TSVV5 – Neutral gas dynamics in the edge

Intermediate progress report KUL

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Outline

- Status advanced fluid and hybrid neutral models for fast simulations

- Highlights inclusion n-n collisions
  - Theoretical derivation (Hilbert expansion)
  - Practical extension to SOLPS-ITER
  - Application to AUG and ITER modeling, incl. extended grids
  - Error analysis for DEMO modeling

- Summary and next steps

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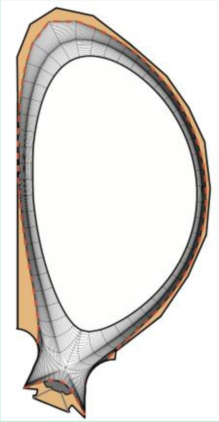
A hierarchy of neutral models

Advanced fluid neutral models (AFN)

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

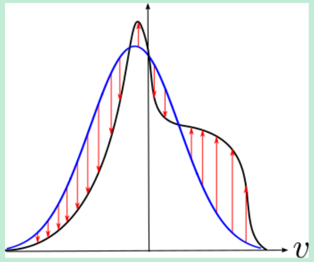
Hybrid fluid-kinetic models

Spatially (SpH)



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

micro-Macro (mMH)



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

- 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

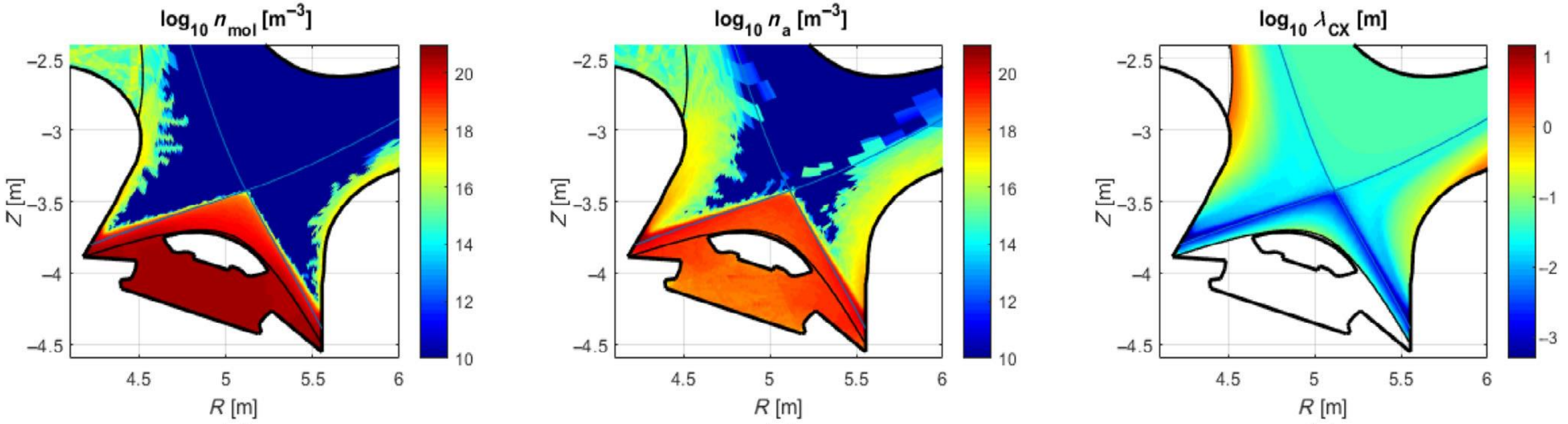
CPU × 1/10?

Summary achievements AFN: mature models!

- 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], including neutral-neutral collision effects [W. Dekeyser et al, PSI, 2024.]
  - Boundary conditions consistent with kinetic EIRENE treatment [N. Horsten et al., NF 57, 2017], incl. fast/thermal reflection (approximate effect of molecules) and TRIM data (effect of wall materials)
  - Separate neutral energy equation to extend validity range of fluid (and SpH) model towards lower recycling conditions [W. Van Uytven et al., CPP 60, 2020]
  - Inclusion of plasma drift effects [W. Van Uytven et al. NME 2022]
- Made widely available to users through implementation 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 [W. Dekeyser et al, NME 27, 2021]
- Already successfully applied to various machines, incl. AUG, JET [N. Horsten et al., NME 2022], ITER [W. Van Uytven et al, NF 62, 2022] and DEMO (link WP-DES) [W. Van Uytven et al, CPP, 2024]
- Support provided for implementation of AFN models in European turbulence codes (TOKAM3X, GRILLIX – link TSVV3).

Achievements spatially hybrid modeling (SpH)

- Combine AFN model in high-collisional regions with kinetic treatment in low collisional regions [W. Van Uytven, CPP, 2022]
    - Improved accuracy compared to pure fluid
    - Improved speed compared to kinetic (factor 5-20 depending on regime)
- Accurate treatment of molecular and (kinetic) impurity effects
- Fully integrated in extended grids version of SOLPS-ITER for simulations up-to-the-wall



Status of two-phases hybrid method and boundary conditions

- Overview of practical boundary condition implementation strategies for fluid neutral models
  - Matching moments and fluxes (Marshak, most used in practise)
  - Adjoint source iteration method (Golse, Klar)
  - Moment model approach (Kainz, Titulaer, Borsche, Klar)
- Comparison of the different strategies is WIP

- Two-phases hybrid method with particle tracing phase and fluid phase
- For a given error tolerance, the most cost-effective two-phases hybrid method is a domain decomposition (spatial hybrid) method
- Implementation of an adaptive spatial hybrid method with error-based interface position is WIP

Status of hybrid method based on KDMC

- Aim: investigate alternative, fully particle-based, hybrid method
- Basic particle tracing scheme implemented in EIRON
- Eiron updated to use BGK operator
  - KDMC depends on certain assumptions of the physics to work
  - EIRON used simple rotation after collision, which violated those assumptions
  - Initial results look ok, but more tests needed
- Estimation of QoIs through fluid model based on particle positions
  - Error analysis of 1D homogeneous background is now more rigorous.

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Introducing neutral-neutral collisions

Nonlinear kinetic equation:

$$\partial_t f(x,v,t) + v\partial_x f(x,v,t) = R_{cx}(x)\left(M_{cx}(v|x)\int f(x,v',t)dv' - f(x,v,t)\right)$$
$$+R_{nn}(x)\left(M_{nn}(v|x)\int f(x,v',t)dv' - f(x,v,t)\right)$$

With

$$M_{cx}(v|x) = \frac{1}{\sqrt{2\pi T_p(x)}} e^{-\frac{1}{2}\frac{\left(v-u_p(x)\right)^2}{T_p(x)}} \qquad M_{nn}(v|x) = \frac{1}{\sqrt{2\pi T_n(x)}} e^{-\frac{1}{2}\frac{\left(v-u_n(x)\right)^2}{T_n(x)}}$$

→ $M_{nn}(v|x)$ depends on the neutral particle distribution itself!

Make a fluid model in a systematic way?

