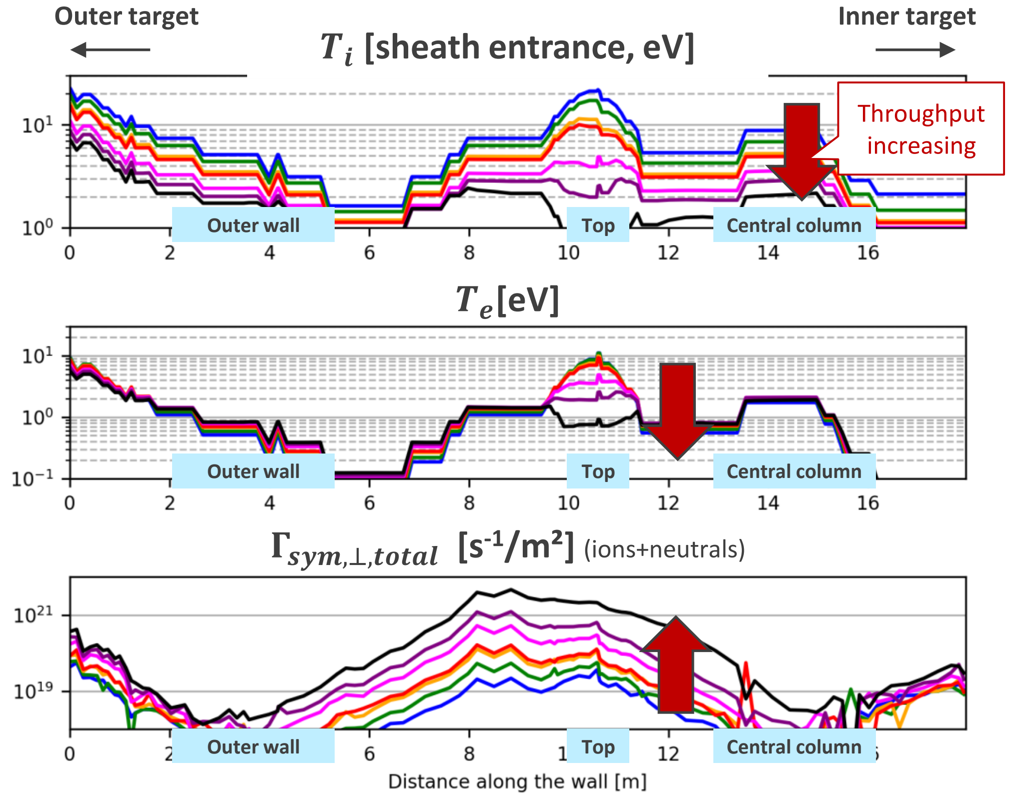
SOLPS-ITER domain



SOLEDGE3X domain







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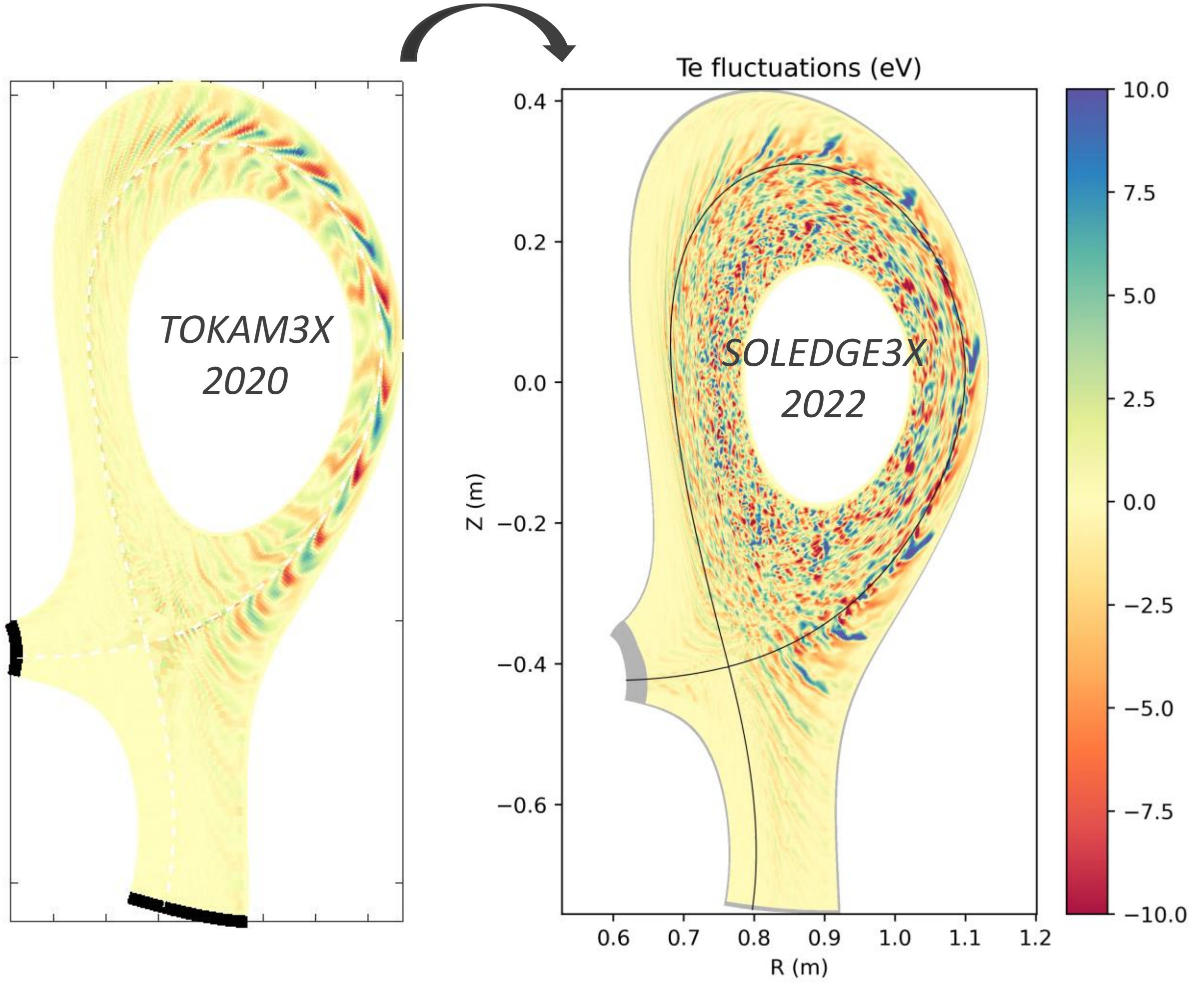
The path to reactor scale simulations

- Challenge for 3D turbulence codes: **time to solution**
  - Already issue for 2D mean-field high recycling cases in large machines
    - JET H-mode case ~ 1 week
    - ITER H-mode full power case ~ months
  - Some acceleration schemes (e.g., FCI) currently incompatible with self-consistent divertor physics
- **Important progress** in last few years thanks to investment in numerical optimization => **realistic MST cases accessible** (TCV, ASDEX) in 3D turbulence
- Progress of **HPC hardware both an opportunity and a threat**
  - GPU-ization promising but large investment and no clear standard yet

Realistic collisionality, x10 resolution



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Conclusion

- Progress in exhaust modelling towards reactor relevant simulations goes through **self-consistent integration of divertor physics (neutrals / impurities) and geometric flexibility in 3D turbulence codes**

- **Integration largely achieved in SOLEDGE3X** code
