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Introduction

Two types of fluid models are widely used to model edge plasma:

- 2D transport codes such as SOLPS, UEDGE or SOLEDGE2D assuming plasma axi-symmetry and where cross-field turbulent transport is emulated by empirical diffusion. These codes account for neutrals (fluid or kinetic) and impurities and are key tools to interpret experiments. They lack predictability due to their poor description of turbulence.
- 3D turbulent codes such as BOUT++, GBS or TOKAM3X which are able to self-consistently model turbulent transport but often rely on idealistic plasmas. The description of realistic tokamak geometry, neutrals or impurities is not always addressed.

We propose here to capitalize on the experience in developing SOLEDGE2D and TOKAM3X at CEA to create a new code SOLEDGE3X integrating the advantages of the two codes and thus being able to simulate complex multi-species plasma in realistic geometry, either in transport mode (2D) or turbulent mode (3D).

Description of the model

SOLEDGE3X solves:

- **Mass balance [for each ion species (α)]:**

$$\partial_t n_\alpha + \vec{\nabla} \cdot (n_\alpha \vec{v}_\alpha) = S_\alpha^n \quad \text{where} \quad \vec{v}_\alpha = v_{\parallel,\alpha} \vec{b} + \vec{v}_{E \times B} + \vec{v}_\alpha^* - \frac{D_\alpha \vec{\nabla}_\perp n_\alpha}{n_\alpha} + \vec{v}_\alpha^p$$

- **Parallel momentum balance [for each ion species (α)]:**

$$\partial_t (m_\alpha n_\alpha v_{\parallel,\alpha}) + m_\alpha \vec{\nabla} \cdot (n_\alpha v_{\parallel,\alpha} \vec{v}_\alpha - v_\alpha n_\alpha \vec{\nabla}_\perp v_{\parallel,\alpha}) = -\nabla_\parallel p_\alpha - \vec{b} \cdot \vec{\nabla} \cdot \overline{\tau_\alpha} + Z_\alpha e n_\alpha E_\parallel + R_{\parallel,\alpha} + S_\alpha^T$$

- **Energy balance [for each ion species (α) and electrons]:**

$$\partial_t E_\alpha + \vec{\nabla} \cdot (E_\alpha \vec{v}_\alpha + p_\alpha v_{\parallel,\alpha} \vec{b} + q_{\parallel,\alpha} \vec{b} - \frac{m_\alpha}{2} v_\alpha n_\alpha \vec{\nabla}_\perp v_{\parallel,\alpha}^2 - \chi_\alpha n_\alpha \vec{\nabla}_\perp T_\alpha) = Z_\alpha e n_\alpha v_{\parallel,\alpha} E_\parallel + v_{\parallel,\alpha} R_{\parallel,\alpha} + Q_\alpha + S_\alpha^E$$

- **Charge balance:**

$$\vec{\nabla} \cdot (j_\parallel \vec{b} + \vec{j}^* + \vec{j}^p) = 0$$

$$\text{where} \quad j_\parallel = -\sigma_\parallel \left(\nabla_\parallel \phi - \frac{\nabla_\parallel p_e}{n_e} - \frac{R_{\parallel,e}^T}{n_e} \right) \quad \vec{j}^* = \sum_{i,e} Z_\alpha n_\alpha \vec{v}_\alpha^* \quad \vec{j}^p = \sum_i Z_\alpha n_\alpha \vec{v}_\alpha^p$$

$$\text{with} \quad n_\alpha \vec{v}_\alpha^p = -\partial_t \vec{\omega}_\alpha - \vec{\nabla} \cdot (\vec{v}_\alpha \otimes \vec{\omega}_\alpha) \quad \text{where} \quad \vec{\omega}_\alpha = \frac{m_\alpha}{Z_\alpha B^2} \left(n_\alpha \vec{\nabla}_\perp \phi + \frac{1}{Z_\alpha} \vec{\nabla}_\perp p_\alpha \right)$$

- **Electron density (from quasi-neutrality):** $n_e = \sum_i Z_\alpha n_\alpha$

- **Parallel electron velocity (from parallel current):** $n_e v_{\parallel,e} = \sum_i Z_\alpha n_\alpha v_{\parallel,\alpha} - j_\parallel$

- **Neutrals:** EIRENE or fluid neutrals (diffusive)

In green are shown diffusive cross-field transport which can be used to emulate turbulence when the code is used as a transport code. In red are shown collisional closure terms (see below). In blue are shown terms not yet implemented.

