Extended grids in SOLPS-ITER: status and new code features

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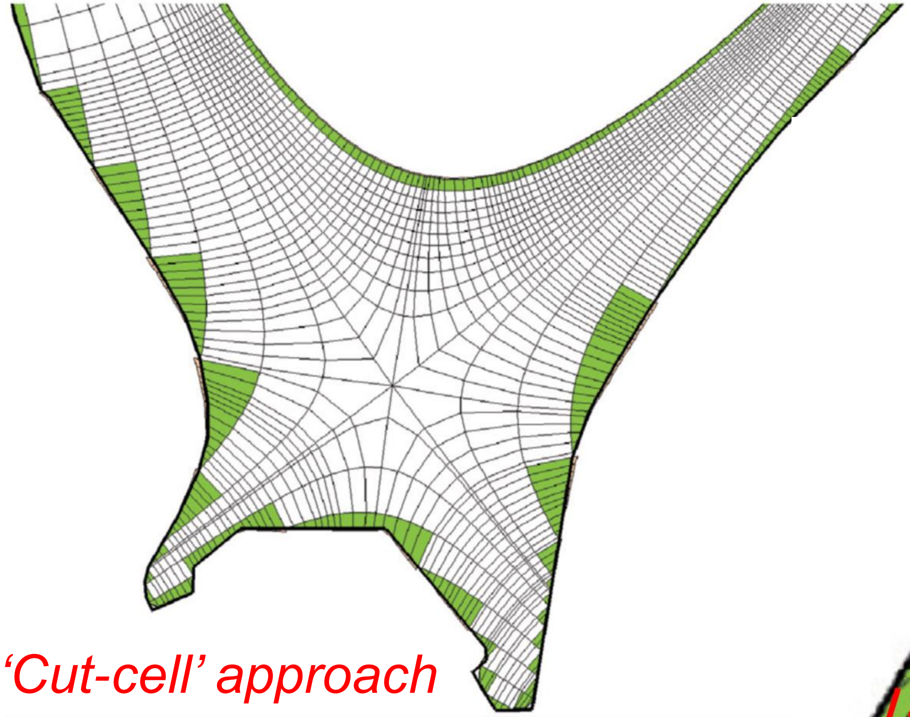
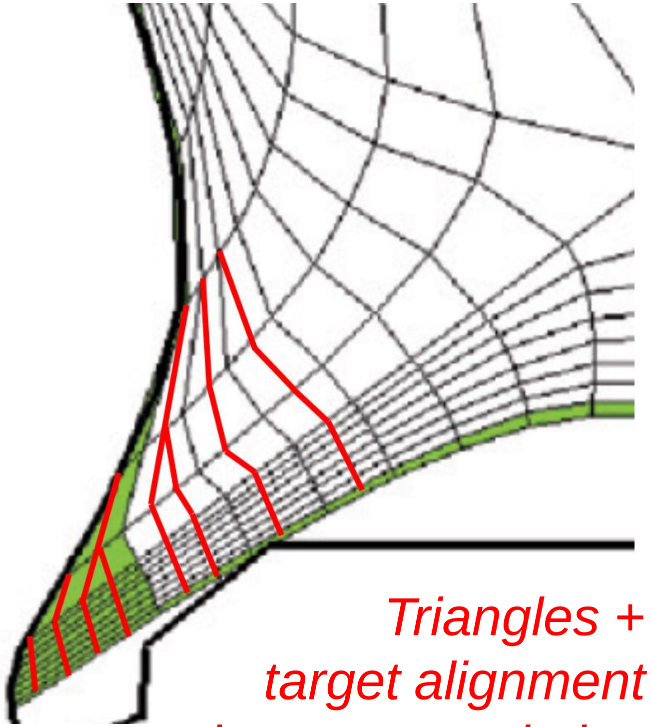
New SOLPS-ITER: unstructured finite volume solver

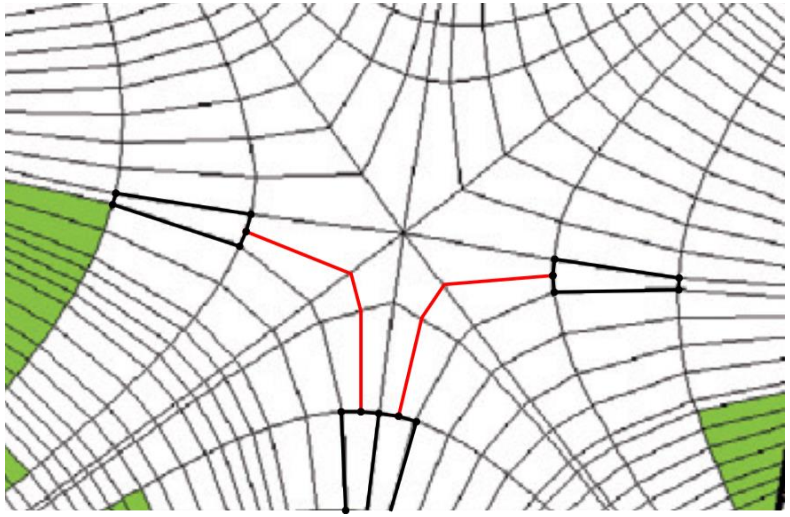
[W. Dekeyser et al., NME, 2021]



'Cut-cell' approach to resolve full vessel



Triangles + target alignment to improve resolution



Improved resolution at X-point using pentagonal cells

Base carre2 grids: Klingshirn et al., JNM, 2013.

Arbitrary polygonal cells in poloidal plane possible, w. arbitrary connectivity
Arbitrary (toroidally symmetric) magnetic topology
… but still 1st order discretization schemes => alignment needed as much as possible

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Status extended grids version of SOLPS-ITER

- Extended grids functionality implemented for default SOLPS-ITER model
  - SOLPS5.2 drifts and currents model (except some smaller current/drift terms) – v3.0.6
  - Default: correct treatment of grid non-orthogonality; can be turned off for structured cases (not recommended!)
  - Basic treatment of impurities converted
  - Basic feedback schemes available
- Remaining work
  - Some of the smaller drift terms, incl. adapted stencil for perp. visc. current
  - Non-default BCs
  - Feedback schemes
  - Various specific model options
  - Various input/output options (*b2time.nc*-traces, movies, IDS interfaces,…)

Coupling to EIRENE

- EIRENE version based on SOLPS-ITER v3.0.6
- Coupling routines adapted to unstructured format
  - Implicit geometry assumptions in interface with B2.5 removed (mainly: sheath model)
    $\Rightarrow$ (small) restart effects possible
- Scoring of tallies directly in (polygonal) plasma cells (instead of triangles)
- Considerations for merging with EIRENE from SOLPS-ITER master:

  => several updates done in SOLPS-ITER master version likely not included
  => further updates related to hybrid modeling included
  => merging with more recent EIRENE version will take careful checking

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Status extended grids version of SOLPS-ITER

- Core solver verified on various cases, incl. MMS
- Fully backwards compatible* for existing, structured grids

  *except for bugfixes, and when not using improved stencil options

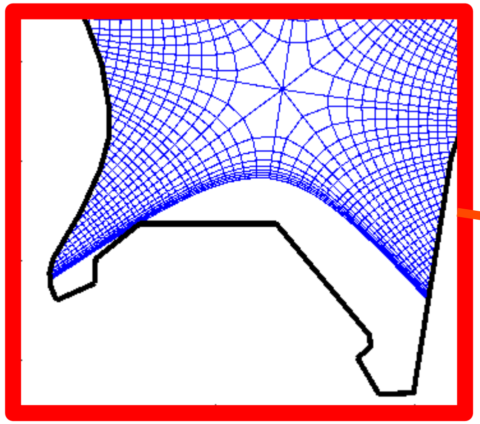
  *in some places, implicit geometric assumptions removed (e.g. interface to EIRENE)
- Grid generation remains bottleneck
  - Code can handle CARRE2 grids, but CARRE2 needs revival (documentation)
  - TIARA under development at ITER, but not interfaced to the solver

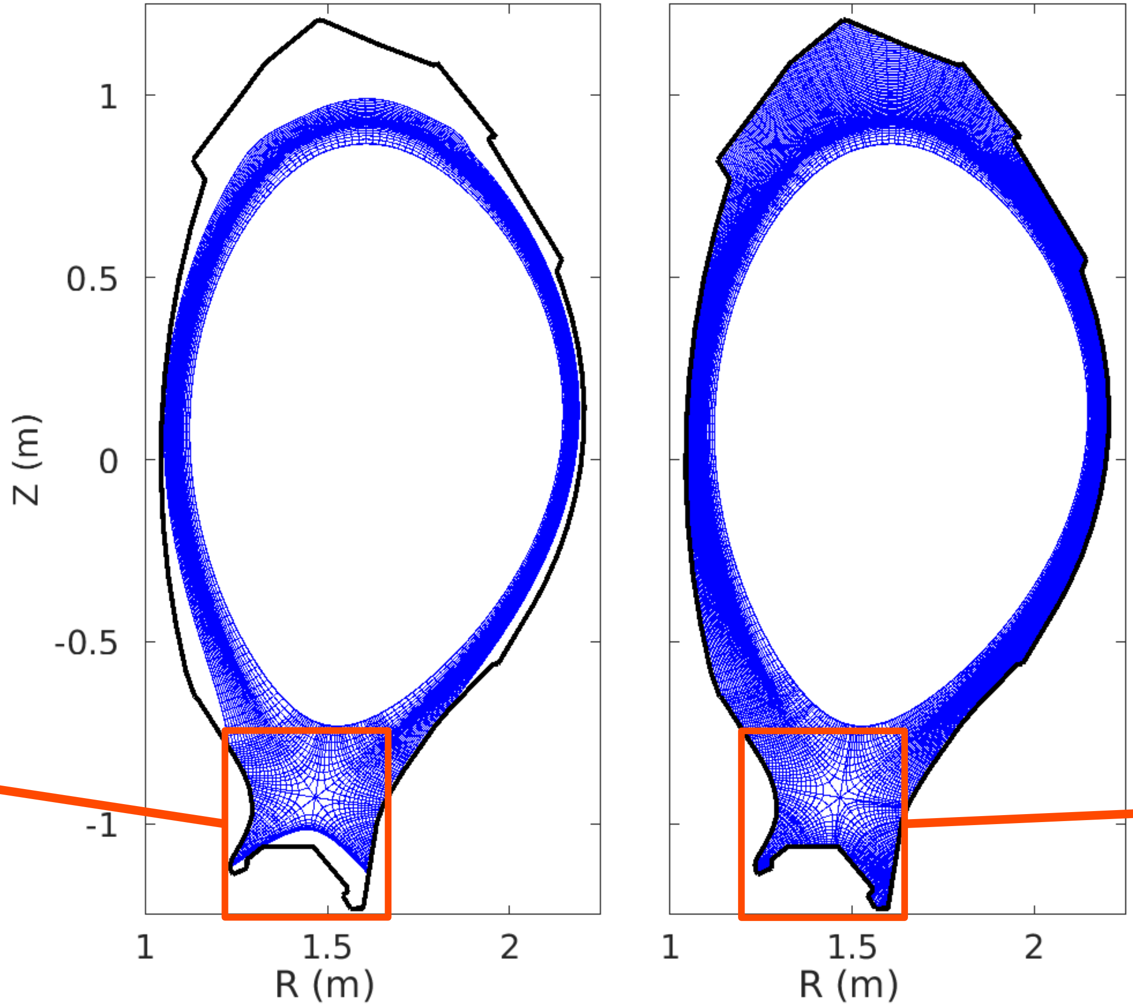
CARRE2: ‘Target mode’ and ‘vessel mode’ grids

[W. Dekeyser et al., NME 2021.]

Target mode

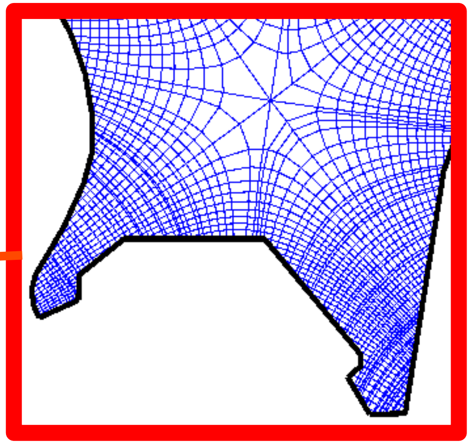
- Non-extended
- Internally orthogonal
- No bunching problems due to strong shaping,…