→ Explicit in time: $M_{nn}(v|x)$ is known from previous time step

→ Hilbert expansion

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Hilbert expansion

Hilbert expansion ansatz[1]:
Introducing a scaling parameter $\varepsilon \ll 1$

$$f(x,v,t) \approx f_0(x,v,t) + \varepsilon f_1(x,v,t) + \varepsilon^2 f_2(x,v,t) + \ \dots$$

→ The particle distribution is an equilibrium f_0 plus higher order perturbations

Rank terms by importance by scaling them with $\varepsilon^k \ll 1$
(larger k → less important term) and equate per order in ε

[1] H. Grad 1958

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Results

[E. Andoni, MSc thesis, KU Leuven]

$$\partial_t(\rho(x,t)) + \partial_x(u_A(x,t)\rho) - \partial_x\left(D(x,t)\partial_x\left[\rho \mathrm{Var}_B(x,t)\right]\right) = 0$$

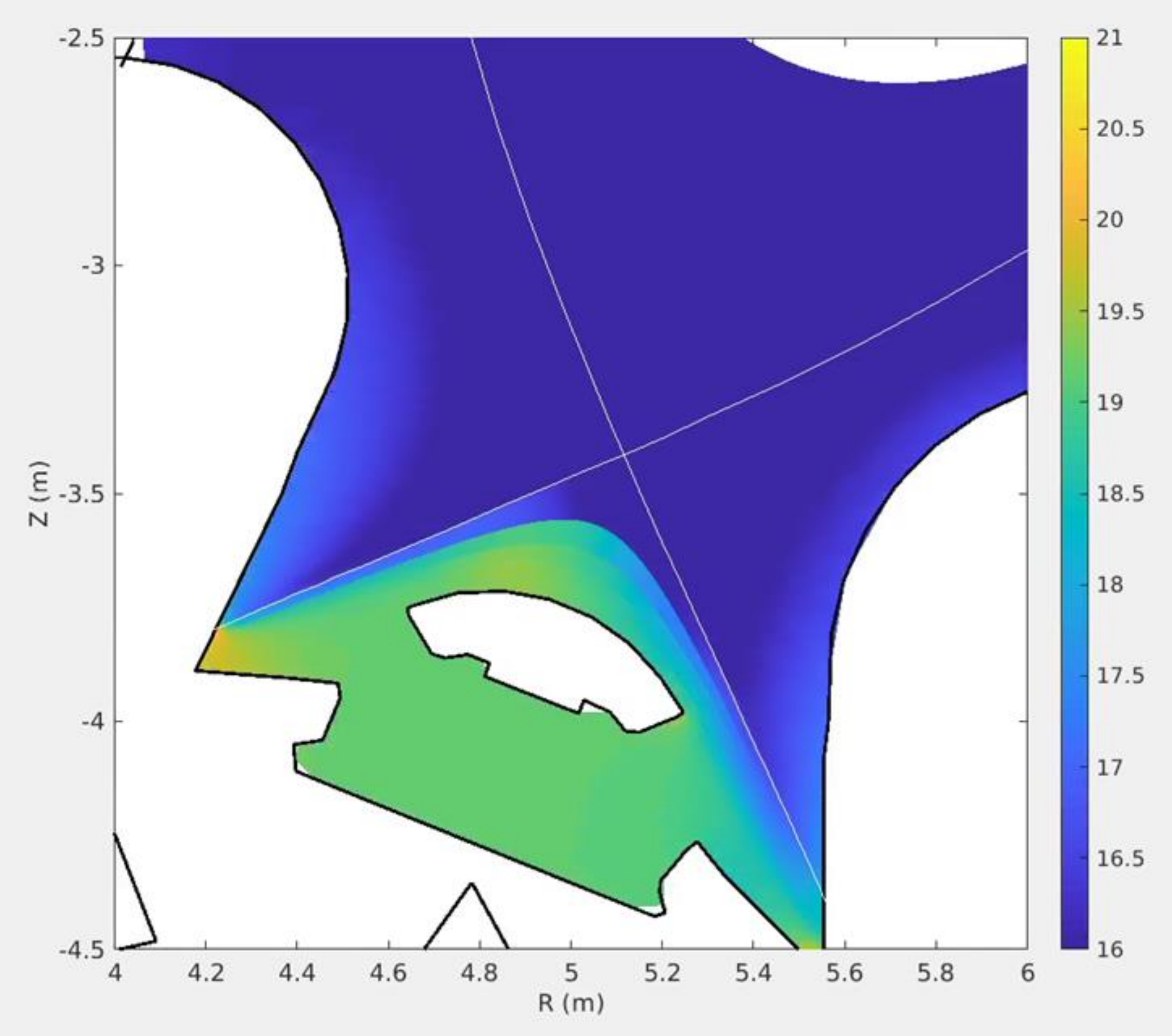
Hydrodynamic scaling:

$R_{nn} = \epsilon^k R_{cx}$	$u_A(x,t)$	$D(x,t)$	$\mathrm{Var}_B(x,t)$
$k = 0$	u_R	0	0
$k > 0$	u_p	0	0

Diffusive scaling:

$R_{nn} = \epsilon^k R_{cx}$	$u_A(x,t)$	$D(x,t)$	$\mathrm{Var}_B(x,t)$
$k = 0$	u_R	$\frac{1}{R_{nn}(x,t)+R_{cx}(x,t)}$	$\mathrm{Var}_{M_R}(x,t)$
$k = 1$	$u_p + \frac{R_{nn}}{R_{cx}}(u_n - u_p)$	$\frac{1}{R_{cx}(x,t)}$	σ_p^2
$k > 1$	u_p	$\frac{1}{R_{cx}(x,t)}$	σ_p^2

AFN model including n-n collisions in SOLPS-ITER



- 'Standard' AFN model assumes dominant CX collisions for transport of atoms, but:
  - n-n collisions may be as frequent as CX in case $n_i \approx n_n$
  - No plasma below dome, far-SOL,…
- Add n-n collision contribution to diffusion coefficient (and viscosity/conductivity) *(rate based on Kotov 2007 (thesis))*

$$D_0^n = \frac{T_n}{m_n(\nu_{ion} + \nu_{CX} + \nu_{n-n})}$$

- Split into (perpendicular) pressure diffusion and (isotropic) density diffusion based on relative collision frequencies

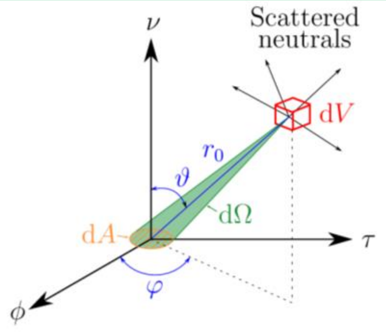
$$D_p^n = \frac{(\nu_{ion}+\nu_{CX})D_0^n}{\nu_{ion}+\nu_{CX}+\nu_{n-n}}, \qquad D_n^n = \frac{\nu_{n-n}D_0^n}{\nu_{ion}+\nu_{CX}+\nu_{n-n}}$$

AFN boundary conditions including n-n collisions

Speed- and angular-dependent particle flux density

$\Gamma^{\mathrm{n}}_{\nu-}(v,\vartheta,\varphi)$ Incident neutrals: diffusion approx. or Maxwellian approx.

