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Model advancements in mean-field plasma edge codes to enable computationally achievable simulations of the ITER and DEMO reactors

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EUROfusion

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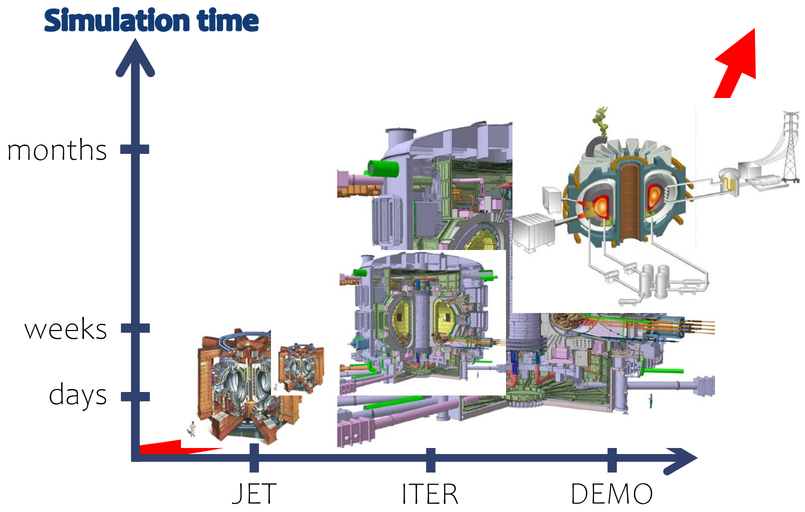
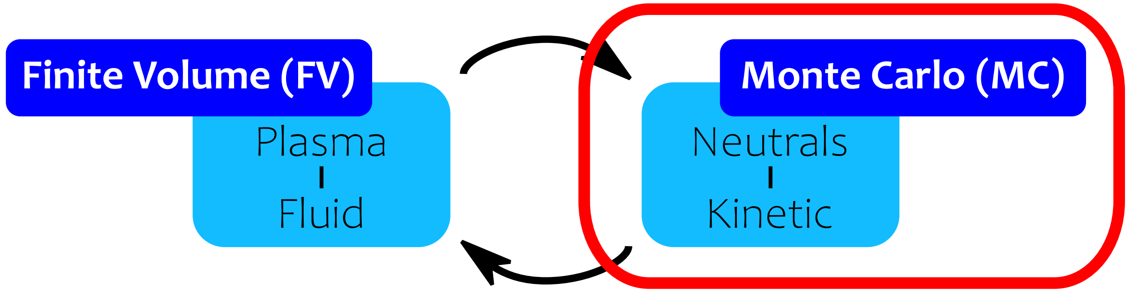
Important issues with mean-field plasma edge simulations

1. Simulation time with kinetic neutral model strongly increases for reactor-scale devices



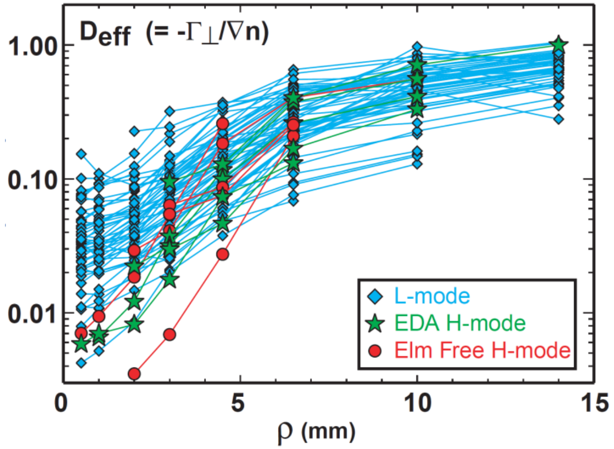


Intense plasma-neutral interactions for detached divertor conditions

2. Ad-hoc model for anomalous turbulent transport

Simple anomalous transport assumptions (constant coefficients; radial profile; …) vs. complex poloidal transport behavior

Dependence on plasma regime/conditions?



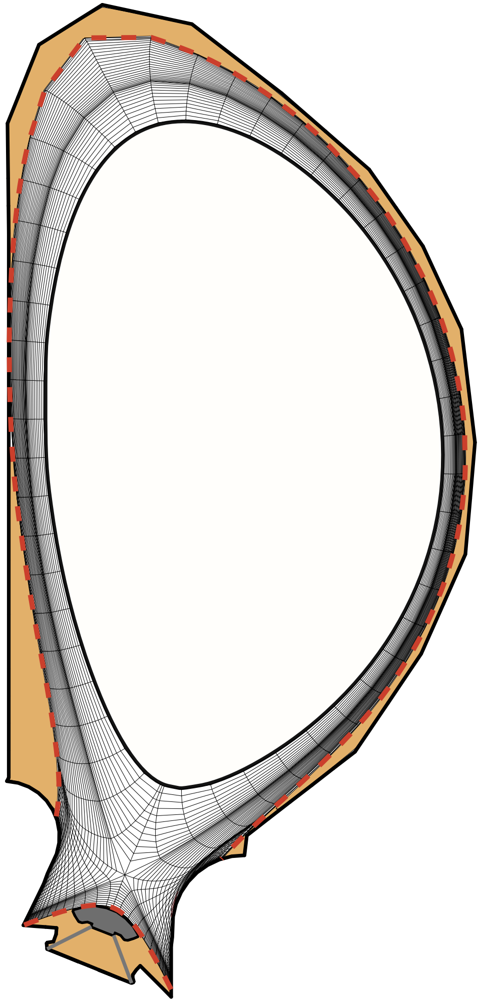
[B. LaBombard et al., NF 40 (2000) 2041]

Important issues with mean-field plasma edge simulations (2)

3. Plasma mesh typically does not extend to the vessel wall

Ad-hoc boundary conditions at limiting flux surface

No realistic (far-SOL) background for neutrals, and erosion, migration and redeposition studies



Outline

- Introduction
- Speed-up of simulations with fluid and hybrid neutral models
- Self-consistent anomalous transport models
- Extending grids to the vessel wall
- Conclusions & perspectives for DEMO

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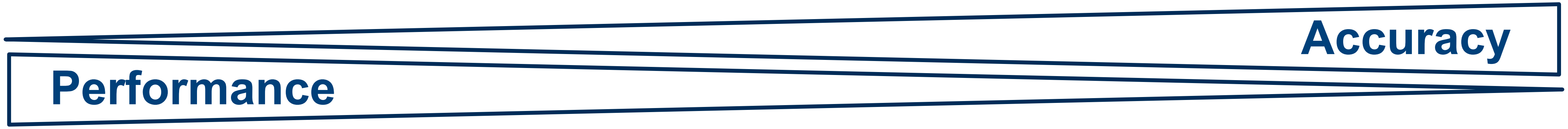
Hierarchy of neutral models



Purely fluid	Hybrid	Fully kinetic
Improvement of existing fluid neutral models	Combination of fluid and kinetic descriptions	
Advanced Fluid Neutral (AFN) models	More **accurate** than fluid **Faster** than kinetic	Most complete description; ‘reference’

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AFN models more consistent with kinetic counterpart

[N. Horsten et al., NF 57 (2017) 116043]

Equilibration by dominant CX process – **no tuning parameters**!

1. **Boundary conditions:** impose macroscopic neutral moment fluxes (moments $\boldsymbol{\mu}(\mathbf{v})$ ➔ particle, momentum and energy)

$$\begin{aligned}\boldsymbol{\Gamma}_{\mathrm{n}} &= \int_{\mathbf{v}\cdot\boldsymbol{\nu}<0} \boldsymbol{\mu}(\mathbf{v}) f_{\mathrm{n}}(\mathbf{v})(\mathbf{v}\cdot\boldsymbol{\nu})\mathrm{d}\mathbf{v} \\ &\quad - \int_{\mathbf{v}\cdot\boldsymbol{\nu}\geq 0} \boldsymbol{\mu}(\mathbf{v}) \int_{\mathbf{v}'\cdot\boldsymbol{\nu}\leq 0} \boxed{R(\mathbf{v}' \to \mathbf{v})} \left(f_{\mathrm{i}}(\mathbf{v}') + f_{\mathrm{n}}(\mathbf{v}')\right)(\mathbf{v}'\cdot\boldsymbol{\nu})\mathrm{d}\mathbf{v}'\end{aligned}$$

→ Incident part

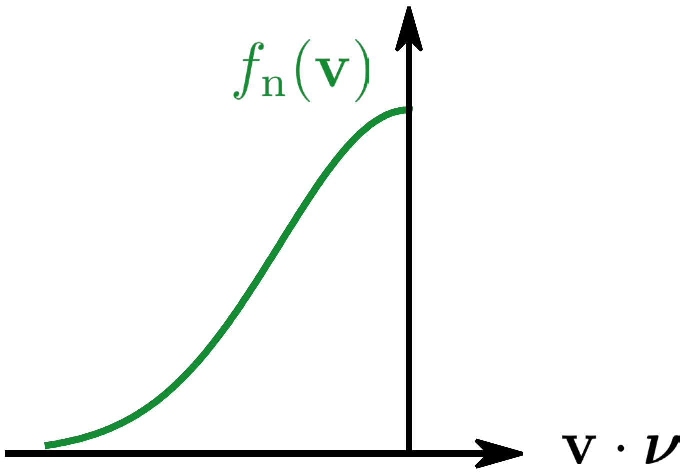
→ Recycled/ reflected part

TRIM reflection database

$\mathbf{v}$	Particle velocity vector
$\boldsymbol{\nu}$	Surface normal (pointing inward the plasma domain)

$f_{\mathrm{i}}(\mathbf{v})$ Ion distribution ➔ Maxwellian (possibly accelerated by sheath)