Boundary conditions on the wall (Bohm-Chodura):

- **Velocity:** $|\vec{v}_\alpha \cdot \vec{n}_{wall}| \geq c_{s,\alpha} |\vec{b} \cdot \vec{n}_{wall}|$
- **Energy flux:** $\Phi_{E,\alpha} = \left(\gamma_\alpha T_\alpha + \frac{1}{2} m_\alpha v_{\parallel,\alpha}^2 \right) \Phi_{n,\alpha}$ where γ_α is sheath transmission factor
- **Current:** $j = [\sum_{ions} Z_\alpha \Phi_{n,\alpha}] \times [1 - \exp(\Lambda - \frac{\phi}{T_e})]$

Multi-species Zhdanov closure

- For simple hydrogen plasmas, Braginskii or Balescu provides clear closure expression for conductive heat fluxes or friction forces, for example:

$$q_{\parallel,e} = -\kappa_e^0 T_e^2 \nabla_\parallel T_e + 0,71 n_e T_e (v_{\parallel,e} - v_{\parallel,i}) \quad \text{or} \quad R_{\parallel,e} = -0,71 n_e \nabla_\parallel T_e - 0,51 \frac{m_e}{\tau_e} n_e (v_{\parallel,e} - v_{\parallel,i})$$

- Explicit expressions exist for friction forces for trace impurities [see Stangeby, Plasma boundary of magnetic fusion devices (2000)]

- Zhdanov closure [Transport processes in multicomponent plasmas (2002)] provides linear relation between temperature gradients, velocities and heat fluxes and friction forces.

Pros: No trace impurity assumption, no light species assumption

Cons: No explicit expression for forces and heat fluxes. Requires linear system inversion

$$\begin{cases} \frac{5}{2} n_\alpha k T_\alpha = \sum_\beta \left[\frac{5}{2} \frac{\mu_{\alpha\beta}}{m_\alpha} \bar{G}_{\alpha\beta}^{(2)} (\bar{w}_\alpha - \bar{w}_\beta) + \bar{G}_{\alpha\beta}^{(5)} \frac{\bar{h}_\alpha}{p_\alpha} + \bar{G}_{\alpha\beta}^{(6)} \frac{\bar{h}_\beta}{p_\beta} + \frac{\mu_{\alpha\beta}}{kT} \left(\bar{G}_{\alpha\beta}^{(9)} \frac{\bar{r}_\alpha}{p_\alpha} + \bar{G}_{\alpha\beta}^{(10)} \frac{\bar{r}_\beta}{p_\beta} \right) \right] \\ 0 = \sum_\beta \left[\frac{35}{2} \left(\frac{\mu_{\alpha\beta}}{m_\alpha} \right)^2 \bar{G}_{\alpha\beta}^{(8)} (\bar{w}_\alpha - \bar{w}_\beta) + 7 \frac{\mu_{\alpha\beta}}{m_\alpha} \left(\bar{G}_{\alpha\beta}^{(9)} \frac{\bar{h}_\alpha}{p_\alpha} + \bar{G}_{\alpha\beta}^{(10)} \frac{\bar{h}_\beta}{p_\beta} \right) + \frac{m_\alpha}{kT} \bar{G}_{\alpha\beta}^{(11)} \frac{\bar{r}_\alpha}{p_\alpha} + \frac{m_\beta}{kT} \bar{G}_{\alpha\beta}^{(12)} \frac{\bar{r}_\beta}{p_\beta} \right] \end{cases}$$

Where $\bar{G}_{\alpha\beta}^{(n)}$ can be computed explicitly from local plasma parameters

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A word about the numerics

SOLEDGE3X numerical scheme is based on a 2nd order finite volume scheme with a mixed implicit/explicit time stepping. One uses structured grid aligned on magnetic flux surfaces + domain decomposition to treat X-points. The following discretization is used:

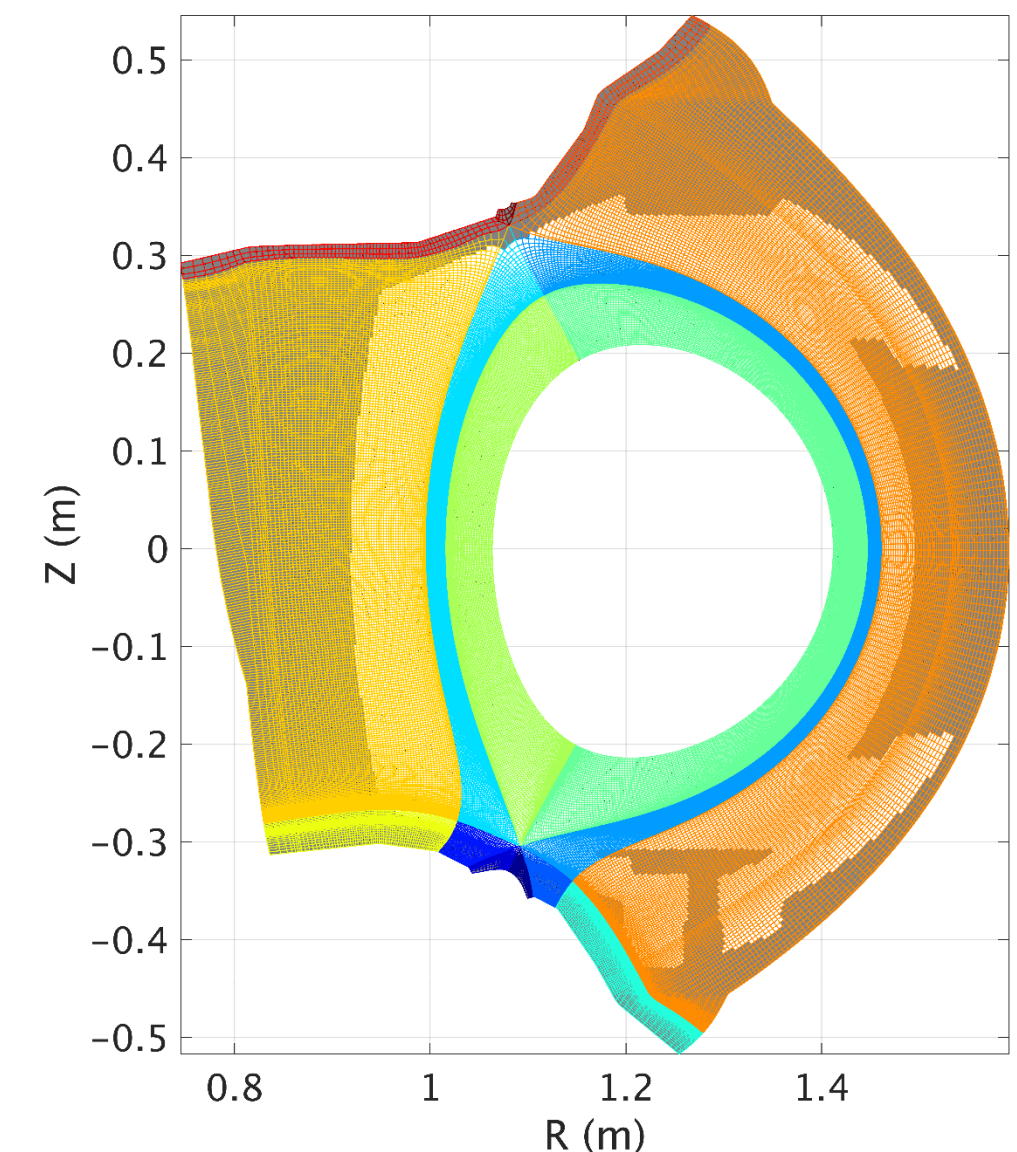
- Donat-Marquina fluxes + WENO interpolation for advection [JCP 125, 42-58 (1996)]
- Günter scheme for parallel diffusion in the flux surface [JCP 209, 354-370 (2005)]

A mask function χ is used to define the wall location. Boundary conditions are imposed at the interface $\chi = 1 | \chi = 0$.