Vessel mode

- Extended
- Internally orthogonal



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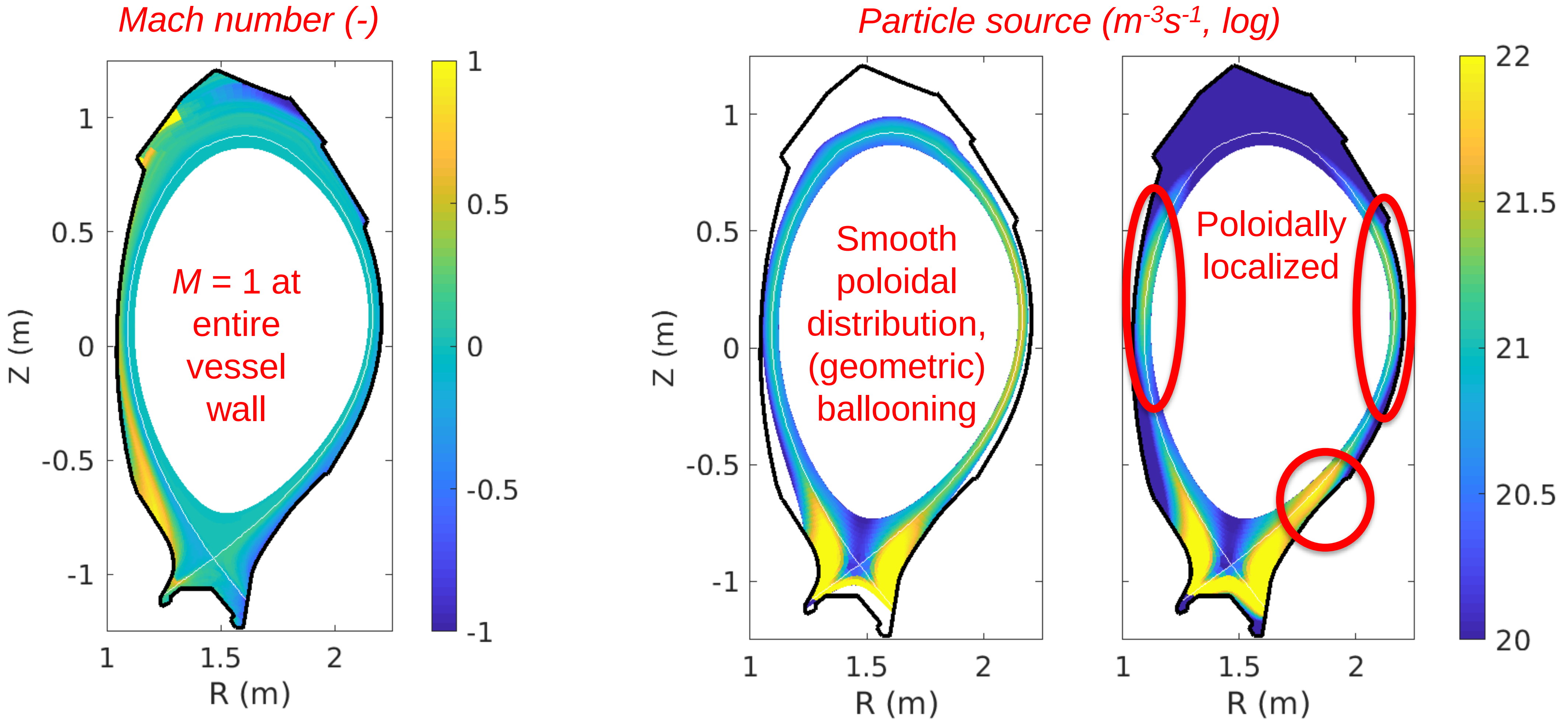
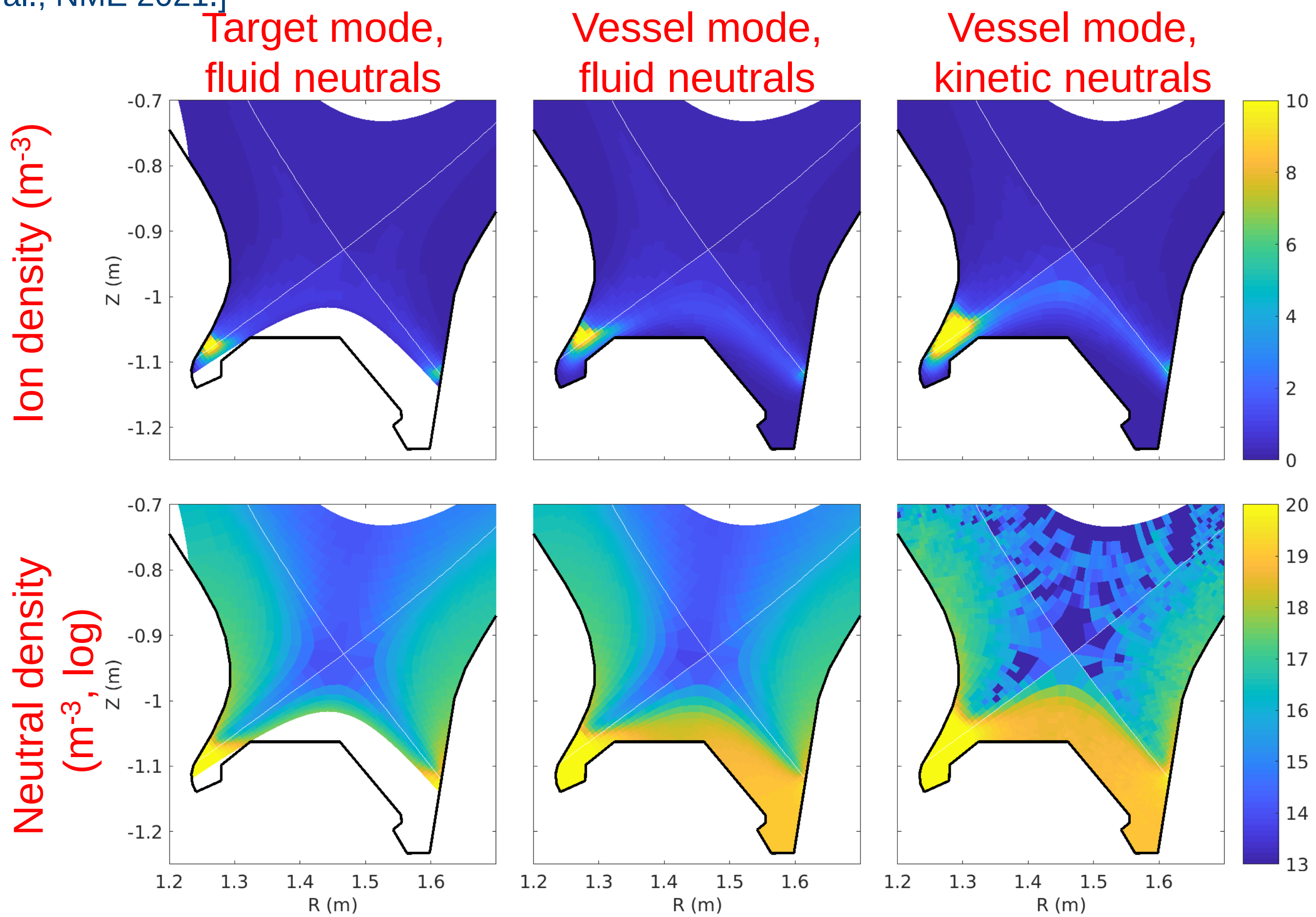
Poloidally localized MC recycling and heat/particle fluxes

[W. Dekeyser et al., NME 2021.]



Divertor solution

[W. Dekeyser et al., NME 2021.]



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Additional code features in extended grids code

- By default: correct treatment of grid non-orthogonality using 9-point stencil
  - More complete and robust implementation compared to v3.1.0
- Advanced fluid and hybrid neutral models
  - AFN, incl. option of separate neutral energy equation
  - SpH in different flavors, incl. coupling to molecules
  - mMH
  - See a.o. recent work presented at PET21 [Van Uytven et al., Horsten et al.]
- *k(-enstrophy)* models for improved description of anomalous transport
- Framework for optimization/calibration of unknown model parameters from experiment (nonlinear regression + MAP estimates)

$\kappa_\perp$ model in extended grids code

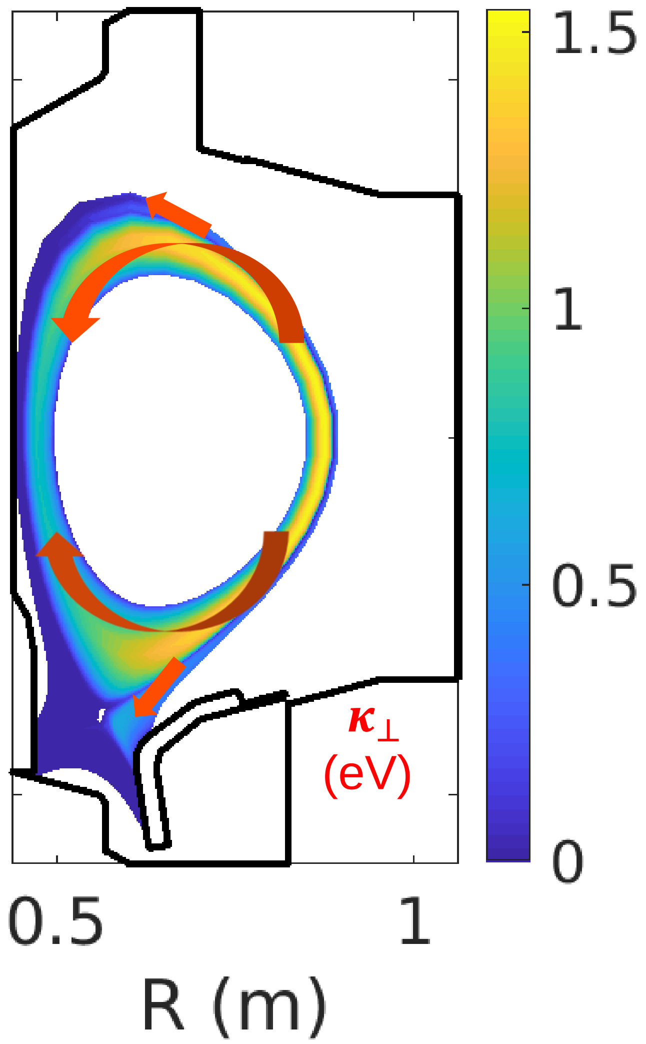
- $\kappa_\perp$ equation for 2D electrostatic interchange turbulence

$$\frac{\partial}{\partial t}\bar{n}\kappa_\perp + \nabla \cdot \overline{\boldsymbol{\Gamma}}_{\kappa_\perp} = \bar{S}_{\kappa_\perp}$$

  - Source/sink of $\kappa_\perp$: $\bar{S}_{\kappa_\perp} \approx \bar{S}_{IC} + \bar{S}_{||} + \bar{S}_{RS}$
  - Transport: $\overline{\boldsymbol{\Gamma}}_{\kappa_\perp} \approx \nabla \cdot \left(\overline{\boldsymbol{\Gamma}}\kappa_\perp + \frac{1}{2}\overline{mn\boldsymbol{V}''V''^2_{E\times B}} + \overline{\boldsymbol{\phi}'\boldsymbol{J}'_{||}}\right)$
- Coupled to 'regular' mean field equations
  - Transport coefficients determined by local value of $\kappa_\perp$

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

  - Energy conservation (mean field + turbulent + RS-drift)
- More details: [Coosemans et al., Dekeyser et al., PET 21]



Status of optimization tools in extended grids code

- Gradient calculation through Algorithmic Differentiation (AD – TAPENADE [Inria])
  - Tangent mode: cost proportional to number of inputs, gradient verified on finite differences
    [Carli et al., Nucl. Mater. and Energy **18** (2019) 6-11.]
  - Adjoint mode: cost independent on number of inputs, gradient verified on finite differences, memory efficiency through reverse accumulation
- Optimization framework implemented in B2.5 through coupling to external libraries for large-scale optimization (IPOPT, PETSC/TAO)
- Results verified on simple cases (scalar diffusion coefficients)
- Framework for MAP estimation recently implemented (Bayesian setting), and parameter identification in the presence of measurement noise achieved
  [Carli et al, PET 21]

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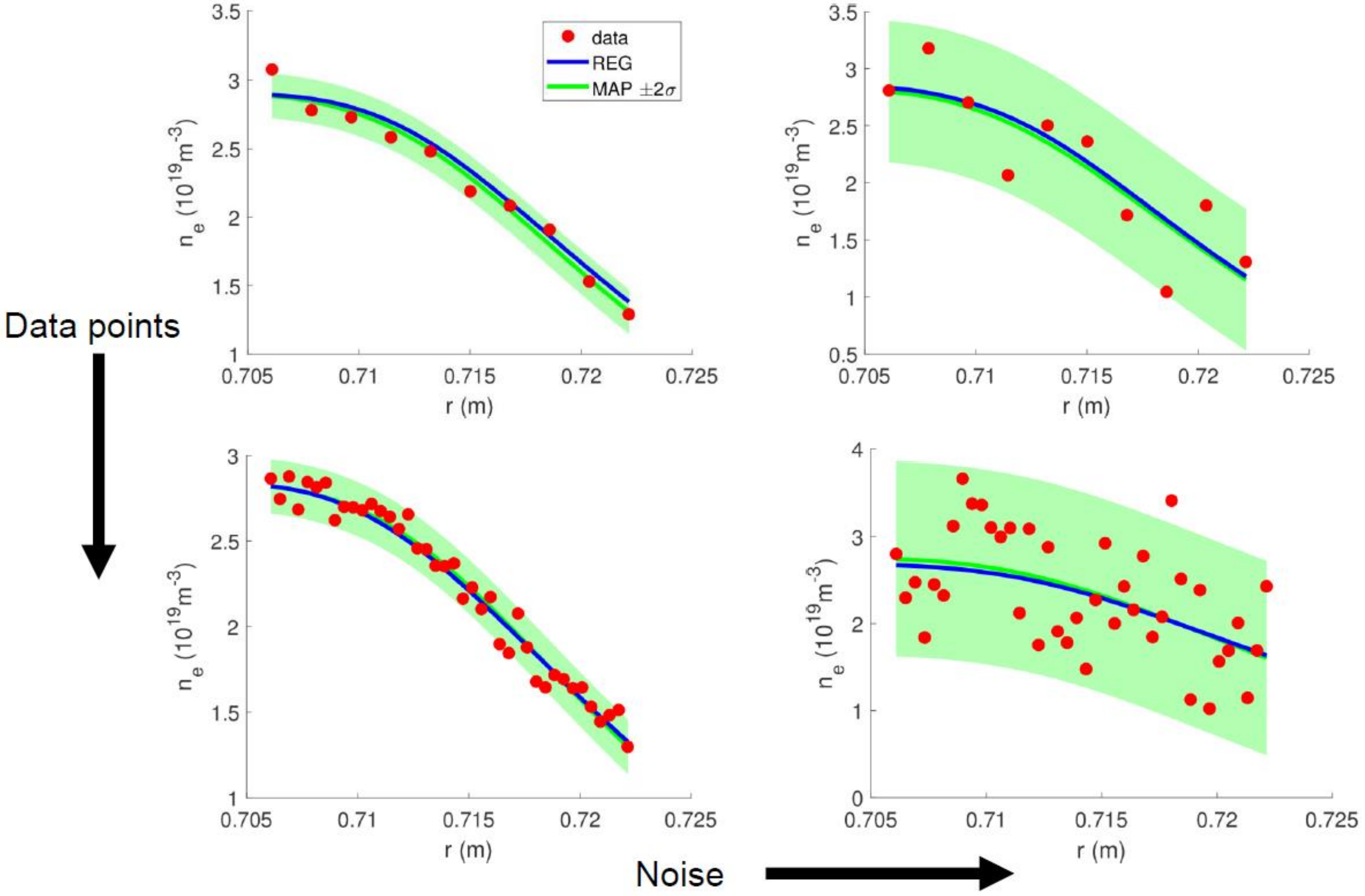
Bayesian MAP-estimation of k-model parameters

[Carli et al., PET 21]



Regression:

$$\min \quad \frac{1}{\Omega}\int_{\Omega} \omega_q \left(\frac{1}{\overline{\mathcal{D}}^2}\left(q(\theta)-\mathcal{D}\right)^2\right) d\Omega$$

MAP:

$$\max \quad \pi(\theta|\mathcal{D},\mathcal{M}) = \frac{\mathcal{L}(\mathcal{D}|\theta,\mathcal{M})\pi(\theta|\mathcal{M})}{\pi(\mathcal{D}|\mathcal{M})}$$

$$\mathcal{L}(\mathcal{D}|\theta,\mathcal{M}) = \prod_{i=1}^{N_{\mathcal{D}}} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{\epsilon_i^2}{\sigma^2}\right)$$

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Extended grids: workflow for structured cases

- Structured case set-up following usual procedure:

  divgeo => carre(2) => … => b2ag => b2ah => b2ar => b2ai

- Conversion to unstructured format:

  b2us: converts *b2fstati, b2fgmtry, b2.boundary.parameters, b2.neutral.parameters* and *input.dat*

  (*b2frates* and *b2fpardf*: unchanged)

- With converted files: set up new *baserun* and *run* directories
- Run simulation using unstructured solver (*b2mn*)
- Back-conversion to structured format:

  b2uf: creates *b2fstate_st, b2fplasmf_st* in structured format, for use in *b2plot*

  (minor adaptations to b2run-script (and b2plot) still needed to read b*2fstate_st/ b2fplasma_st/ b2fgmtry_st)*

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SOLPS-ITER extended grids version (v3.2.0): route to code release

- Code robust and backwards compatible for ‘standard’ grids
- Ready to be handed to users for testing after minor updates to workflow
- Further conversion of various code features based on user demand
- Further development of true extended grids functionality, incl. grid generation and post-processing capabilities, can be developed in parallel (after initial release)
- Several interesting model and code features under active development (AFN / hybrid / k-enstrophy / AD)

Back-up

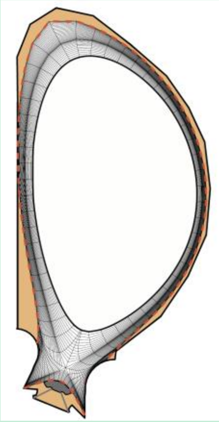
A hierarchy of neutral models

Advanced fluid neutral models (AFN)

- Efficient (direct) coupling to plasma equations, no MC noise
- Basis for hybrid methods
- Good accuracy in highly collisional regimes

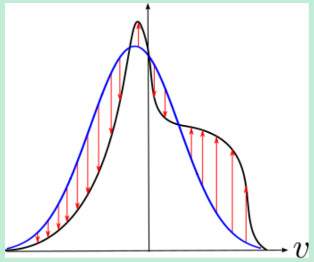
Hybrid fluid-kinetic models

Spatially (SpH)



- F-K transition based on location
- User-defined transition criteria

micro-Macro (mMH)



$$f_n(v) = f_{n,f}(v) + f_{n,k}(v)$$

- Decomposition in velocity space
- Can be made **fully equivalent** to kinetic model

Kinetic model

- Most complete physical description
- Flexibility w.r.t. geometry, collisional processes, sources, boundary conditions,…
- Very expensive in highly collisional regimes

Model accuracy →

← Computational efficiency

CPU × 1/10?