$f_{\mathrm{n}}(\mathbf{v})$ Neutral distribution ➔ assumed to be a Maxwellian for incident neutrals



AFN models more consistent with kinetic counterpart (2)

[N. Horsten et al., NF 57 (2017) 116043]

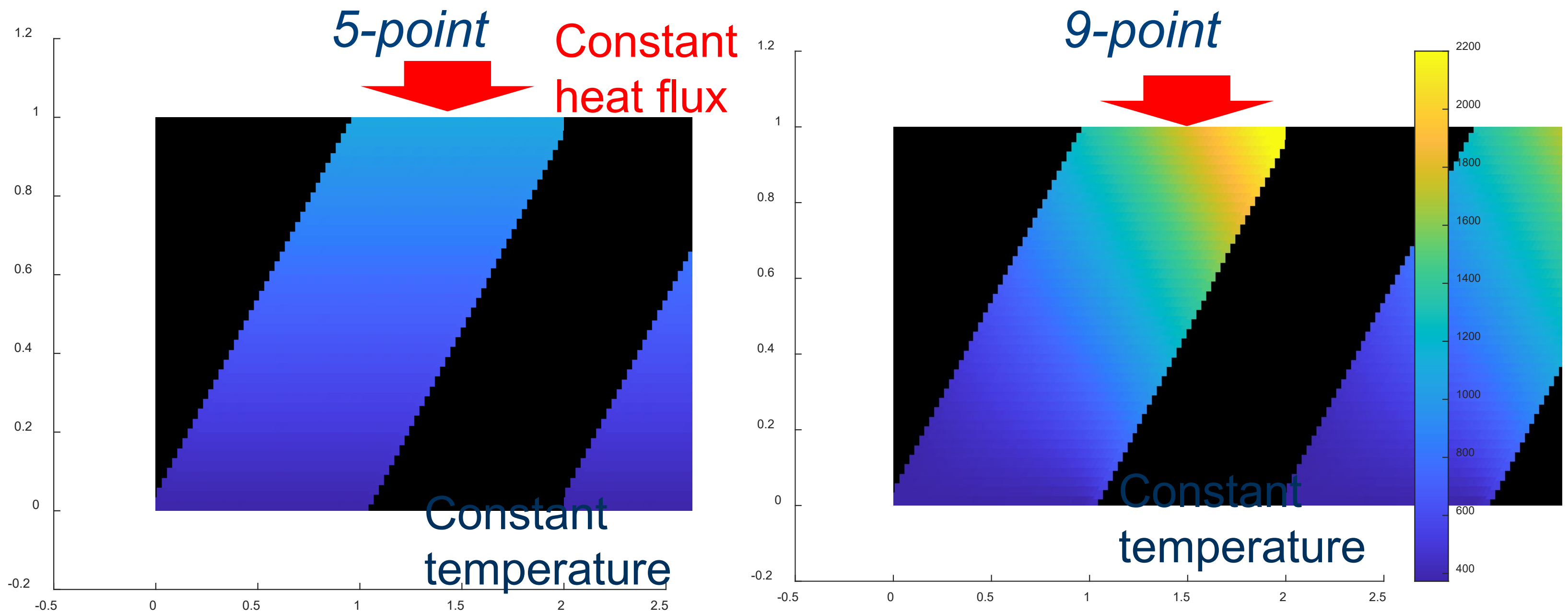
2. **Transport coefficients:** derived from AMJUEL/HYDHEL databases

3. **9-point stencil:** improved numerical solution

[W. Dekeyser et al., NME 18 (2019) 125-130]

E.g. effect for simple heat conduction equation

Required by isotropic character of neutrals!



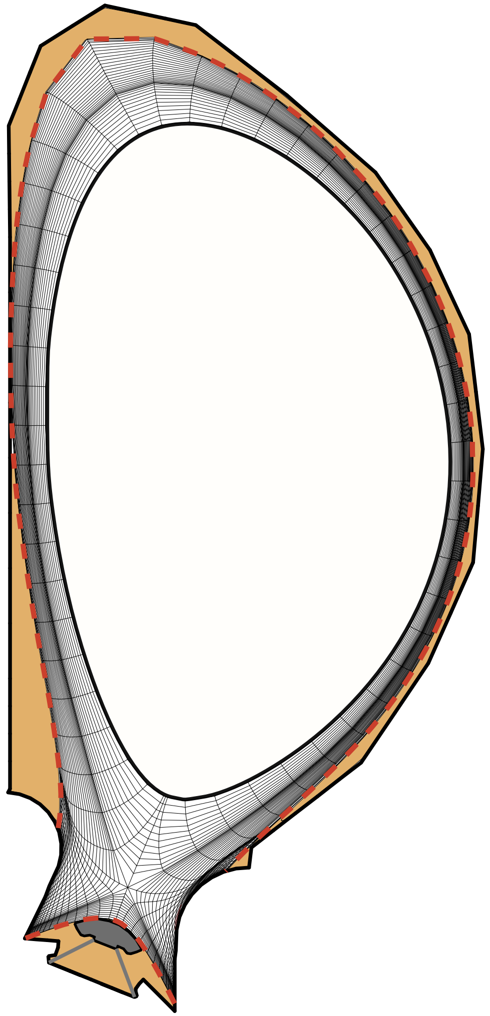
Remaining shortfalls of AFN models

1. **No transport in void regions**

2. **Only hydrogenic atoms:** molecules and impurities do typically not reach the fluid limit

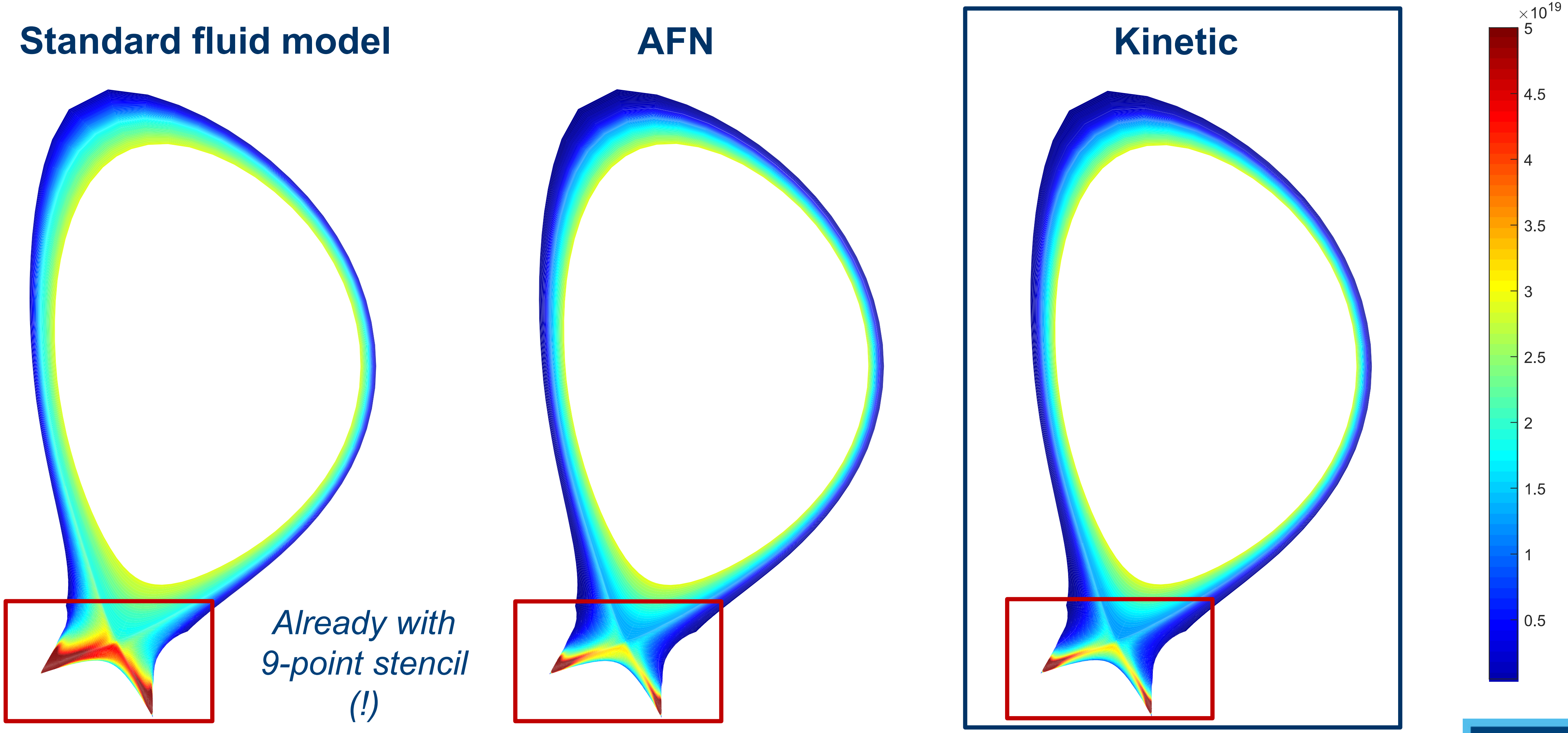
Fluid – kinetic comparison in next slides: **ITER case** with only D atoms without voids and no drifts

Molecules are assumed to dissociate at the surface ➔ Resulting atoms get energy of 2 eV (Franck-Condon dissociation)



AFN model significantly reduces fluid-kinetic discrepancies

[W. Van Uytven et al., NF 62 (2022) 086023]