$\Gamma^{\mathrm{i}}_{\nu-}(v,\vartheta,\varphi)$ Incident ions: truncated Maxwellian + sheath acceleration



Reflected/recycled neutrals

$$\Gamma^{\mathrm{n}}_{\nu+}(v_{\mathrm{R}},\vartheta_{\mathrm{R}},\varphi_{\mathrm{R}}) = \int_{v=0}^{\infty}\int_{\vartheta=0}^{\pi/2}\int_{\varphi=0}^{2\pi} R(v,\vartheta,\varphi \rightarrow v_{\mathrm{R}},\vartheta_{\mathrm{R}},\varphi_{\mathrm{R}}) \sin\vartheta_{\mathrm{R}} \left(\Gamma^{\mathrm{n}}_{\nu-}(v,\vartheta,\varphi)+\Gamma^{\mathrm{i}}_{\nu-}(v,\vartheta,\varphi)\right)\mathrm{d}v\mathrm{d}\vartheta\mathrm{d}\varphi$$

TRIM database

Moments total distribution: particle, momentum and energy flux densities *[N. Horsten et al., NF* ***57*** *(2017)]*

Diffusion approx.:

- Original BCs: consider neutrals from CX-collisions only
- Modified: neutrals from both CX and n-n collisions

Maxwellian approx.:

- Assume (drifting) Maxwellian based on T_n and $u_{||n}$

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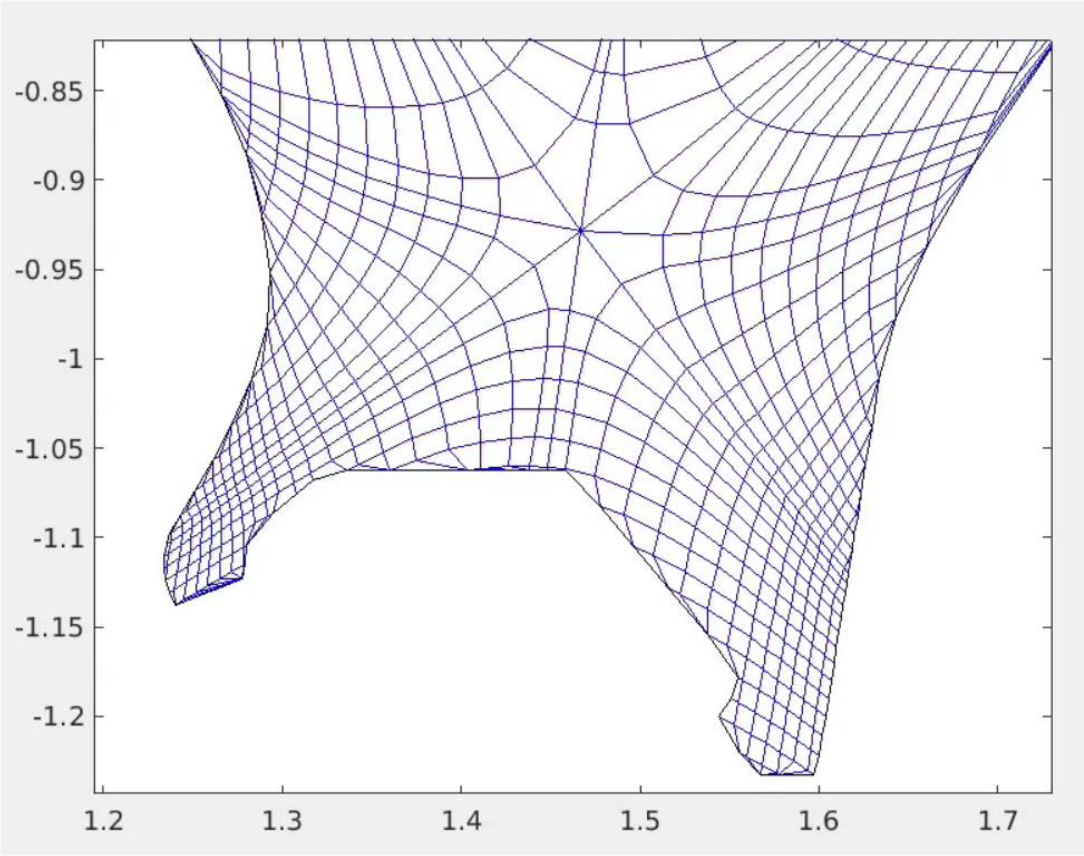
AUG 16151

- A standard SOLPS-ITER equilibrium/geometry, but full W wall
- Grid created with carreMode=3 and GOAT
- BCs:
  - Core: $T_i=T_e=300$eV, $n_i=2.8e19\ m^{-3}$
  - Walls: sheath BCs
  - Recycling 1.0; no puff/pump
- Setup:
  - D only, no drifts, but with parallel currents
  - AFN model, incl. n-n collisions, with and w/o separate neutral energy equation
  - Ref.: full kinetic neutrals (atoms, molecules, n-n collisions)