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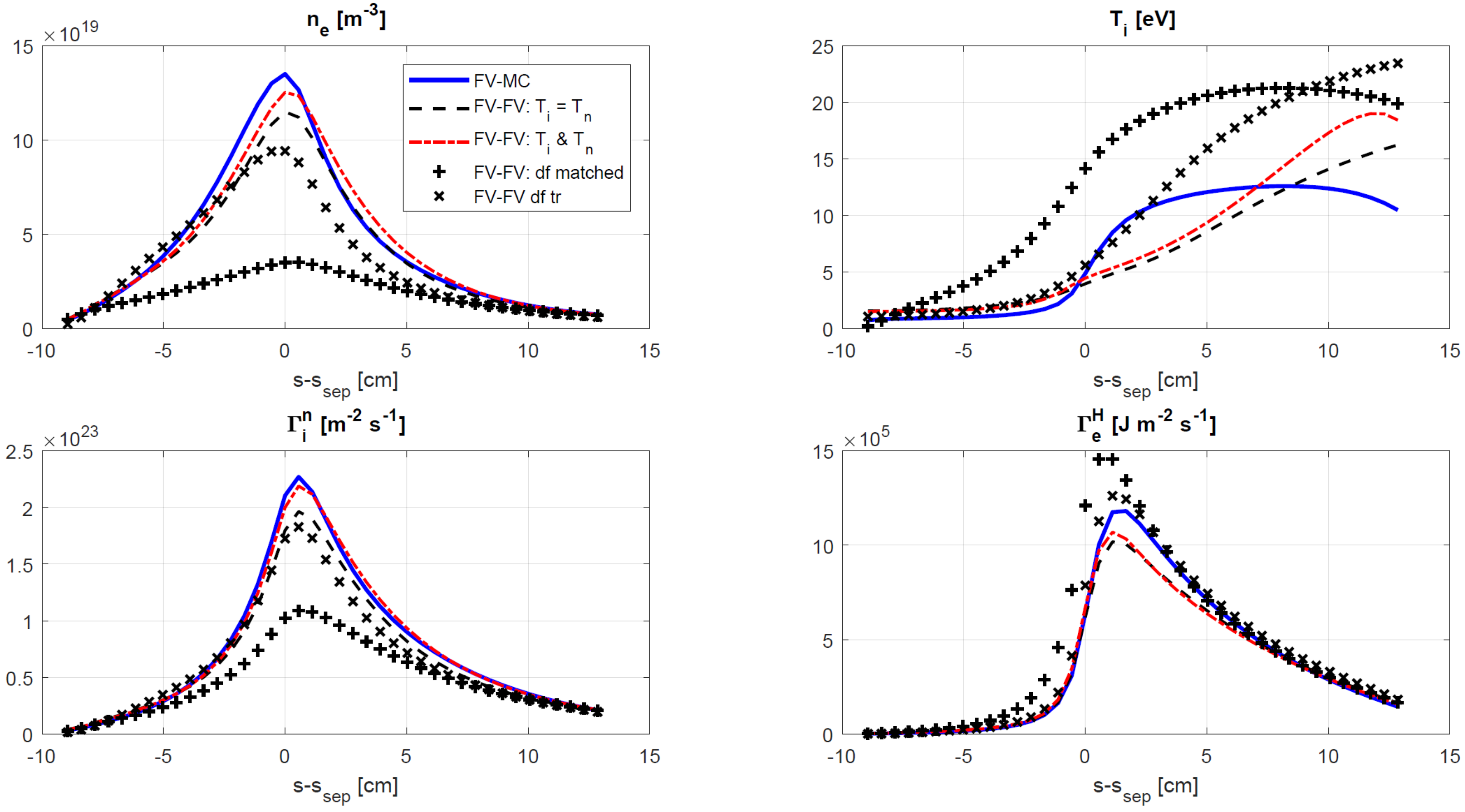
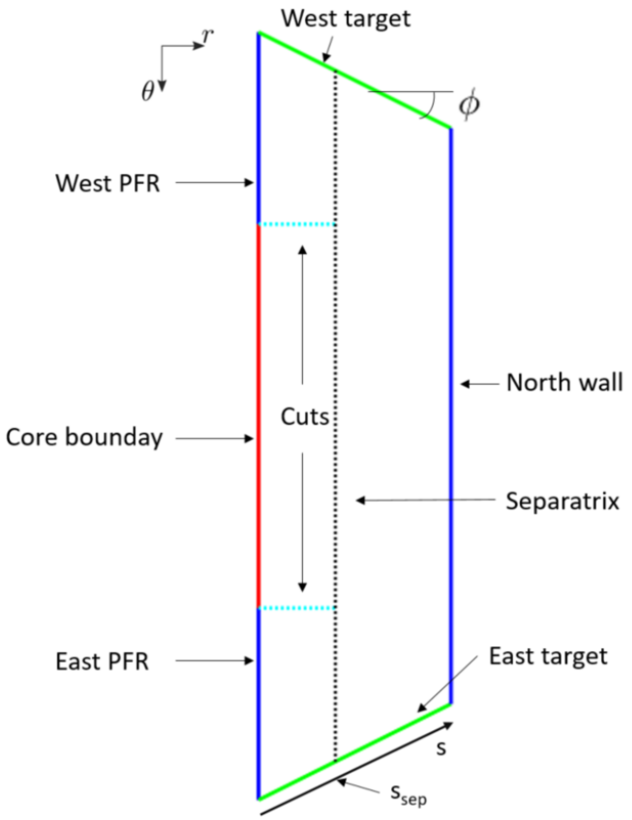
Achievements AFN

- Significant model improvements compared to ‘standard’ fluid neutral models
  - Transport coefficients consistent with collisional processes used by EIRENE (AMJUEL/HYDHEL) [N. Horsten et al., NF, 2017]
  - Boundary conditions consistent with kinetic treatment in EIRENE [N. Horsten et al., NF, 2017], incl.
    - fast/thermal reflection (approximate effect of molecules)
    - TRIM (effect of wall materials)
  - Separate neutral energy equation to extend validity range of fluid (and SpH) model towards lower recycling conditions (+ expect increased efficiency mMH) [W. Van Uytven et al., CPP 60, 2020]
- Implementation of AFN, incl. separate T_n equation, in new extended grids version of SOLPS-ITER
  - correct treatment of grid non-orthogonality [W. Dekeyser et al, NME 18, 2019]
  - simulations up-to-the-wall

‘Standard fluid neutrals’ vs. AFN vs. kinetic

[W. Van Uytven et al., in preparation.]





AFN outperforms original fluid model, without need for parameter tuning compared to kinetic simulation!

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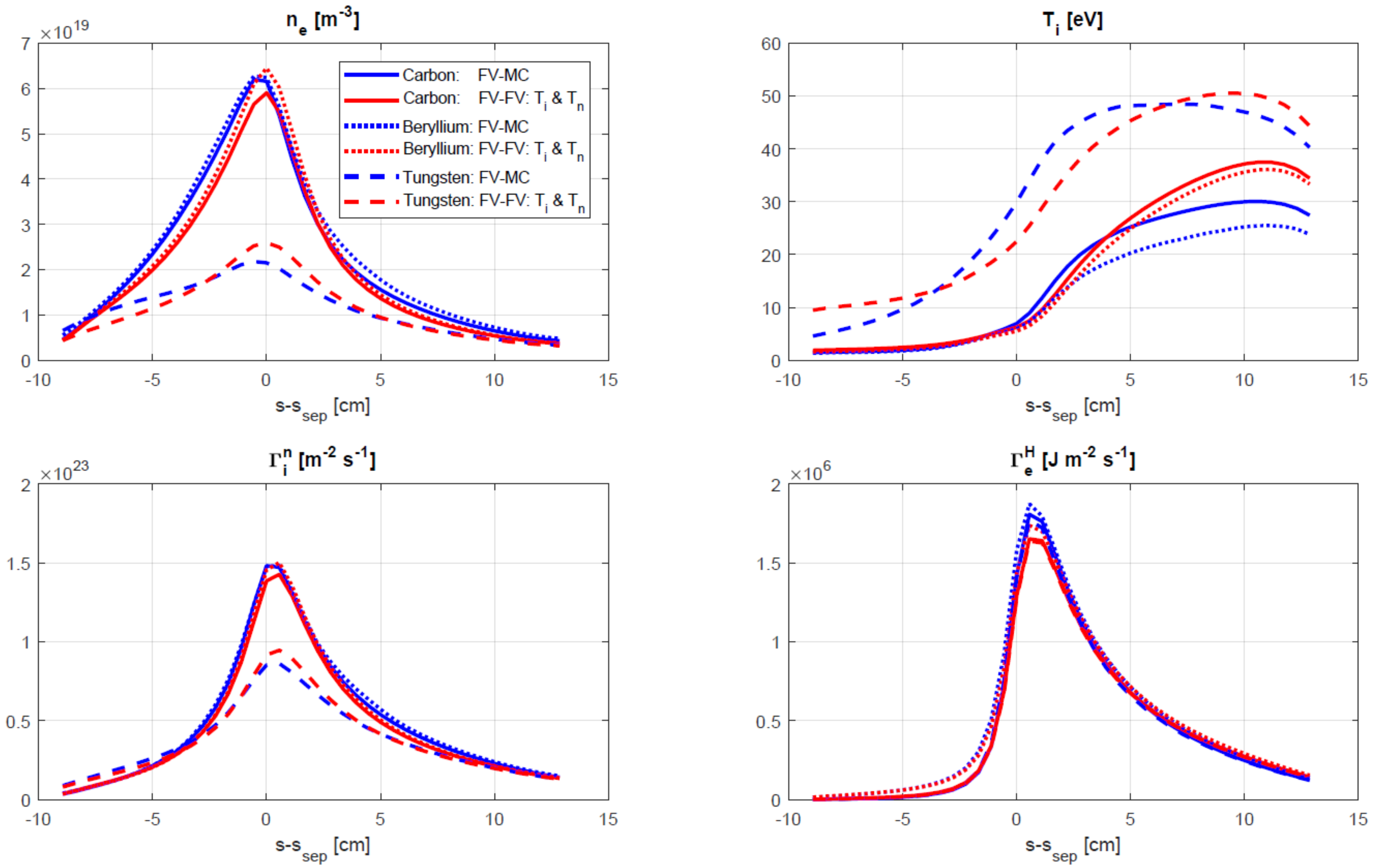
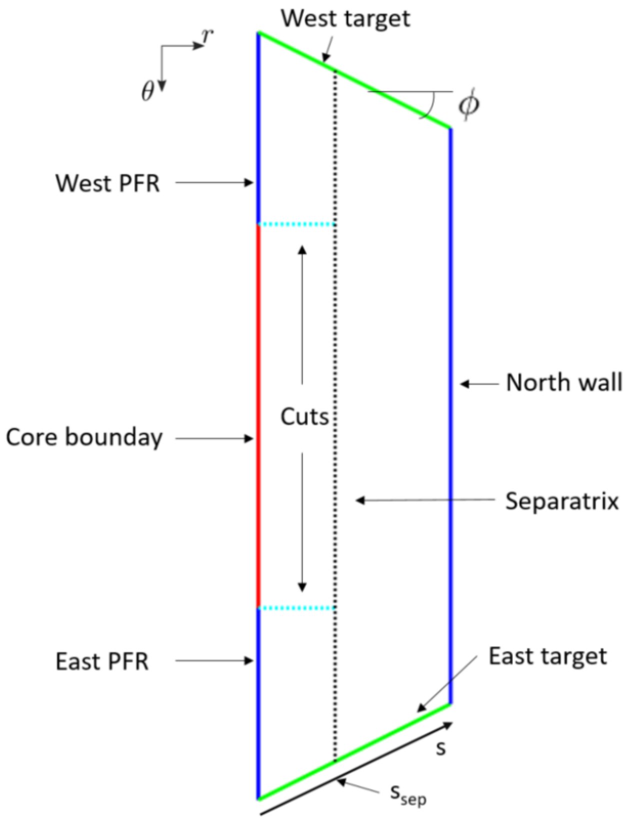
AFN: impact of wall material

[W. Van Uytven et al., in preparation.]





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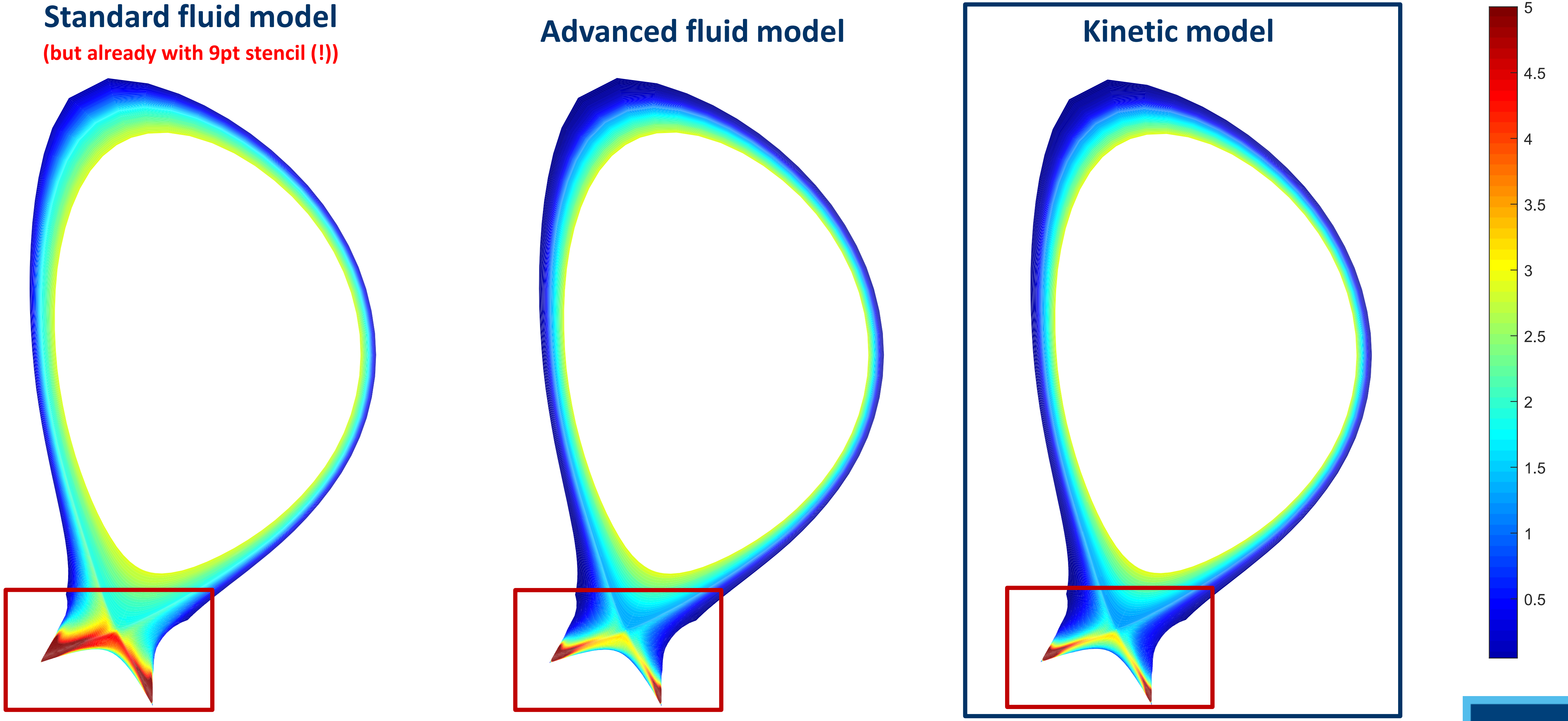
AFN: application to ITER

[W. Van Uytven et al., in preparation.]



