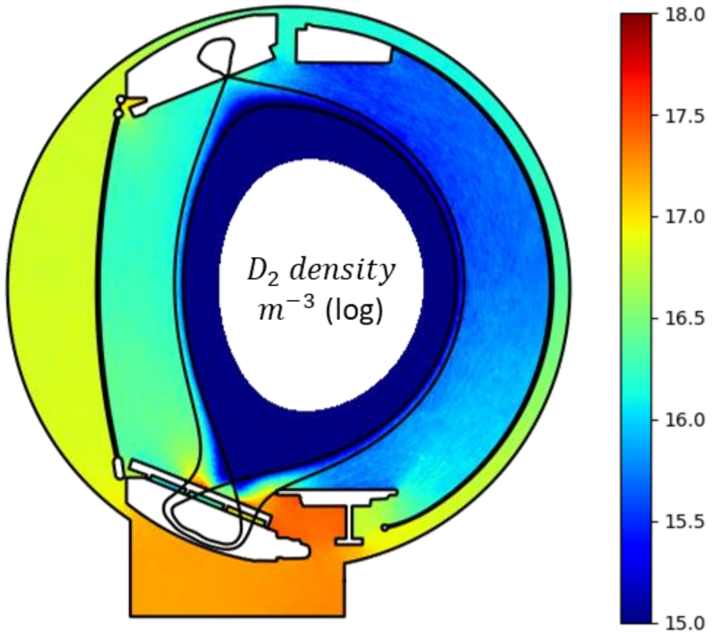
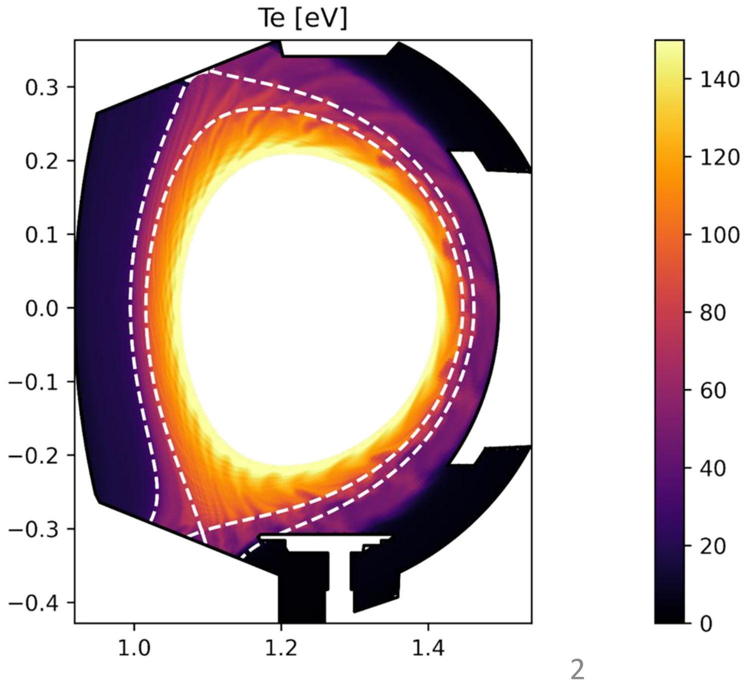
Investigation of transport barrier formation in edge turbulent simulations

Hugo Bufferand, G. Ciraolo, G. Falchetto, N. Fedorczak, Ph. Ghendrih, Y. Marandet, E. Serre, P. Tamain

The SOLEDGE3X code

- Merging of the transport code SOLEDGE2D and the turbulence code TOKAM3X
  → Can be used in 2D (transport) or 3D (3D transport or turbulence simulations)
- Solves fluid equations for multi-species plasma based on Zhdanov closure [Raghunathan et al., PPCF, 2021]
- Electrostatic at the moment – Electromagnetic version under development
- Implements several neutral models:
  - Fluid neutrals (diffusive): very crude but fast and robust
  - Kinetic neutrals: EIRENE – high fidelity





The SOLEDGE3X drift-ordering fluid model

Collisional closure terms
Ionization terms
External sources
“Anomalous” diffusion for transport simulations

- **Mass balance** (for all ion species – quasi-neutrality for electrons)

$$[1] \qquad \partial_t n + \vec{\nabla} \cdot (n\vec{v}) = S_n^{iz}$$

- Velocity decomposition $\vec{v} = v_{\parallel}\vec{b} + \vec{v}_{drifts} - \frac{D\vec{\nabla}_{\perp} n}{n}$

- Ionization/recombination sources involving neutrals are computed by the “neutral solver”, for instance EIRENE when using kinetic neutrals.

