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Fluid neutral models including CX and n-n collisions and application to AUG and ITER

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Overview

- Hilbert-expansion based fluid neutral models including n-n collisions
- AFN model including n-n collisions in SOLPS-ITER
- Application to AUG and ITER

Setting

Linear kinetic equation:

$$\underbrace{\partial_t f(x,v,t)}_{\text{Transient}} + \underbrace{v\partial_x f(x,v,t)}_{\text{Transport}} = \underbrace{R_{cx}(x)\left(M_{cx}(v|x)\int f(x,v',t)dv' - f(x,v,t)\right)}_{\text{Charge exchange collisions}}$$

Post-collisional velocity distribution: Maxwellian

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

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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!

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Introducing neutral-neutral collisions

Nonlinear kinetic equation:

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

Make a fluid model in a systematic way?

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

→ Hilbert expansion

Hilbert expansion

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

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

→ 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

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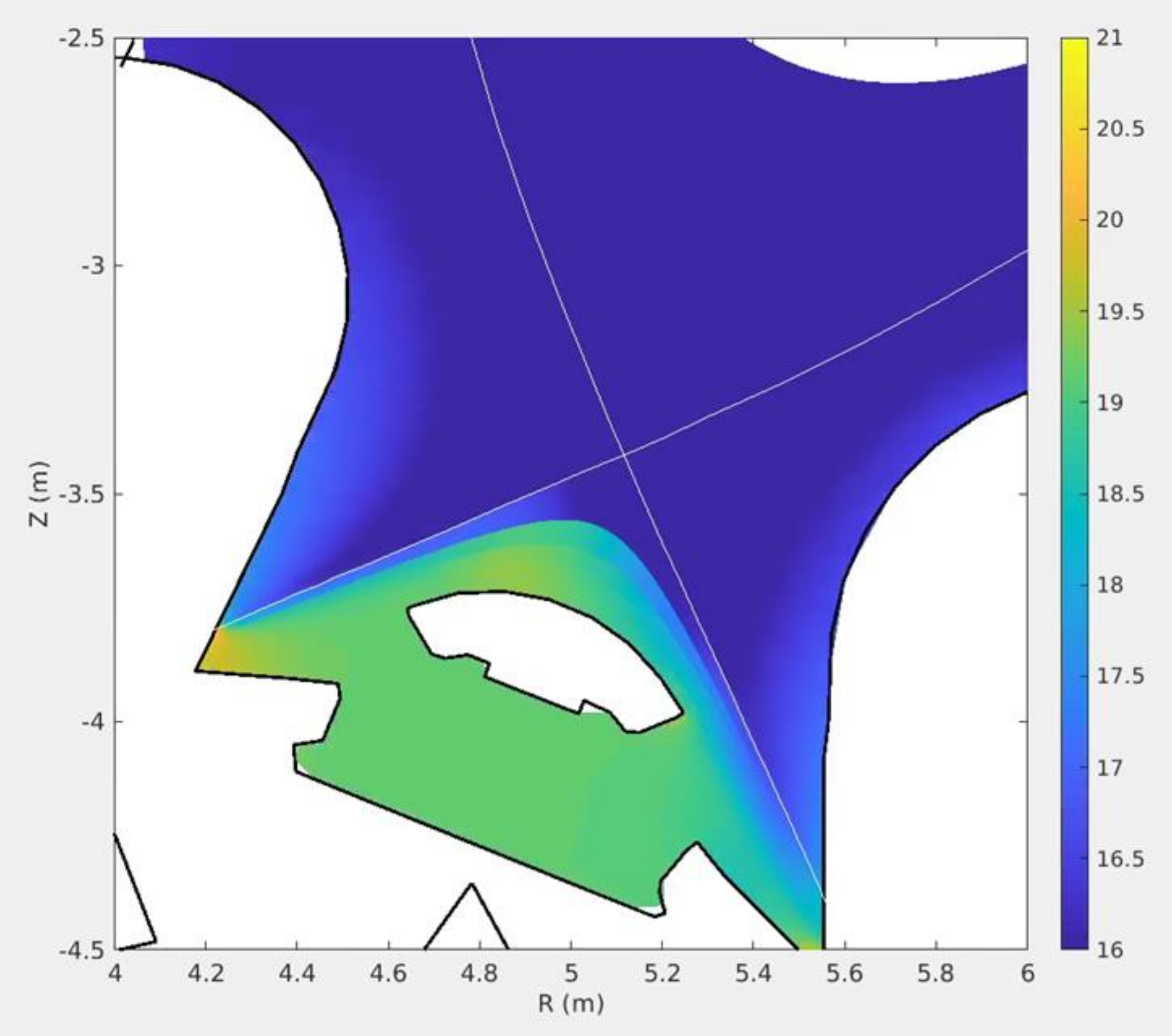
AFN model including n-n collisions