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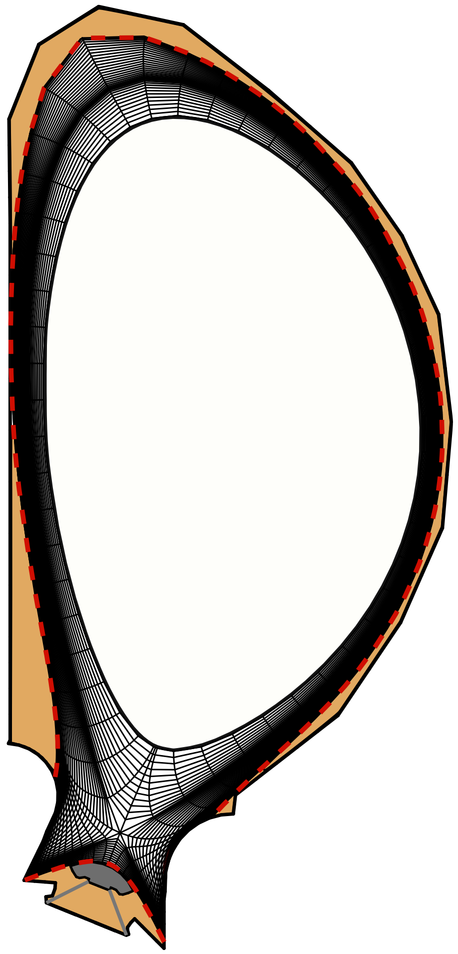
The need for SpH methods

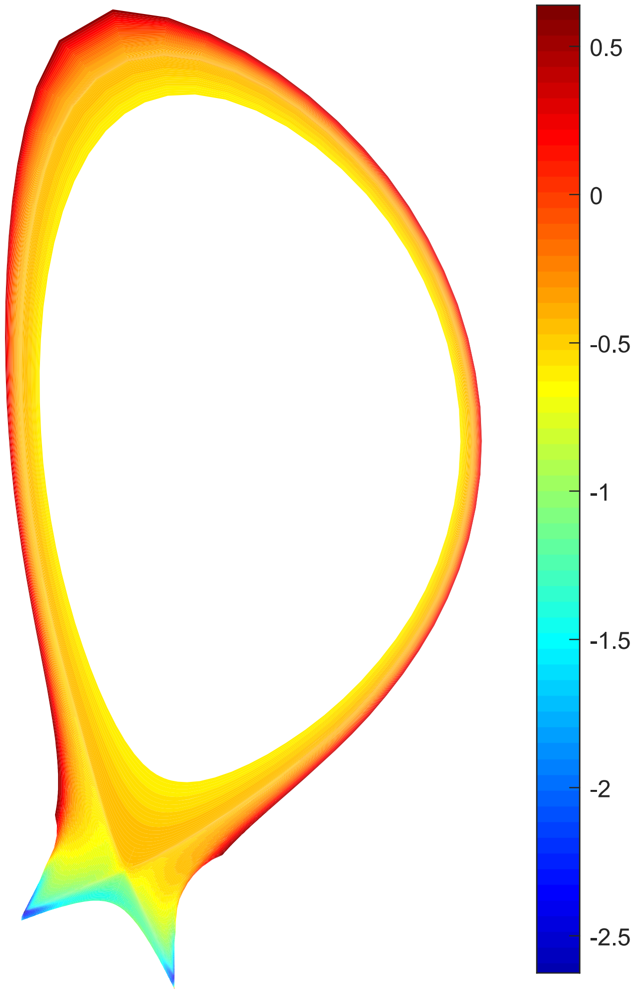
Voids not in fluid simulation



$$Kn = \frac{\lambda}{L}$$

λ: Mean-free path
L: Characteristic length scale for transport

Knudsen number high in main chamber



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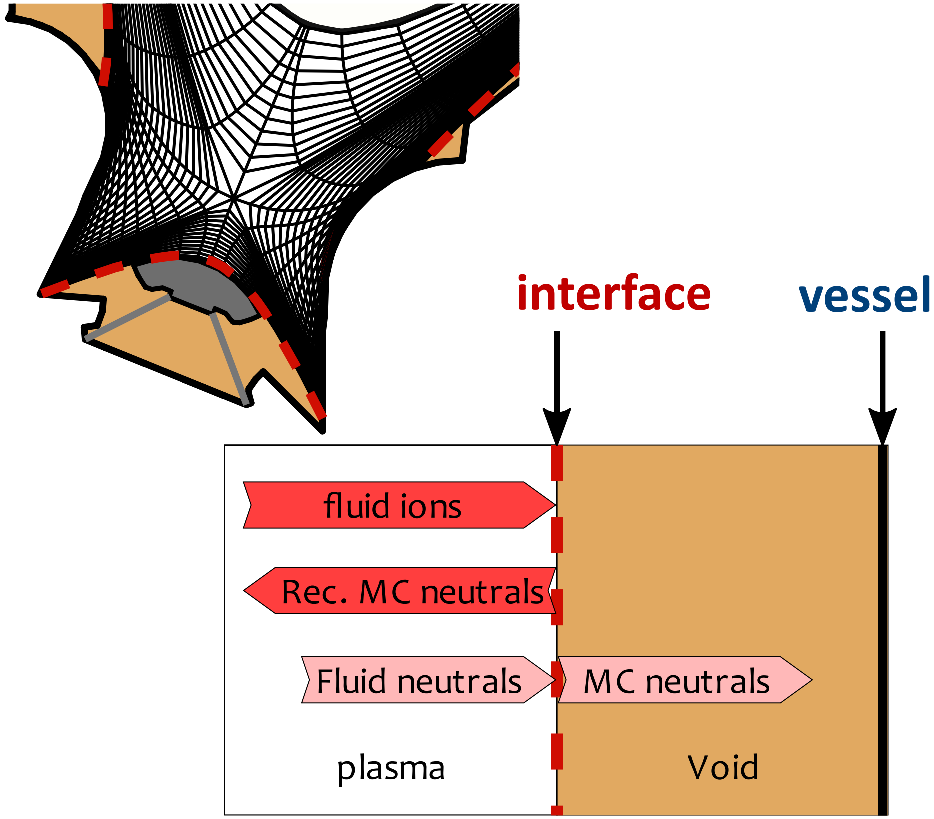
Spatially hybrid: interface conditions

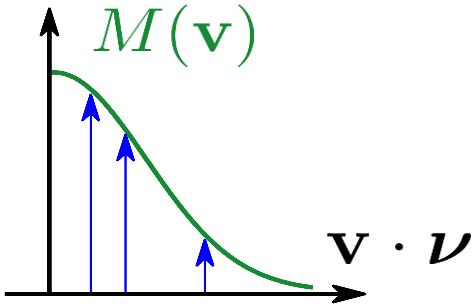
[M. Blommaert et al., NME, 2019.]



Note: approach not restricted to voids only; can decide at each boundary to treat recycling as 'fluid' or 'kinetic'

Fluid ➔ kinetic

Surface source in EIRENE sampled from **truncated Maxwellian** fluid neutral distribution



Kinetic neutrals are followed until ionization

Fluid neutral boundary condition

Moments of Maxwellian ➔ imposed fluxes

$$\Gamma^{\mathrm{n}}_{\mu} = \int_{\mathbf{v}\cdot\boldsymbol{\nu}>0} \mu(\mathbf{v})M(\mathbf{v})\mathrm{d}\mathbf{v}$$

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Achievements SpH

- Determine for each boundary whether to treat recycled/reflected particles as fluid or kinetic
  - Improved accuracy compared to pure fluid
  - Improved speed compared to kinetic

- Coupling to molecules
  - Purely kinetic treatment of molecules, SpH for atoms
  - After dissociation of molecule: choice whether to continue with fluid or kinetic treatment of the resulting atom(s) (more reliable treatment based on local ‘fluid limit’ under investigation)
  - Adaptations to B2.5-EIRENE interface to decide which part of the incident fluxes should be recycled as kinetic atom/molecule (=> EIRENE) or fluid atom (=> B2.5)
  - Speed up compared to fully kinetic simulation: ~order of magnitude (JET L-mode, N. Horsten, NME)

- Integration in extended grids version of SOLPS-ITER

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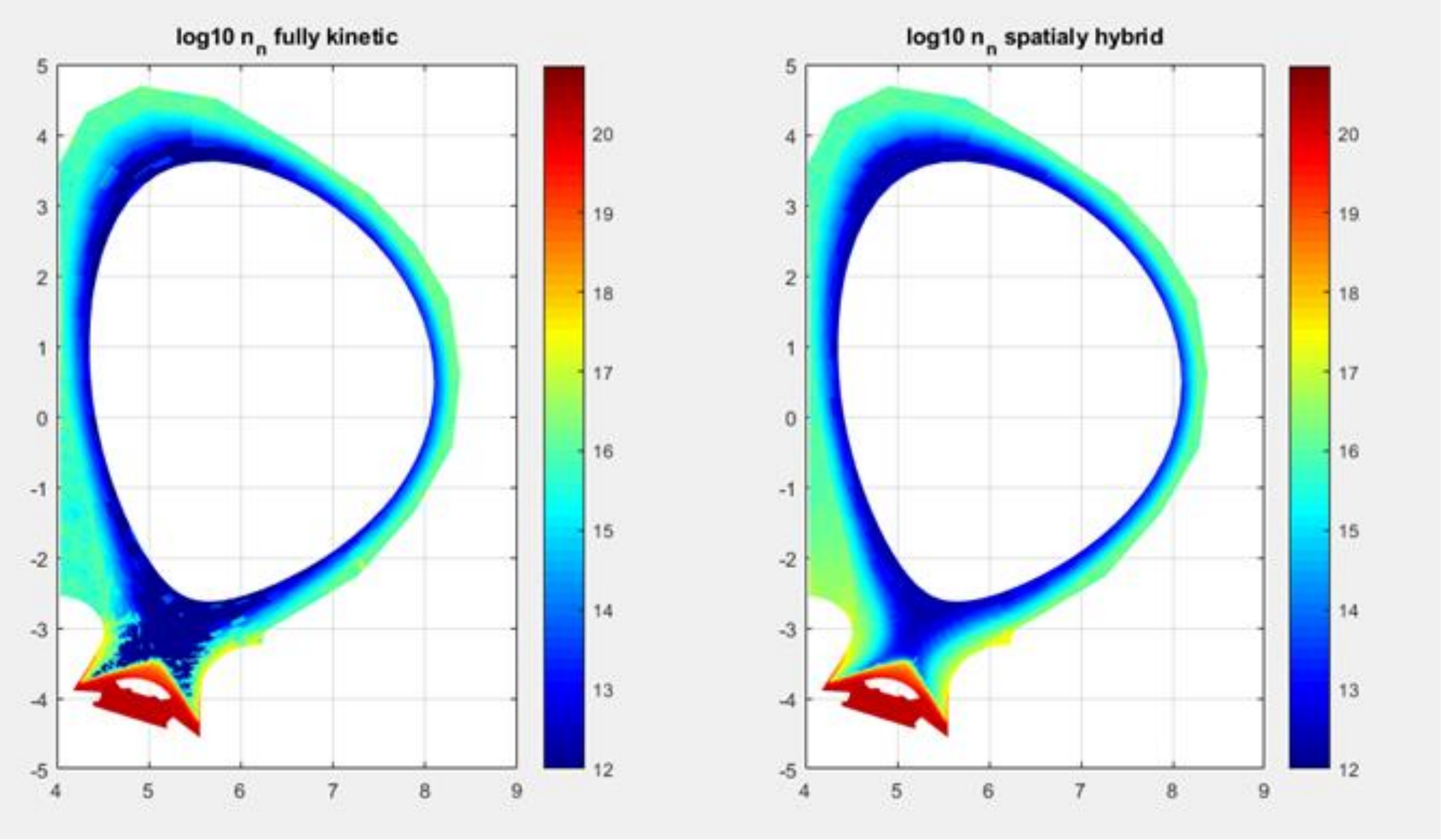
SpH: first application to ITER, fixed plasma (*prelim.*)



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Application 3: matching experimental data

[Baelmans et al., Plasma Phys. Control. Fusion **56** (2014) 114009.]

Cost functional

$$J(\phi, \mathbf{q}) = \frac{1}{2} \int_{\mathrm{t,OM}} \frac{1}{L_0} \left(\frac{1}{n_0^2} \left(n - n^{\mathrm{exp}}\right)^2 + \frac{1}{T_0^2} \left(T - T^{\mathrm{exp}}\right)^2 \right) \mathrm{d}s$$

ϕ : transport coefficients and plasma edge model constants

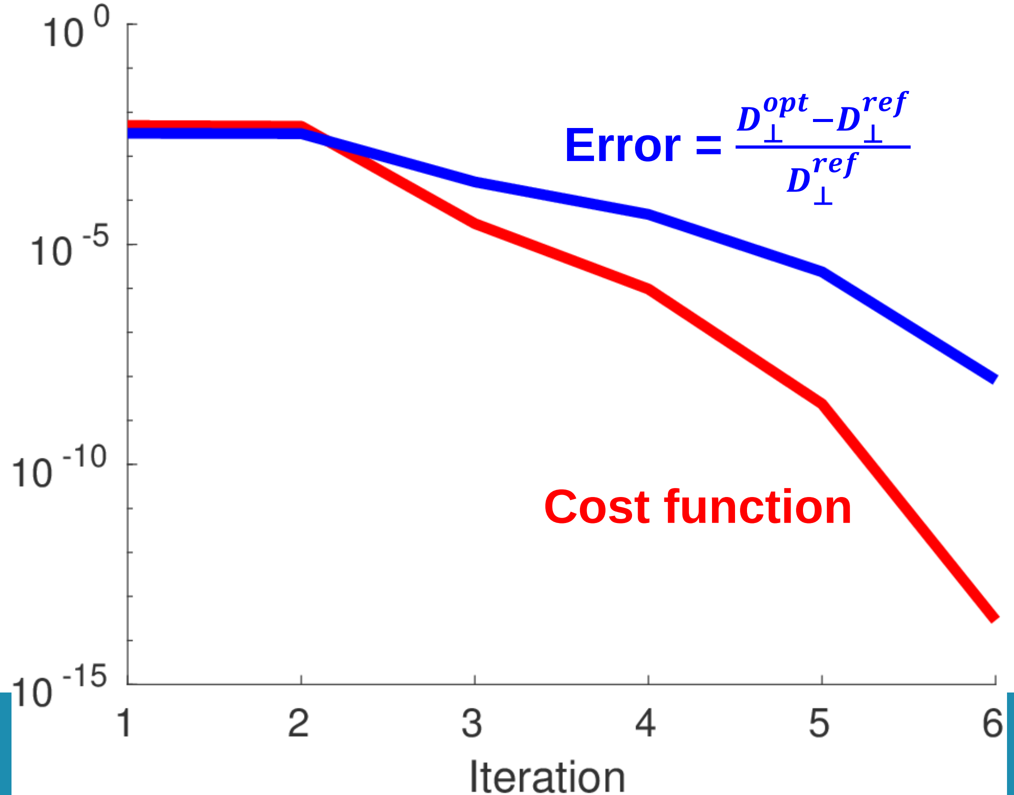
$\mathbf{q}$: ‘state’ variables (plasma density, temperature,…)

