Numerical modeling of core-edge turbulent transport in realistic tokamak geometry by an advanced numerical tool

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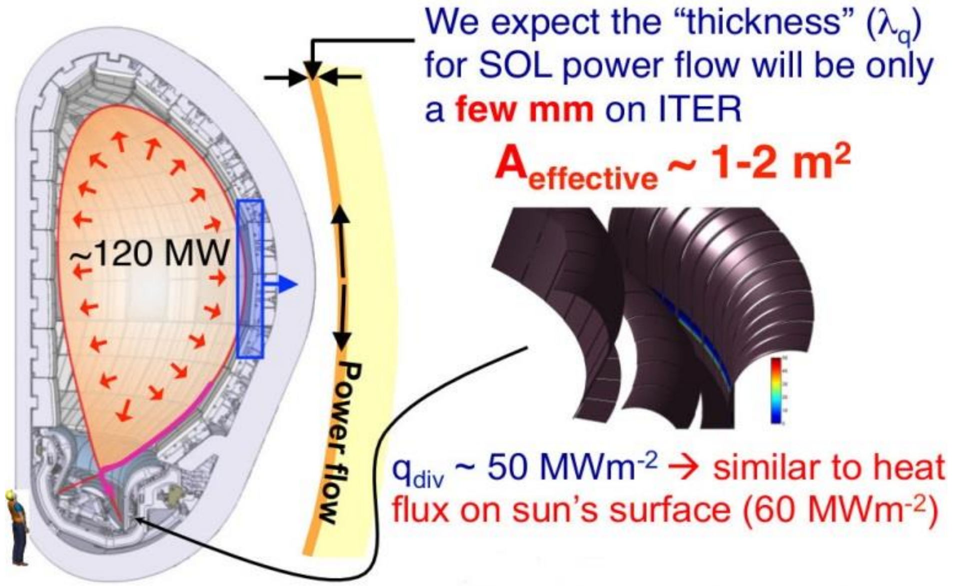
Introduction

- **Energy from fusion in magnetically confined devices**
  - → The heat and particle exhaust issues in ITER
  - → Investigation and prediction of the perpendicular turbulent transport
- **Numerical modeling:**
  - → Support and interpretation of experimental measures
  - → Become predictive
- **Challenges in the plasma numerical modeling:**
  - → Complex magnetic (X-point, close-open field lines) and wall geometries
  - → Multiphysics and multiscale problem: from fluid turbulence to atomic physics
  - → Strong anisotropy
- **Different level of analysis:**
  - → Model Hierarchy



Courtesy of **A. Loarte**

6D/5D kinetic/Gyrokinetic model: **~O(10⁹) DoF**

$$\partial_t f + v.\nabla x f + F/m.\nabla v f = C$$ **[Chang. Et al. PRL 2017]**

$$\partial_t < f >_{cyclo} + ...$$

2D/3D Fluid model: **~O(10⁵ -10⁷) DoF**

Moment distribution function + closure

Integrated: 1D model

richness of information ↑

computational cost ↓

Current 2D/3D fluid approach: flux-aligned scheme

- Drift-reduced fluid model: $\lambda_c \gg \rho_L,\ \omega \ll \Omega_{c,i}$

- Current state-of-the-art averaged fluid codes based on flux aligned discretization, SE3X **[H. Bufferand, NF, 2015]**, SOLPS-ITER **[S. Wiesen et al., JNM, 2015]**