The following linear solver are used:

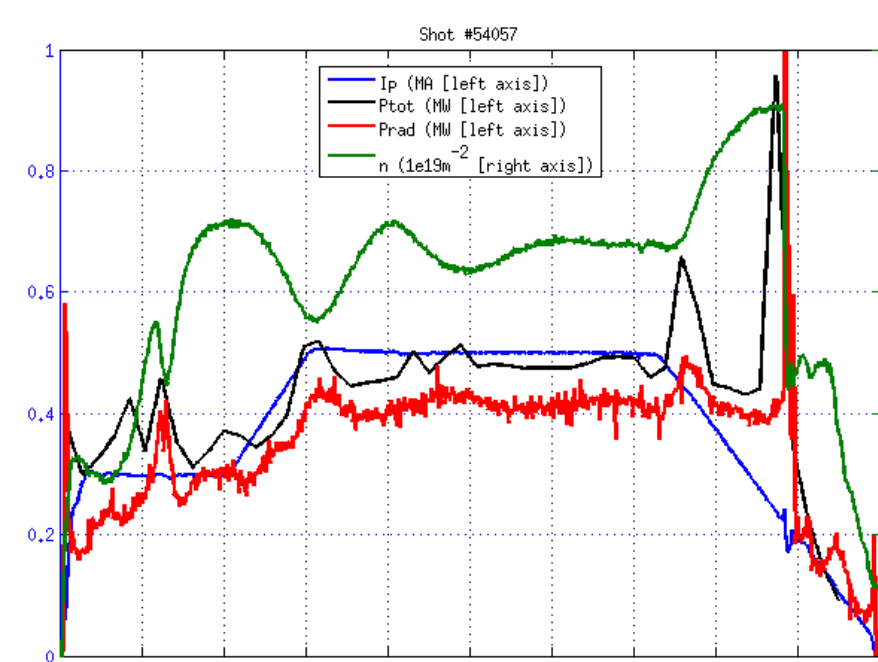
- LAPACK for small linear problems (1D)
- PASTIX (direct solver) for medium size problems (2D diffusion or 3D diffusion on small grids)
- AGMG (algebraic multigrid iterative solver) for 2D and 3D diffusion [agmg.eu]
- PETSC for 2D and 3D diffusion

An hybrid MPI/OpenMP parallelization is used to solve in parallel different sub-domains. An OpenMP layer is used to solve species in parallel.



Application to 2D transport modelling

SOLEDGE3X is used here as a transport code to help interpret experiments, namely WEST Ohmic shot #54057 at $B_T = 3,83T$, $I_p = 500kA$, $P_{Ohm} \approx 500kW$, $n_e(lid) = 2 \cdot 10^{19} m^{-2}$.

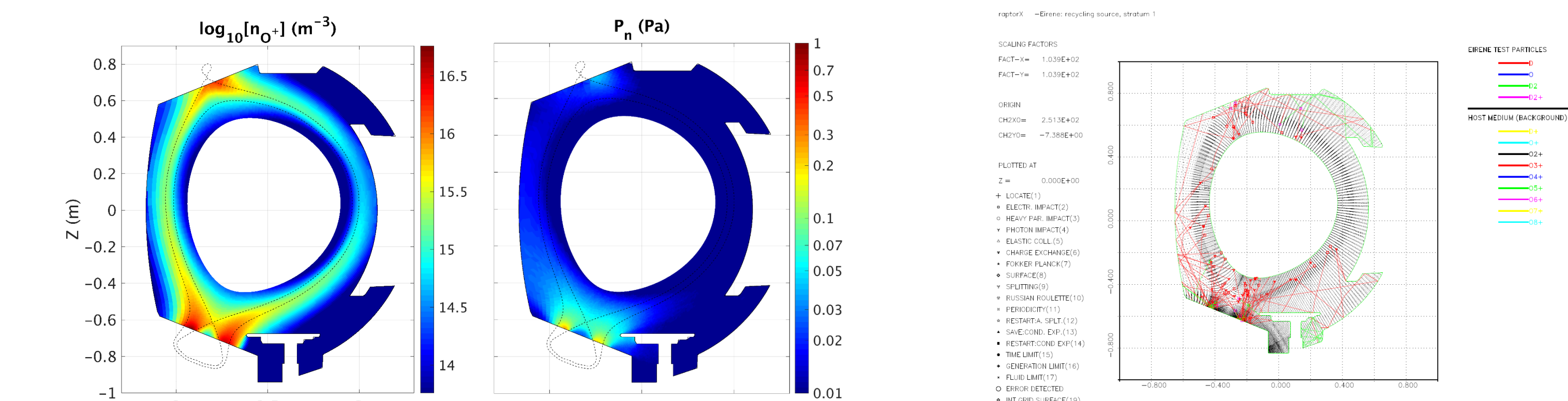


The shot is simulated with the following parameters:

$D = v$	$\chi_e = \chi_i$	composition	R_n	Neutrals
$1 m^2 s^{-1}$	$2 m^2 s^{-1}$	D + O (2%)	98 %	EIRENE

BC at core side: $n_{D^+} = 9 \cdot 10^{18} m^{-3}$; $n_{\Sigma O^{n+}} = 1,8 \cdot 10^{17} m^{-3}$
 $P_e = 250kW$; $P_{D^+} = 250kW$

Grid resolution: $[N_\theta \times N_\psi] \approx [260 \times 100]$



- Code ability to simulate multi-component plasma with EIRENE coupling well tested
- Next step: validation with experimental data from WEST campaigns

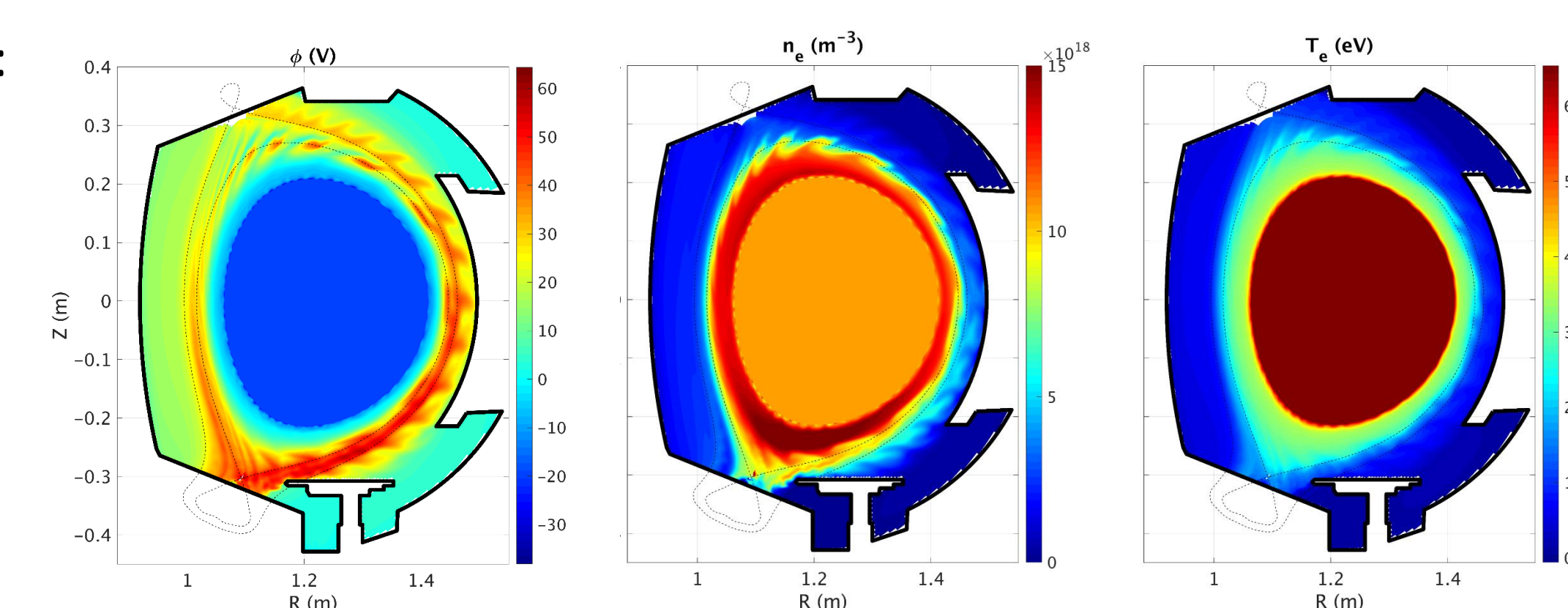
Application to 3D turbulence modelling

First attempt to perform turbulence modelling in realistic WEST wall geometry. Machine size is reduced by a factor 2. Parallel resistivity is multiplied by 10.