- ‘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

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

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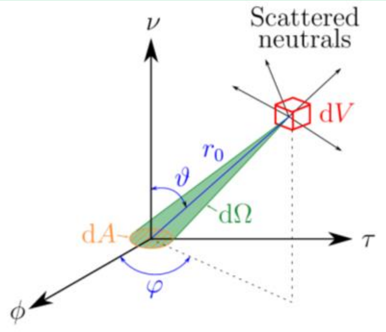
AFN boundary conditions including n-n collisions

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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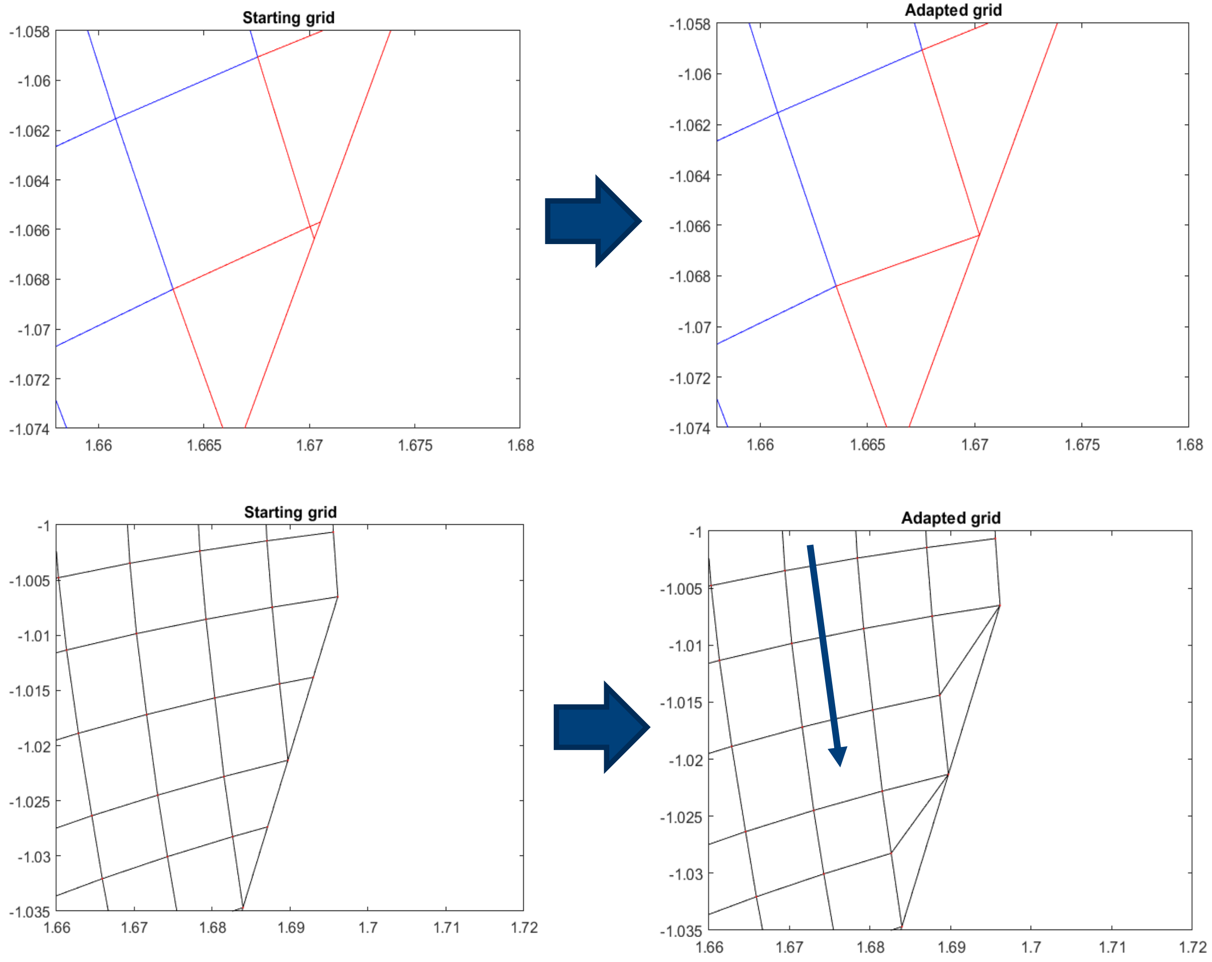
Improved extended grid exploiting GOAT

