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TSVV5 – Neutral gas dynamics in the edge

Progress report KUL-TME 2023 & Workplan 2024

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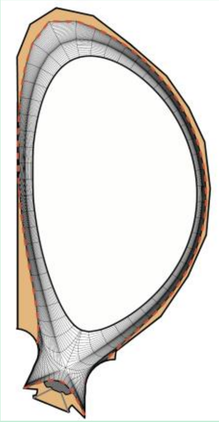
A hierarchy of neutral models

Advanced fluid neutral models

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

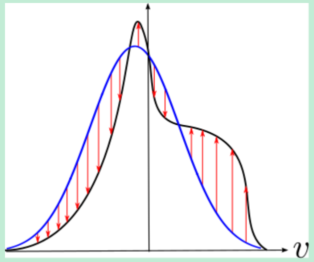
Hybrid fluid-kinetic models

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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Summary of recent achievements

- Application Advanced Fluid Neutral (AFN) models to ITER case, realistic wall materials [W. Van Uytven et al. NF 2022]
  - Consistent numerics essential for good agreement with kinetic results (9pt stencil, isotropic flux limits,…)
  - Impact wall material: more fast reflection with metallic wall (W) => larger kinetic corrections needed compared to low-Z materials (C, Be)
- Extension AFN models to account for drifts [W. Van Uytven et al. NME 2022]
  - Additional advective transport term in AFN model
  - Correctly includes effect of drifts on neutral transport compared to kinetic simulation (link with ion neutral current)
  - But: impact of drifts on background plasma solution is by far most dominant contributor compared to direct impact of drifts on neutral transport
- Extension AFN models towards n-n collisions and H/D/T mixtures (validation ongoing)
  - Ad-hoc correction term to transport coefficients for n-n collisions
  - Generalization of AFN models for H/D/T mixtures in extended grid version of SOLPS-ITER
  - Independent continuity & momentum equation for each hydrogenic atom, common T
  - Application to ITER, incl. extended grids, under investigation
- Application to ITER and DEMO reference cases (link WP-DES; [W. Van Uytven, PET 2023])