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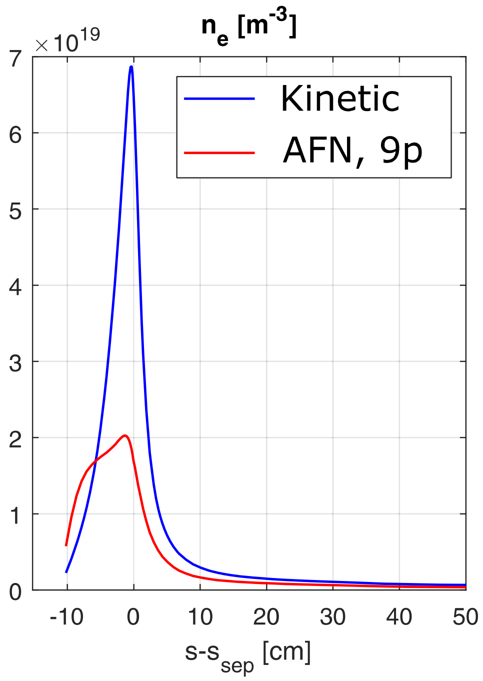
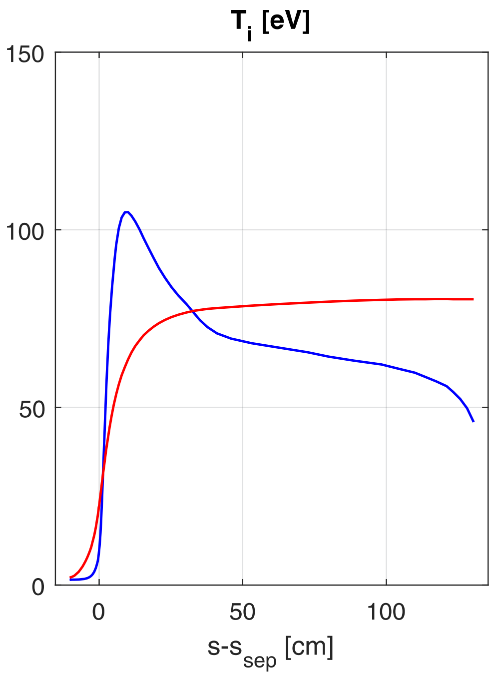
Fluid approximation becomes valid for high-recycling conditions

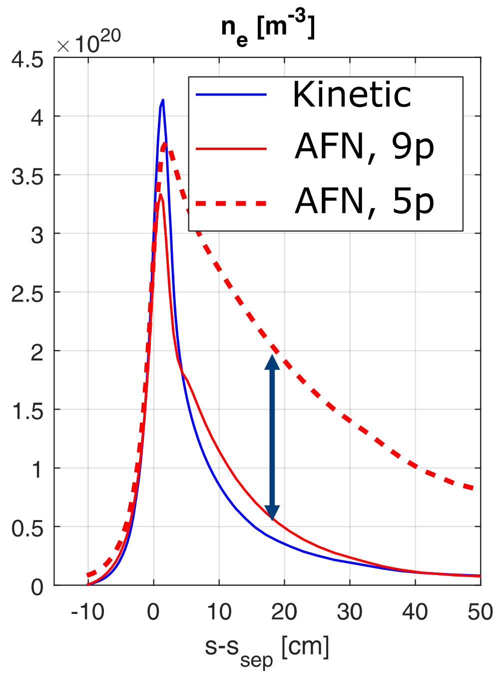
[W. Van Uytven et al., NF 62 (2022) 086023]

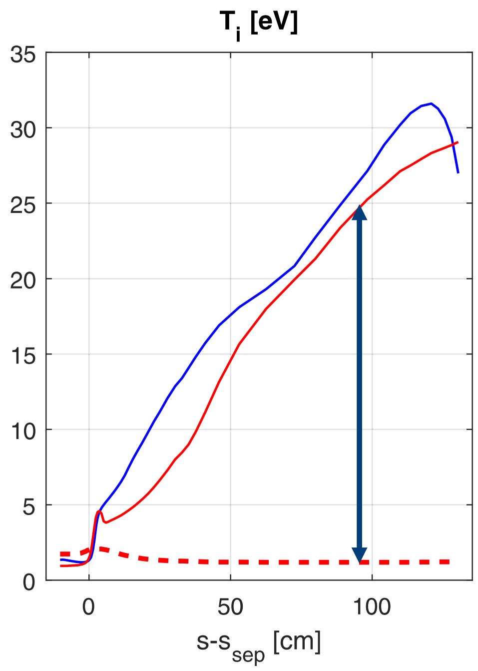
Low recycling





High recycling





Effect of 9-point stencil!

➡ Further improvements with hybrid approach

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  - **Hybrid neutral models**
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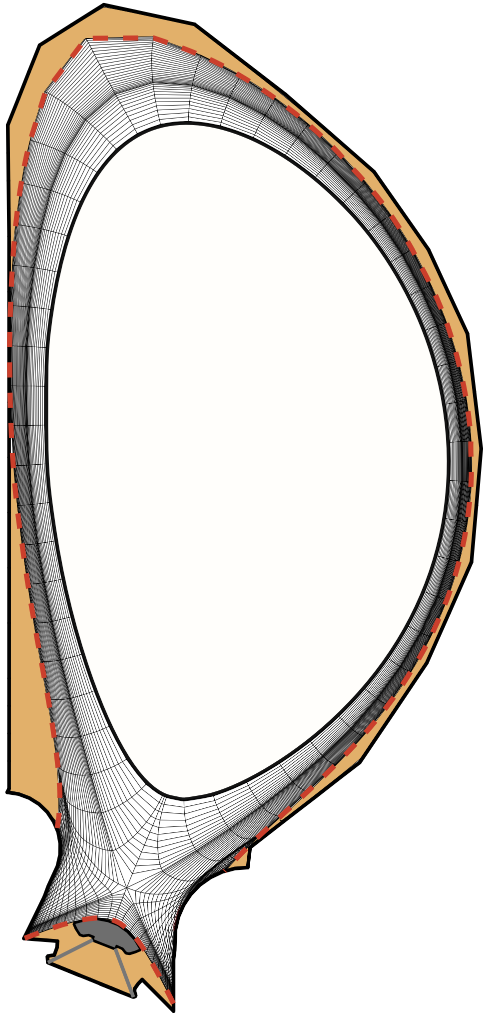
Methods in plasma edge neutral community

- Spatially hybrid [M. Blommaert et al., NME 19 (2019) 28-33]
- Evaporation/condensation [M. Valentinuzzi et al., NME 18 (2019) 41-45]
- Micro-macro decomposition [N. Horsten et al., JCP 409 (2020) 109308]
- Kinetic-diffusion Monte Carlo schemes [B. Mortier et al., CPP 60 (2020) e201900134]

Combined in
[W. Van Uytven et al., CPP (2022) e202100191]

This presentation

Hybrid approach includes void regions and a fully kinetic treatment for the molecules



- **Void regions**: fully kinetic treatment of neutrals by sampling at the plasma-void interfaces

- **Plasma fluid grid**: atoms are transferred from the kinetic to fluid population when

$$Kn^{\mathrm{p}} < Kn^{\mathrm{t}}$$

Local particle Knudsen number

User-defined transition criterion

- Fully kinetic treatment of **molecules** in the whole domain

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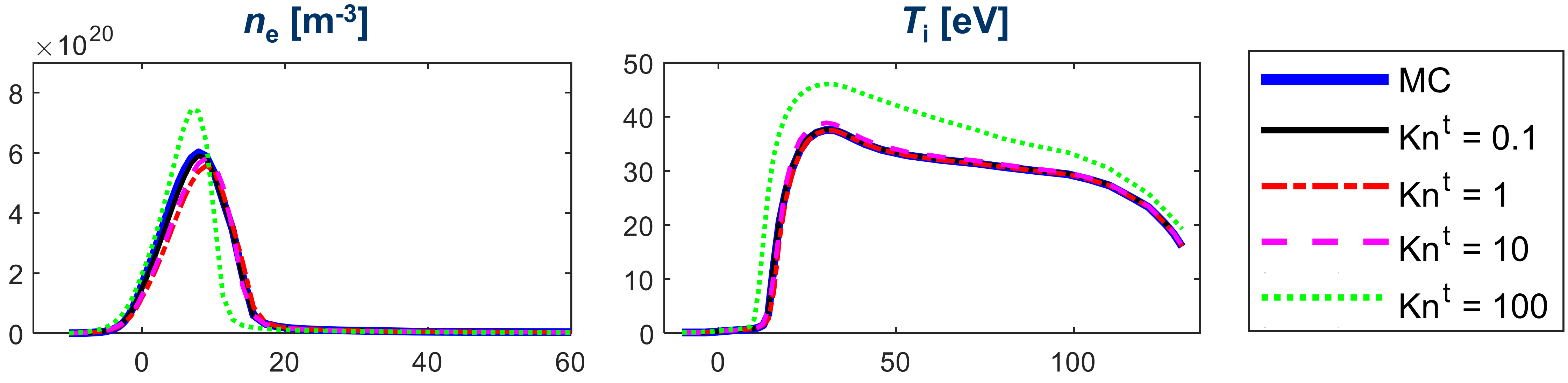
Hybrid model with Kn^t = 10 gives accurate results with factor 5 speed-up

Outer target profiles:



Speed-up compared to fully kinetic simulation:

Kn^t	0.1	1	10	100
	1.20	3.05	4.86	4.93

Speed-up still limited due to fully kinetic treatment of molecules!