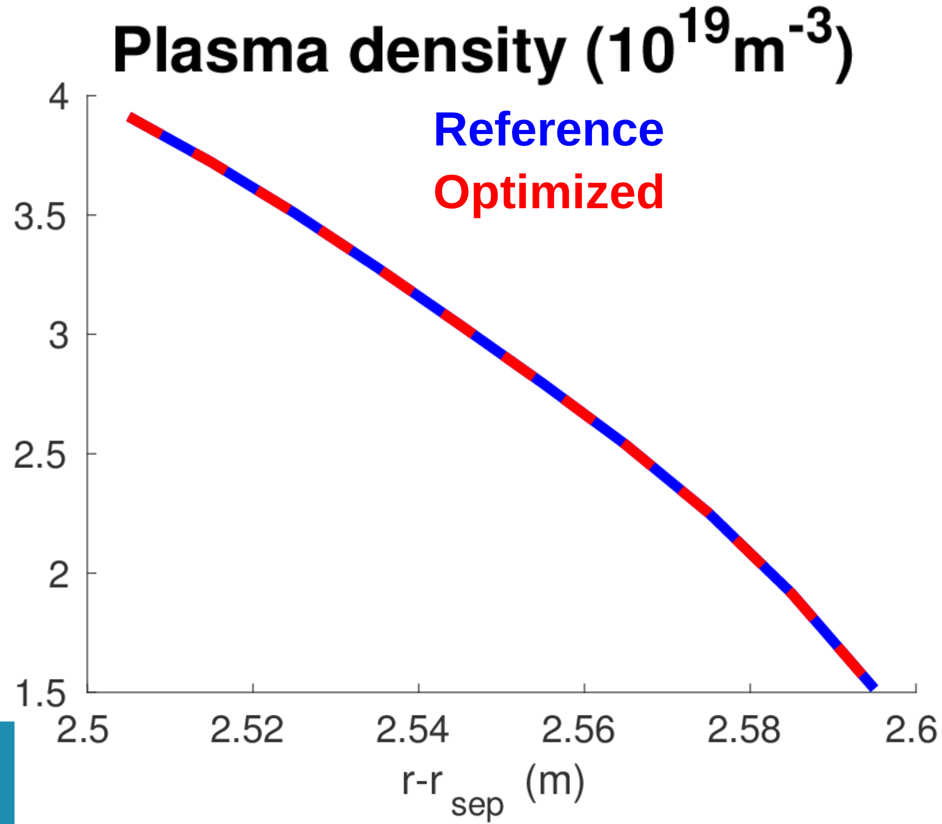
Control variables: unknown parameters ϕ to match

Additional constraints: ϕ within specified range

Proof of principle parameter estimation

- Slab case, pure D plasma with AFNs
- Scalar $D_\perp \in [0.5, 2.5]$, only n_e in cost functional
- Fictitious experimental data: SOLPS result with scalar $D_\perp^{ref}$





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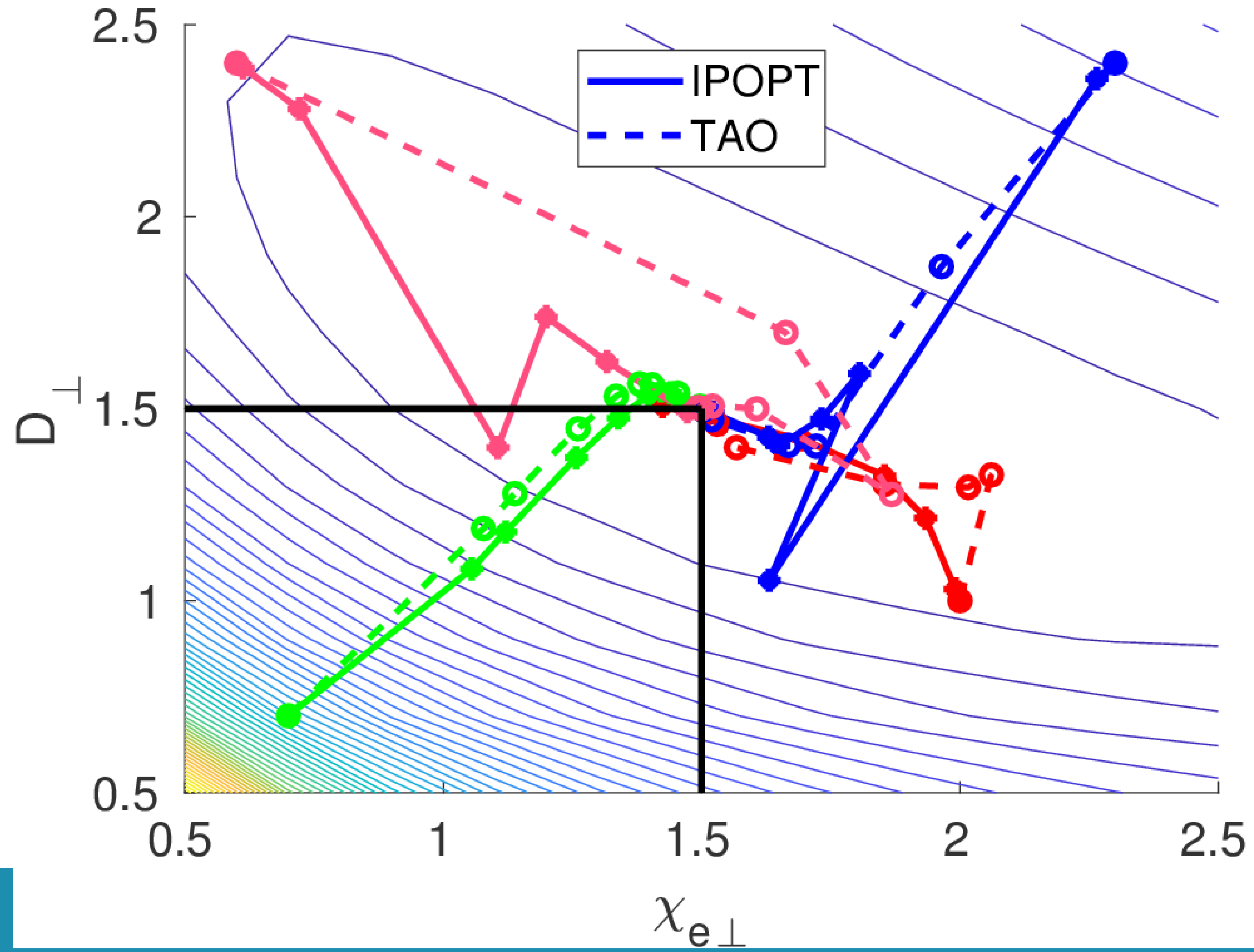
Scalar $D_{\perp}$ and $\chi_{e\perp}$ estimation, n_e and T_e in cost function



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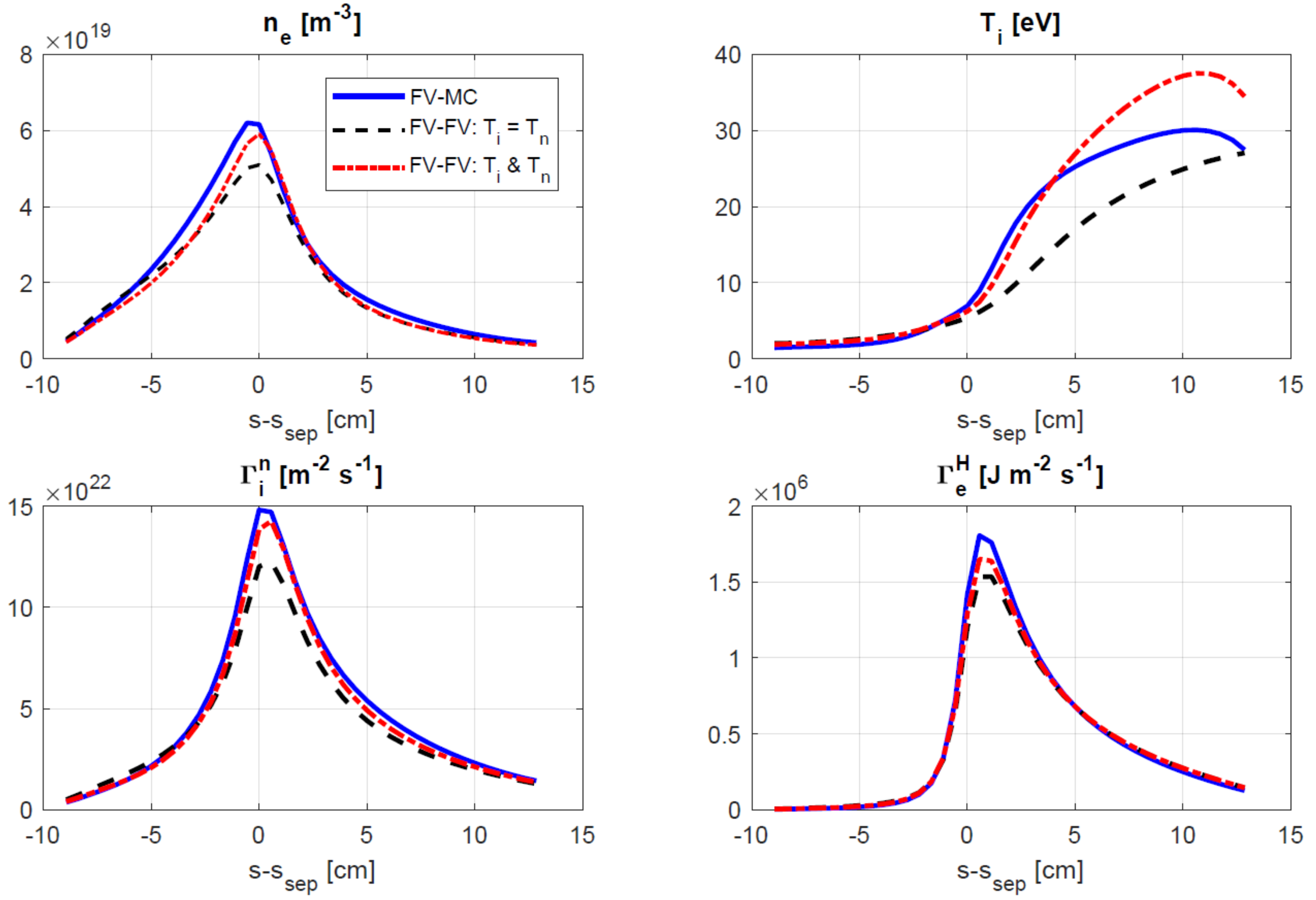
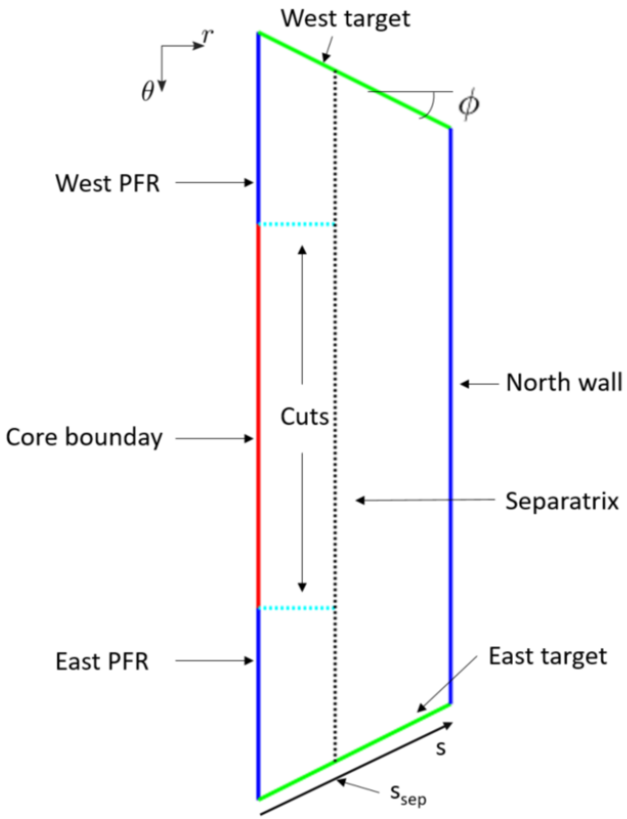
AFN: impact of separate T_n equation

[W. Van Uytven et al., in preparation.]





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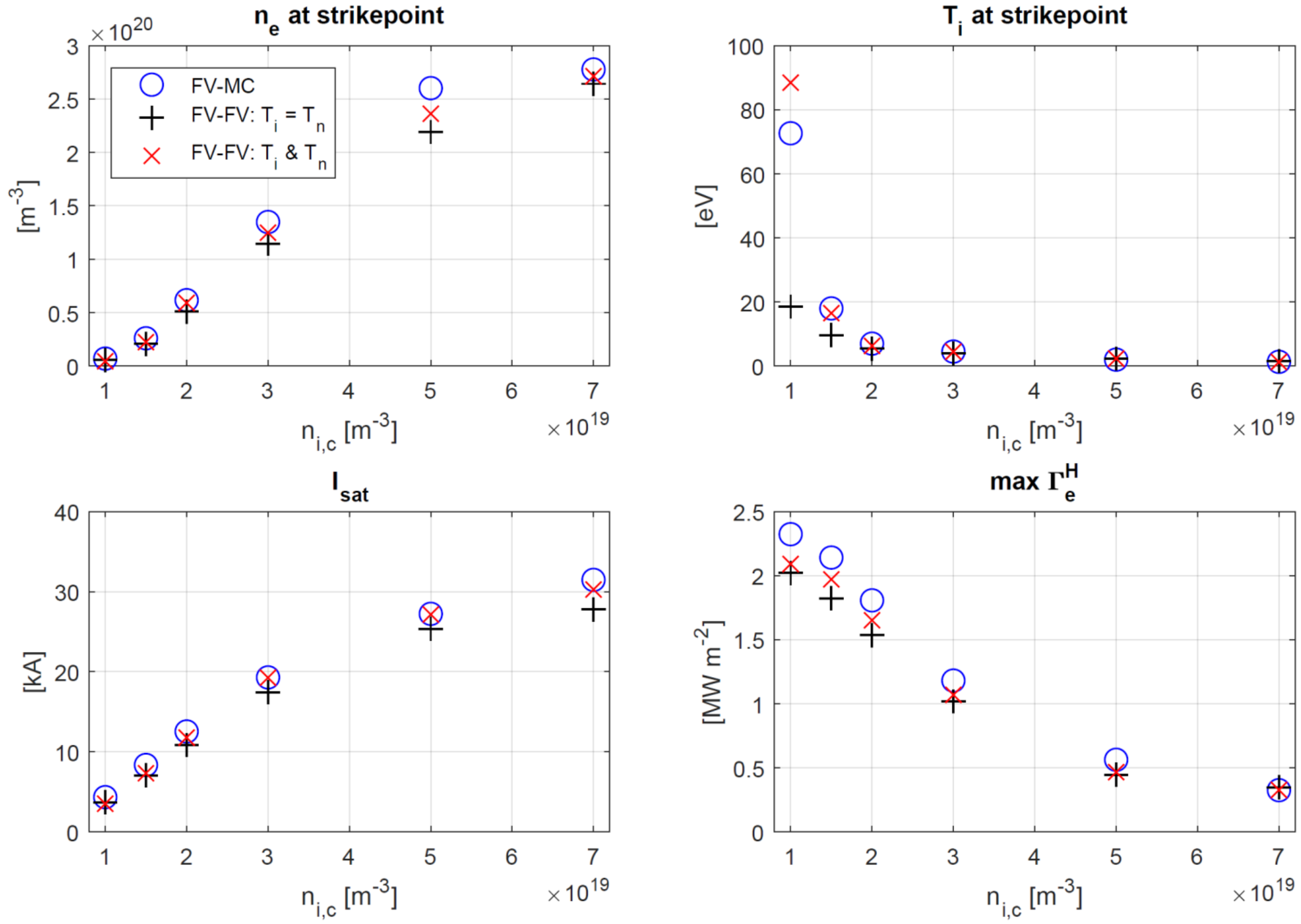