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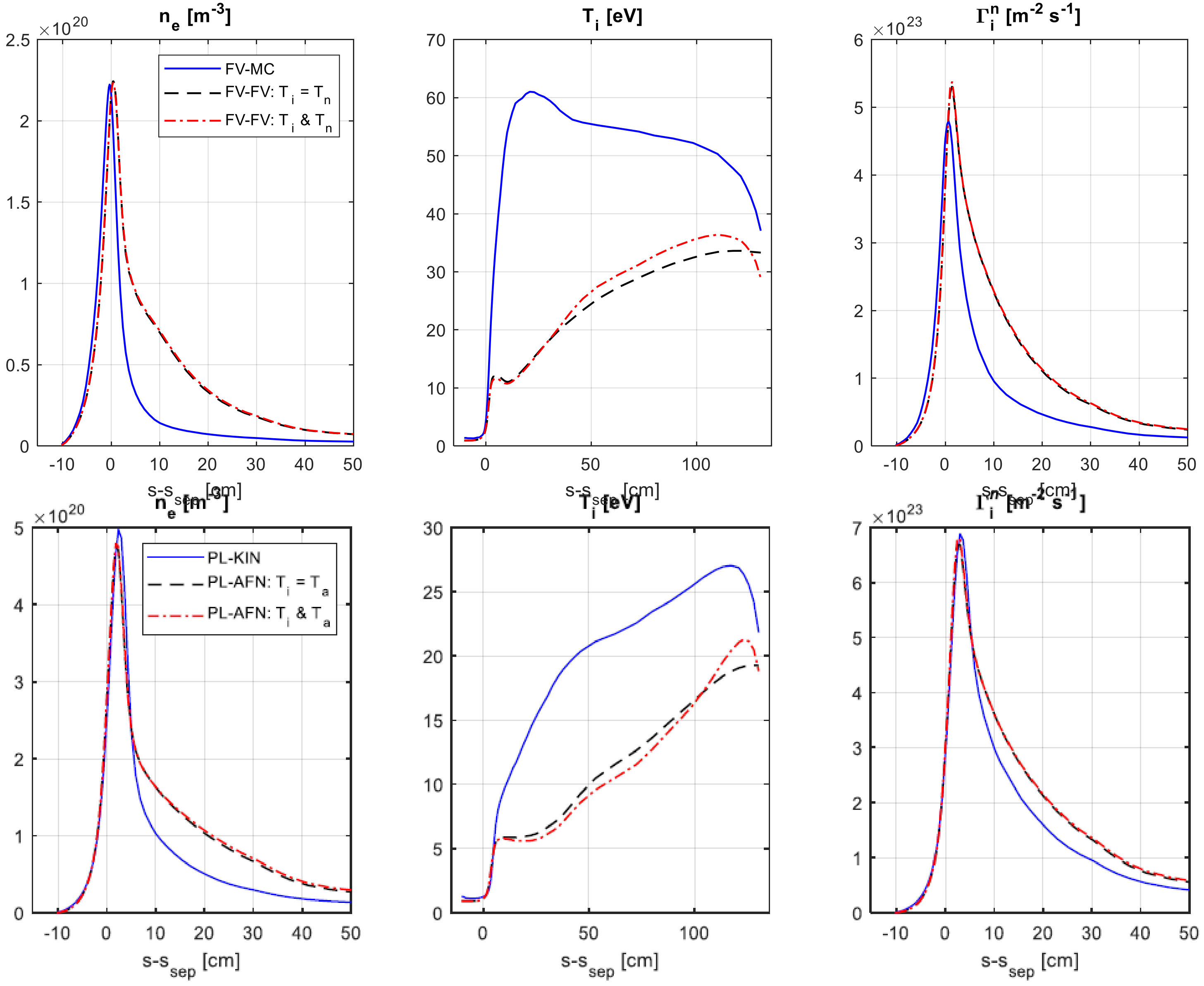
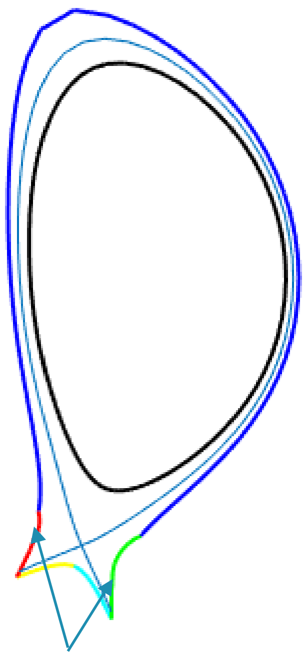
Application AFN to ITER case, W-Be wall