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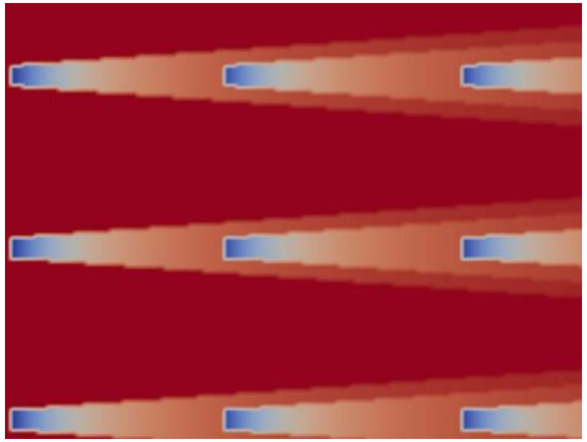
Hydrodynamic turbulence

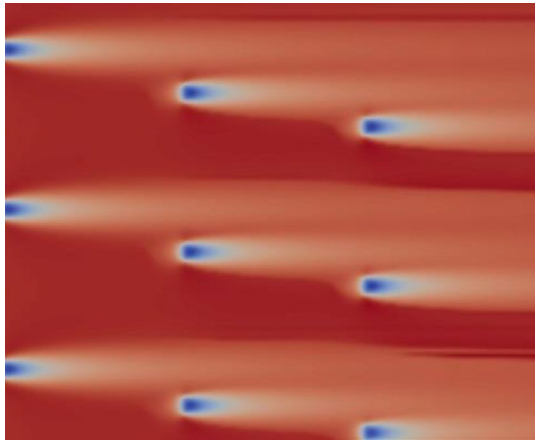
Wide range of simulation strategies…

Model accuracy →

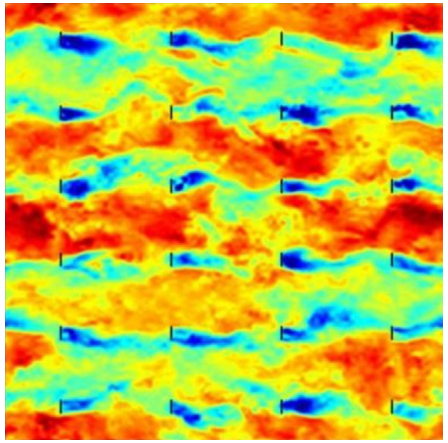
← Computational efficiency

Analytical models	*Reynolds-Averaged Navier-Stokes (RANS)*	*Large-Eddy Simulation (LES)*	*Direct Numerical Simulation (DNS)*

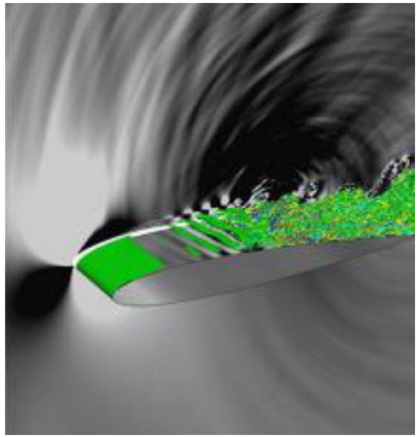




[Schmidt (2014)]



[Calaf et al. (2010)]



[Sandberg & Jones (2011)]

[Courtesy W. Munters]

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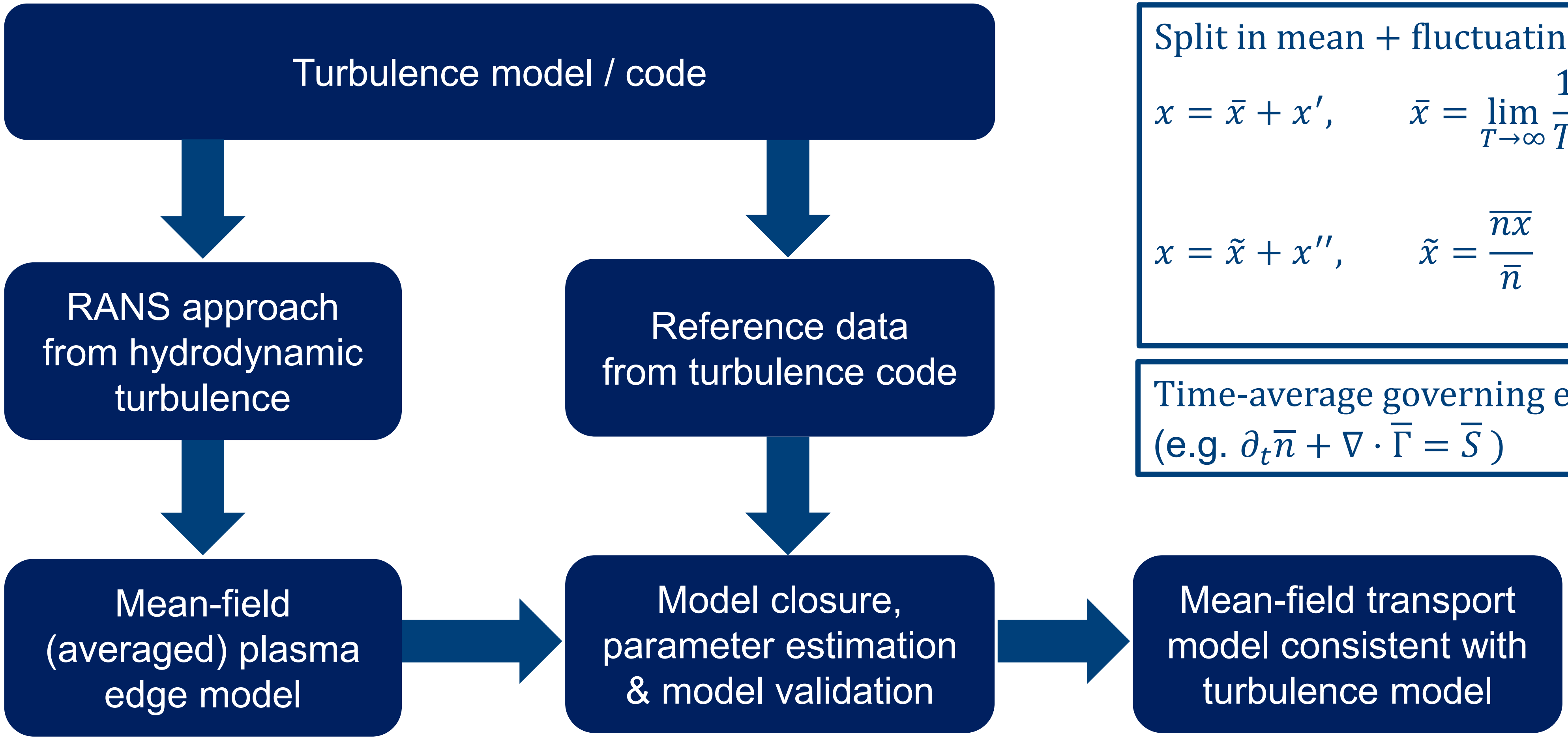
Approach



Split in mean + fluctuating components

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

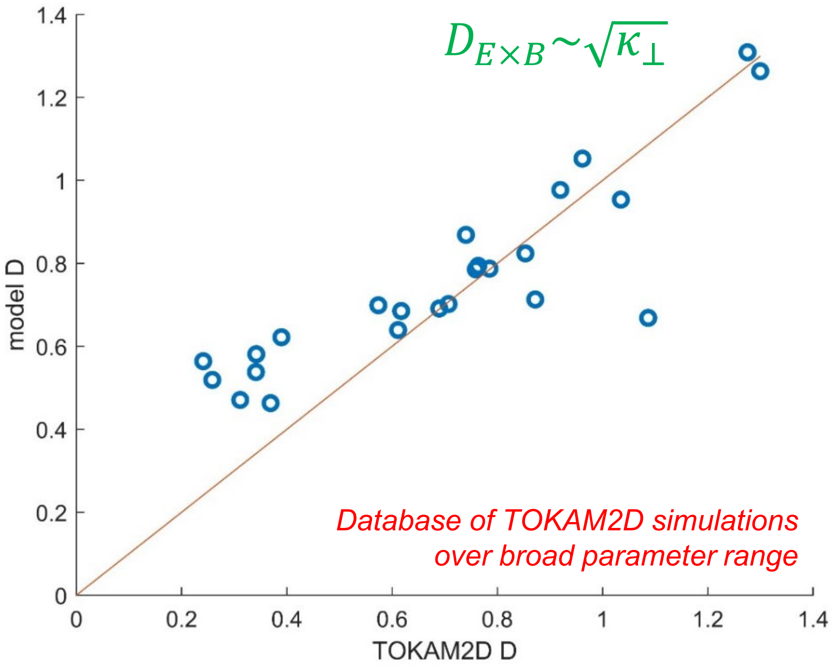
$$x = \tilde{x} + x'', \qquad \tilde{x} = \frac{\overline{nx}}{\bar{n}}$$