The SOLEDGE3X drift-ordering fluid model

- **Momentum balance**

Collisional closure terms
Ionization terms
External sources
"Anomalous" diffusion for transport simulations

[2] $$\partial_t(mn\vec{v}) + \vec{\nabla}\cdot(mn\vec{v}\otimes\vec{v}) = -\vec{\nabla}p - \vec{\nabla}\cdot\bar{\bar{\Pi}} + Zen(\vec{E}+\vec{v}\times\vec{B}) + \vec{R} + \vec{S}_v^{iz} + \vec{S}_v^{ex}$$

$$\bar{\bar{\Pi}} = \pi_\parallel\left(\vec{b}\otimes\vec{b} - \frac{1}{3}\bar{\bar{I}}\right) + \bar{\bar{\Pi}}^{FLR}$$ where $$\pi_\parallel = -3\eta_\parallel\left(\nabla_\parallel v_\parallel - \vec{\kappa}\cdot\vec{v} - \frac{1}{3}\vec{\nabla}\cdot\vec{v}\right)$$

- Parallel projection ($\vec{b}\cdot[2]$)

[3] $$\partial_t(mnv_\parallel) + \vec{\nabla}\cdot(mnv_\parallel\vec{v}) = -\nabla_\parallel p - \vec{b}\cdot(\vec{\nabla}\cdot\bar{\bar{\Pi}}) + ZenE_\parallel + R_\parallel + S_{v_\parallel}^{iz+ex} + m\vec{\nabla}\cdot(n\eta_\perp\vec{\nabla}_\perp v_\parallel)$$

- Perpendicular momentum: ($\vec{b}\times[2]$)

$$\vec{v}_\perp = \frac{\vec{E}\times\vec{B}}{B^2} + \frac{\vec{B}\times(\vec{\nabla}p + \vec{\nabla}\cdot\bar{\bar{\Pi}})}{ZenB^2} - \frac{\vec{B}\times(\vec{R}_\perp + \vec{S}_{v_\perp}^{iz+ex})}{ZenB^2} + \frac{\vec{b}}{n\omega_c}\times\left[\partial_t(n\vec{v}) + \vec{\nabla}\cdot(n\vec{v}\otimes\vec{v})\right]$$

Drift ordering (assuming $\omega_c^{-1}d_t \ll 1$ and $\omega_c^{-1}\tau_{col}^{-1} \ll 1$):

$$\vec{v}_\perp^0 = \frac{\vec{E}\times\vec{B}}{B^2} + \frac{\vec{B}\times\vec{\nabla}p}{ZenB^2}$$

E cross B *Diamagnetic*

$$\vec{v}_\perp^1 = \frac{\vec{b}}{n\omega_c}\times\left[\partial_t(n\vec{v}^0) + \vec{\nabla}\cdot(n\vec{v}^0\otimes\vec{v}^0)\right] + \frac{\vec{B}\times\vec{\nabla}\cdot\bar{\bar{\Pi}}}{ZenB^2} - \frac{\vec{B}\times(\vec{R}_\perp + \vec{S}_{v_\perp}^{iz+ex})}{ZenB^2}$$

Polarization *Non-linear drifts (function of $\vec{v}^0$)*

The SOLEDGE3X drift-ordering fluid model

Collisional closure terms
Ionization terms
External sources
"Anomalous" diffusion for transport simulations

- **Current balance** (Equation on ϕ – vorticity equation)

[4] $\vec{\nabla} \cdot \vec{j} = 0$ with $\vec{j} = \sum Zn\vec{v} = j_\parallel \vec{b} + \vec{j}^\star + \vec{j}_\Pi + \vec{j}_{pola} + \vec{j}^{ex}$

  - Parallel current expression obtained from parallel electron momentum balance (Generalized Ohm's law)

$$j_\parallel = -\sigma_\parallel \left(\nabla_\parallel \phi + \frac{-\nabla_\parallel p_e + R^T_{e,\parallel}}{en_e} \right)$$