$n_{i,c} = 4{\cdot}10^{19}$ m^{-3}

$n_{i,c} = 8{\cdot}10^{19}$ m^{-3}

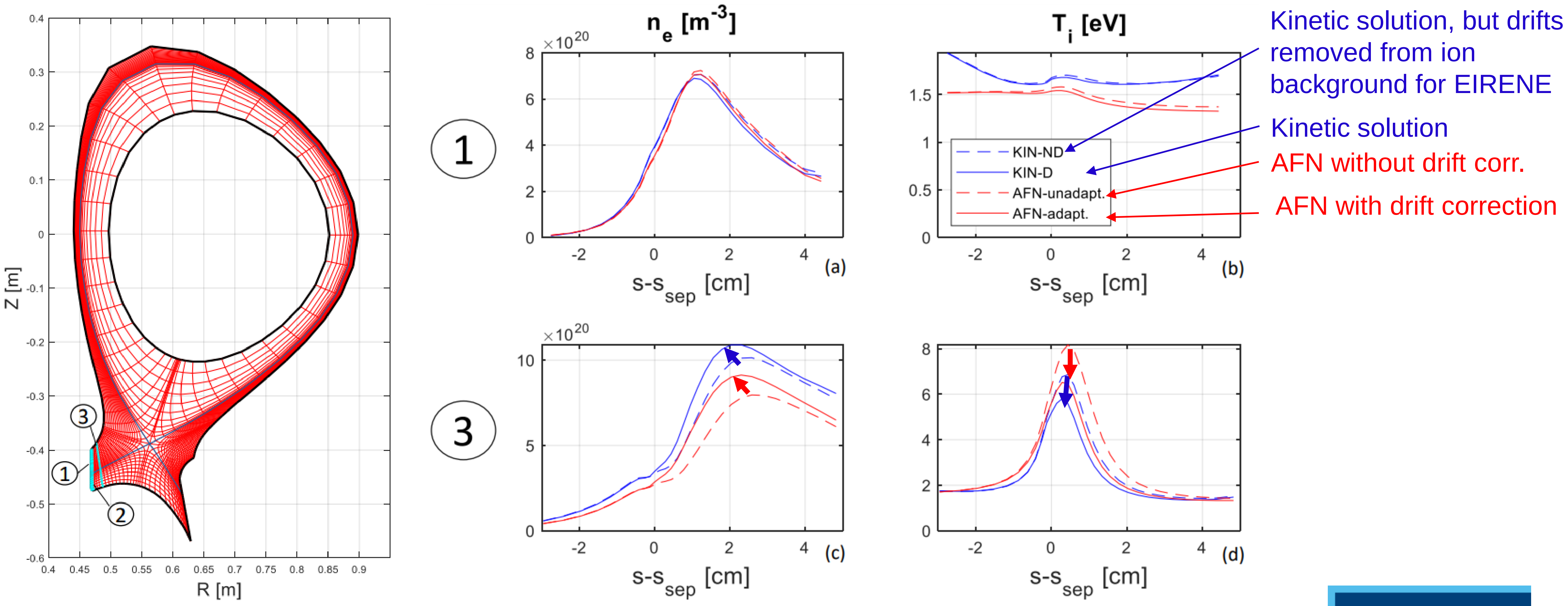




Tungsten

Tungsten
→ more fast reflection
→ higher T and Kn
→ reduced validity fluid neutrals
→ correct with hybrid approach

Application AFN to Alcator C-mod case with drifts



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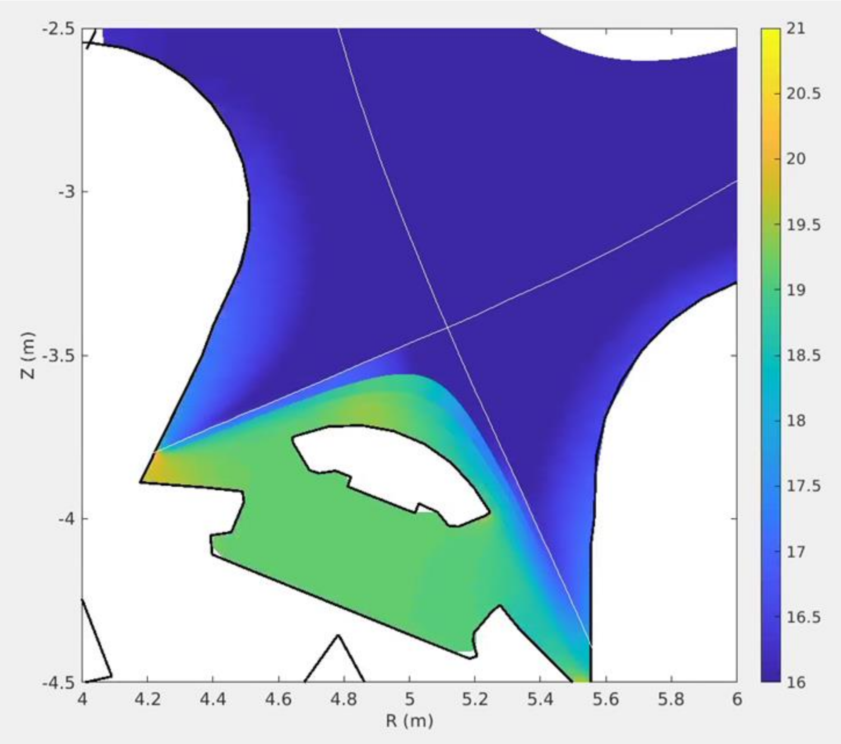
Application AFN models to ITER with extended grid