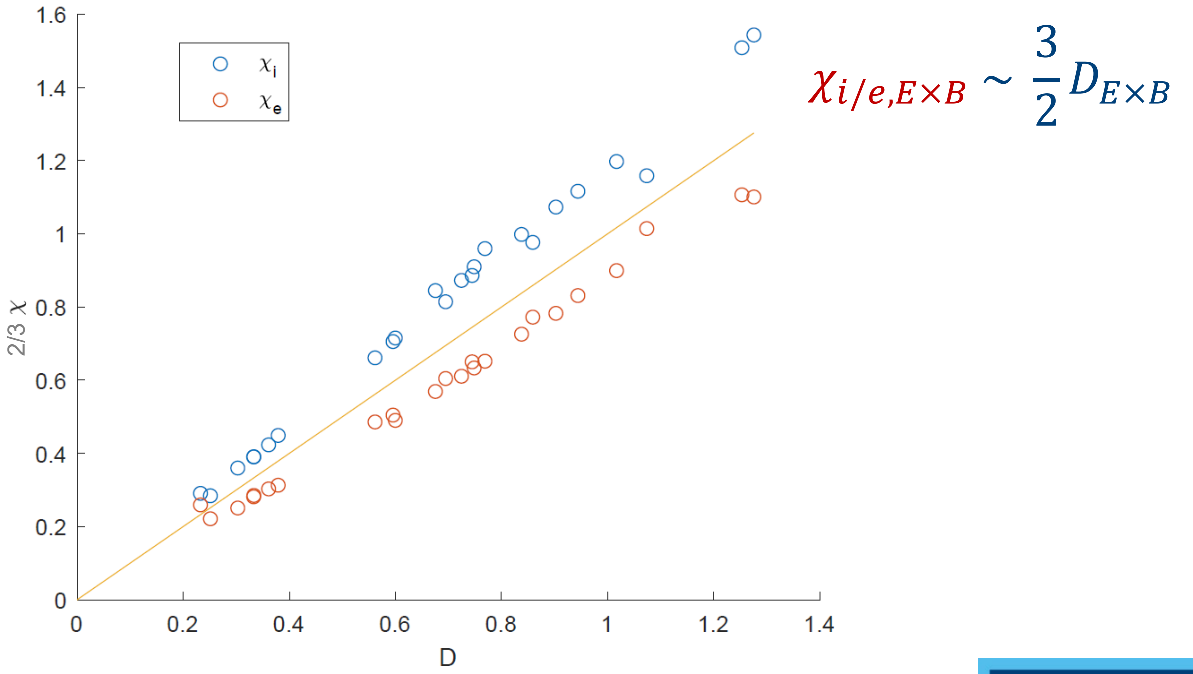
Time-average governing equations (e.g. $\partial_t \bar{n} + \nabla \cdot \bar{\Gamma} = \bar{S}$)

RANS approach for electrostatic interchange turbulence

- Average fluxes, electrostatic turbulence: fluctuating $E \times B$-terms need closure
  - $\overline{\boldsymbol{\Gamma}}_{i/e,E\times B} = \overline{n_i' \boldsymbol{u}_{E\times B}'} \sim -D_{E\times B} \nabla_\perp \bar{n}_i$
  - $\overline{\boldsymbol{Q}}_{i/e,E\times B,c} = \frac{3}{2} \overline{n_i \boldsymbol{u}_{E\times B}'' T_i''} \sim -\chi_{i/e,E\times B}\, \bar{n}_{i/e} \nabla_\perp \tilde{T}_i$
- Proposal: relate to turbulent kinetic energy $\kappa_\perp$ as measure of local intensity of the turbulence/transport
- Diffusive transport model based on 2D interchange simulations [Coosemans et al., CPP 2022, e202100193.]

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





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Sources and transport of $\kappa_\perp$ for interchange turbulence

[R. Coosemans, PhD thesis, 2022]

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

$$\frac{\partial}{\partial t}\bar{n}\kappa_\perp + \nabla\cdot\left(\overline{\mathbf{\Gamma}}_i\kappa_\perp + \overline{\phi' J'_{||}}\right) = \overline{S}_{IC} + \overline{S}_{||} + \overline{S}_{RS}$$

  - Total heat flux due to $E \times B$ fluctuations drives production of $\kappa_\perp$ [Coosemans et al., CPP 2022, e202100193.]

$$\overline{S}_{IC} = -\frac{2}{3}\overline{\boldsymbol{Q}}_{i+e,E\times B}\cdot\nabla\ln B^2 \quad \text{(exact)}$$

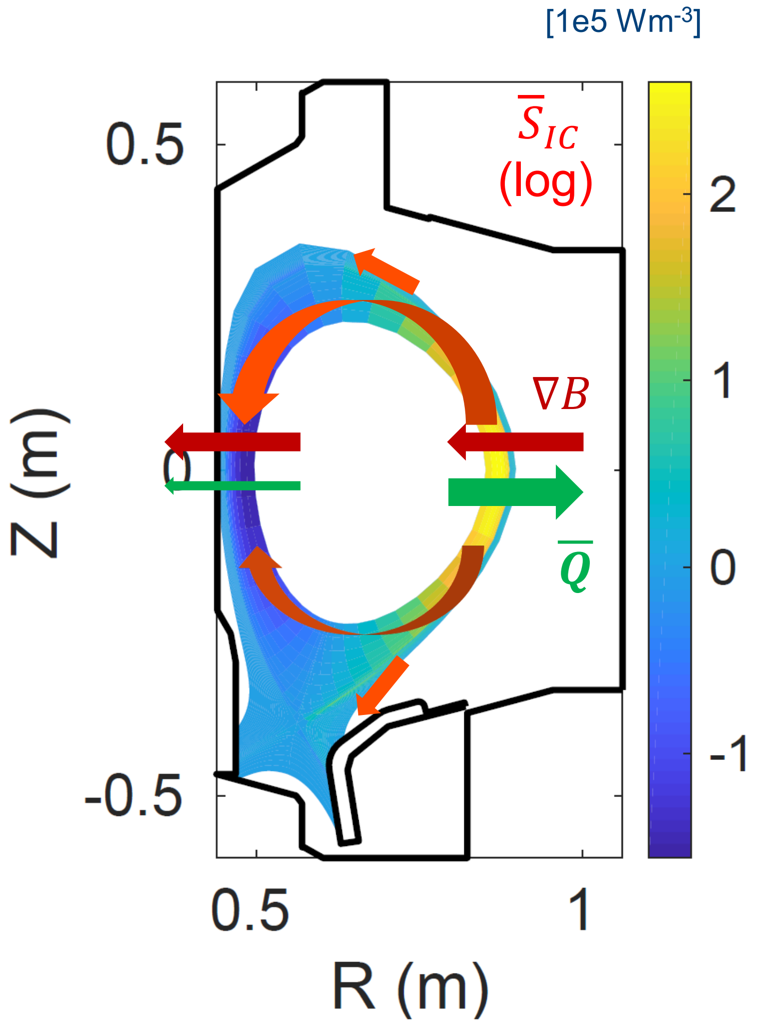
    - Source in 'bad-curvature' regions, sink in 'good-curvature' regions

  - Parallel transport of $\kappa_\perp$ governed by plasma conductivity
    - *Strongly exceeds parallel convection with $\tilde{u}_{||}$!*

  - Turbulence suppression due to flow shear: negative viscosity model

…coupled to 'regular' mean field equations [Dekeyser et al., CPP 2022, e202100190.]

⇒ towards self-consistent description of mean-field transport mechanisms (parallel, drifts, anomalous)



Intrinsic ballooning character and 'self-saturation'

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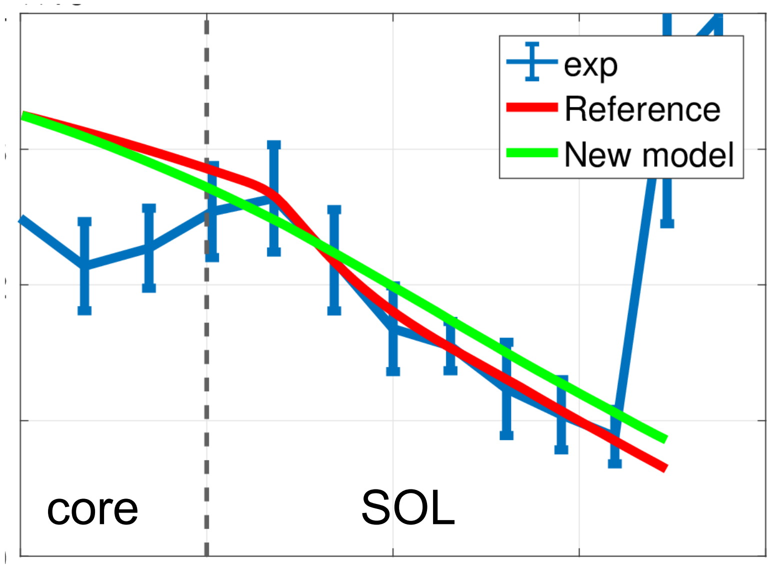
First comparison to experiments: COMPASS

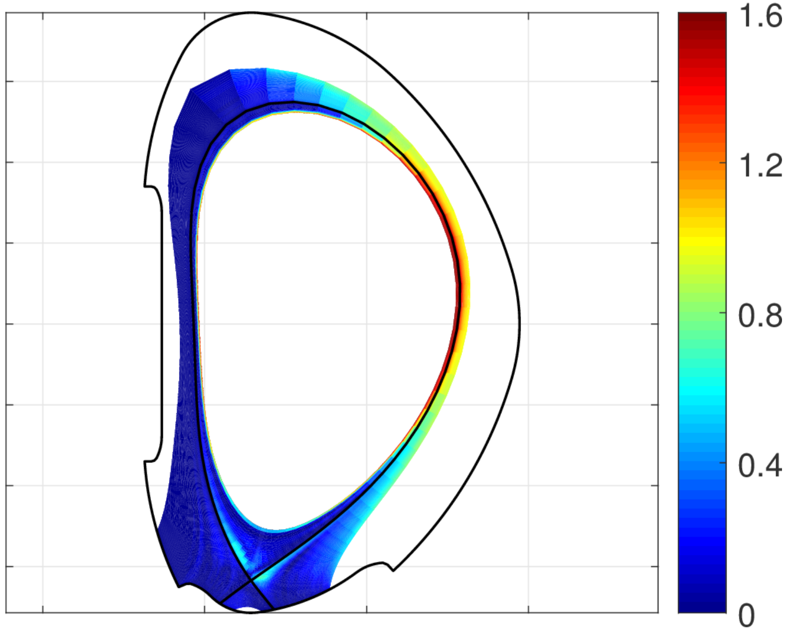
[S. Carli et al., CPP 60 (2020) e201900155.]