- “Grid Optimization and Adaptation” Tool

- Adaptation, e.g.:
    - Small triangles (Carre2 artefacts) removed
    - ‘Stacked triangles’ to avoid flux tube splitting / trapezoidal cells
- Optimization:
    - Grid smoothing to improve cell size distribution/skewness/…

- Essential for accuracy and stability of the simulations



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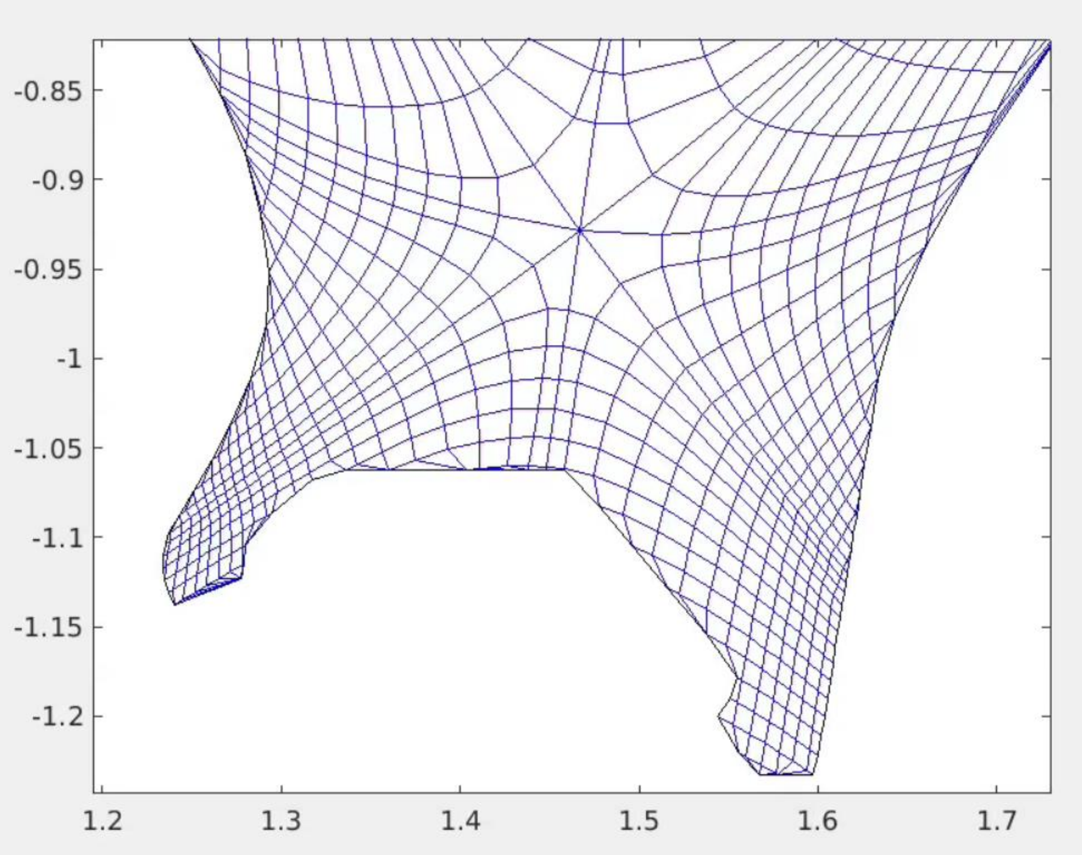
AUG 16151