  - Given zeroth order drift expression, polarization current can be expressed: $\vec{j}_{pola} = -\partial_t \vec{\omega} - \vec{\nabla} \cdot (\vec{v}^0 \otimes \vec{\omega})$ where:

$$\vec{\omega} = \frac{m_i}{B^2}\left(n\vec{\nabla}_\perp \phi + \frac{1}{Ze}\vec{\nabla}_\perp p_i \right)$$

$\vec{\nabla} \cdot \vec{\omega} = \Omega$ so called vorticity

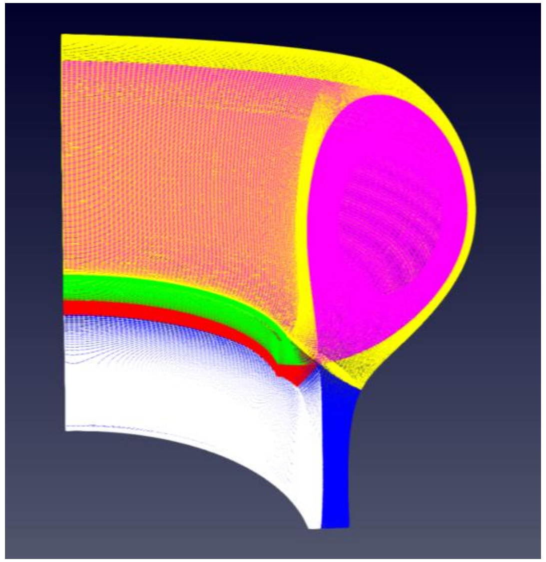
  - Shape of ϕ equation :

$$\vec{\nabla} \cdot \left(\partial_t \left[\frac{m_i n}{B^2} \vec{\nabla}_\perp \phi \right] + \sigma_\parallel \nabla_\parallel \phi \vec{b} \right) = RHS$$

- **Energy balance** $\mathcal{E} = \frac{3}{2} nT + \frac{1}{2} mnv_\parallel^2$

[5] $$\partial_t \mathcal{E} + \vec{\nabla} \cdot \left(\mathcal{E}\vec{v} + pv_\parallel \vec{b} + v_\parallel \bar{\bar{\Pi}} \cdot \vec{b} + \vec{q} \right) = Zne v_\parallel E_\parallel + v_\parallel R_\parallel + Q + S_\mathcal{E}^{iz+ex} + \vec{\nabla} \cdot \left(mnv_\parallel \eta_\perp \vec{\nabla}_\perp v_\parallel + n\chi_\perp \vec{\nabla}_\perp T \right)$$

The SOLEDGE3X implementation



- Numerical scheme
  - Finite volumes with multi-domain structured grid aligned with magnetic flux surfaces
  - **Spatial discretization**: - Advection [$\mathcal{A}$]: Donat & Marquina scheme [JCP 1996] + WENO interpolation
    - Parallel diffusion [$\mathcal{D}_{\parallel}$]: Günter scheme [JCP 2005]
    - Perpendicular diffusion [$\mathcal{D}_{\perp}$]: Sharma & Hammet scheme [JCP 2007]
  - **Temporal discretization**: Explicit except parallel diffusion terms treated implicitly

$$\frac{X(t+\delta t)-X(t)}{\delta t}+\mathcal{A}(X(t))+\mathcal{D}_{\parallel}(X(t+\delta t))+\mathcal{D}_{\perp}(X(t))=\mathcal{S}(X(t))$$

Exception: Electric potential equation mixing parallel Laplacian and perpendicular Laplacian treated both implicitly (3D problem – potential **bottleneck** for linear solvers):

$$\frac{1}{\delta t}\left(\mathcal{D}_{\perp}(\phi(t+\delta t))-\mathcal{D}_{\perp}(\phi(t))\right)+\mathcal{D}_{\parallel}(\phi(t+\delta t))=\mathcal{S}(t)$$

The SOLEDGE3X implementation

- Focus on electric potential equation

$$\frac{1}{\delta t}\left(\mathcal{D}_\perp\left(\phi(t+\delta t)\right) - \mathcal{D}_\perp\left(\phi(t)\right)\right) + \mathcal{D}_\parallel\left(\phi(t+\delta t)\right) = \mathcal{S}(t)$$

Anisotropic 3D Laplacian: $\frac{1}{\delta t}\mathcal{D}_\perp \ll \mathcal{D}_\parallel$