- Promising results w.r.t. reference case and experiment, despite ‘crude’ dissipation model
- Ballooning nature of transport retrieved

Upstream density profile



$D_{\perp}$ distribution



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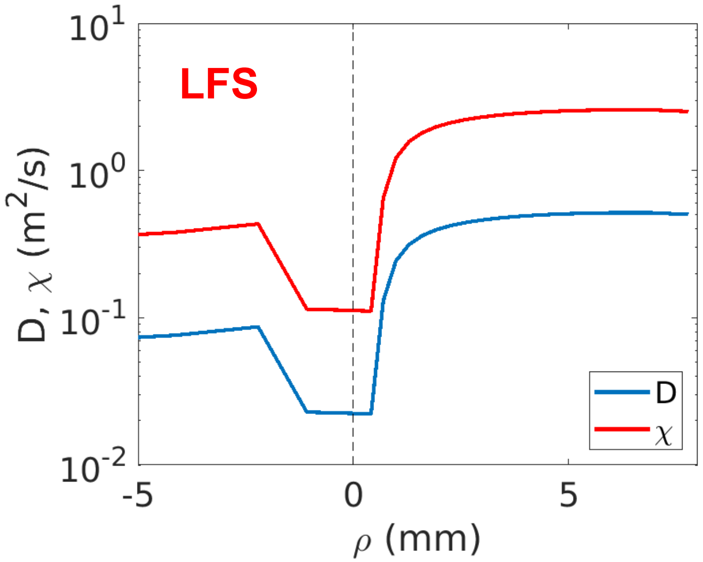
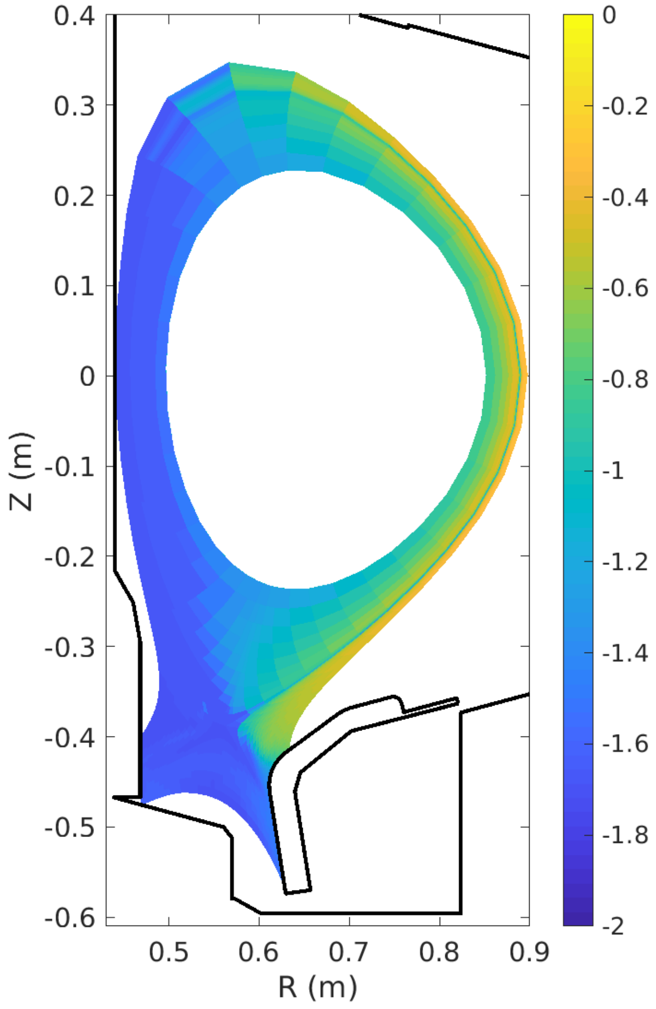
First comparison to experiments: C-Mod

[W. Dekeyser, PSI-25, Jeju, Korea, 2022.]

- With **few parameters**, the RANS-model can reproduce radial transport coefficients at the LFS midplane similar to those found through manual tuning…
  - …but now providing also full poloidal description, incl. suppression at HFS & separatrix!
  - …consistent variation with regime (?)





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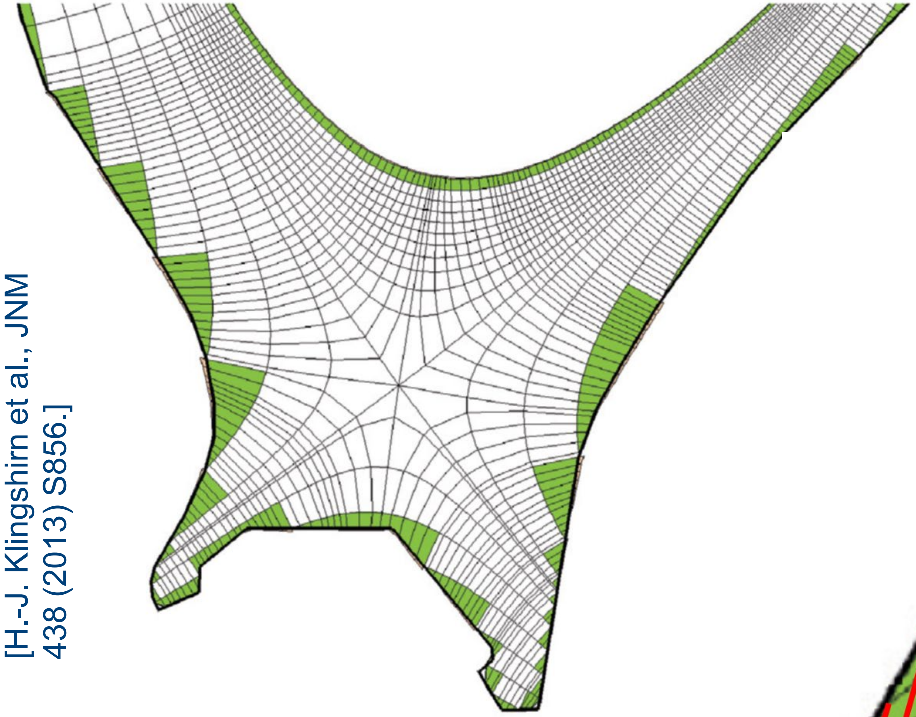
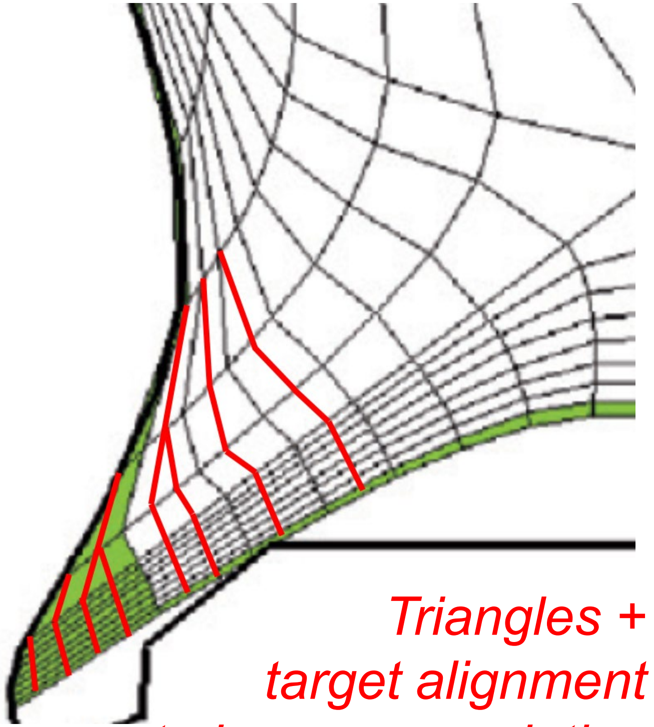
New unstructured finite volume solver for SOLPS-ITER



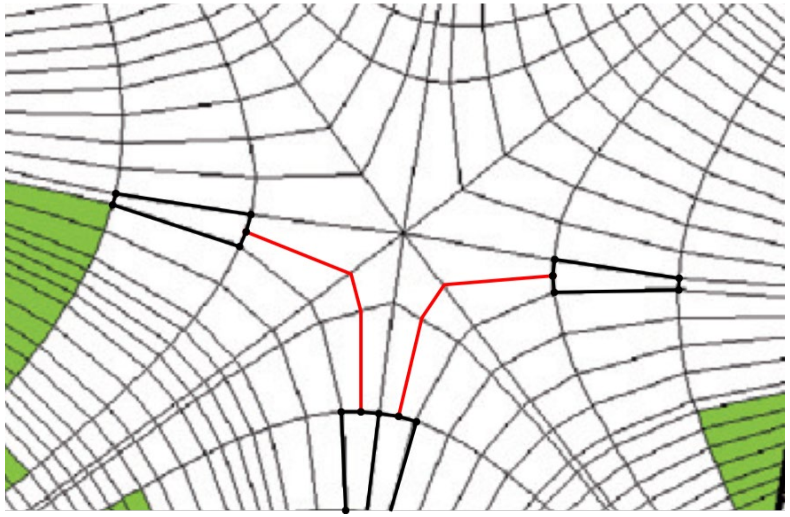
[H.-J. Klingshirn et al., JNM 438 (2013) S856.]

'Cut-cell' approach
to resolve full vessel

[M. Baelmans et al., Nucl. Fusion 51 (2011) 083023.]