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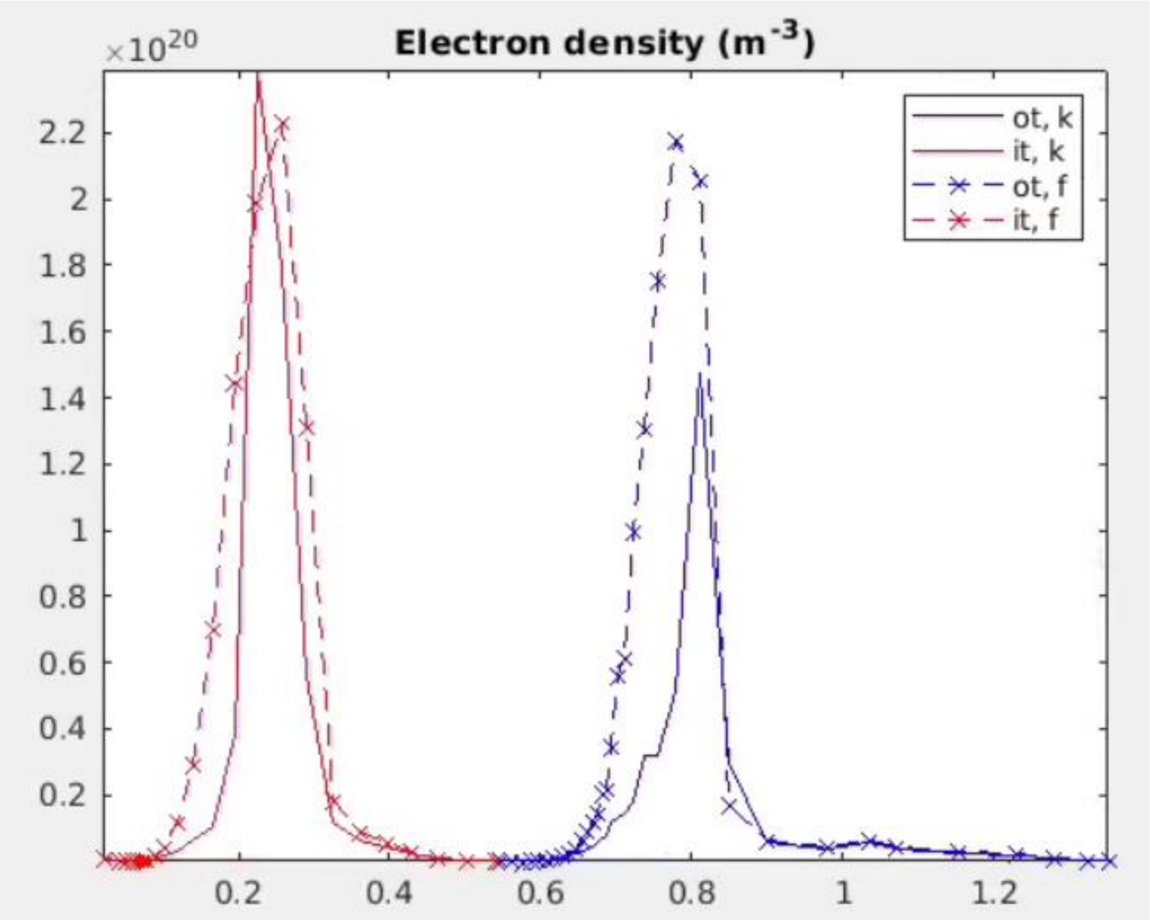
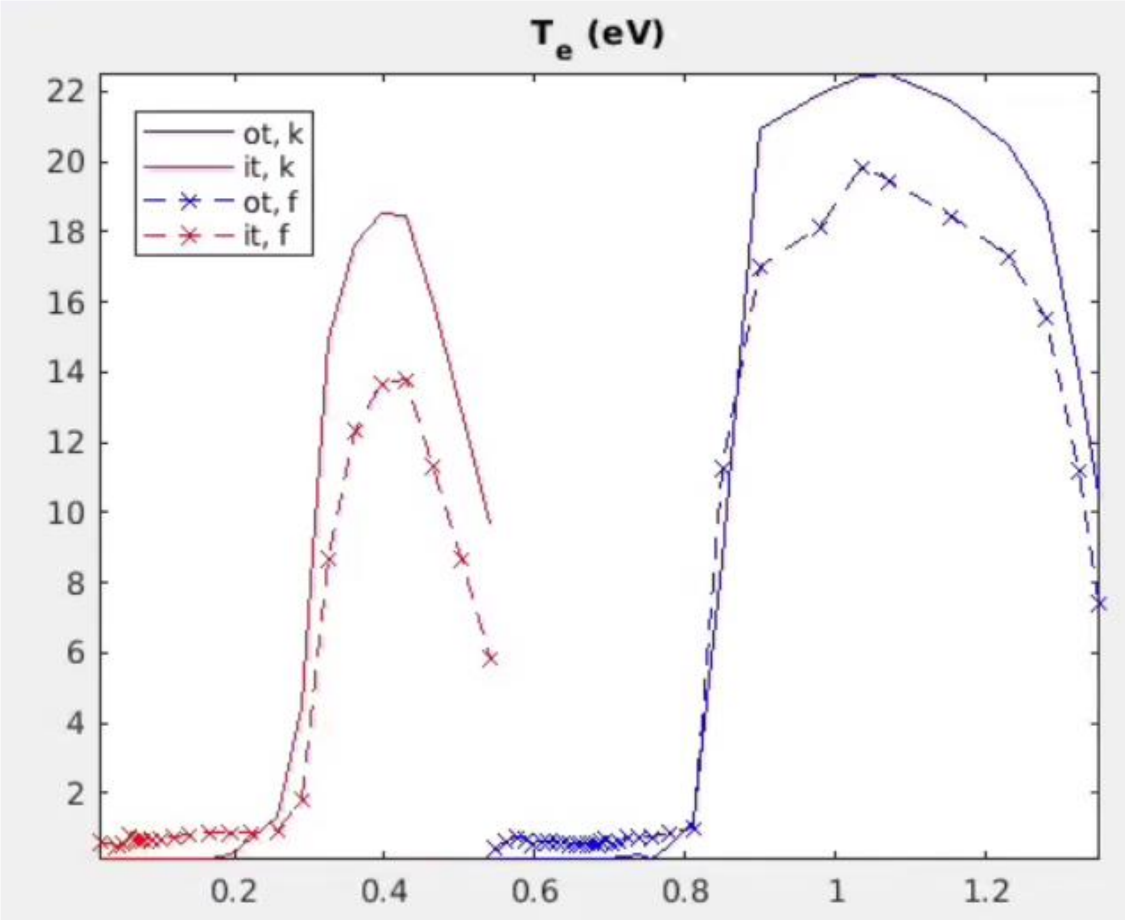
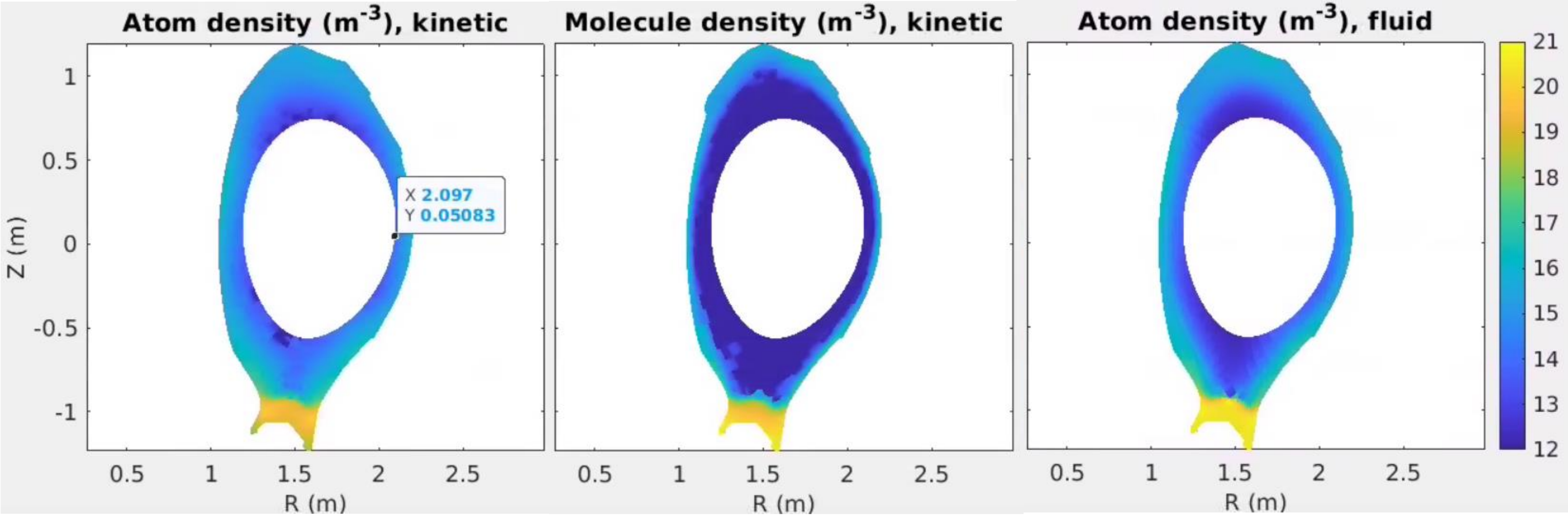
Target profiles