- Near Neuman BC (ill-defined problem):

$$j_\parallel^{BC} = j^{sat}\left(1 - \exp\left(\Lambda - \frac{\phi}{T_e}\right)\right) \rightarrow \nabla_\parallel \phi + \alpha\phi = \beta \quad \text{with } \alpha \ll 1$$

- Matrix of the problem poorly conditioned
- Problem too big for direct solvers. Iterative solver are used → need for a good preconditioner

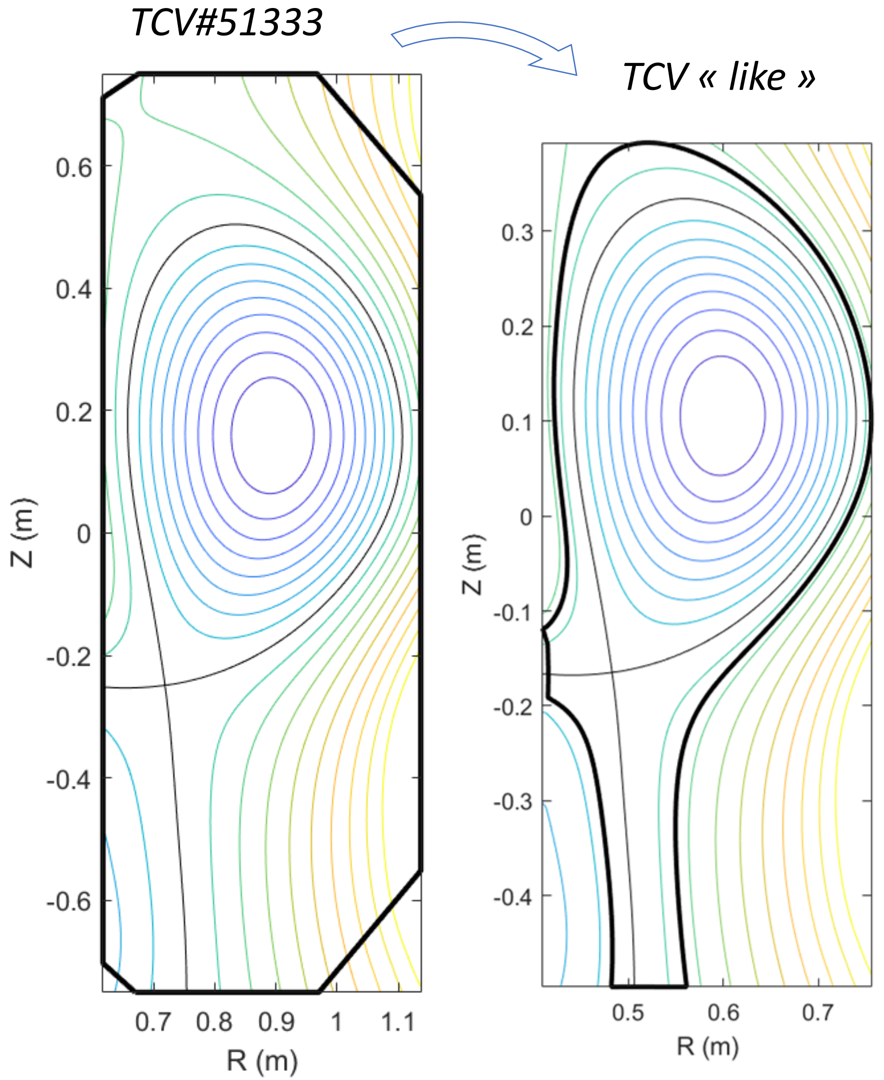
→Best solution found so far: Algebraic multigrid preconditioner combined with Krylov solver (GMRES, BiCGS)

- Implementation based on "on the shelf" libraries: PETSc with gamg preconditioner, HYPRE with BoomerAMG preconditioner, AGMG (ULB) – only CPU platform used so far, possible extension to GPU platform foreseen.