  - Freedom to run in **2D/3D and mean-field/turbulent** mode => any progress benefits all applications
  - Arbitrary axisymmetric plasma geometry, **arbitrary wall geometry** including 3D
  - **Multi-component plasmas** with Zhdanov closure, available for turbulence within some approx.
  - **Kinetic neutrals** in 2D with most advanced A&M model, **fluid neutrals** for 3D mode

- Some **challenges** remain:
  - Robustness in turbulence mode in high density regimes to be assessed (on-going)
  - **Performances of kinetic neutrals solver** are bottleneck => acceleration / memory footprint critical
  - **Up-scaling** of simulations to reactors while keeping compliance with rest of physics requires large investment

- Code **readily applicable to large variety of applications and machines**, available on request

https://www.soledge3x.com
https://gitlab.eufus.psnc.pl/tsvv3/soledge3x

Appendices

Modelling turbulence without DNS (1)

- Heuristic **k-epsilon model** inspired from RANS models in CFD *[S. Baschetti, NF 2021]*

Turbulence energy κ: $$\partial_t \kappa + \nabla_{\|}(\kappa u_{\|} b) - \nabla_{\perp} \cdot (D_\kappa \nabla \kappa) = \gamma_\kappa \kappa - \frac{1}{D_\omega}\kappa^2 - \varepsilon$$