Benefits

→ More efficient numerically in term of DoF and implementation

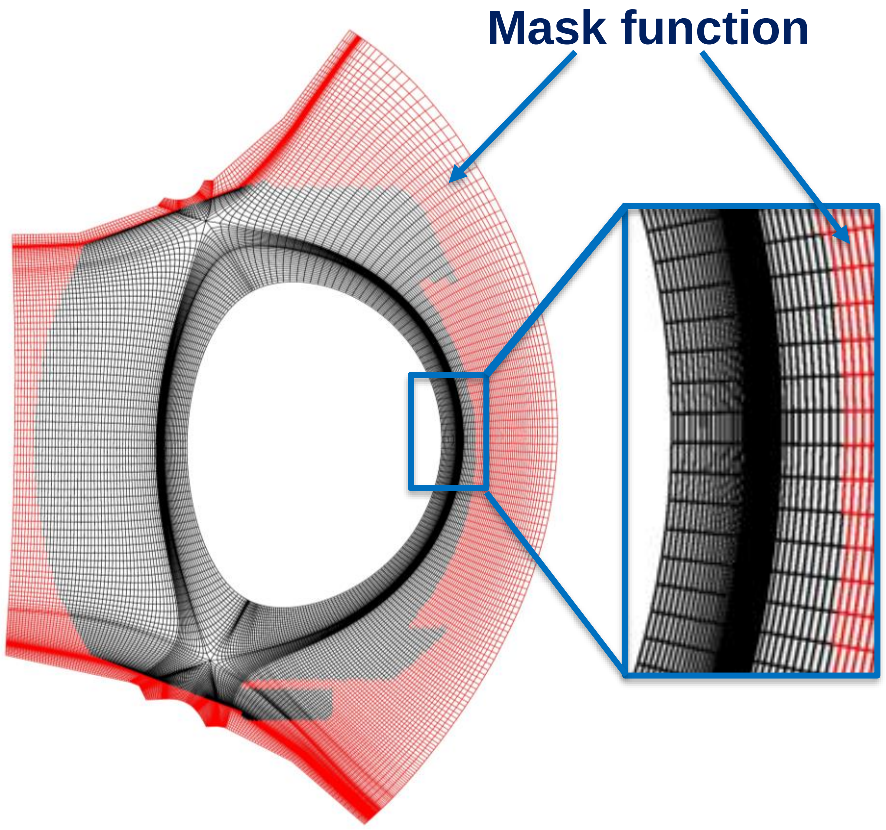
→ Alignment to reduce numerical diffusion induced by anisotropy

Disadvantages

→ Inaccurate description of complex tokamak geometry

→ Difficulty to handle singularity in the magnetic field: X point, core center

→ Static magnetic equilibrium



Flux Aligned Mesh of SE3X

An original approach

- Development of an high-order finite elements method (Hybrid Discontinuous Galerkin HDG) + implicit time integration **[Giorgiani *et al*. J. Comp. Phys. 2018]** in the SOLEDGE3X suite of codes

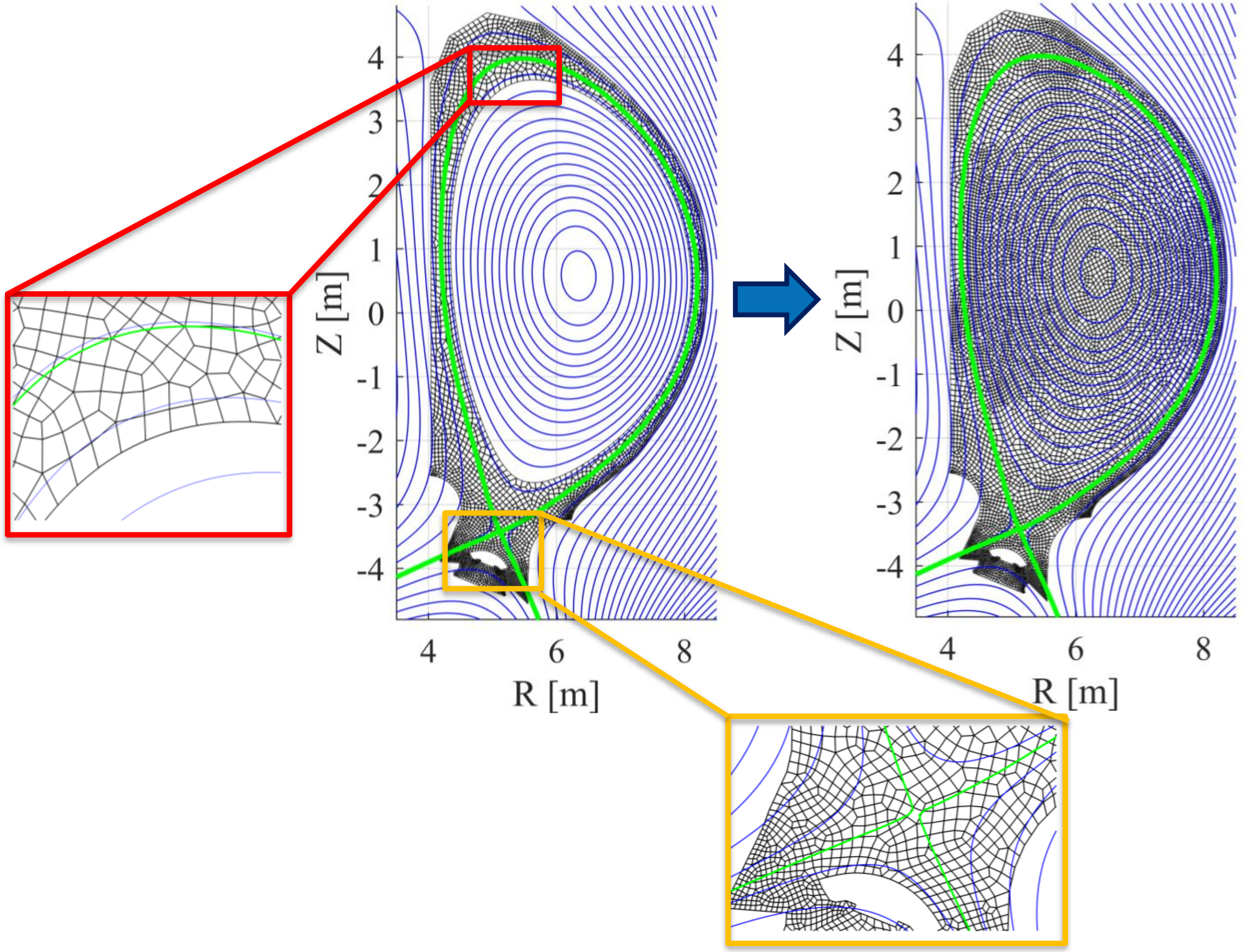
→ MPI-OMP SOLEDGE3X-HDG
[Giorgiani *et al*. Comp. Phys. Com. 2020]