Application to a TCV-like turbulent simulation

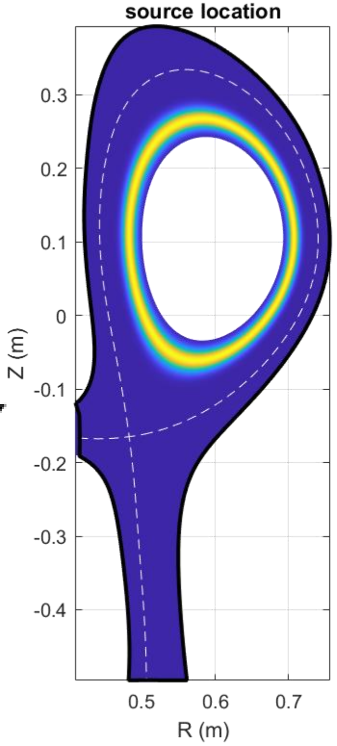
Purpose: test code ability to simulate turbulent plama in divertor geometry including neutrals

- Equilibrium based on TCV#51333 (magnetic field rescaled by ½)
- Wall geometry modified to fit a flux surface
  (to avoid potential artefacts due to a non-aligned wall
  – consequence: more closed divertor in the simulation)



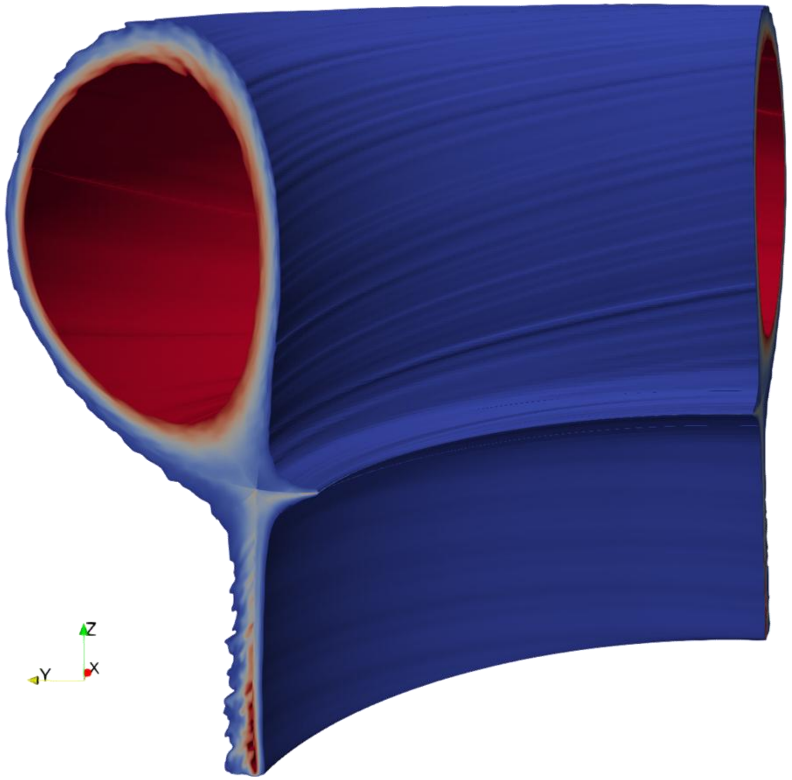
Simulation setup:

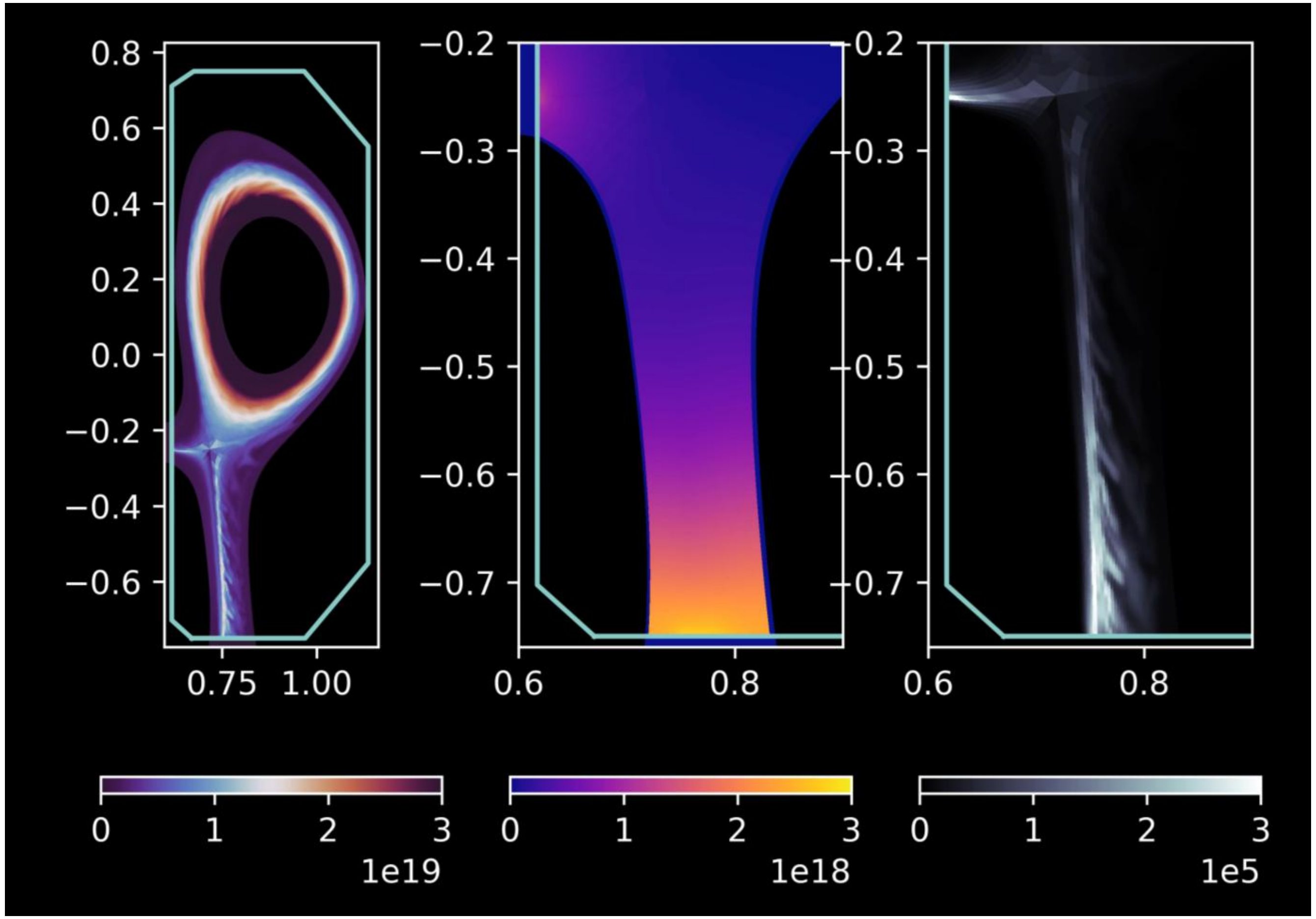
- Pure D plasma with fluid neutrals
- Anomalous diffusivities set to $10^{-2} m^2 s^{-1}$ (classical collisional level)
- Energy source at $\frac{r}{a} \approx 0.75$
  Power scanned between $50kW$ and $200kW$
- Recycling on the wall set to 80%
  Gas puff in the midplane adjusted to get $n_e \approx 10^{19} m^{-3}$ at the separatrix
- Parallel resistivity × 10 artificially