Dissipation rate ϵ: $$\partial_t \varepsilon + \nabla_{\|} \cdot (\varepsilon u_{\|} b) - \nabla_{\perp} \cdot (D_\varepsilon \nabla \varepsilon) = \gamma_\varepsilon \varepsilon - \frac{V}{\kappa^{3/2}}\varepsilon^2$$

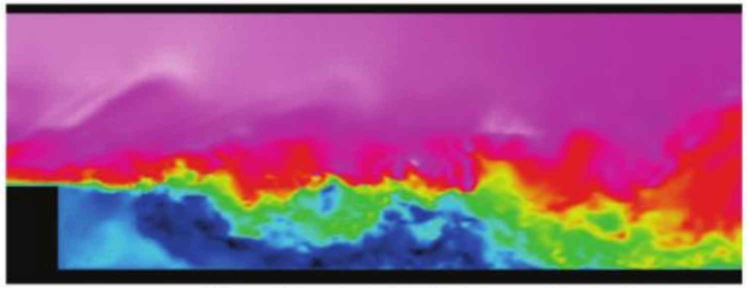
$$D_n = C_\nu \frac{\kappa^2}{\epsilon}$$

- Closure relying on:
  1. Theoretical considerations on leading instabilities (interchange here) and dissipation (Kolmogorov cascade here)
  2. Experimental scaling laws for λ_q

  $\Rightarrow$ **Single free parameter** (C_ν) for self-consistent determination of transport at every point in space at **negligible extra computing cost**

Source: Rémy Fransen, 3rd INCA colloquium, ONERA, Toulouse (2011)

RANS

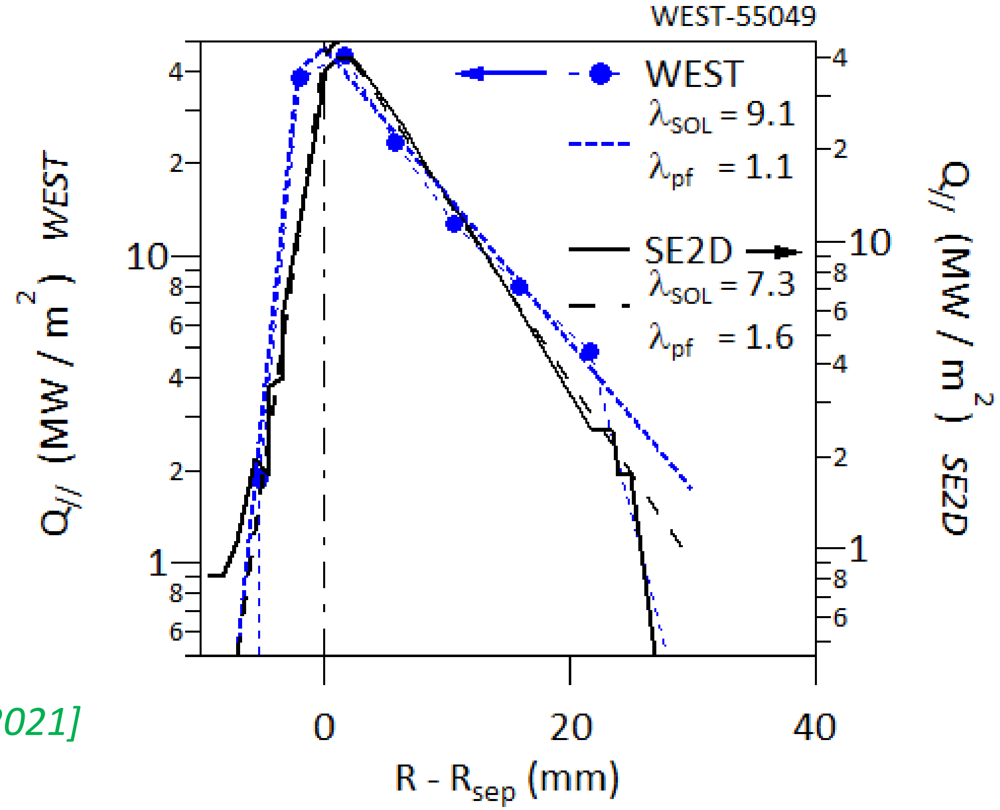


Source: Rémy Fransen, 3rd INCA colloquium, ONERA, Toulouse (2011)