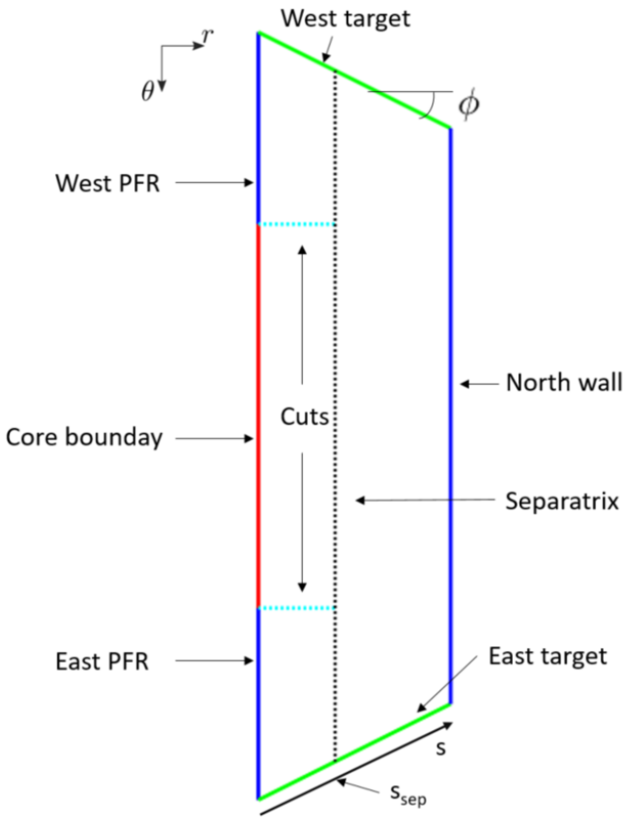

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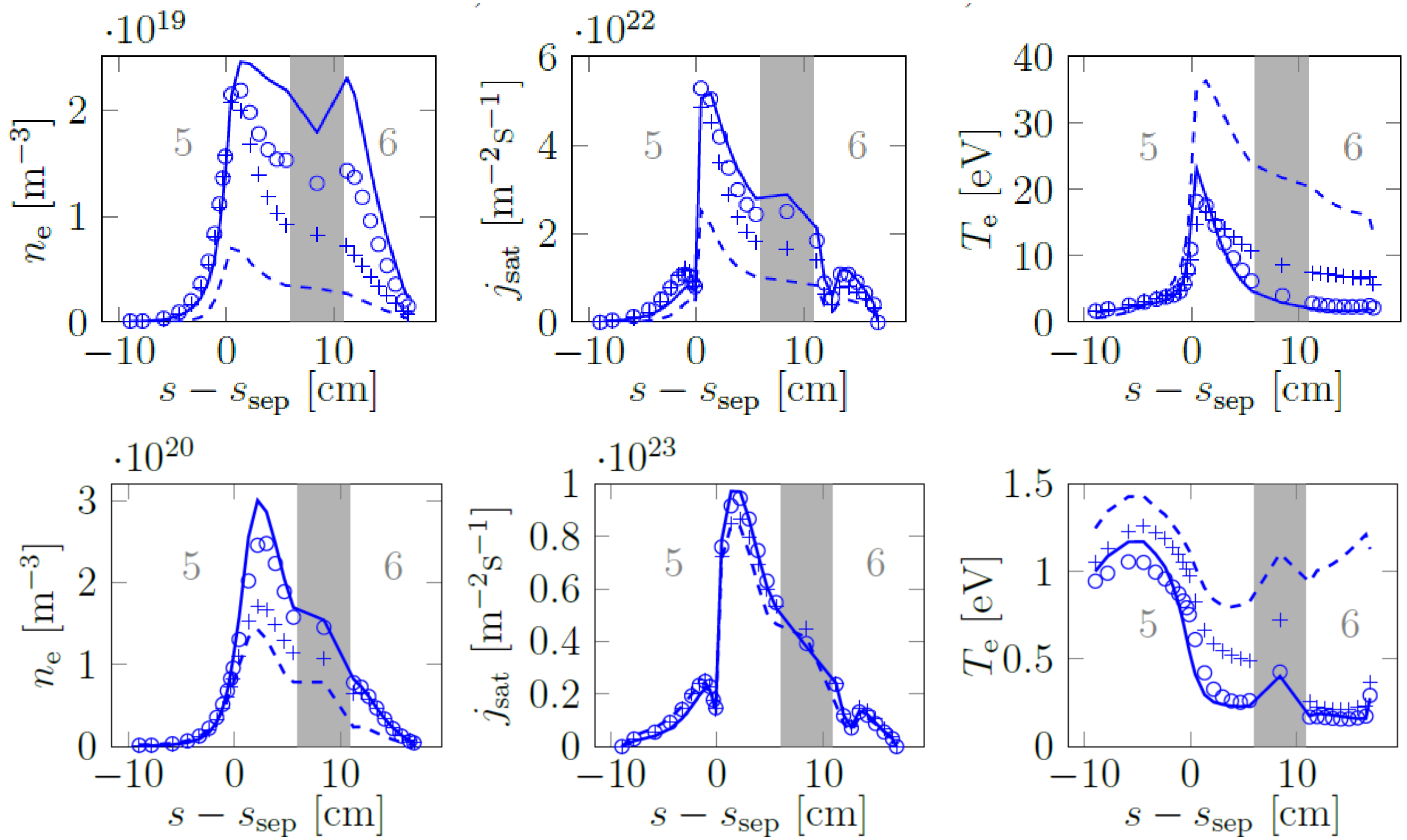
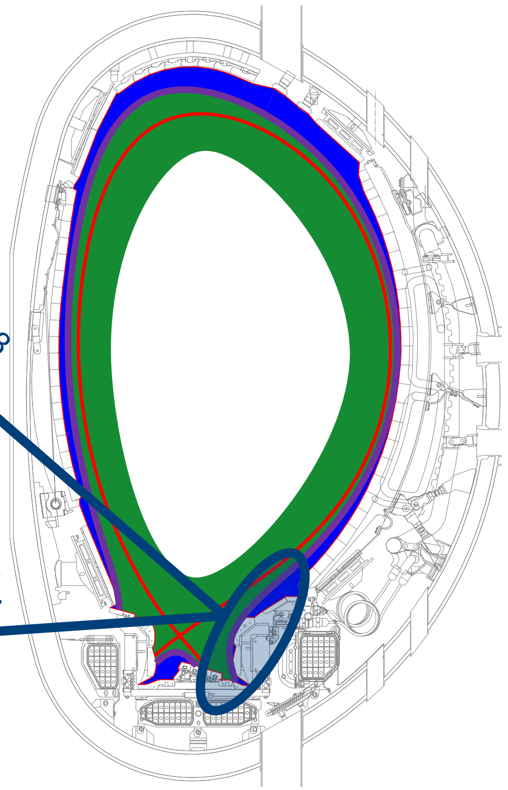
SpH: coupling to molecules

[N. Horsten et al., submitted to NME.]

Medium recyc.

High recyc.





n_{core} = 2.0e19 m^{-3}

n_{core} = 4.0e19 m^{-3}

—— Fully kinetic	○ Hybrid, atoms from dissociation kinetic
- - - Purely fluid	+ Hybrid, atoms from dissociation fluid

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SpH: coupling to molecules, speed-up

[N. Horsten et al., submitted to NME.]

Variance reduction at equal # particles

	$A_{n_{e,it}}$	$A_{n_{e,ot}}$	$A_{T_{e,it}}$	$A_{T_{e,ot}}$
$n_{core} = 2.0 \cdot 10^{19}$ m^{-3}				
Kinetic	4.19	5.23	5.39	5.00
Hybrid 1	3.69	1.42	2.94	1.72
Hybrid 2	1.52	1.36	1.73	1.68
$n_{core} = 4.0 \cdot 10^{19}$ m^{-3}				
Kinetic	1.72	3.07	6.25	9.61
Hybrid 1	1.41	3.86	2.24	2.18
Hybrid 2	1.24	1.04	1.68	1.11

Hybrid 1: diss. mol. kin.
Hybrid 2: diss. mol. fluid

- Speed-up: ~ $(A_{kin}/A_{hyb})^2$
  - Hybrid 1: ~ 6…7
  - Hybrid 2: ~ 10…20
- Trade-off hybrid 2: speed-up vs. model accuracy; further optimization possible:
  - Improved redistribution of particles for hybrid methods
  - Improved choice between fluid/kinetic treatment dissociated molecules based on stratum/location/…

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The interchange source of $\kappa_\perp$

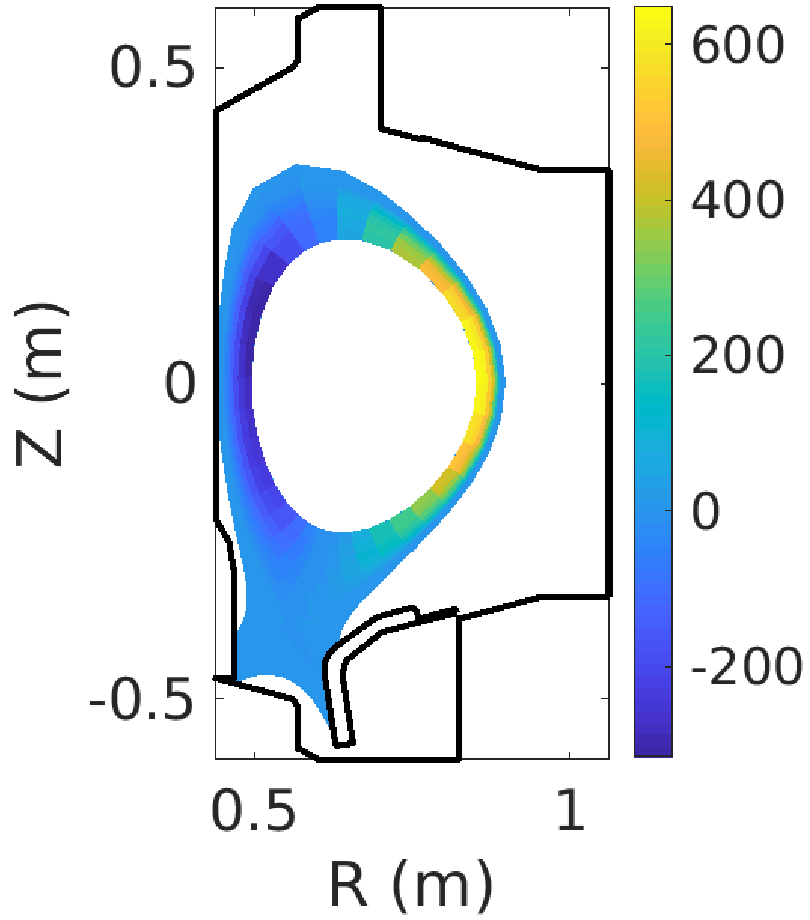
- Total heat flux due to $E \times B$ fluctuations drives production of $k_\perp$
  [Coosemans et al., prev. talk.]

$$\overline{S}_{IC} = -\frac{2}{3}\left(\overline{\boldsymbol{\Gamma}}_{i,E\times B}\tilde{T}_i + \overline{\boldsymbol{\Gamma}}_{e,E\times B}\tilde{T}_e + \overline{\boldsymbol{Q}}_{i,E\times B} + \overline{\boldsymbol{Q}}_{e,E\times B}\right)\cdot\nabla \ln B^2$$

  - Source in 'bad-curvature' regions
  - Sink (!) in 'good-curvature' regions
  - Internal saturation mechanism
  - Energy conservation: coupling with ion/electron internal energy equations

- Neglect transport contributions (cancel exactly in 1D)

$$\nabla\cdot\left(\overline{\phi' J'_*} + \overline{p' V'_{E\times B}}\right) \approx 0$$



Transport of $\kappa_\perp$ due to parallel current fluctuations

- Parallel current fluctuations:

$$j'_{||} \approx -\sigma_{||}\nabla_{||}\phi' + \frac{\sigma_{||}}{e n_e}\nabla_{||}p'_e + \frac{0.71\sigma_{||}}{e}\nabla_{||}T'_e$$

- Model for transport of $\kappa_\perp$:

$$\overline{\phi' j'_{||}} \sim -\sigma_{||}\nabla_{||}\frac{\overline{\phi'^2}}{2} \sim -C_{\sigma 1}\sigma_{||}\rho_L^2\nabla_{||}\kappa_\perp$$

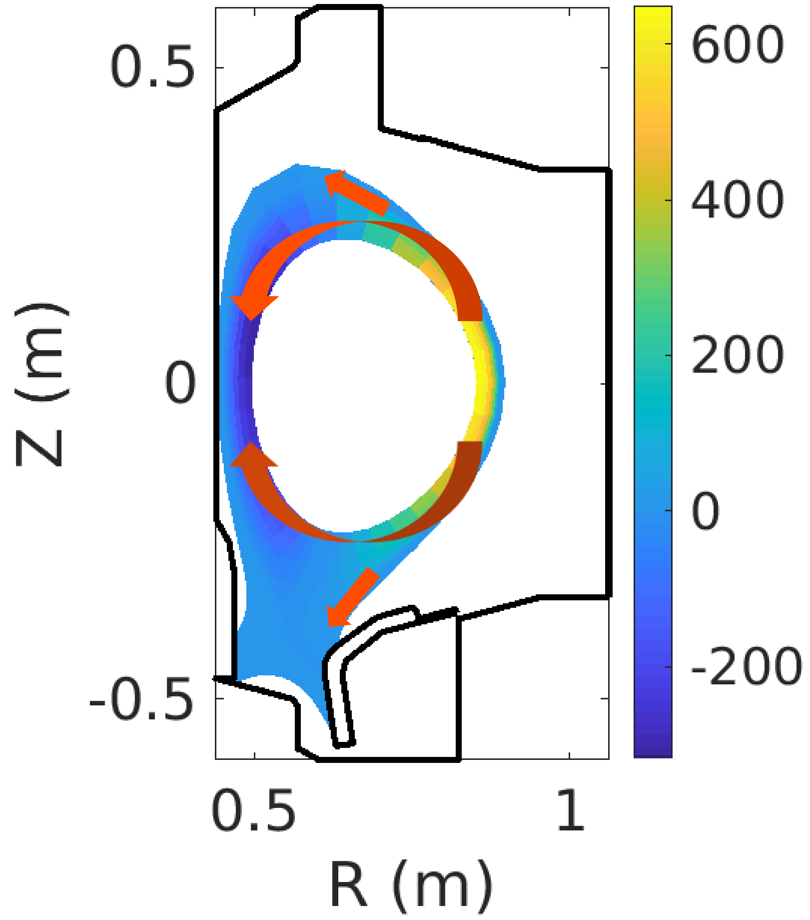
Strongly exceeds parallel convection with $\tilde{u}_{||}$!