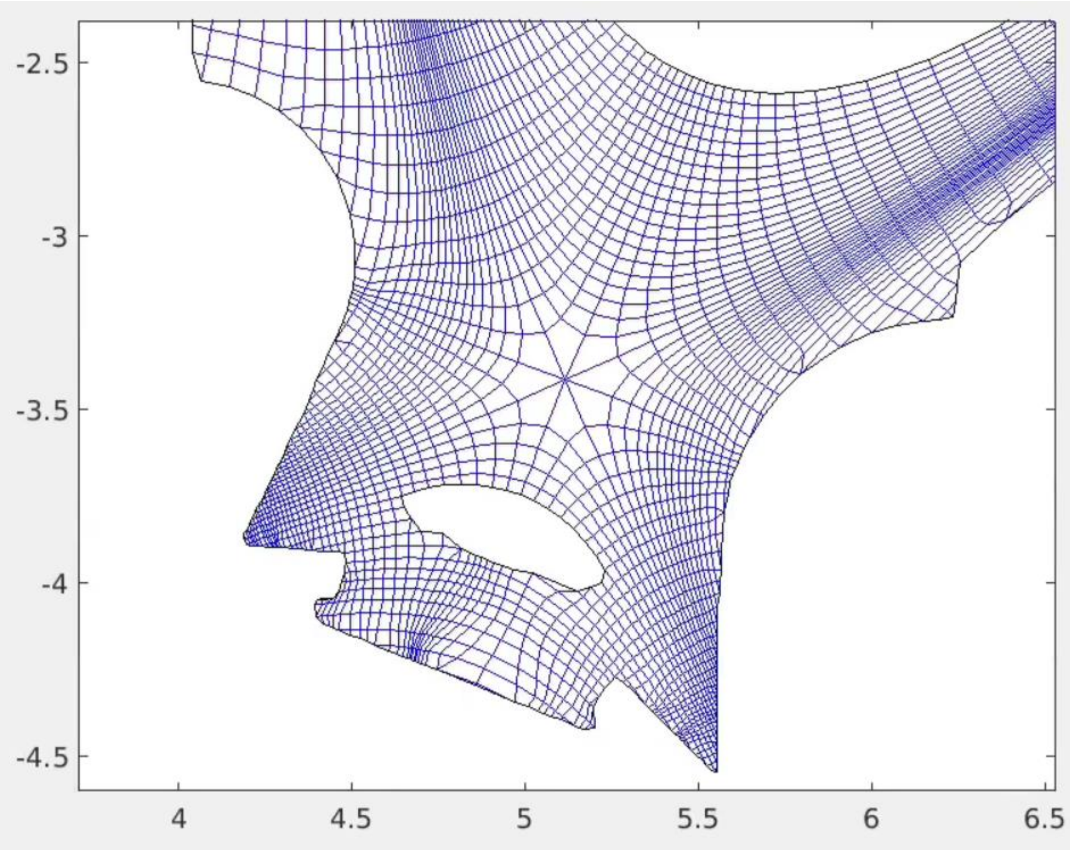


Neutral density



ITER

- Case based on ITER 2275, but full W wall
- Grid created with carreMode=3 and GOAT
- BCs:
    - Core: T_i=T_e=300eV, n_i=2.8e19 m^{-3}
    - Walls: sheath BCs
    - Recycling 1.0; puff 1e22 s^{-1};pump beneath dome
- Setup:
    - D only, no drifts, no parallel currents
    - AFN model, incl. n-n collisions, with and w/o separate neutral energy equation
    - Ref.: full kinetic neutrals (atoms, molecules, n-n collisions)



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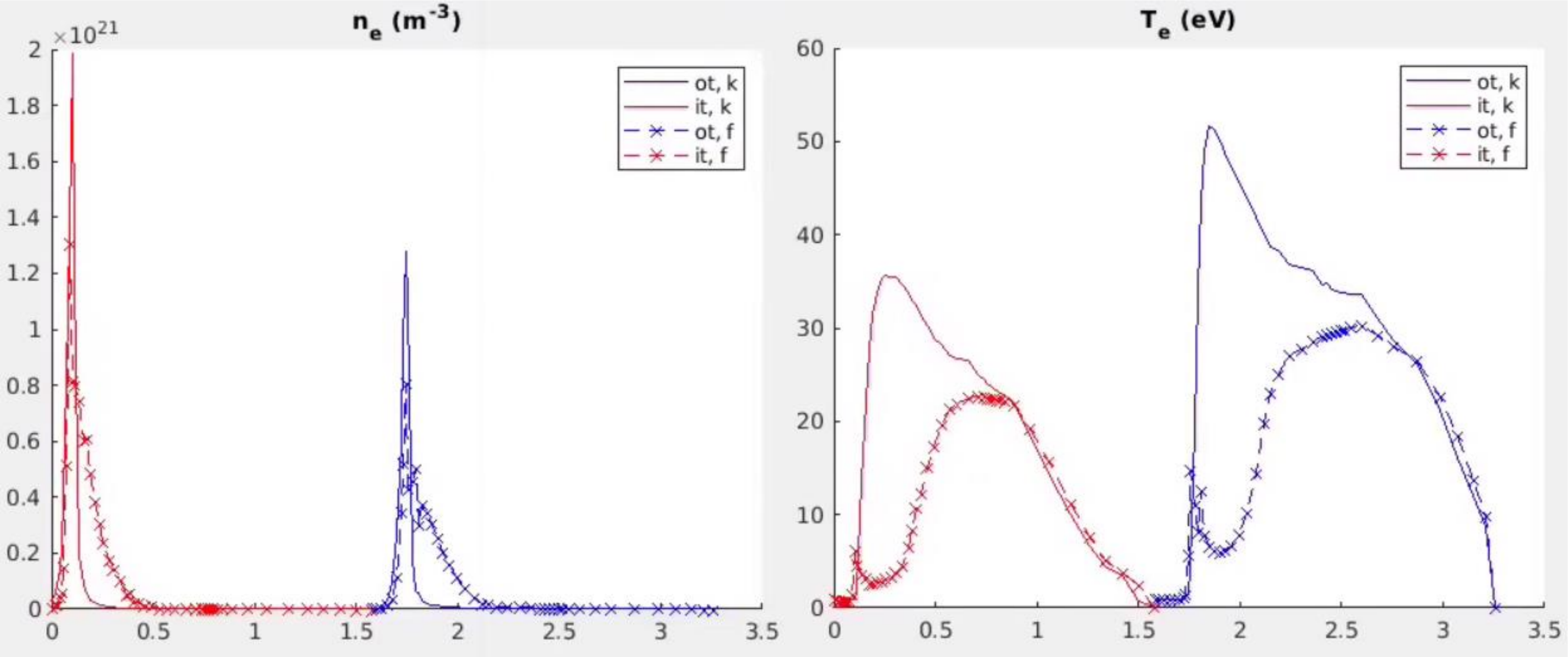
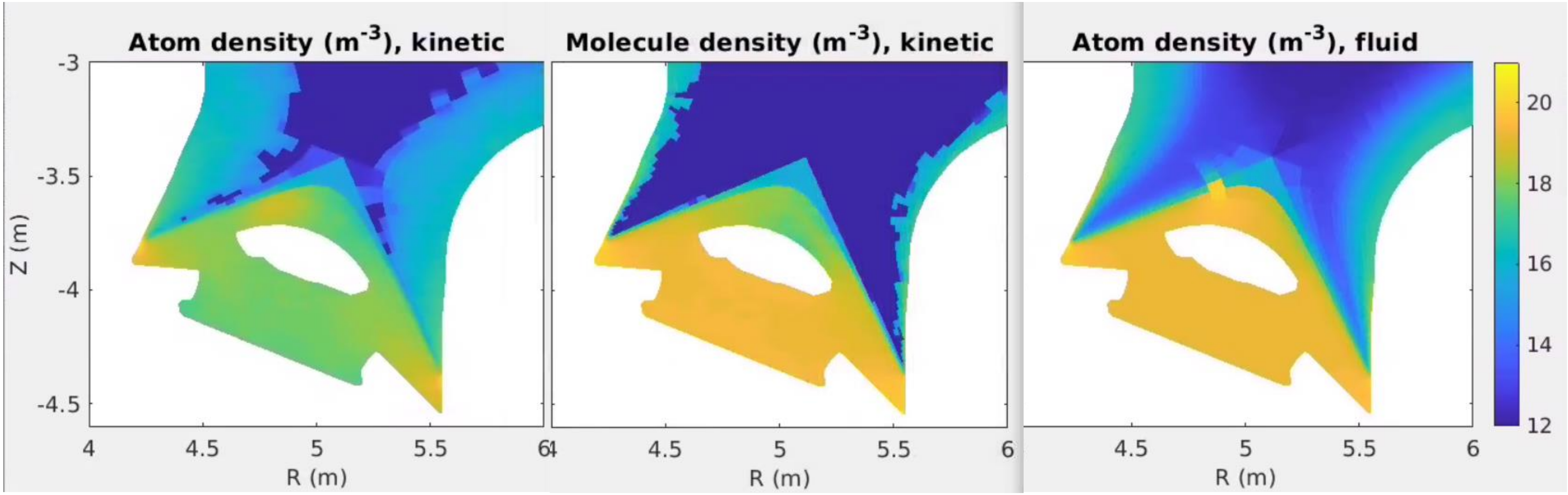