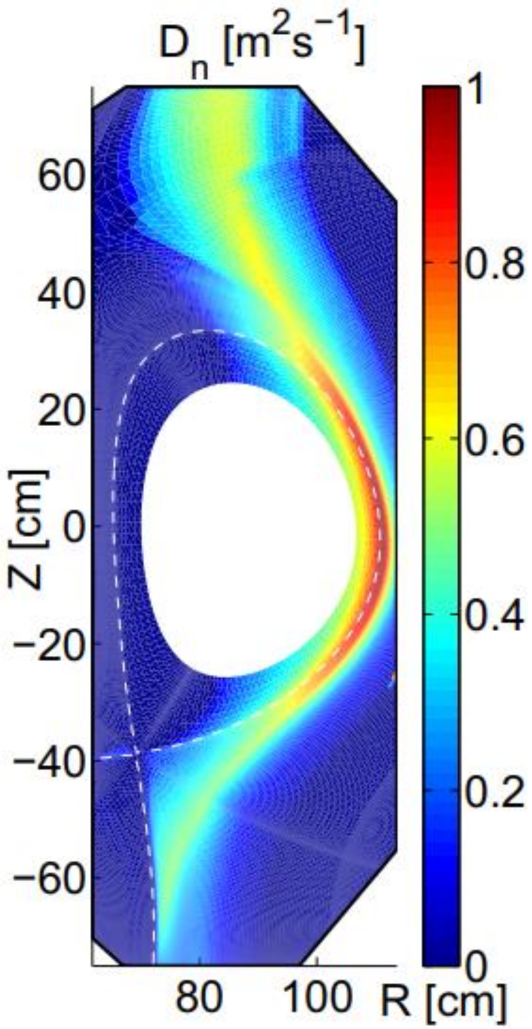
LES

Modelling turbulence without DNS (2)

- Model results **confronted to experiments** on **TCV** and **WEST**
  - **Remarkable agreement** in both machines in several configuration once C_ν tuned (once and for all)
  - Recovers spatial distribution (ballooning) of turbulent transport



[S. Baschetti, NF 2021]



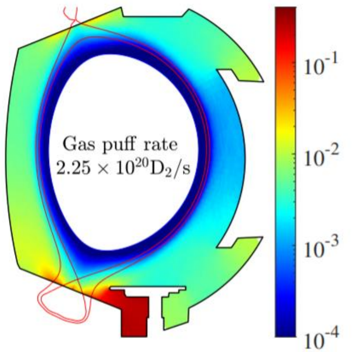
[S. Baschetti, J. Phys.: Conf. Series 2018]

In practise: same model, different parameters

- Example of particle balance:

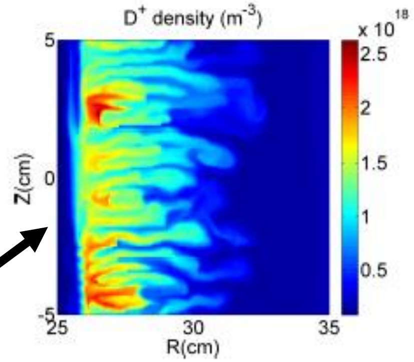
$$\partial_t n_i + \vec{\nabla} \cdot \left(n_i u_{i\parallel} \vec{b} + n_i \vec{u}_{i\perp} \right) = S_{n_i} + \vec{\nabla} \cdot \left(\boldsymbol{D_{\perp n_i}} \vec{\nabla}_\perp n_i \right)$$

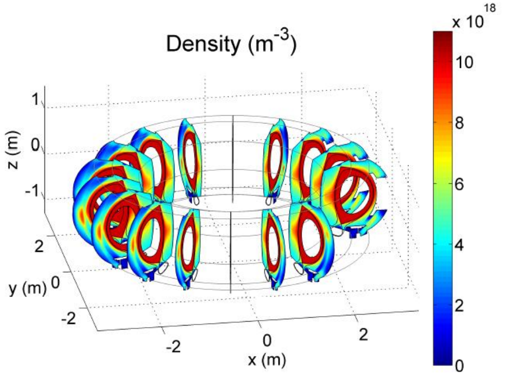
- **Same equation** is solved whatever mode is used, **only input parameters change**