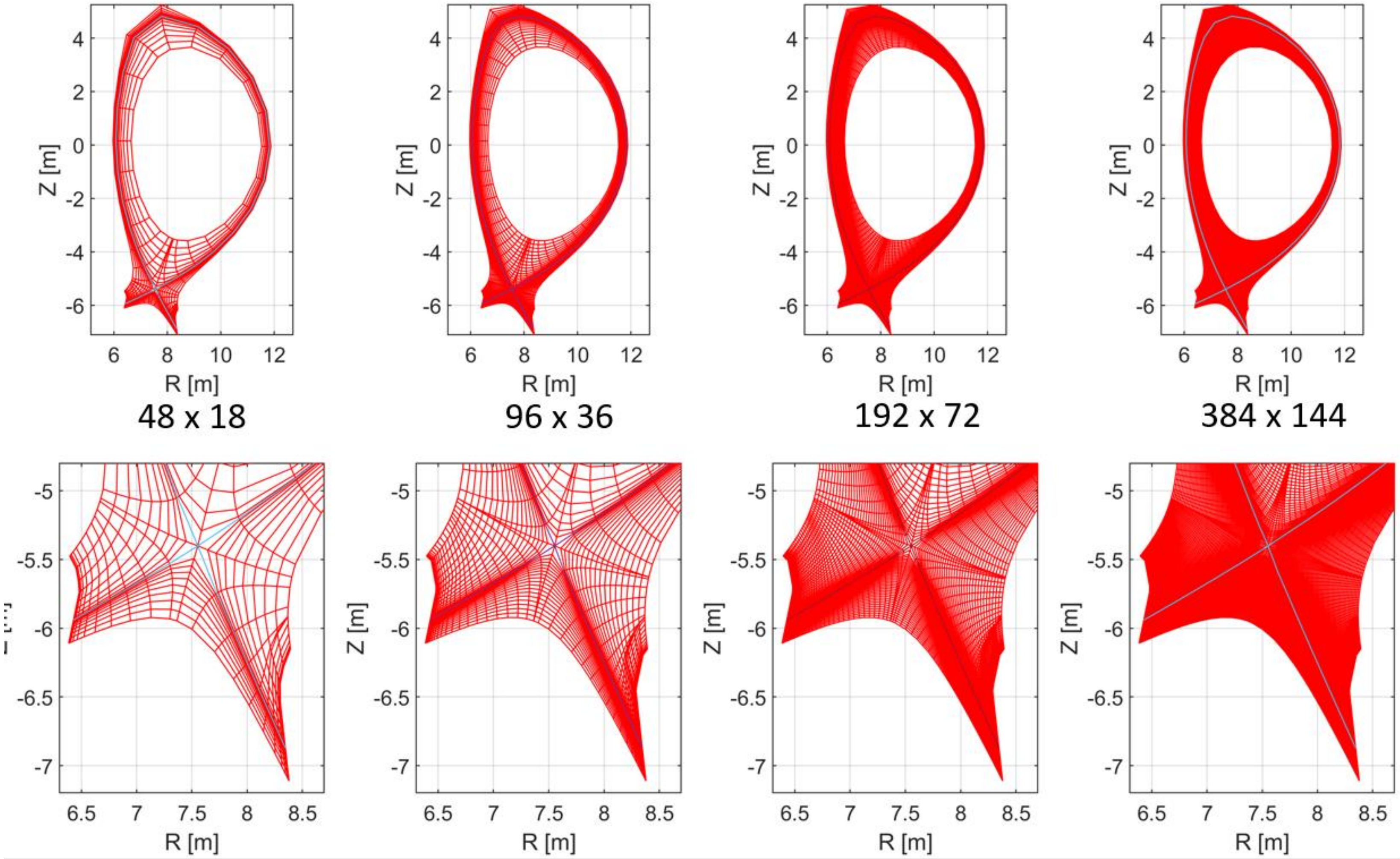


- 'Standard' AFN model assumes dominant CX collisions for transport of atoms: invalid below dome (no plasma)
    - Added ad-hoc n-n collision contribution to pressure diffusion coefficient (and viscosity/conductivity) *(rate based on Kotov 2007 (thesis))*

$$D_p^n = \frac{1}{m_n(\nu_{ion} + \nu_{CX} + \nu_{n-n})}$$

    - Need for adapted BCs to be studied
- Inner-outer divertor communication below dome now 'technically possible'