- A standard SOLPS-ITER equilibrium/geometry, but full W wall
- Grid created with carreMode=3 and GOAT
- BCs:
  - Core: T_i=T_e=300eV, 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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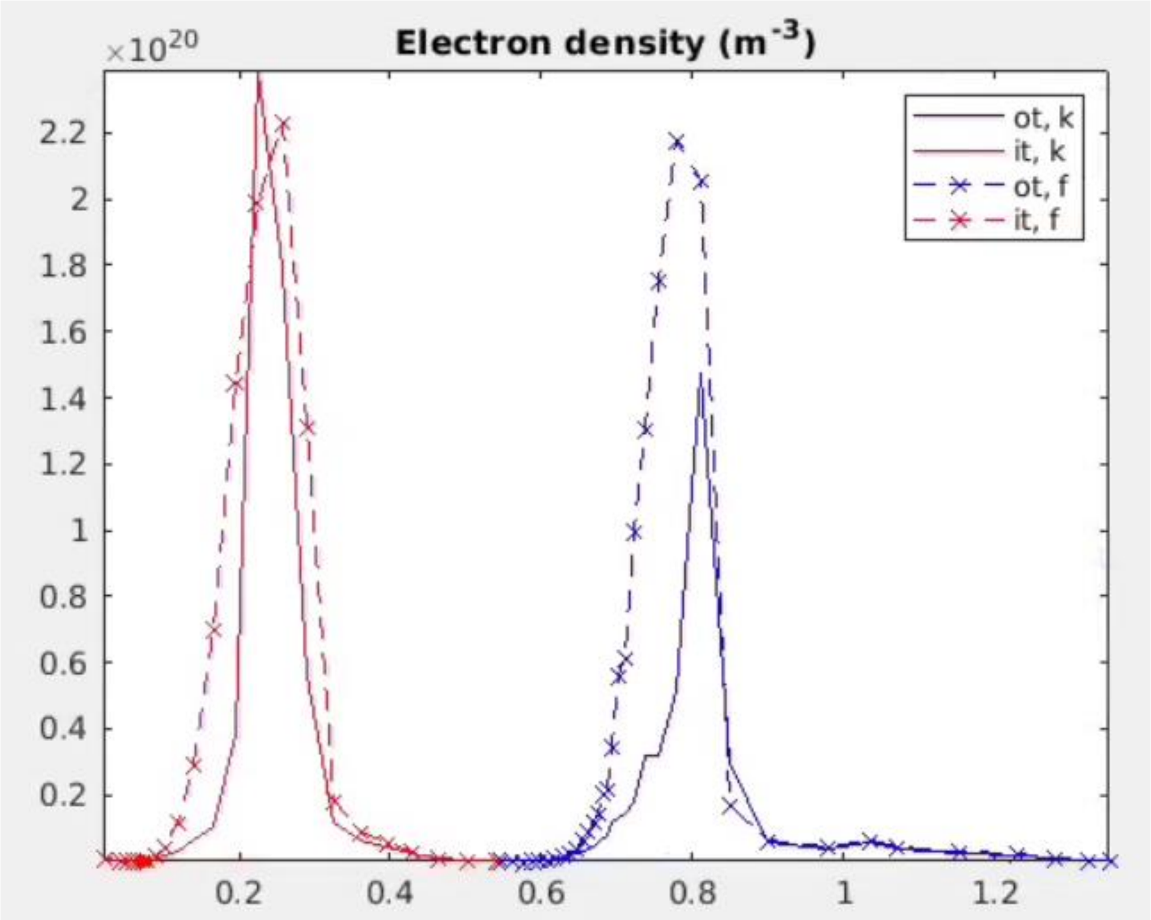
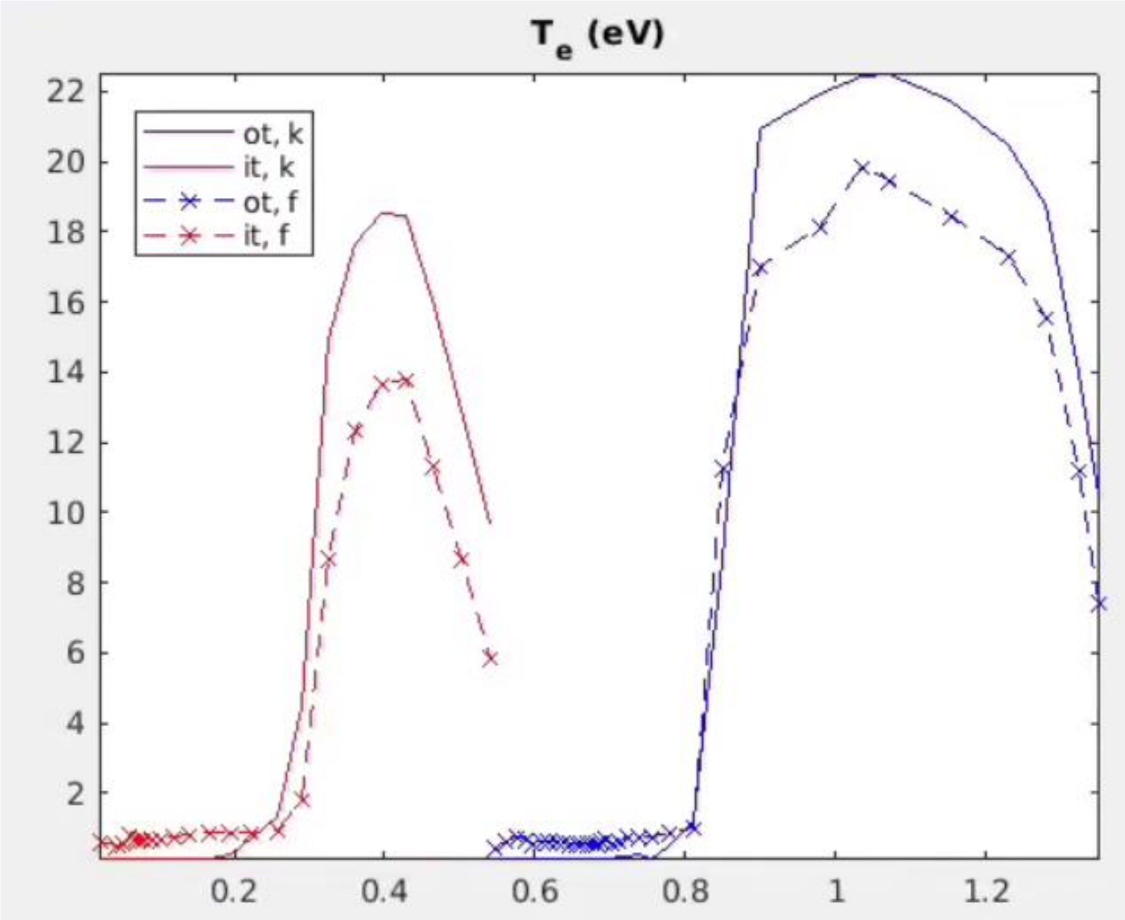
Target profiles