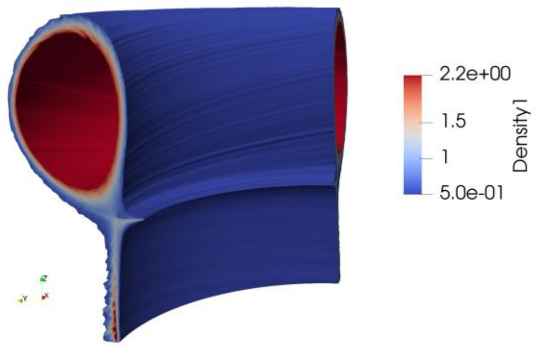


(a) $n_{neu}[10^{19} m^{-3}]$

	Mean-field	Turbulence
2D	$D_{\perp n_i} \sim$ anomalous $\partial_\varphi = 0,\ \vec{b} = \frac{B^\theta}{B}\vec{e}_\theta + \frac{B^\varphi}{B}\vec{e}_\varphi$	$D_{\perp n_i} \sim$ classical $\partial_\varphi = 0,\ \vec{b} = \frac{1}{\lvert\vec{e}_\varphi\rvert}\vec{e}_\varphi$
3D	$D_{\perp n_i} \sim$ anomalous * $\partial_\varphi \neq 0,\ \vec{b} = \frac{B^\theta}{B}\vec{e}_\theta + \frac{B^\varphi}{B}\vec{e}_\varphi$	$D_{\perp n_i} \sim$ classical $\partial_\varphi \neq 0,\ \vec{b} = \frac{B^\theta}{B}\vec{e}_\theta + \frac{B^\varphi}{B}\vec{e}_\varphi$