Neutral density



Towards accurate and efficient DEMO simulations in SOLPS

- Goal: acceptable numerical errors for DEMO SOLPS cases (e.g. < 10%) as cheaply as possible
- Start from error analysis framework of PhD K. Ghoos

$$\boldsymbol{\epsilon_{\mathrm{num}} = \epsilon_{\mathrm{d}} + \epsilon_{\mathrm{c}} + \epsilon_{\mathrm{b}} + \epsilon_{\mathrm{s}}}$$

- ϵ_s: statistical error — direct result of noisy MC sources
- ϵ_b: finite sampling bias error — deterministic error due to noise + non-linearities
- ϵ_c: convergence error — non-zero residuals
- ϵ_d: discretization error — finite grid resolution

- But, some unanswered questions:
  - Q1: effect of Δt on bias? (*[M. Baeten et al., CtPP, 2018]:* statistical error ~ $\sqrt{\Delta t}$ (0D+1D cases))
  - Q2: effect of n-n collisions (NNC) on error scaling?
  - Q3: effect of impurities?

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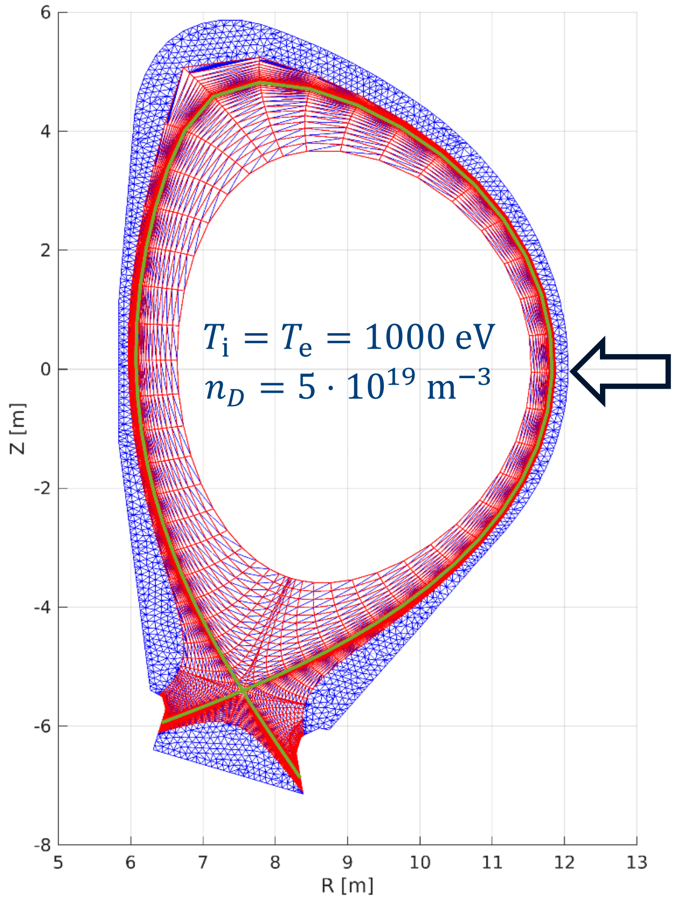
Case set-ups

D-only

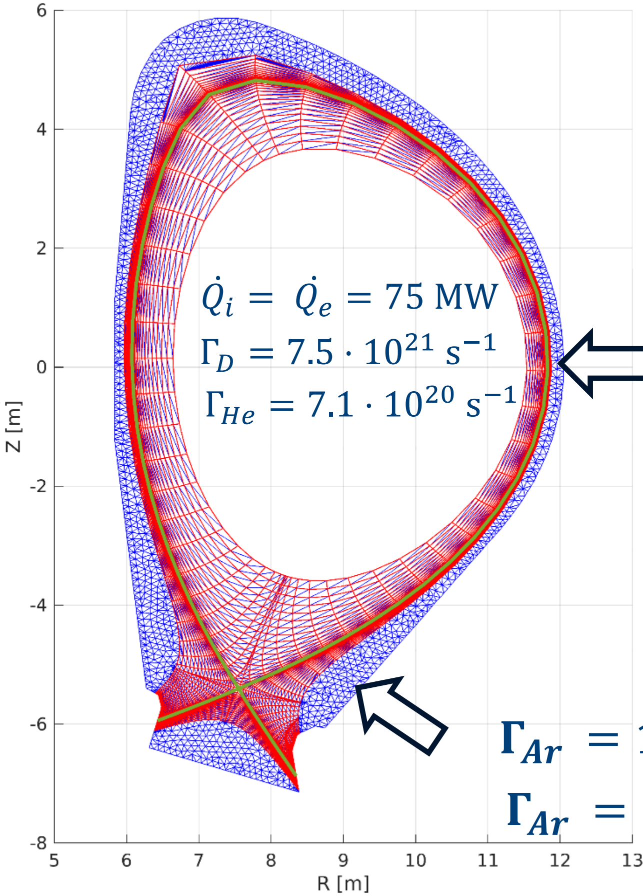


$T_{\mathrm{i}} = T_{\mathrm{e}} = 1000\ \mathrm{eV}$

$n_D = 5 \cdot 10^{19}\ \mathrm{m}^{-3}$

$\Gamma_{D_2} = 1 \cdot 10^{23}\ \mathrm{s}^{-1}$

D + He + Ar



$\dot{Q}_i = \dot{Q}_e = 75\ \mathrm{MW}$

$\Gamma_D = 7.5 \cdot 10^{21}\ \mathrm{s}^{-1}$

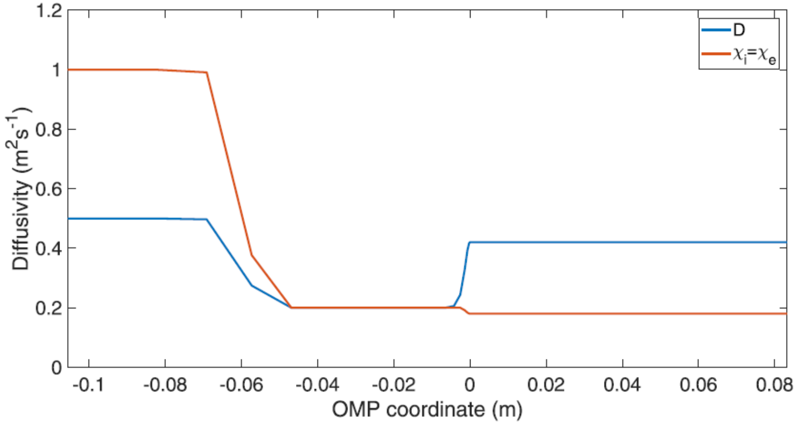
$\Gamma_{He} = 7.1 \cdot 10^{20}\ \mathrm{s}^{-1}$