    - Comparison with kinetic simulation to be done
- Significant progress on gridding exploited, enabling simulations up to the full vessel [N. Vervloesem, PET2023]
    - Collaboration with S. Van den Kerkhof (EEG)
- Convergence AFN model on fixed plasma background achieved. Coupling to plasma to be analyzed.

Grid convergence study for EU-DEMO with AFN (I)



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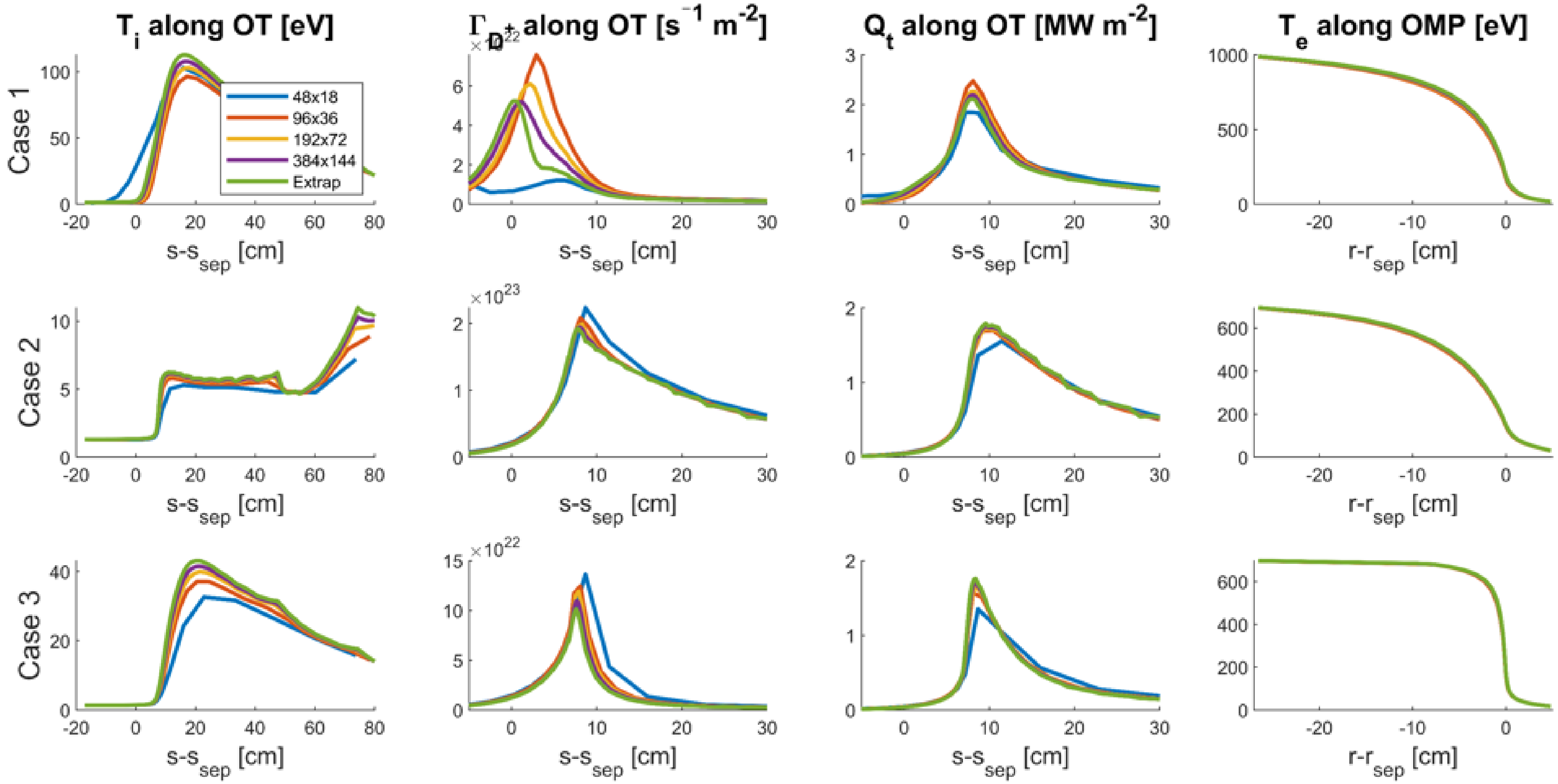
Grid convergence study for EU-DEMO with AFN (II)