Triangles +
target alignment
to improve resolution



Improved resolution at X-point
using pentagonal cells

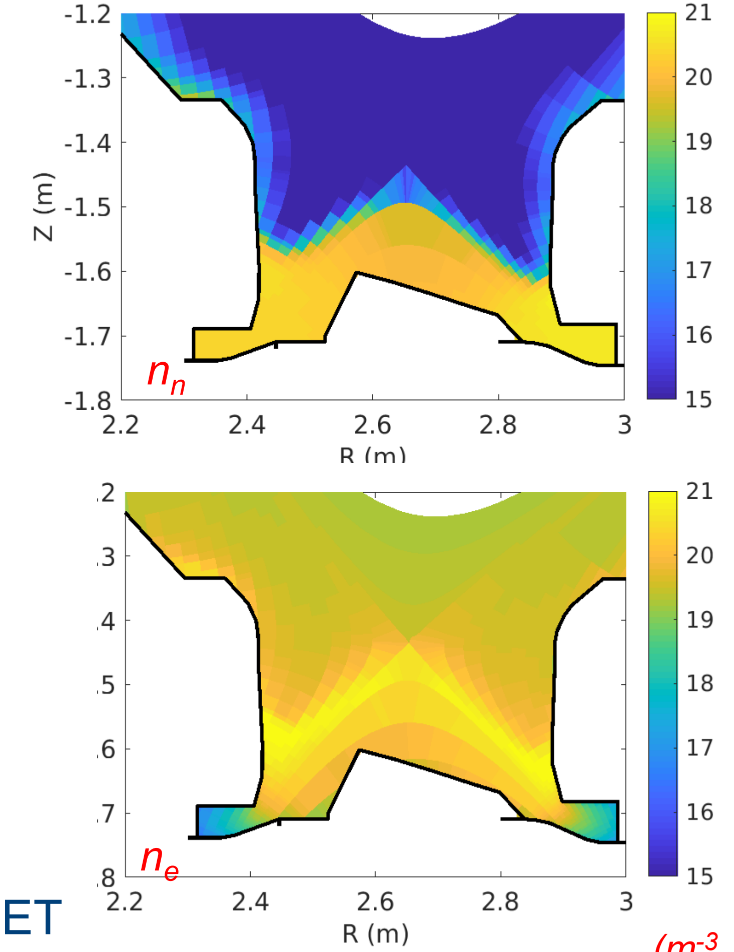
Large grid flexibility needed to meet conflicting resolution requirements
⇒ choice for unstructured FV solver (*)

(*) work performed under ITER-contract 2017-2019

New unstructured finite volume solver for SOLPS-ITER

- Arbitrary poloidal grid and cell topologies now possible (toroidally symmetric)
  - SN, DN, limiter,…
  - Advanced Divertor Configurations (multiple X- and O-points,…)
  - New configurations, e.g. without confined plasma, enabled

- Grid generation
  - Carre2 restricted to ‘standard’ configurations (SN, DN)
  - Flexible TIARA grid generator under development @ ITER



JET
SP@ horizontal plates
AFN model

(m^{-3}, log)

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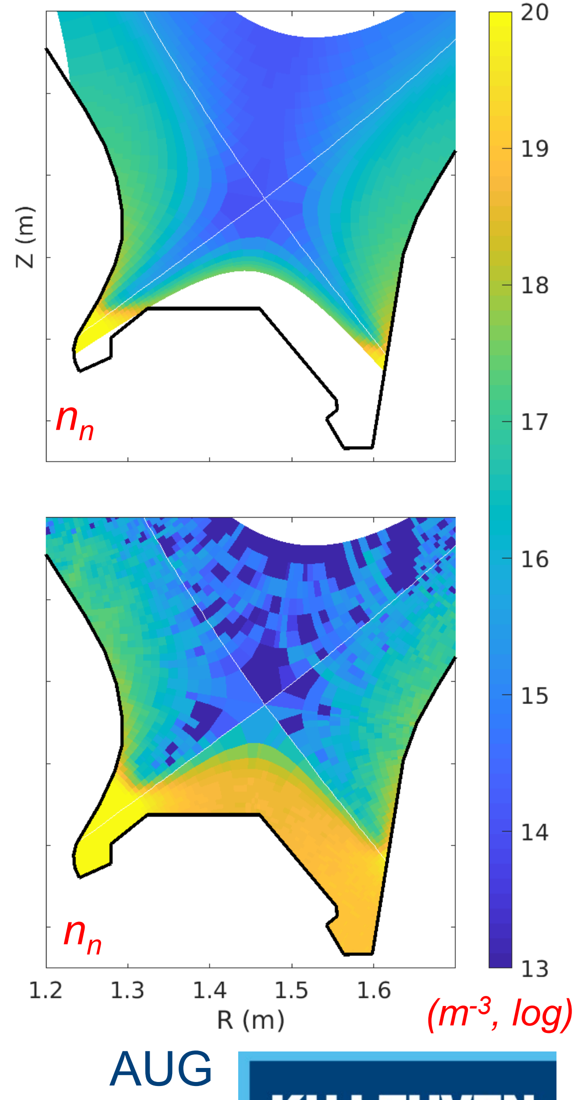
Status extended grids version of SOLPS-ITER

- Extended grids functionality implemented for default SOLPS-ITER model (model based on v3.0.6)
  - Incl. drifts and currents
  - Solver verified on various cases, incl. MMS

- Fully backwards compatible* with v3.0.6 for default model options on existing, non-extended, structured grids

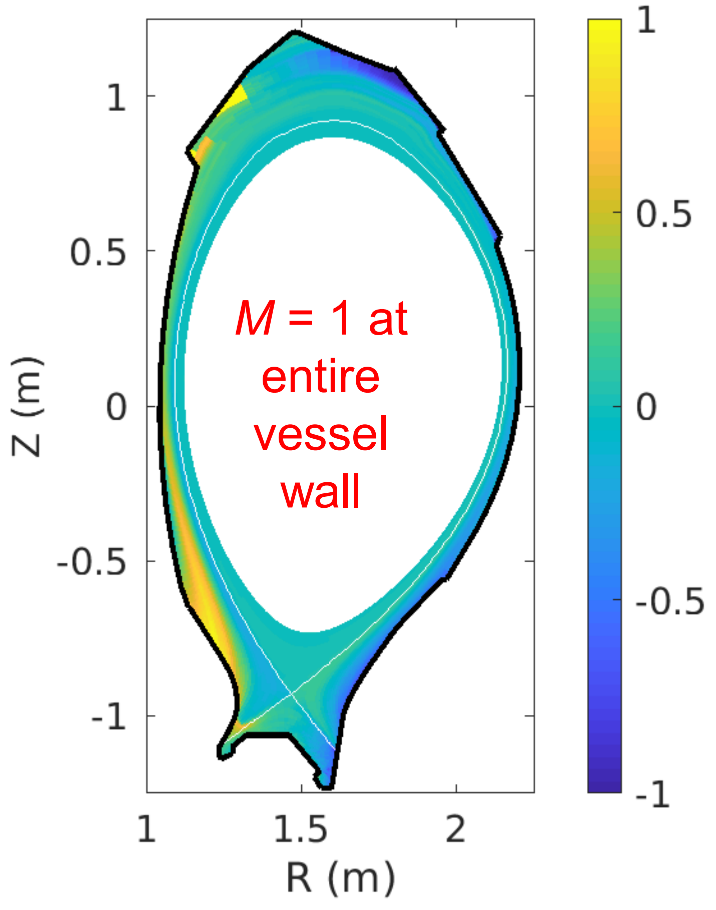
  *except for bugfixes, implicit geometry assumptions, and when not using improved stencil

- New features available
  - Improved numerical schemes (in particular, *9-point stencil*)
  - Advanced fluid and hybrid neutral models
  - Anomalous transport models based on RANS approach
  - Parameter estimation and optimization framework (see talk W. Dekeyser)