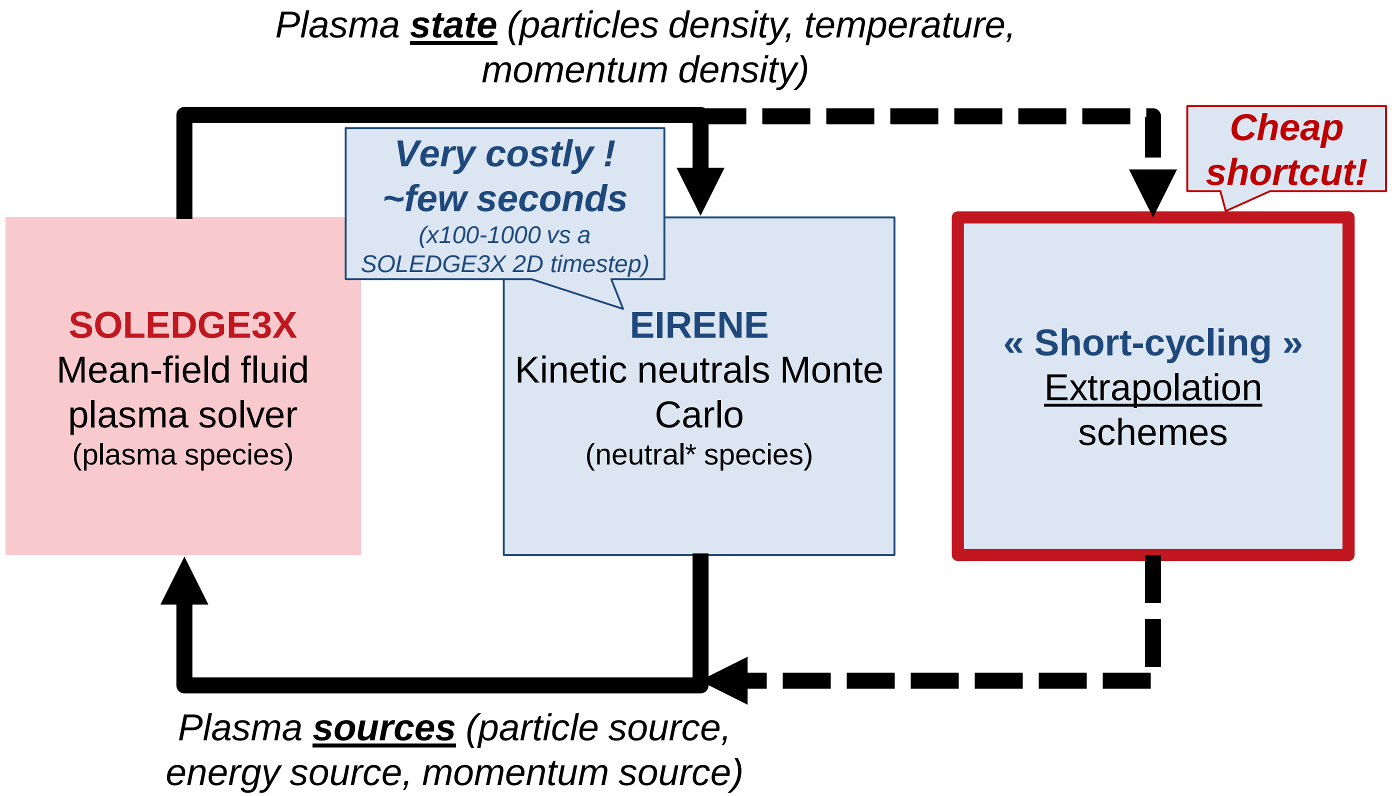




** Instabilities can kick-in when solving in 3D with drifts even at high diffusion*

SOLEDGE3X coupled to kinetic neutrals model via EIRENE

- Kinetic neutrals models mandatory for high-recycling / detached regimes in reactor relevant conditions
- **SOLEDGE3X coupled to EIRENE** via STYX interface
  - Immediate access to **up-to-date A&M models**
  - STYX enables **complex coupling schemes** to save computing time while ensuring stability



- Time step ~10^{-7}s (CFL)
- ITER solution equilibrium time: ~ 1s
- **Requires "shortcuts" i.e. extrapolations**

Sources extrapolation:

- $S_n = n_{atom}\, n_e < \sigma_{iz} v >$

Updated from plasma background (n_e, $< \sigma_{iz} v >$)

Keep spatial distrib. (n_{atom})

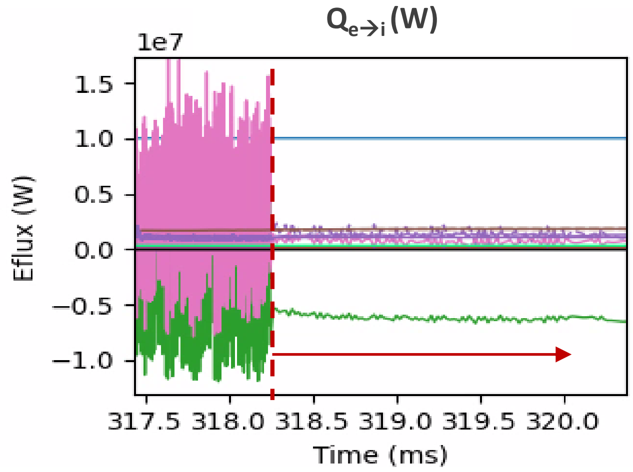
Extrapolated source from neutrals (S_n)

Lessons learned from application of kinetic neutrals for ITER cases

- **Coupling to neutrals is extremely stiff** in ITER scenarios ≠ medium sized tokamaks
  - Explicit coupling to EIRENE constrains stability and time step => **advanced coupling schemes** can help
  - Need to call EIRENE often => >95% of computing time => **faster kinetic neutrals solver** needed! (GPU?)

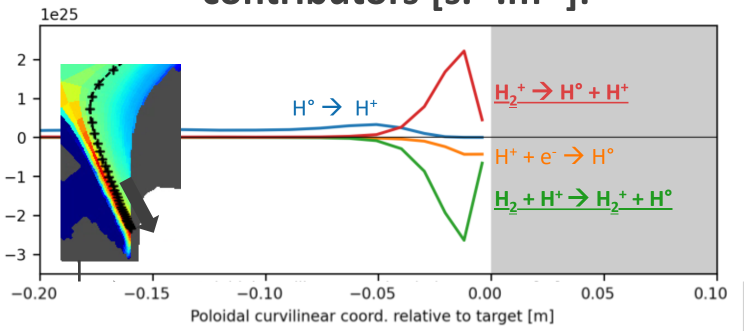
- Divertor conditions challenging require **specific numerical schemes for robustness**
  - E.g.: dense and cold plasma conditions => short time scales for collision terms => implicit treatment mandatory

$$Q_{e\to i} = \frac{m_e Z^2 e^4 \Lambda}{m_i (2\pi)^{\frac{3}{2}} \varepsilon_0^2 \sqrt{m_e}} n_e n_i \frac{1}{T_e^{\frac{3}{2}}} (T_i - T_e)$$