→ Non-aligned discretization: unstructured meshes
- Accurate description of PFCs
- Full tokamak cross section
- Magnetic equilibrium free

→ High-order
- Reduced DoF

→ Full implicit time
- Long time integration for full experimental discharges

ITER



Outlines

- **Mathematical and numerical model**
- Verification and validation
- Core-edge coupling and sources
- Preliminary investigation of a detached plasma
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- Steady vs transient

The mathematical model

- Braginskii 2D fluid reduced model **[Braginskii 1965]**

$$
\begin{cases}
\partial_t n + \nabla\cdot(nu\mathbf{b}) - \nabla\cdot(D\nabla_\perp n) = S_n \\
\partial_t(m_i nu) + \nabla\cdot(m_i nu^2\mathbf{b}) + \nabla_\parallel(k_b n(T_e + Ti)) - \nabla\cdot(\mu\nabla_\perp(m_i nu)) = S_\Gamma \\
\partial_t\left(\frac{3}{2}k_b nT_i + \frac{1}{2}m_i nu^2\right) + \nabla\cdot\left(\left(\frac{5}{2}k_b nT_i + \frac{1}{2}m_i nu^2\right)u\mathbf{b}\right) - nueE_\parallel - \nabla\cdot\left(\frac{3}{2}k_b(T_i D\nabla_\perp n + n\chi_i\nabla_\perp T_i)\right) \\
-\nabla\cdot\left(-\frac{1}{2}m_i u^2 D\nabla_\perp n + \frac{1}{2}m_i\mu n\nabla_\perp u^2\right) - \nabla\cdot(k_{\parallel i}T_i^{\frac{5}{2}}\nabla_\parallel T_i\mathbf{b}) + \frac{3}{2}\frac{k_b n}{\tau_{ie}}(T_e - T_i) = S_{E_i} \\
\partial_t\left(\frac{3}{2}k_b nT_e\right) + \nabla\cdot\left(\frac{5}{2}k_b nT_e u\mathbf{b}\right) + nueE_\parallel - \nabla\cdot\left(\frac{3}{2}k_b(T_e D\nabla_\perp n + n\chi_e\nabla_\perp T_e)\right) - \nabla\cdot(k_{\parallel e}T_e^{\frac{5}{2}}\nabla_\parallel T_e\mathbf{b}) \\
-\frac{3}{2}\frac{k_b n}{\tau_{ie}}(T_e - T_i) = S_{E_e}
\end{cases} \tag{1}
$$