Main conclusions:

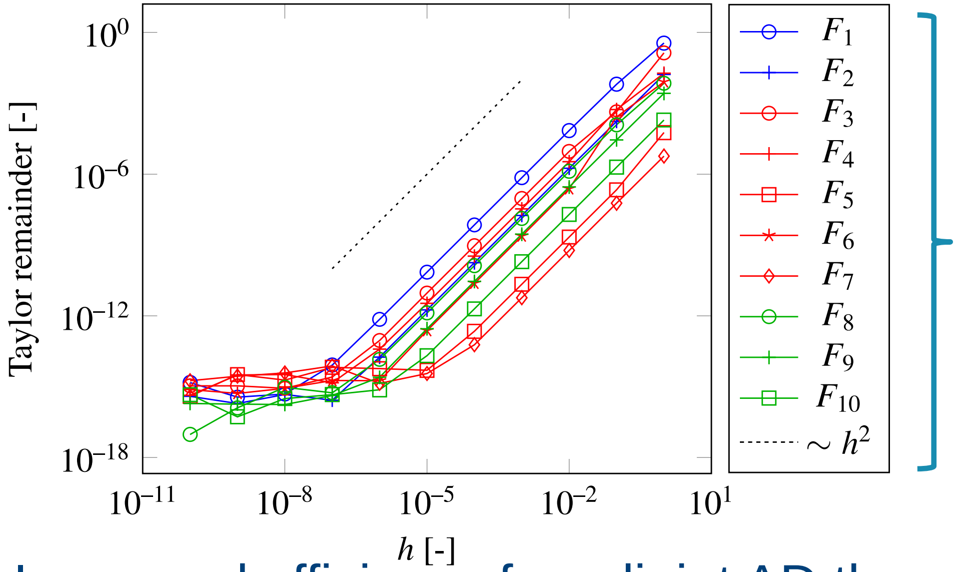
- “standard” 96x36 grid is acceptable for scoping studies
- good practice to perform grid refinement for subset of cases
- grid refinement encouraged when making final claims about peak heat loads