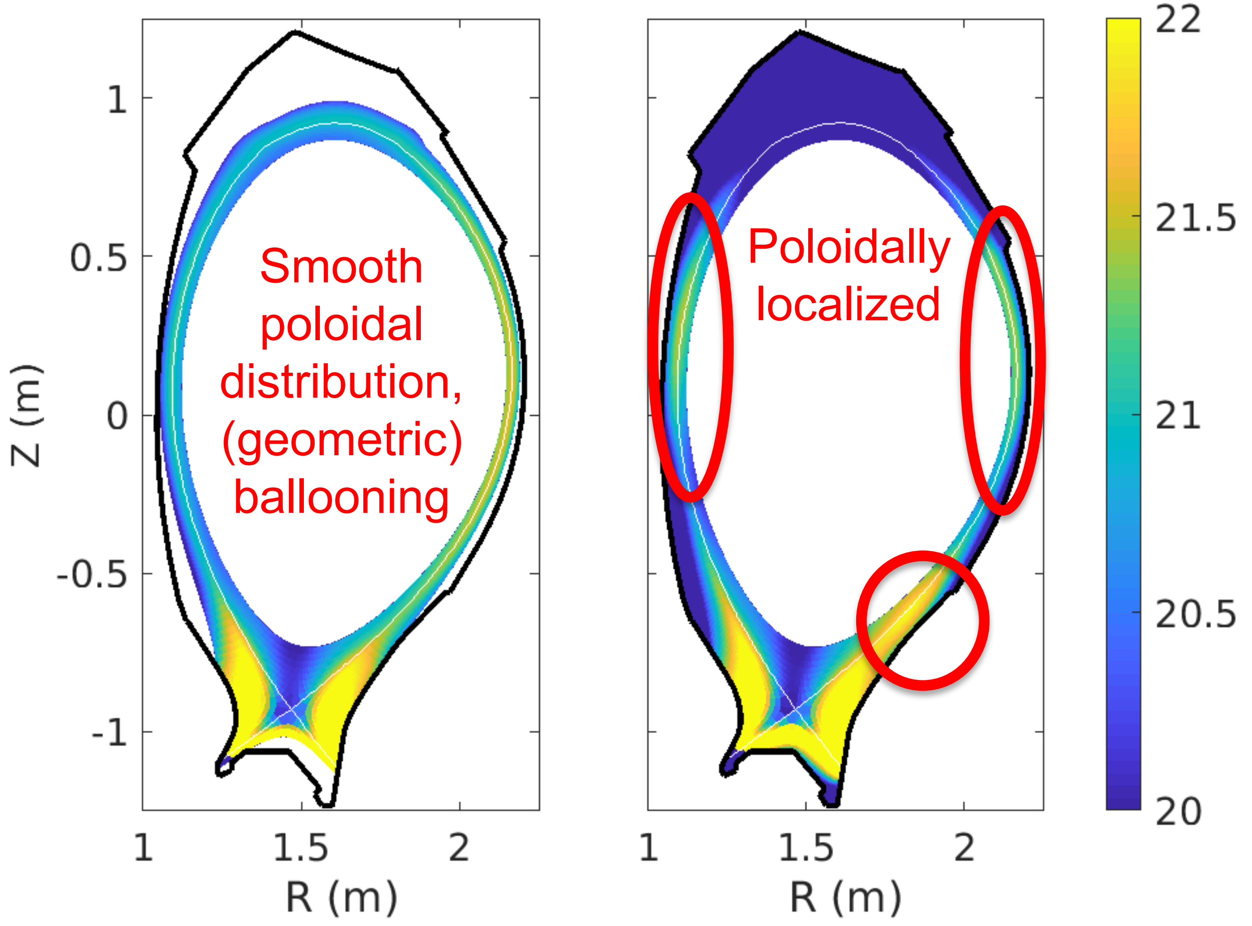


Poloidally localized MC recycling

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



Mach number (-)



Particle source ($m^{-3}s^{-1}$, log)

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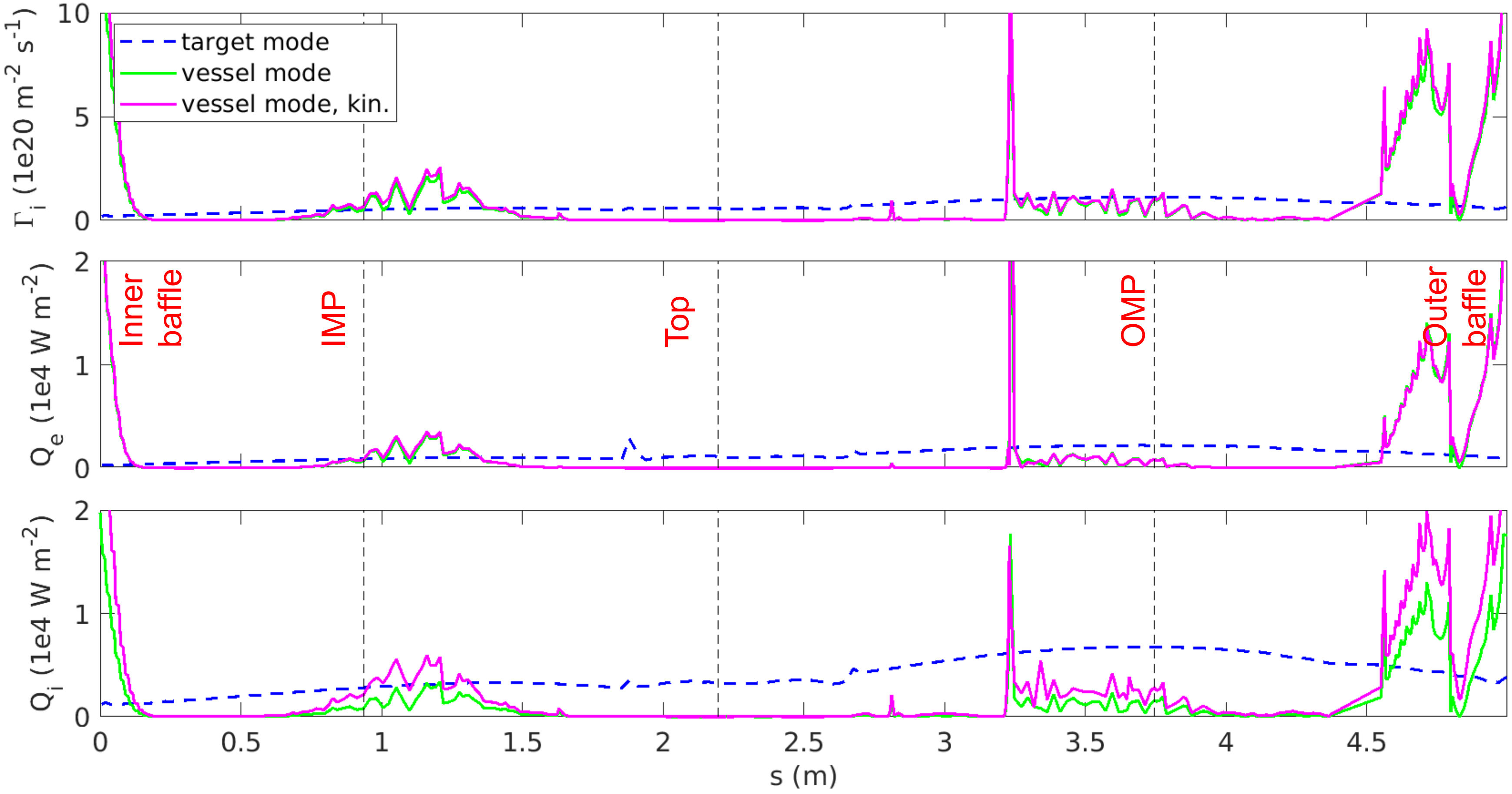
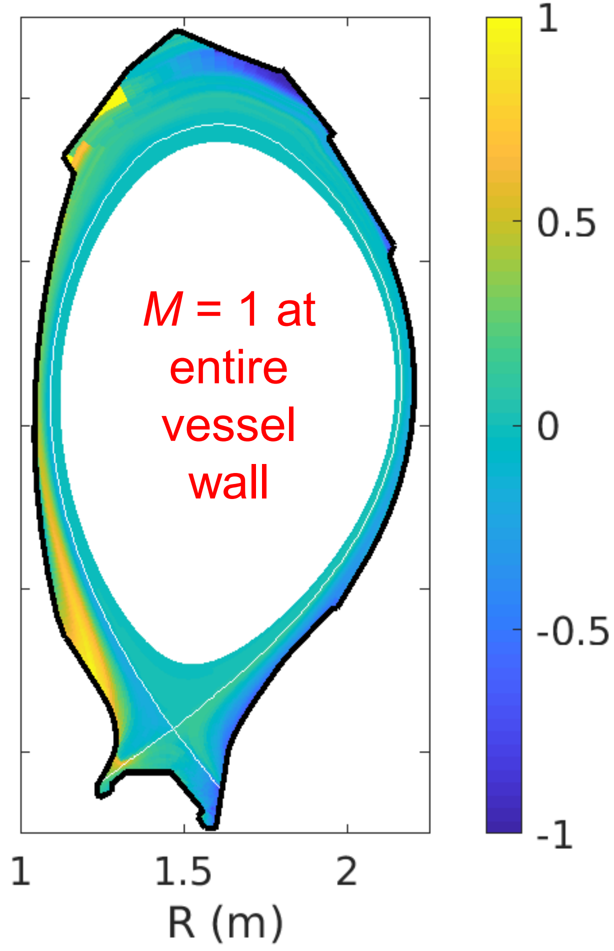
Simulation of wall fluxes

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





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Conclusions

- Advanced fluid and hybrid neutral models can provide significant speed-up compared to fully kinetic simulations of reactors
  - AFN qualitatively correct for high-density conditions
  - Hybrid approach able to correct remaining fluid-kinetic discrepancies

- Anomalous transport models based on RANS-approach may provide consistent description of mean field transport mechanisms (parallel, drifts, anomalous)
  - Some basic transport features (ballooning) reproduced inherently by the models
  - Successful first comparisons to experiment

- Simulations up to the wall enabled with SOLPS-ITER
  - Providing consistent plasma backgrounds for erosion studies
  - Facilitating far-SOL transport studies

Challenges and perspectives for DEMO

- Advanced fluid and hybrid neutral models
  - Ready to be applied to DEMO
  - Even more accurate results expected due to increased ion-neutral collisionality
  - Speed-up limited by fully kinetic treatment of molecules ➔ fluid/hybrid model, e.g. [A. Holm, et al., NME 19 (2019) 143-148]
- Extension of RANS models towards reactor-relevant turbulence regimes
  - Improved description of impact fluctuations in parallel direction (in particular, *drift waves*)
  - Effect of neutrals and recycling conditions
  - Extensive model validation & calibration needed (incl. 3D turbulence simulations)
- Extended grids
  - Potential to provide consistent plasma backgrounds for various reactor studies
  - Combination with AFN models may further reduce fluid-kinetic discrepancies by removing the voids $\Rightarrow$ extended range of applicability of AFN?

Challenges and perspectives for DEMO

- Rigorous model validation framework:
  - Combining data & errors from all available diagnostics
  - Estimating the error bars on the unknown model parameters
  - Propagating expected model errors to DEMO predictions

- Do we have sufficient experimental data to validate/extrapolate all the model aspects? E.g.
  - 2D (poloidal-radial) resolved data?
  - Turbulence characteristics for the RANS models?
  - …

- Can we fill some gaps by calibrating parameters with scaling laws?

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Thank you! Questions?