where $\boldsymbol{\nabla}_\parallel = \boldsymbol{b}\cdot\boldsymbol{\nabla}$, $\boldsymbol{\nabla}_\perp = \boldsymbol{\nabla} - \boldsymbol{b}\boldsymbol{\nabla}_\parallel$, and $\boldsymbol{b} = \frac{\mathbf{B}}{\|\mathbf{B}\|}$. D, μ, χ_i χ_e perpendicular diffusion coefficients and $k_{\parallel i}$, $k_{\parallel e}$ parallel heat fluxes diffusion coefficient;

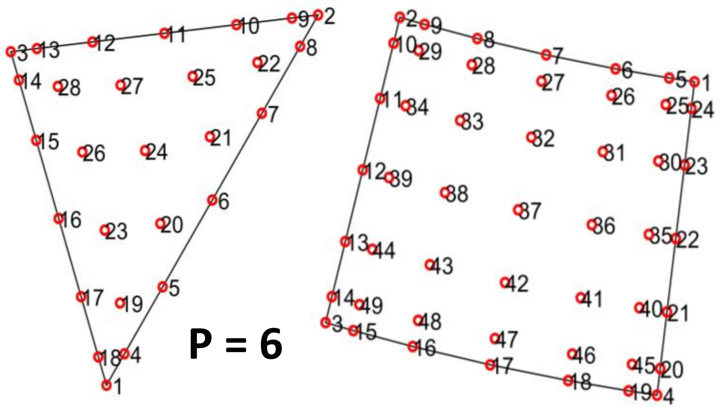
- Plasma-wall interactions prescribed by the Bohm boundary condition:

→ Outgoing supersonic velocity
→ Parallel heat fluxes imposed to the sheat transmission values

$$
\begin{aligned}
u &\geq c_s \qquad if \quad \mathbf{b}\cdot\mathbf{n} > 0 \\
u &\leq -c_s \quad if \quad \mathbf{b}\cdot\mathbf{n} < 0
\end{aligned}
$$

The HDG method

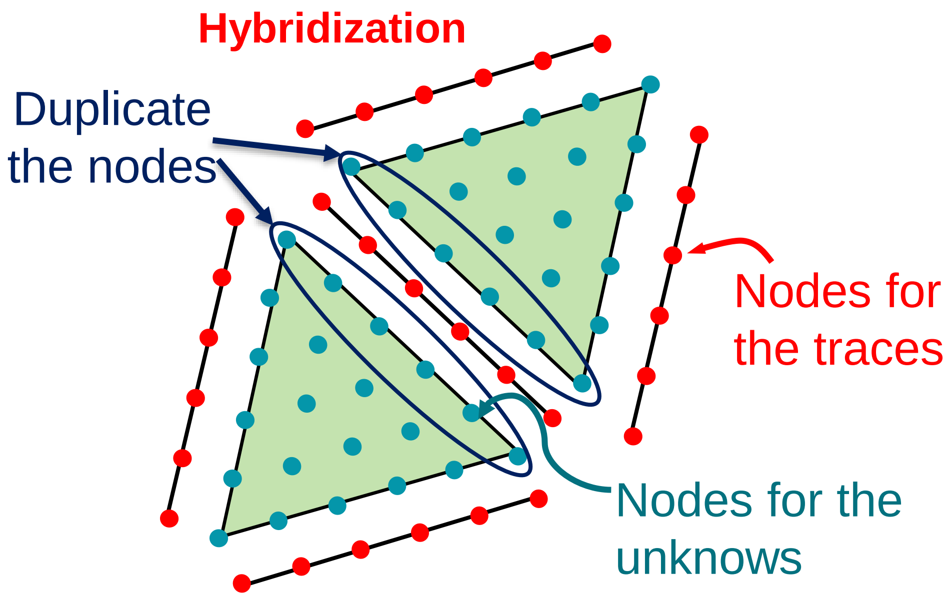
HDG:HIGH ORDER finite element method based on **HYBRID DISCONTINUOUS** Galerkin **[G.Giorgiani,J.C.Physics,2018]**



- **High Order:** the solution is approximated by an high-order polynomial in each element

- **Discontinuous:**
  - Resolution of local problem posed in weak form;
  - Duplication of the nodes at the element borders;
  - Global problem derived by weakly imposing the continuity of numerical fluxes across the borders;

- **Hybrid:** introduction of new unknowns, called trace solutions, defined on the element border. Reduction of DOF.