Application to a TCV-like turbulent simulation

- Turbulence in high recycling regime is observed



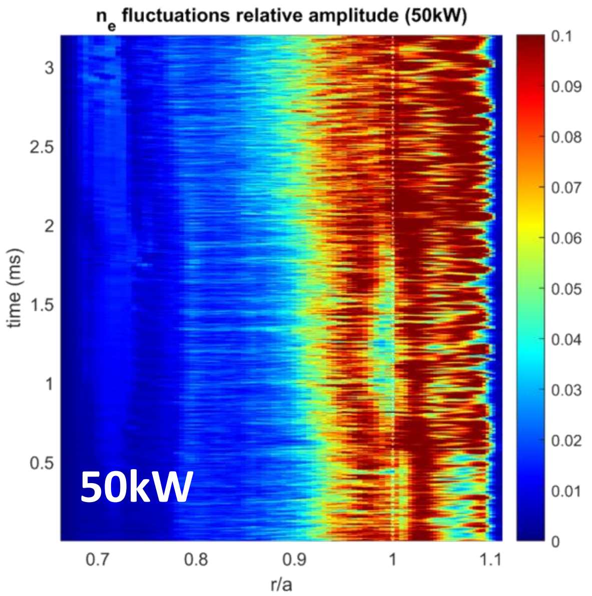


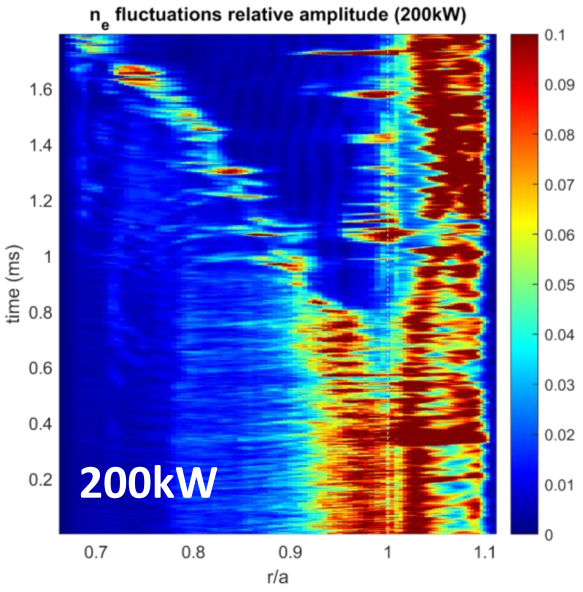
Left: Density in 3D showing filaments. Right: Poloidal map of electron density (/m3) + divertor zoom showing neutrals density (/m3) and Hydrogen radiation (W/m3).

Application to a TCV-like turbulent simulation

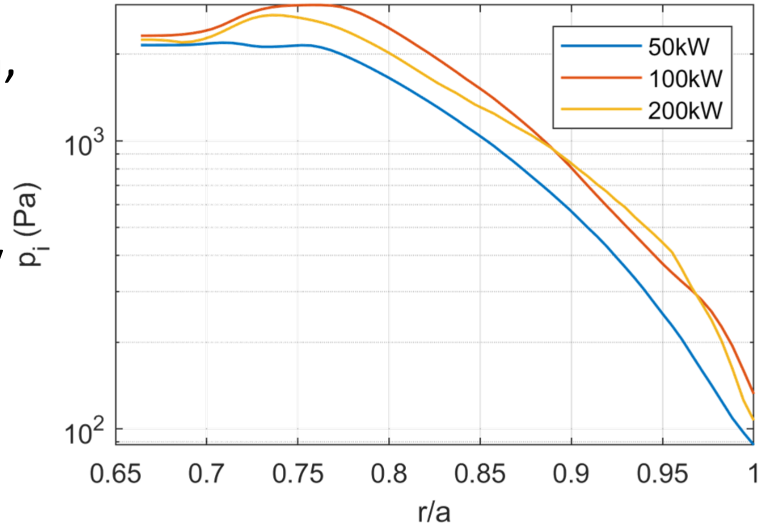
Evidence of turbulent suppression around the separatrix at high power

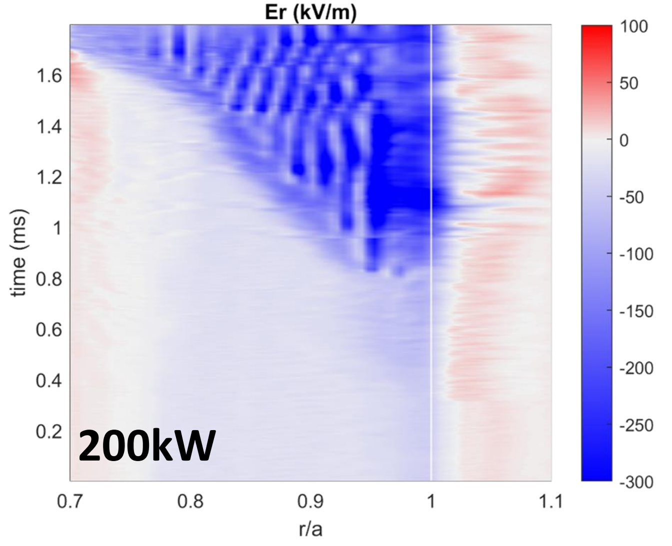
- Well developed turbulence at low power ($50kW$) Avalanches cross the separatrix
- Reduction of fluctuation level around the separatrix at higher power ($100kW$ and $200kW$)
  - The “gap” propagates from separatrix inward
  - Associated with higher $E \times B$ shear
  - Stationary zonal flows observed in the low turbulence region