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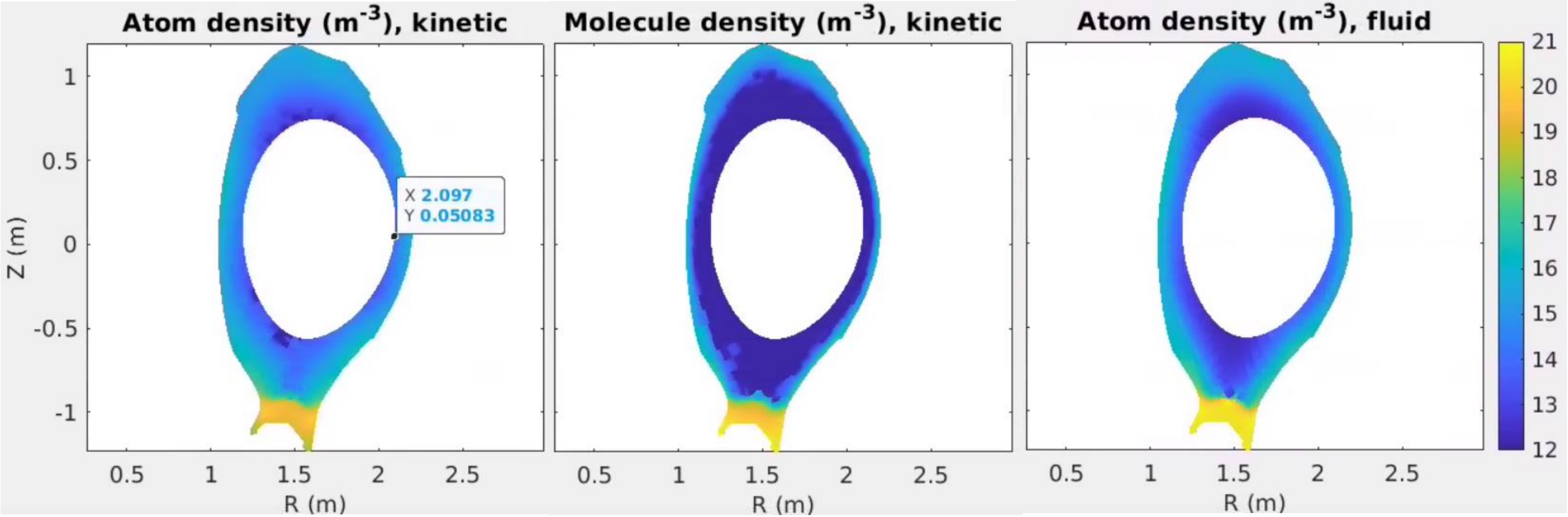
Neutral density