$\Gamma_{D_2} = 1 \cdot 10^{23}\ \mathrm{s}^{-1}$

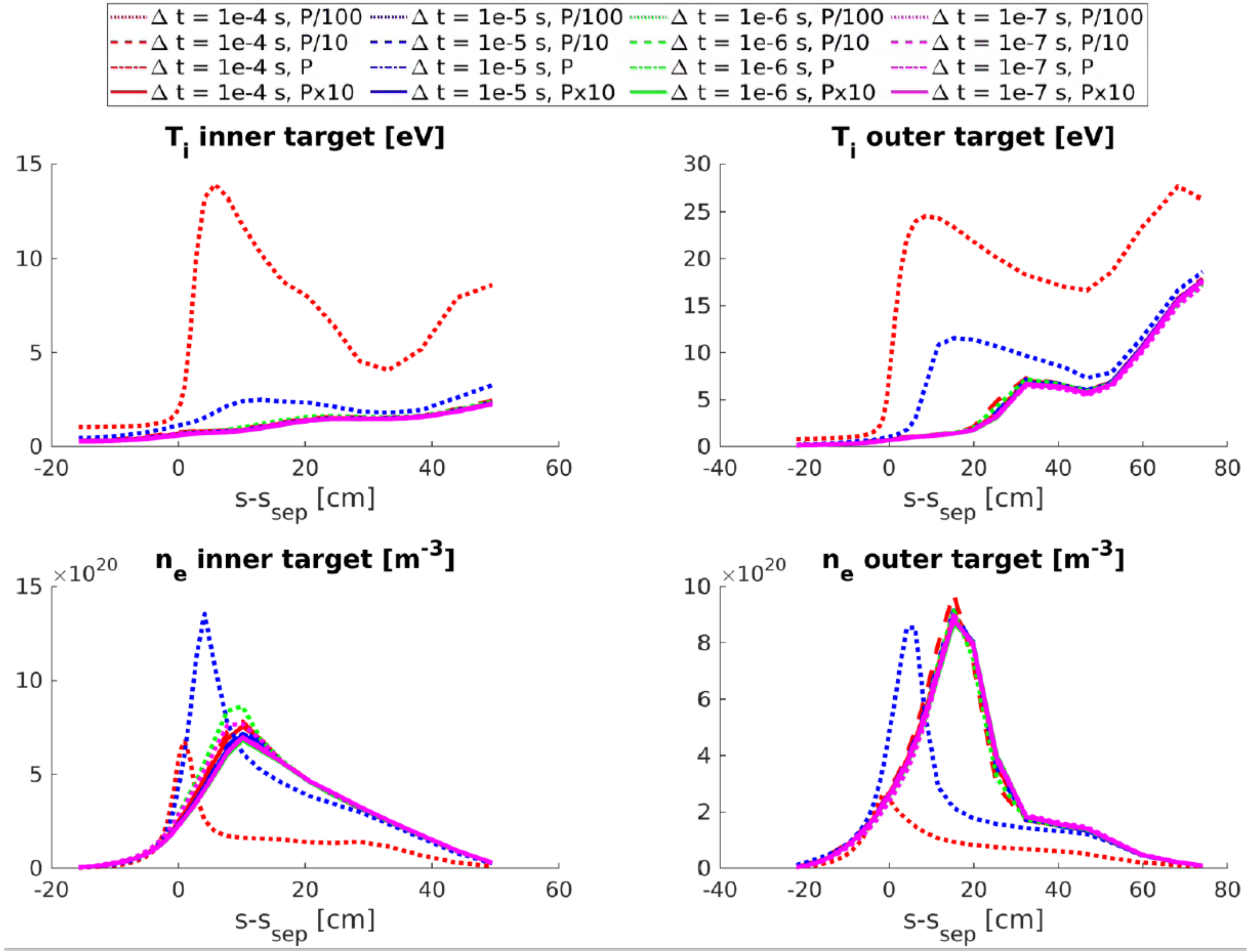
$\boldsymbol{\Gamma_{Ar} = 1 \cdot 10^{19}\ \mathrm{s}^{-1}}$