('ideal' interchange: $\frac{\pi}{2}$ phase shift n'/T'_e and ϕ')

$\left(\kappa_\perp \sim (\nabla_\perp\phi')^2 \sim \frac{\phi'^2}{\rho_L^2}\right)$

- Model for (small) dissipation term for $\kappa_\perp$:

$$\overline{S}_{||} = \overline{j'_{||}\cdot\nabla_{||}\phi'} \sim -\sigma_{||}\left(\nabla_{||}\phi'\right)^2 \sim -C_{\sigma 2}\sigma_{||}\left(\frac{\rho_L}{L_{||}}\right)^2 k_\perp$$



  - Energy balance: coupling with electron energy equation

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Impact of (mean) $E \times B$ flow shear

- Reynolds-stress tensor: negative-viscosity model

$$\Pi_{RS} = \overline{mnV''_{E\times B}V''_{E\times B}} \sim \frac{2}{3}\bar{n}\kappa_{\perp}\mathrm{I} - 2\eta_{E\times B}\left(\nabla\bar{V}_{E\times B} + \nabla\bar{V}_{E\times B} - \frac{1}{3}(\nabla\cdot\bar{V}_{E\times B})\mathrm{I}\right)$$

$$\eta_{E\times B} = -C_\eta m\bar{n}D_{E\times B}$$

- Turbulence suppression due to flow shear

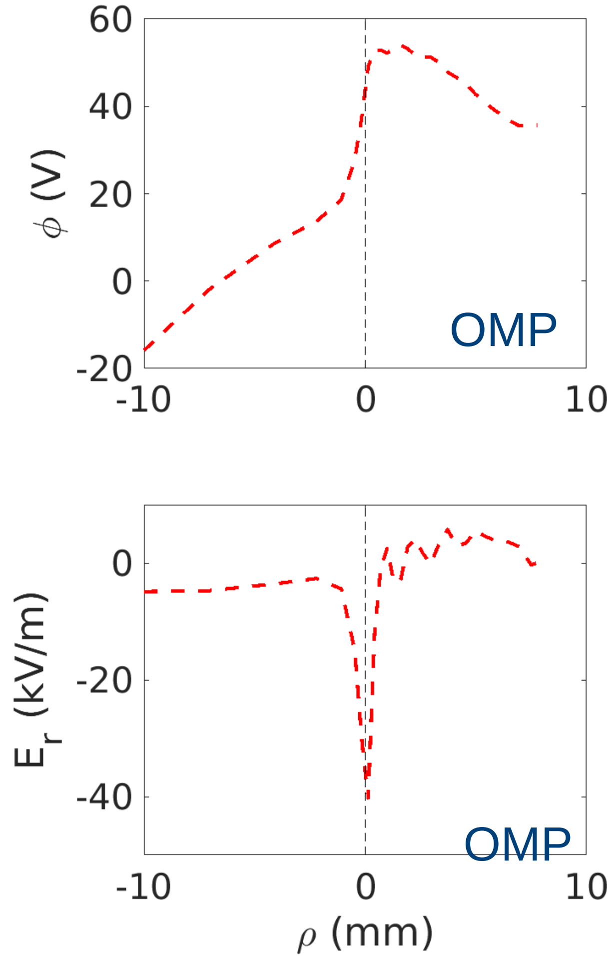
$$\bar{S}_{RS} = -\Pi_{RS}:\nabla\bar{V}_{E\times B} \sim \eta_{E\times B}\left(\frac{\partial\bar{V}_{E\times B,\theta}}{\partial r}\right)^2$$

- Energy conservation: corresponding ion drift/current

$$\mathbf{\Gamma}_{RS} = \frac{m\boldsymbol{b}}{eB}\times\left(\nabla\cdot\overline{nV''_{E\times B}V''_{E\times B}}\right)$$

- Transport reduction due to flow shear: $D_{E\times B} \sim \dfrac{C_D\kappa_\perp}{\sqrt{\kappa_\perp/\mathrm{m}_i}/\rho_L + C_s|\nabla\bar{V}_{E\times B}|}$

[Coosemans et al., J. Phys.: Conf. Series **1785** (2021) 012001.]



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Model summary

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

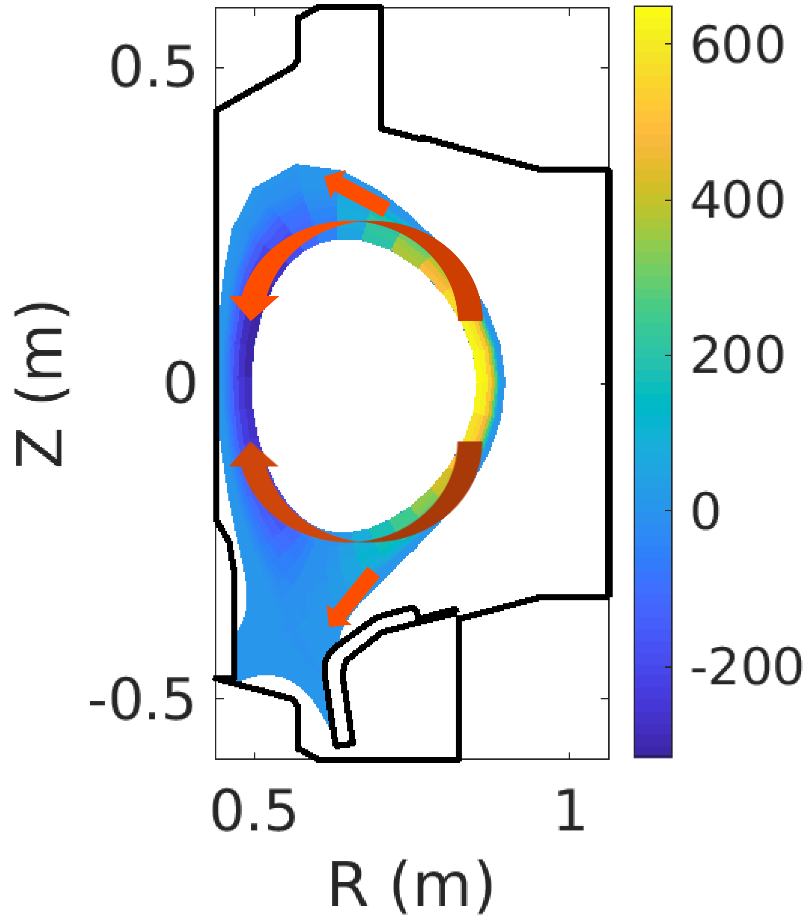
$$\frac{\partial}{\partial t}\bar{n}\kappa_\perp + \nabla\cdot\overline{\boldsymbol{\Gamma}}_{\kappa_\perp} = \bar{S}_{\kappa_\perp}$$

  - Source/sink of $\kappa_\perp$: $\bar{S}_{\kappa_\perp} \approx \bar{S}_{IC} + \bar{S}_{||} + \bar{S}_{RS}$
  - Transport: $\overline{\boldsymbol{\Gamma}}_{\kappa_\perp} \approx \nabla\cdot\left(\overline{\boldsymbol{\Gamma}}\kappa_\perp + \frac{1}{2}\overline{mn\boldsymbol{V}''V''^2_{E\times B}} + \overline{\phi'\boldsymbol{J}'_{||}}\right)$
- Couple to ‘regular’ mean field equations
  - Transport coefficients determined by local value of $\kappa_\perp$

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

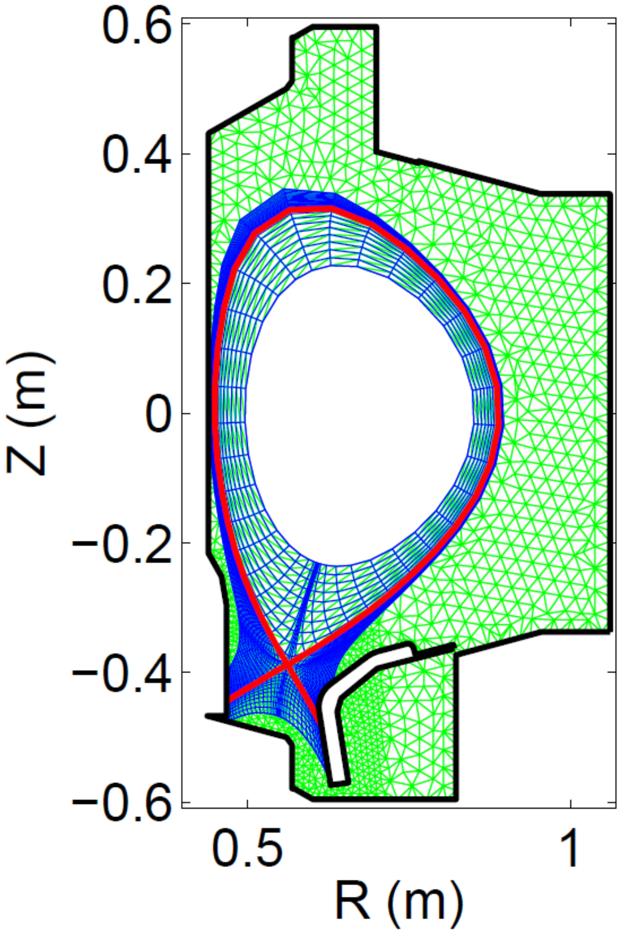
  - Energy conservation (mean field + turbulent + RS-drift)
- Implemented in new ‘extended grids’ version of SOLPS-ITER

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



Test case based on C-Mod shot #1070627009

[Dekeyser et al., NME **12** (2017) 899.]



Model

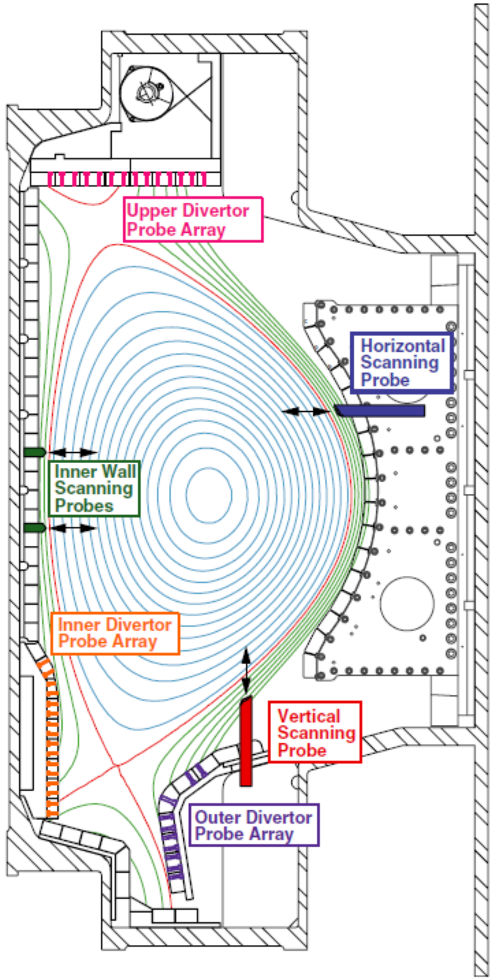
- Single species deuterium plasma
- SOLPS-ITER drifts model incl. (mean-field) ExB and diamagnetic drifts
- Complete kinetic neutral model (atoms + molecules), including n-n collisions
- Newly developed $\kappa_\perp$ model for anomalous transport

Setup and boundary conditions

- Lower Single Null (LSN), ion $B\times\nabla B$ drift towards divertor (“normal” field direction)
- Core: fixed density, power $P_{OH} - P_{rad,core}$ ~ 0.8 MW
- Targets: standard sheath conditions
- Radial boundaries: leakage BCs

Experimental data

- Focus on midplane and target probes



[Smick et al., Nucl. Fusion **53** (2013) 023011.]