- **Details of A&M physics matter** *[N. Rivals, this conference]*
  - E.g., **CX and elastic collisions with molecules** are dominant contributors
  - **Molecular ions dynamics** must be tracked in far SOL and sub-divertor

H^+ particle source main contributors [$s^{-1}.m^{-3}$]:



The "real" issue with self-consistent neutrals recycling

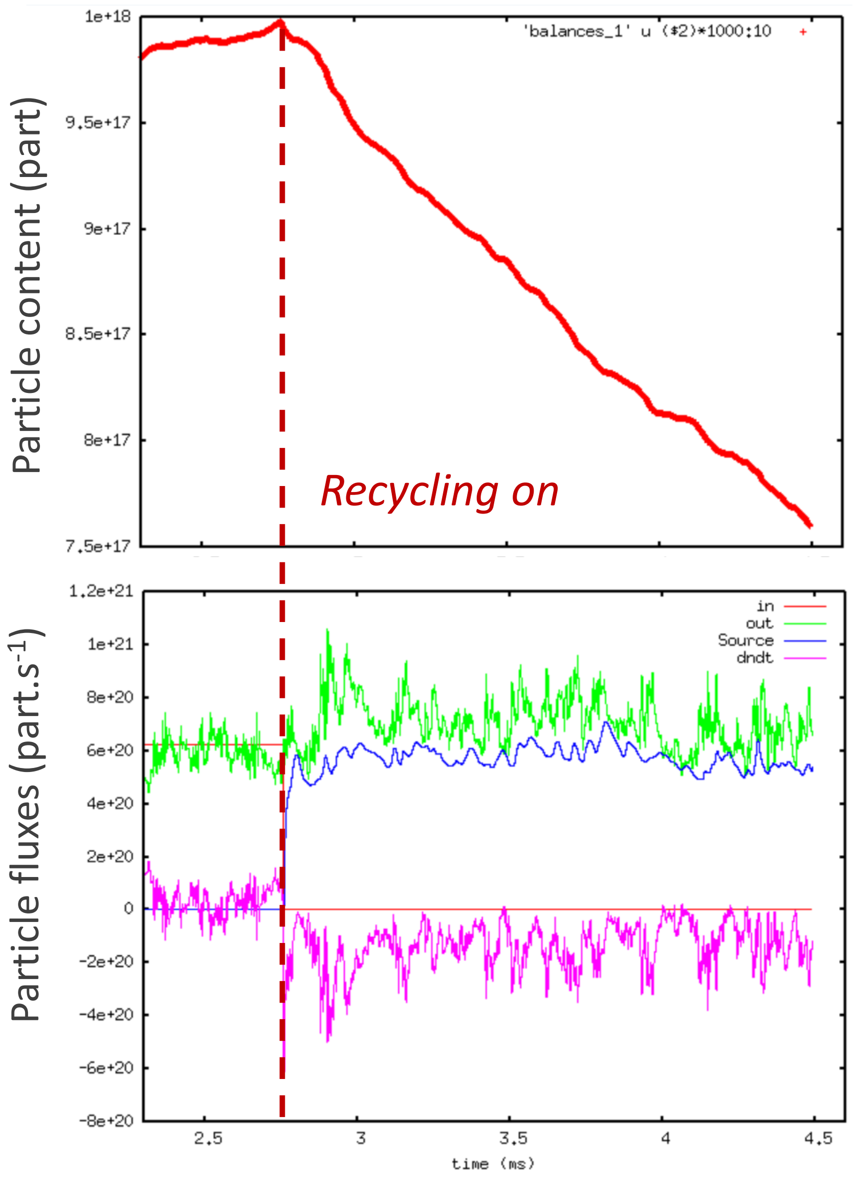
- Self-consistent **recycling adds long time scale** to reach particle balance:

$$\partial_t N = S_{puff} - (1 - R_{eff})\frac{N}{\tau_N(R_{eff})} \quad \Rightarrow \quad \boldsymbol{\tau'_N = \frac{\tau_N(R_{eff})}{1 - R_{eff}}}$$

E.g. , ITER mean-field cases: $[R_{pump} = 0.9928] < R_{eff} < [R_{wall} = 1] \quad \Rightarrow \quad \boldsymbol{\tau'_N > 10 \times \tau_N\ (0) \sim 2 - 3\ \mathrm{s}}$