$\boldsymbol{\Gamma_{Ar} = 1 \cdot 10^{20}\ \mathrm{s}^{-1}}$

Transport barrier

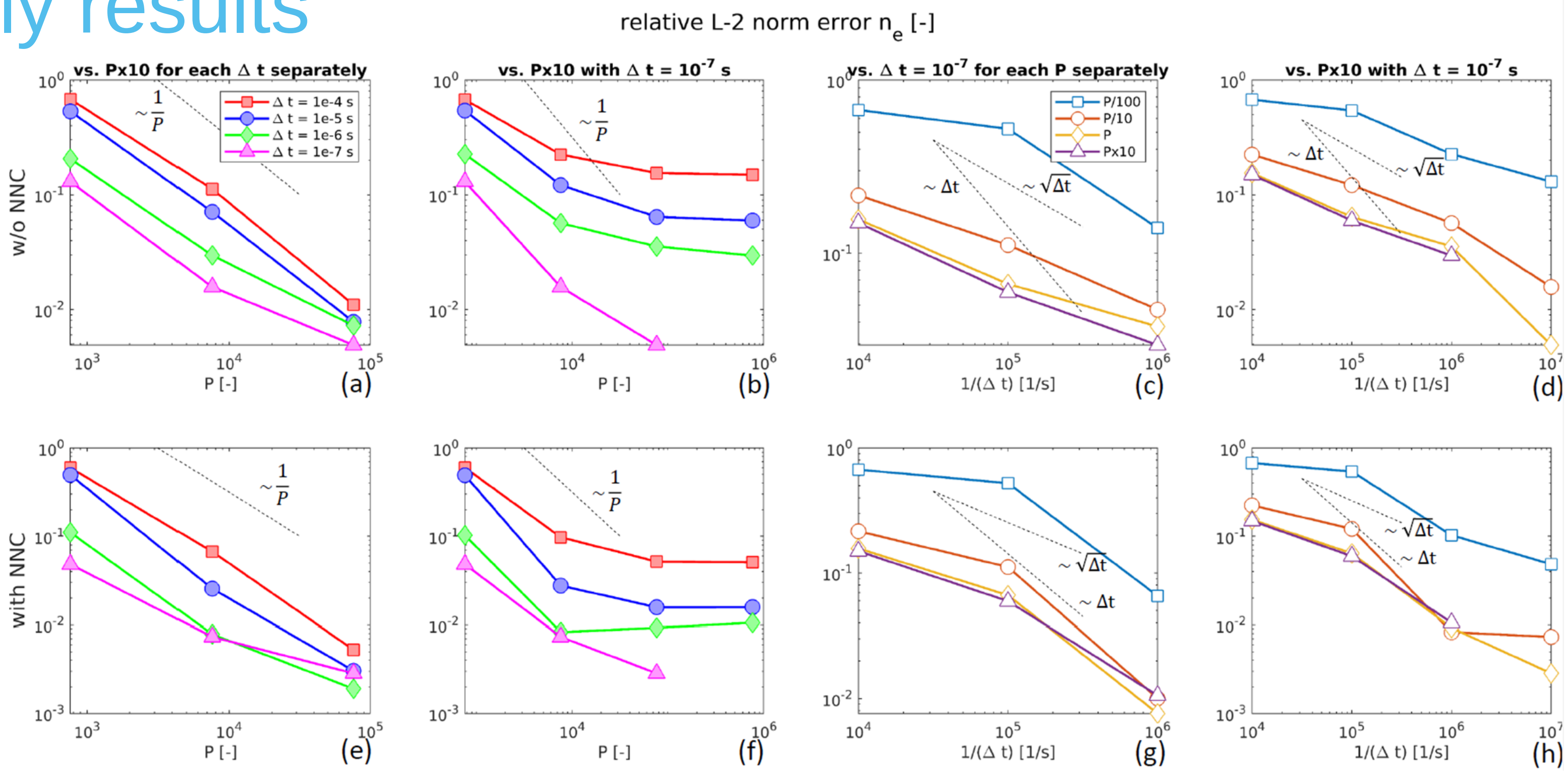


D-only results (with NNCs)



Only 1e-4s and 1e-5s for P/100 lead to a qualitatively wrong solution

D-only results



→ no noticeable effect of NNCs on convergence behavior
→ bias decreases monotinically with Δt

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Prelim. conclusions D + He + Ar cases

- Multi-species cases appear to have much larger bias than D-only case
- Why?
  - Purely case dependent? E.g. much higher core power? higher T's OT?
  - Bad statistics from impurity neutrals themselves?
  - Combination of both?

Conclusions error analysis

- Error reduction w.r.t. P and Δt does not change significantly with NNCs
- Decrease of bias for smaller Δt demonstrated in SOLPS-ITER
  - useful knowledge if Δt is limited by plasma side (e.g. drifts)

- Bias error seems to be much higher for (high-power?) multi-species cases
  - Similar observations in literature
  - Need to better understand why
  - Optimal strategies for D-only may no longer be optimal

→ high priority for future research
→ back to 1D or slab cases? DEMO cases much too slow for efficient research

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FHK modeling based on AFN

- AFN models and hybrid methods (in particular, SpH) reached high level of maturity
  - Including effects of drifts, molecules, n-n collisions,…
  - Coupling with impurity models
- Integration in various codes
  - Default models in SOLPS-ITER extended grids version. Relevant input files automatically generated.
  - Basic AFN models implemented in various European turbulence codes (link TSVV3), incl. SOLEDGE3X, GRILLIX
- Already applied to simulate multiple machines, incl. TCV, AUG, JET, ITER, DEMO (link WP TE, WP DES)
- Next steps
  - Validation n-n collision effects with kinetic simulations
  - Extension to ‘hydrodynamic’ closure model for void regions w/o plasma
  - Fluid model for molecules?

FHK modeling based on KDMC

- Basic particle tracing scheme implemented in EIRON
- Eiron updated to use BKG operator
  - KDMC depends on certain assumptions of the physics to work
  - EIRON used simple rotation after collision, which violated those assumptions
  - Initial results look ok, but more tests needed
- Estimation of QoIs through fluid model based on particle positions
  - Error analysis of 1D homogeneous background is now more rigorous.
- Next steps
  - Extension to heterogeneous background
  - Validation source estimators
  - Integration with multi-level scheme

AD, UQ

- Derivatives based on AD (TAPENADE) in forward mode available
  - EIRENE standalone
- UQ demonstration: applied to study sensitivity of QoIs to uncertainty in reaction rate coefficients
  - Accurate in low/medium recycling regimes
  - Problem of diverging derivatives in high recycling regimes
- Next steps
  - Analysis of derivative problems in high recycling
  - Analysis of impact estimators on accuracy of derivatives
  - Implementation adjoint AD with TAPENADE
  - Adjoint differentiation of couple B2.5-EIRENE solver
- Potential for building implicit coupling to plasma codes (B2.5, SOLEDGE3X) and providing sensitivities (ERO2.0)

References

- N. Horsten et al., Development and assessment of 2D fluid neutral models that include atomic databases and a microscopic reflection model, 2017 Nucl. Fusion 57 116043
- W. Dekeyser et al., Implementation of a 9-point stencil in SOLPS-ITER and implications for Alcator C-Mod divertor plasma simulations, Nuclear Materials and Energy 18 (2019) 125–130
- W. Van Uytven et al., Implementation of a separate fluid-neutral energy equation in SOLPS-ITER and its impact on the validity range of advanced fluid-neutral models, CPP 2020, https://doi.org/10.1002/ctpp.201900147
- W. Dekeyser et al., Plasma edge simulations including realistic wall geometry with SOLPS-ITER, Nuclear Materials and Energy 27 (2021) 100999
- W. Van Uytven et al., Assessment of advanced fluid neutral models for the neutral atoms in the plasma edge and application in ITER geometry, Nucl. Fusion 62 086023
- W. Van Uytven et al., Advanced spatially hybrid fluid-kinetic modelling of plasma-edge neutrals and application to ITER case using SOLPS-ITER, Contrib. Plasma Phys. 2022;e202100191
- W. Van Uytven et al., Discretization error estimation for EU-DEMO plasma-edge simulations using SOLPS-ITER with fluid neutrals, CPP 2024, https://doi.org/10.1002/ctpp.202300125
- N. Vervloesem et al., Error-based grid adaptation methods for plasma edge simulations with SOLPS-ITER,CPP 2024, https://doi.org/10.1002/ctpp.202300126

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References

- W. Dekeyser et al., Divertor target shape optimization in realistic edge plasma geometry, Nucl. Fusion 54 (2014) 073022
- M. Blommaert et al., An automated approach to magnetic divertor configuration design, Nucl. Fusion 55 (2015) 013001
- M. Baelmans et al., Achievements and challenges in automated parameter, shape and topology optimization for divertor design, Nucl. Fusion 57 (2017) 036022
- S. Carli et al., Algorithmic Differentiation for adjoint sensitivity calculation in plasma edge codes, Journal of Computational Physics, Volume 491, 15 October 2023, 112403, https://doi.org/10.1016/j.jcp.2023.112403
- S. Carli et al., Bayesian maximum a posteriori-estimation of κ turbulence model parameters using algorithmic differentiation in SOLPS-ITER, https://doi.org/10.1002/ctpp.202100184
- S. Van den Kerkhof et al., Application of an automated grid deformation tool for divertor shape optimization in SOLPS-ITER, CPP 2024, https://doi.org/10.1002/ctpp.202300134
- Maes, V., Bossuyt, I., Vandecasteele, H., Dekeyser, W., Koellermeier, J., Baelmans, M., Samaey, G. (2024). Predicting the statistical error of analog particle tracing Monte Carlo. arXiv. doi: 10.48550/arXiv.2404.00315