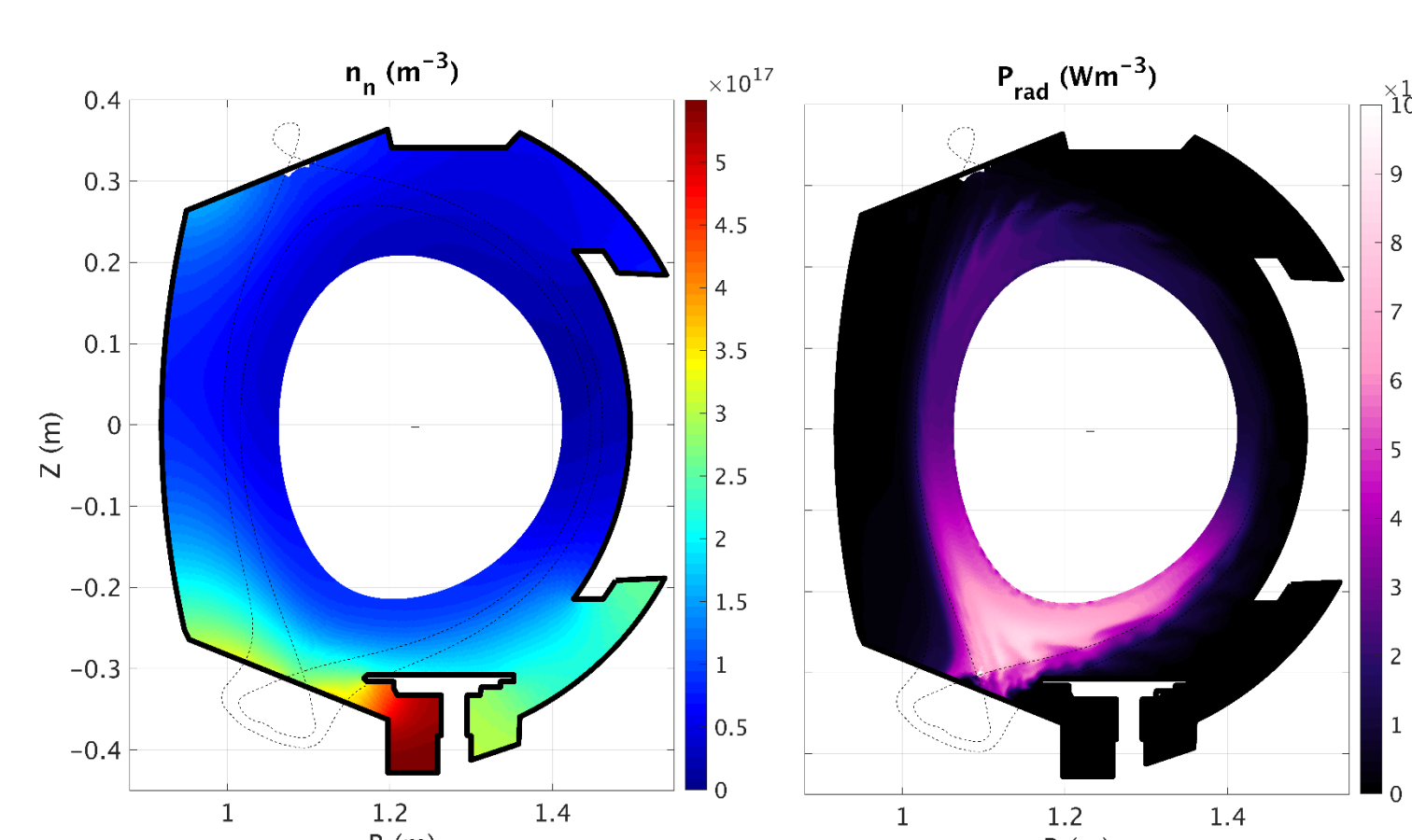
Grid resolution: $[N_\varphi \times N_\theta \times N_\psi] \sim [32 \times 560 \times 130] + \text{core cell (1/4 torus)}$

Main simulation parameters:

$D = v$	$0,2 m^2 s^{-1}$
$\chi_e = \chi_i$	
composition	Pure D
R_n	80%
Neutrals	fluid
Power	125 kW
Puff	$1 \cdot 10^{20} s^{-1}$



Transient showing interchange instability – Drive: energy source in the core cell



- Turbulent results remain preliminary
- Code scaling to higher resolution / real size WEST simulation ongoing
- Code validation with experiments on WEST to be carried out: special focus on core rotation measurements to validate the physical model on current balance.