Summary of achievements

- Validation fluid, (SpH) hybrid and kinetic neutral models for JET ILW L-mode plasmas [N. Horsten et al., NME 2022]
  - Realistic tokamak configuration, incl. voids, molecules,…
  - Large fluid-kinetic discrepancies at low density (factor 2), but smaller discrepancies at higher density (50%)
  - Fluid-kinetic discrepancies in both density regimes successfully corrected by hybrid approach
- Alternative hybrid approach that avoids cancellation errors by construction under development
  - Hilbert expansion based fluid model derived; both diffusive & hydrodynamic scaling investigated [V. Maes, PoP 2023]
  - Corresponding kinetic correction model: optimal distribution between kinetic and fluid particles based on numerical error estimate [V. Maes et al., PET 2023]
- Release of fluid and hybrid approaches in extended grids version of SOLPS-ITER to the community during dedicated workshops
  - KU Leuven, Belgium (Nov. 2022), ORNL, US (Dec 2022), Keio University, Japan (Aug. 2023)
  - Dedicated workflow and example cases available
- Development of alternative hybrid KDMC scheme, fully particle-based
  - Analysis of implementation requirements KDMC scheme in test code EIRON ongoing

Algorithmic Differentiation (AD) for gradient calculation applied to EIRENE

- AD = semi-automatic way to differentiate complex simulation software
- Exact to machine precision
- Rewritten small parts of EIRENE to make the code differentiable by the TAPENADE AD tool
- Verification of gradients with Finite Differences for single particle trajectories



Independent variables

Future application within **optimization** & **uncertainty quantification** framework

[N. Horsten et al., PET 2023]

- Increased efficiency for adjoint AD through reversible random number generators under investigation [E. Loevbak et al., https://arxiv.org/abs/2302.02778]

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Workplan 2024

- Application AFN & SpH to JET/ITER/DEMO [W. Dekeyser, W. Van Uytven, N. Horsten]
  - Application to ITER case
    - Validation AFN in extended grids simulations, incl. sub-divertor area
  - Application to DEMO SN case
    - Incl. error analysis with kinetic neutrals
    - In collaboration with WP-DES
  - Analysis of potential fluid model for molecules
  - Assessment H/D/T isotope effects
    - Linked to invited talk N. Horsten @ PSI2024
- Algorithmic differentiation w. TAPENADE [N. Horsten, S. Carli]
  - Analysis of impact estimator type on accuracy of AD sensitivities
  - Optimization of forward sensitivity computations in standalone EIRENE cases;
  - Differentiation of coupled B2.5-EIRENE code, forward mode
  - Investigation of backward sensitivity computations in standalone EIRENE cases
- Kinetic-diffusion scheme [T. Steel, G. Samaey]
  - Implement estimators for KD in EIRON

Publications and conference contributions 2023

- Van Uytven, W., Dekeyser, W., Subba, F., Wiesen, F., Horsten, N., Vervloesem, N., Baelmans, M. Discretization error estimation for EU-DEMO plasma-edge simulations using SOLPS-ITER with fluid neutrals. Under review for publication in Contributions to Plasma Physics.
- Vervloesem, N., Dekeyser, W., Van den Kerkhof, S., Baelmans, M. Error-based grid adaptation methods for plasma edge simulations with SOLPS-ITER. Accepted for publication in Contributions to Plasma Physics.
- Horsten, N., Carli, S., Dekeyser, W. Sensitivity calculation for Monte Carlo particle simulations of neutrals in the plasma edge . Under review for publication in Contributions to Plasma Physics.
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- Horsten, N., Van Uytven, W., Dekeyser, W., Blommaert, M., Samaey, G., Baelmans, M. (2023). Advanced fluid boundary conditions and hybrid fluid-kinetic approaches to model kinetic effects of atoms in the plasma edge of nuclear fusion devices. NEGF 2023, Date: 2023/03/29-2023/03/31, Location: Eindhoven, the Netherlands.
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- Loevbak, E., Vandewalle, S., Samaey, G. Multilevel Monte Carlo for diffusive Kinetic Equations in Plasma Edge Simulations. NumKin 2022, Date: 2022/11/07-2022/11/10, Location: Garching, Germany.

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