- Though, 1ms after turbulence reduction, no clear steepening in pressure profile
- Er takes very high values: missing term to control plasma rotation? Ion viscosity effects [Sigmar & Helander, Zholobenko et al., PPCF 2021]





Summary

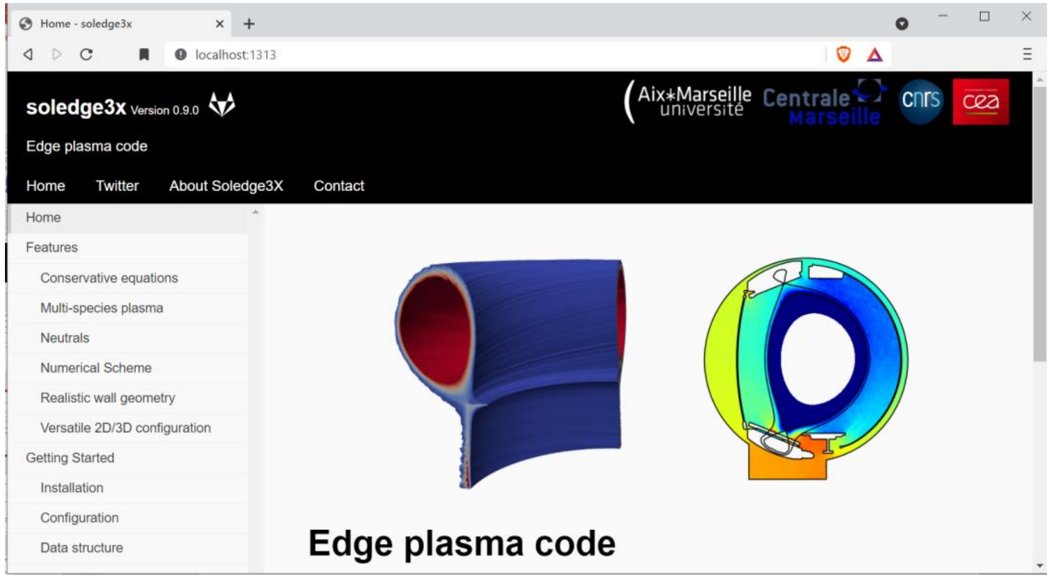
- New SOLEDGE3X code enables 2D/3D transport and 3D turbulent simulations for multispecies plasma.

- First application to power ramp on TCV like case including neutrals shows onset of turbulence reduction around separatrix at high power
  - Similar results with other codes: e.g. GBS [Giacomin et al., J. Plasma Phys., 2020]

→ though ion viscosity effects on current balance missing (ill controlled plasma rotation)

- Missing terms to be implemented and simulations to be re-launched at higher resolution (now possible thanks to better strong and weak scaling with algebraic multigrid iterative solvers)

- More information on code website www.soledge3x.com (under construction)



Drift waves

- Impact of missing polarisation drift in continuity equation
- Full model (B. Scott):

$$\omega = \omega_L = \frac{c_s}{\lambda_p} \frac{k_y \rho_s}{1 + k_\perp^2 \rho_s^2} \qquad \gamma = C \frac{\omega_L^2}{k_\parallel^2} \frac{k_\perp^2 \rho_s^2}{1 + \Gamma k_\perp^2 \rho_s^2}$$

- Without v_{pola} (linear analysis of the system n, $j_\parallel$, ϕ, $u_\parallel$)

$$\omega = \omega_L = \frac{c_s}{\lambda_p} k_y \rho_s \qquad \gamma = C \frac{\omega_L^2}{k_\parallel^2} k_\perp^2 \rho_s^2$$

- Wrong drift waves at the ρ_s scale. For scale smaller than ρ_s, drift growth over estimated. Though, sub Larmor radius scales not really look at or even resolved → filtering

The SOLEDGE3X implementation

- Status of implementation:

✓Code runs routinely in 2D transport and 3D turbulent. 3D transport simulations with non-axisymmetric wall OK.

✓ **Neutrals**: fluid model OK in 2D and 3D, EIRENE 2D transport only for now

✘ **Missing term**: polarization velocity not included in particle, parallel momentum and energy transport

✘ **Missing term**: Drift and current associated to stress tensor divergence (ion viscosity)