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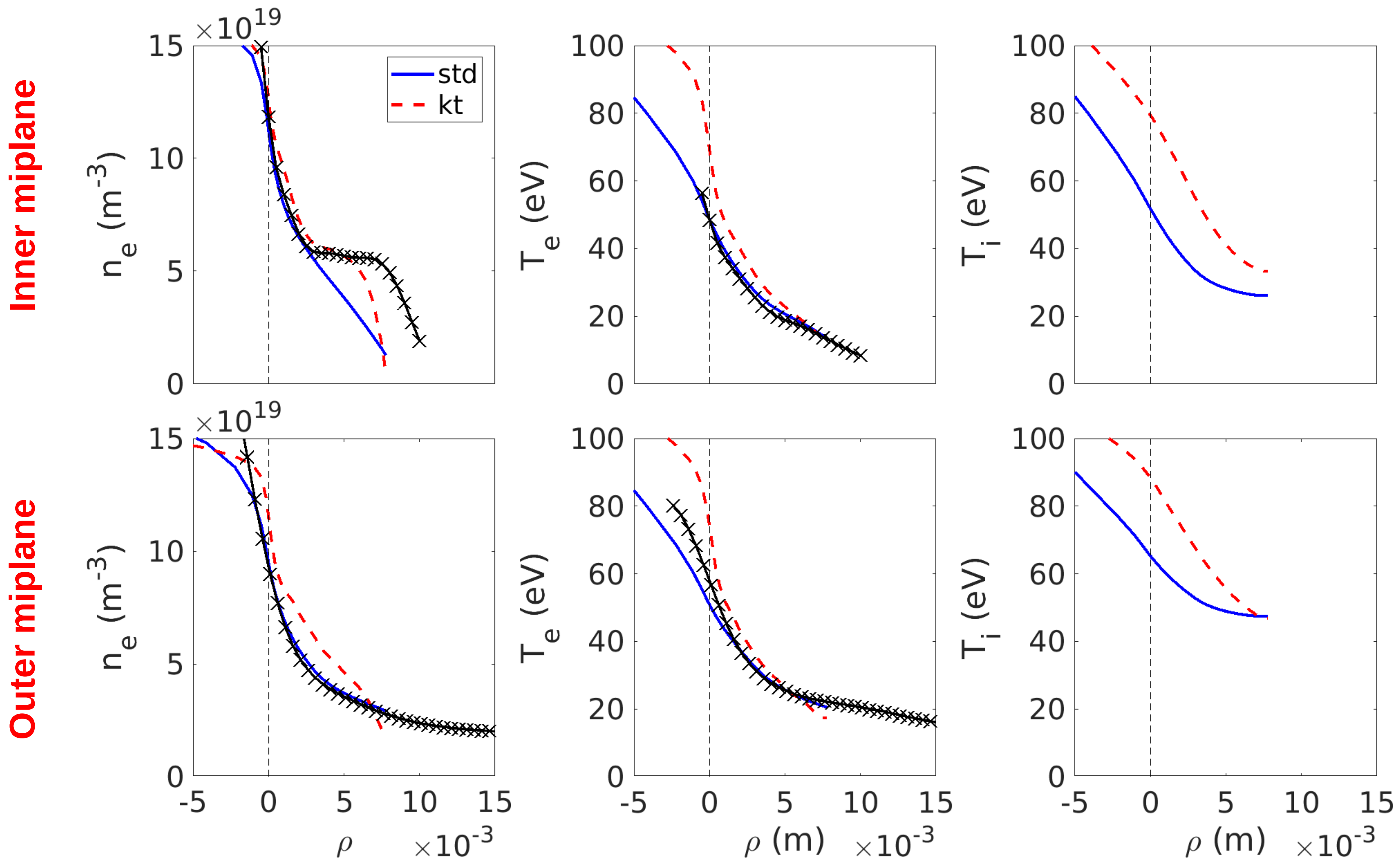
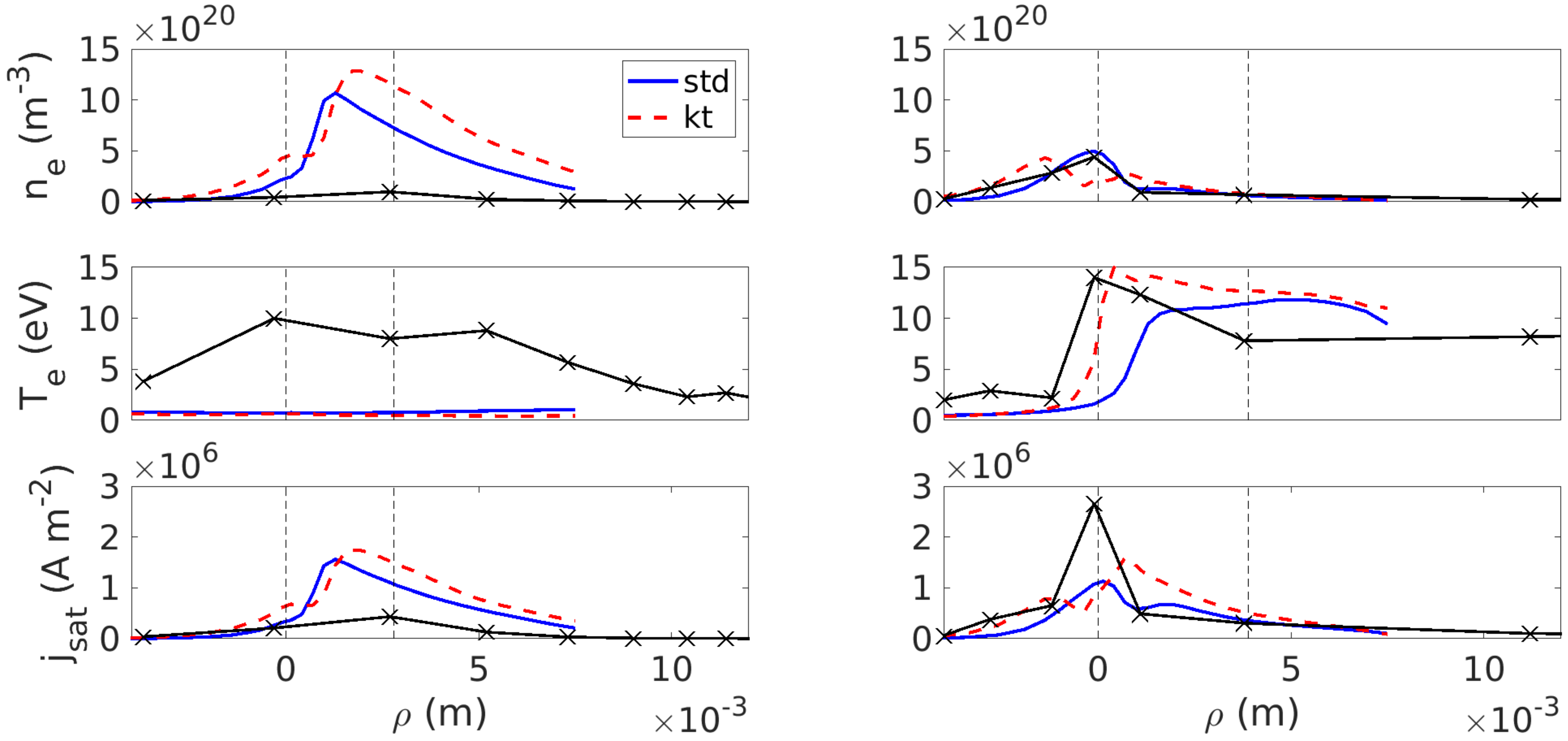
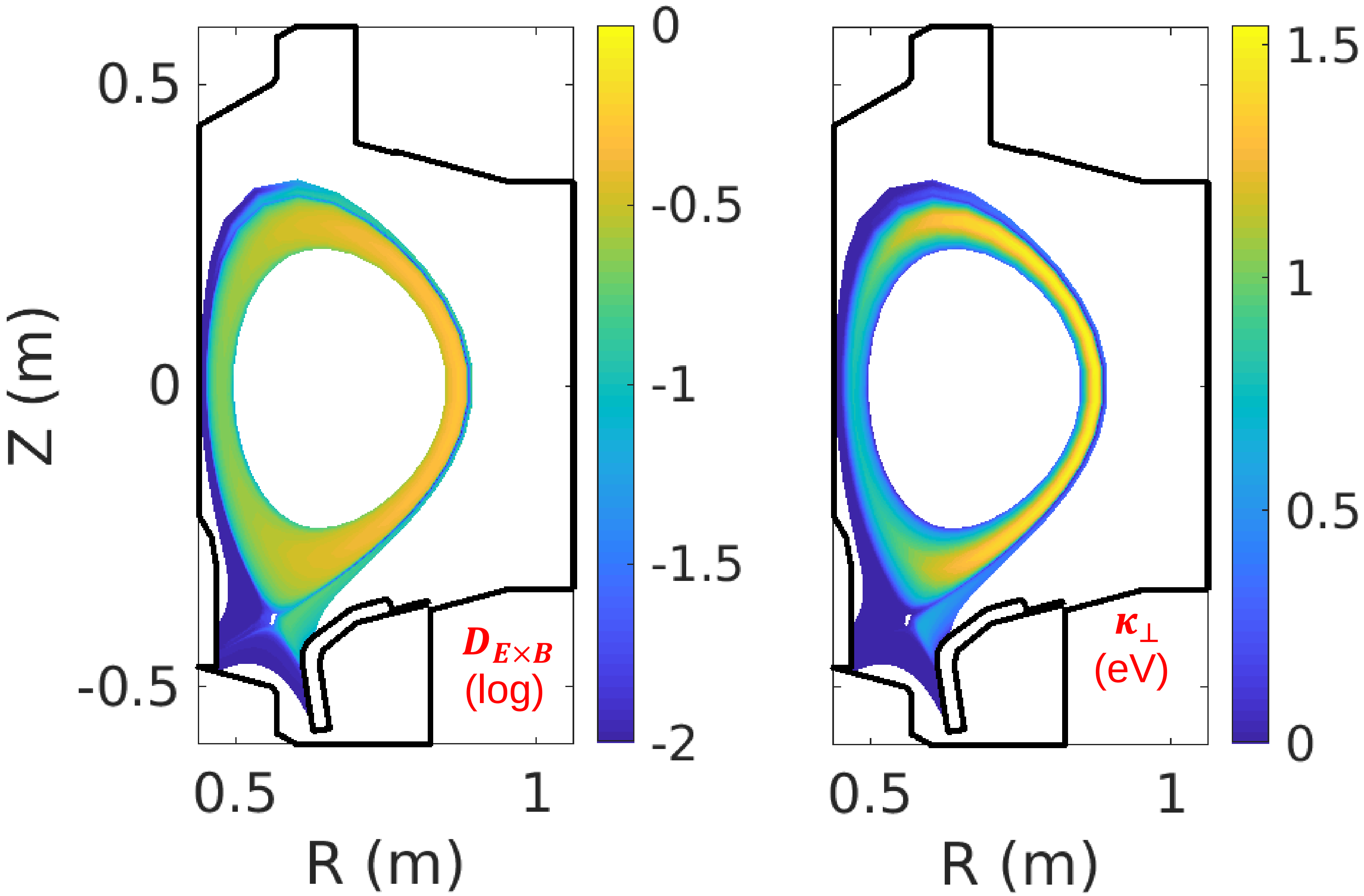
Midplane profiles compared to ‘standard’ approach

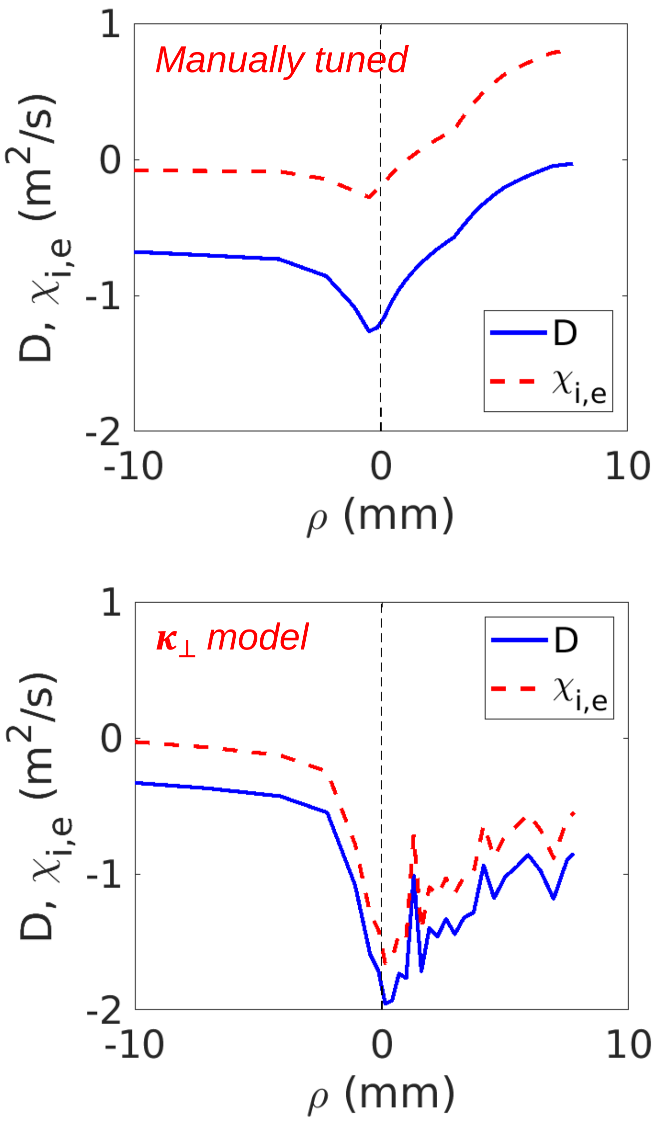


Target profiles compared to ‘standard’ approach



2D profiles of $\kappa_\perp$ and $D_{E\times B}$





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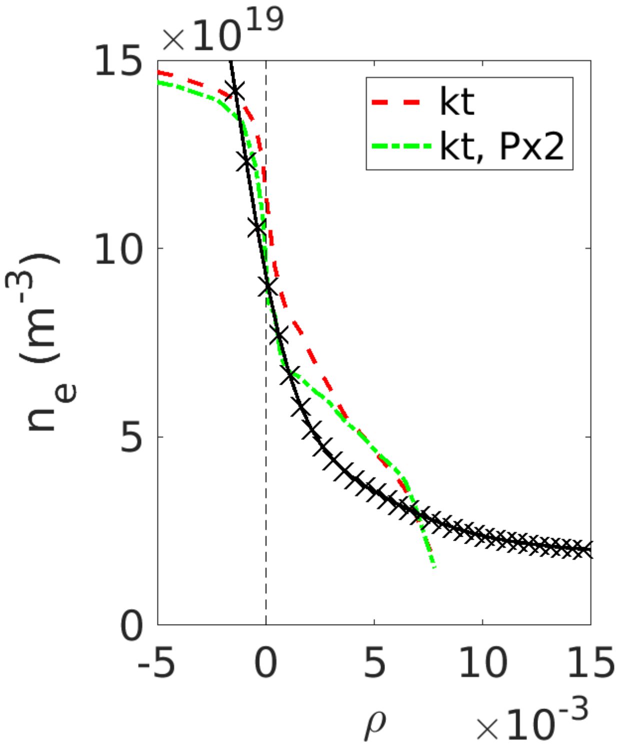
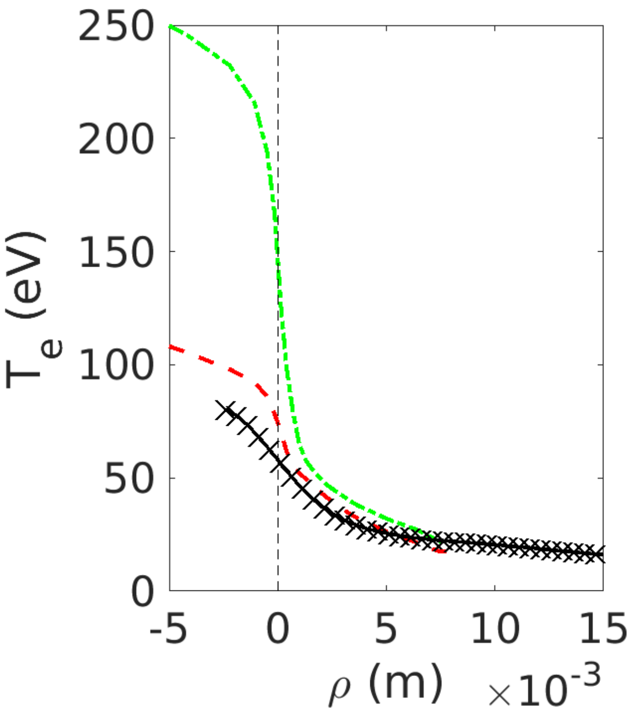
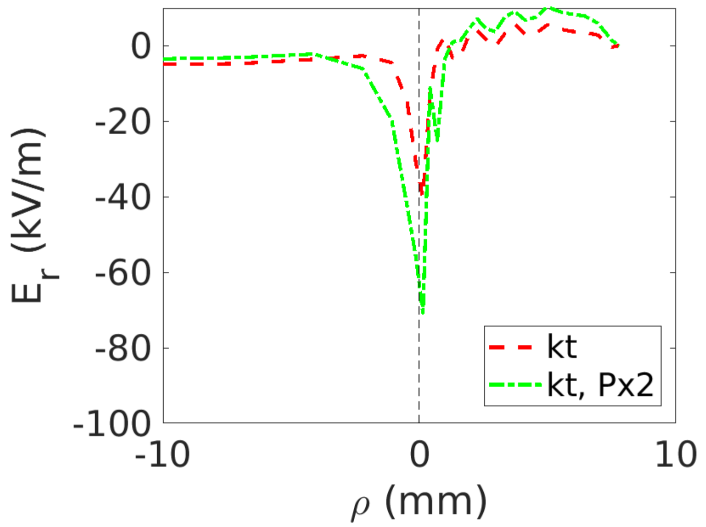
Assessment power dependency

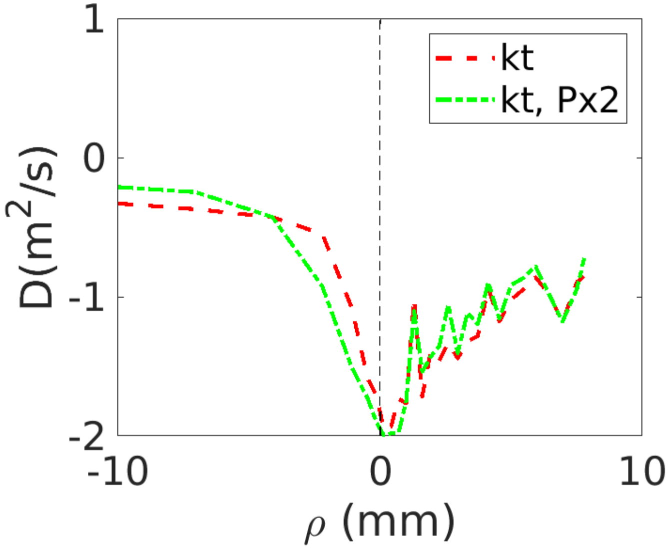
Double power at fixed density

Outer miplane









Similar effect when reducing density at fixed power