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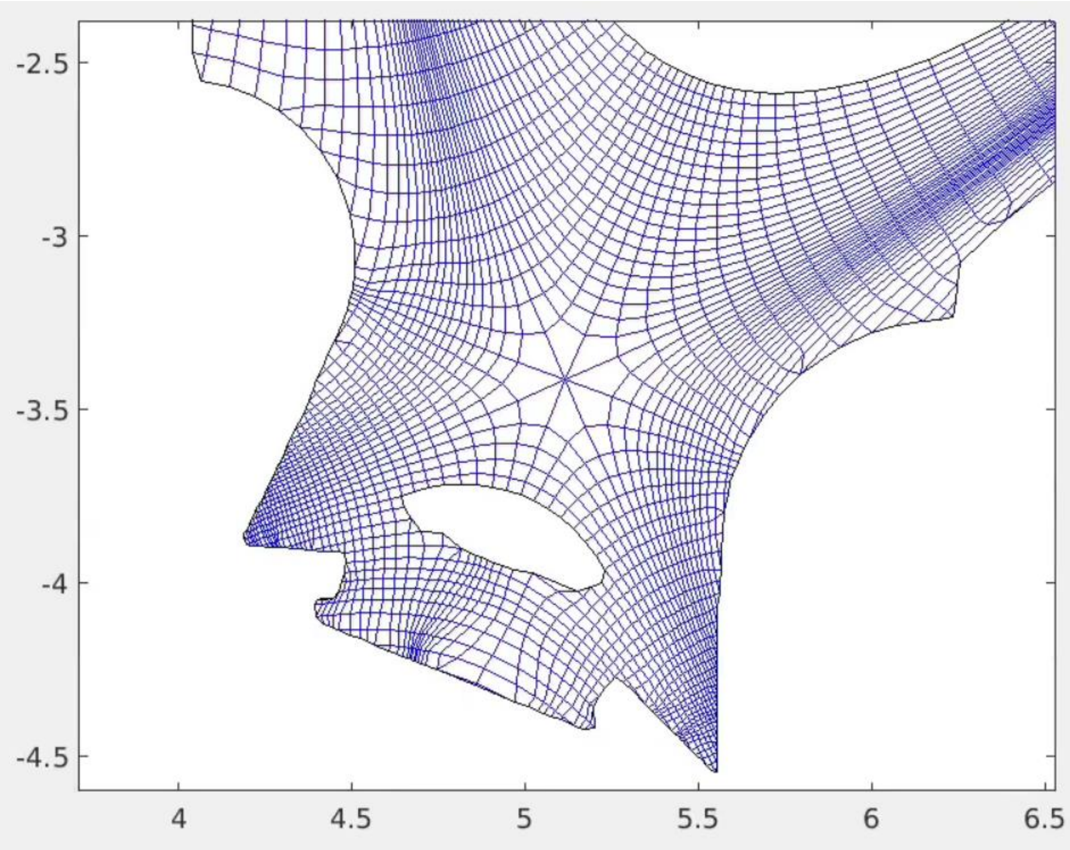
ITER