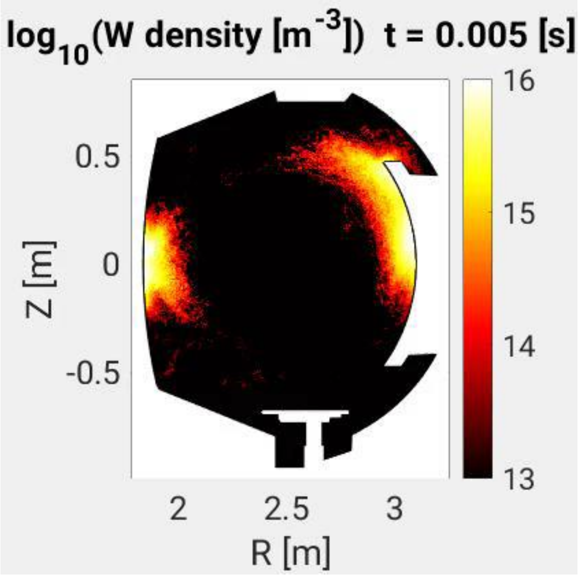
- **Does not preclude investigating turbulence** response to density regime "on the fly" ($\tau_{turb} \ll \tau'_N$)

- But need to **design acceleration schemes** to get to particle balance quasi steady-state
  - Under investigation: use of 2D mean-field simulations as starter for turbulence simulations ($D_\perp$?)



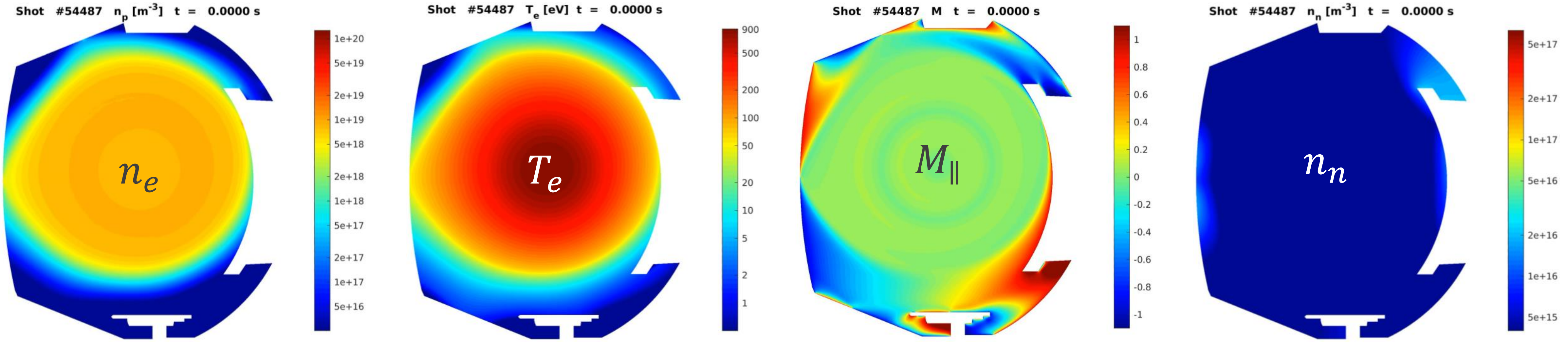
Variable equilibrium simulations in full geometry

- Other approach to geometry problem: **high order finite element methods** (HDG)
  - Implemented in version of SOLEDGE code with simplified plasma and neutrals model
  - Advantage: **total geometrical flexibility**, including time-dependent equilibrium



- Applied to **WEST discharge modelling from start-up to termination**

  [S. Di Genova, NF 2021; M. Scotto d'Abusco, NF 2022]



Conclusion

	2D mean-field	SOLEDGE3X
Turbulent transport		✓
Neutrals	kinetic	✓ Fluid and kinetic 2D ✘ kinetic 3D
Impurities	✓	✓ (approximation)
Plasma geometry	✓	✓ (routine)
Wall geometry	✓ (in general not up to the wall)	✓ (arbitrary, 2D/3D, up to the wall)
Acceptable runtime	~	✓ 2D mean-field MST ~ 2D mean-field reactor ~ 3D turbulence MST ✘ 3D turbulence reactor

- Code **readily applicable to large variety of applications and machines**, available on request

https://www.soledge3x.com
https://gitlab.eufus.psnc.pl/tsvv3/soledge3x

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