- 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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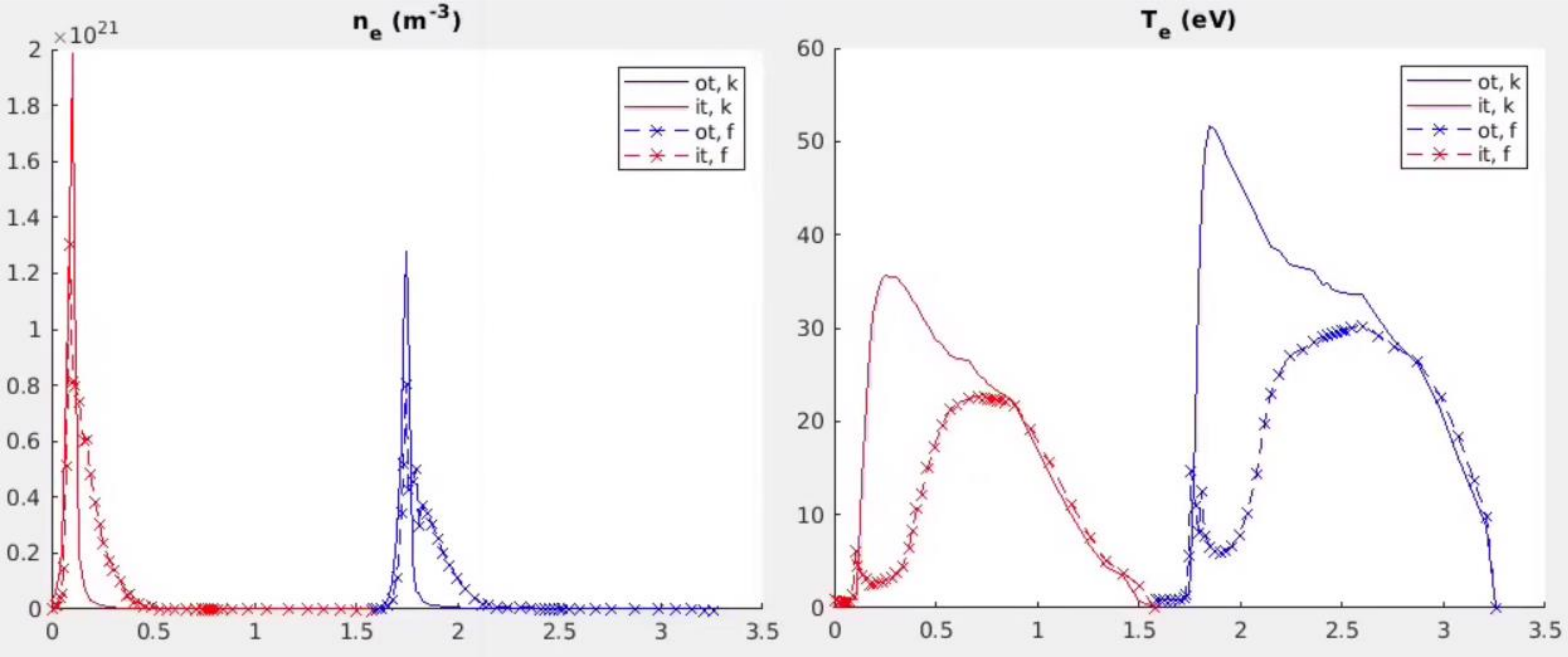
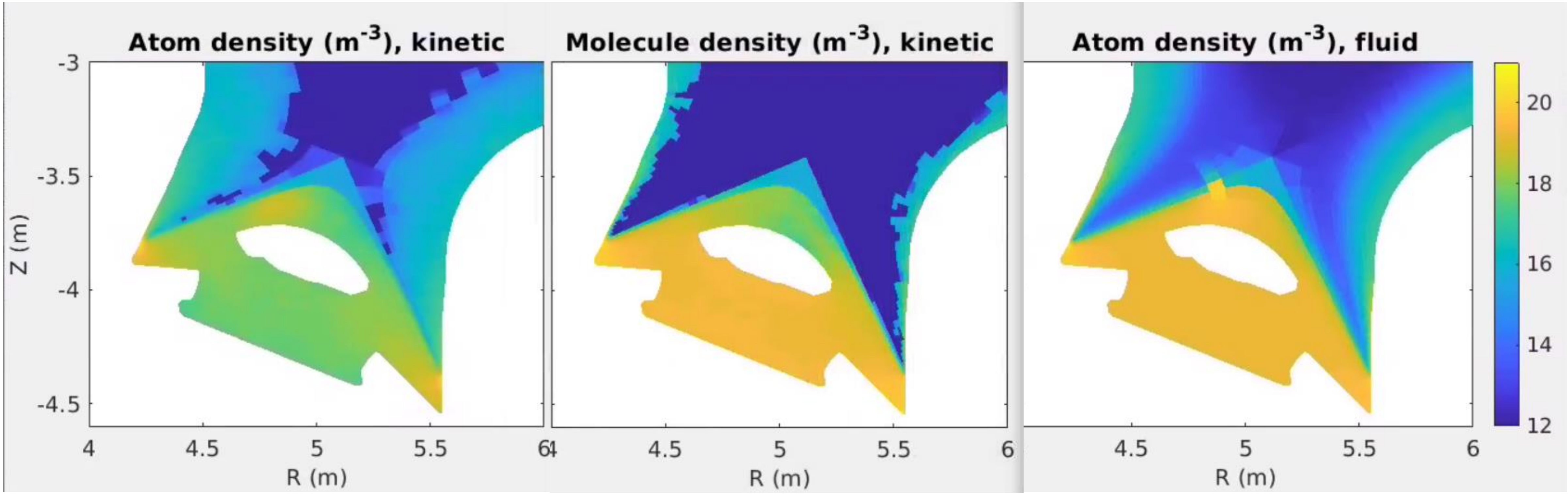
Target profiles



Neutral density



Next steps

- …analysing the results/discrepancies in detail
- Comparison with atom-only kinetic simulation
  - Currently: convergence difficulties
- Fluid model for molecules? Improved fluid approx. for near vacuum?
- Hybrid fluid-kinetic simulation