The HDG formulation: local probelm

- Local problem in each element for the conservative variables $\boldsymbol{U}$, $\mathbf{Q} = \nabla \mathbf{U}$

$$\boldsymbol{U} = \begin{Bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{Bmatrix}, = \begin{Bmatrix} n \\ nu \\ nE_i \\ nE_e \end{Bmatrix} \qquad \mathbf{Q} = \nabla \mathbf{U} = \begin{bmatrix} \nabla \mathbf{U_1}^T \\ \nabla \mathbf{U_2}^T \\ \nabla \mathbf{U_3}^T \\ \nabla \mathbf{U_4}^T \end{bmatrix} = \begin{bmatrix} U_{1,x} & U_{1,y} \\ U_{2,x} & U_{2,y} \\ U_{3,x} & U_{3,y} \\ U_{4,x} & U_{4,y} \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \\ Q_{31} & Q_{32} \\ Q_{41} & Q_{42} \end{bmatrix}$$

$$\begin{cases} \boldsymbol{Q} - \boldsymbol{\nabla U} = 0 & \text{in } \Omega_i \times]0, T_f[\\ \partial_t \boldsymbol{U} + \boldsymbol{\nabla} \cdot (\boldsymbol{F} - D_f \boldsymbol{Q} + D_f \boldsymbol{Qb} \otimes \boldsymbol{b} - \boldsymbol{F}_t) + \\ \qquad \boldsymbol{f}_{E_{||}} + \boldsymbol{f}_{EX} - \boldsymbol{g} = \boldsymbol{s} & \text{in } \Omega_i \times]0, T_f[\\ \mathbf{U}(\mathbf{x}, t) = \hat{\mathbf{U}}(\mathbf{x}, t) & \text{in } \partial\Omega_i \times]0, T_f[\\ \mathbf{U}(\mathbf{x}, 0) = \mathbf{U_0} & \text{in } \Omega_i \end{cases} \qquad (2)$$

convection+diffusion (isotropic part) — $\boldsymbol{F} - D_f \boldsymbol{Q}$

diffusion (anisotropic part) — $D_f \boldsymbol{Qb} \otimes \boldsymbol{b}$

Parallel Diffusion — $\boldsymbol{F}_t$

→ a elemental solution for the vector $\boldsymbol{U}$, $\mathbf{Q}$ is recovered in each element in function of the trace unknown $\hat{\boldsymbol{U}}$

The HDG formulation: global problem

- $\hat{\boldsymbol{U}}$ is the actual unknown of the problem determined by setting up the following global problem:

$$\left\langle \hat{\boldsymbol{v}}, \left(\boldsymbol{F} - D_f \boldsymbol{Q} + D_f \boldsymbol{Q} \boldsymbol{b} \otimes \boldsymbol{b} - \boldsymbol{F}_t\right) \boldsymbol{n} + \boldsymbol{\tau} \left(\boldsymbol{U} - \hat{\boldsymbol{U}}\right) \right\rangle_{\mathcal{T} \setminus \partial\Omega} + \left\langle \hat{\boldsymbol{v}}, \boldsymbol{B}_{BC} \right\rangle_{\partial\Omega} = 0 \qquad (4)$$

→ $\mathcal{T} = \bigcup_{i=1}^{N_{el}} \partial\Omega_i$ mesh skeleton

→ $\boldsymbol{B}_{BC}$ is a flux vector which defines the boundary condition on $\partial\Omega$

- $\boldsymbol{U}$ and $\boldsymbol{Q}$ solution of the local problem Eqs. (3) in function of $\hat{\boldsymbol{U}}$

- **Hybridization**

→ Eq. (4) wakly imposes the normal fluxes at the element boundary and it depends only by the unknown $\hat{\boldsymbol{U}}$

→ reduce the size of the linear system generated by the element discretization

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Verification of the code

- **MMS :** code verification in realistic tokamak geometry → entire 2D cross section
  - → scan in the order of the polynomial of interpolation $p = 1, \ldots, 4$
  - → scan in the characteristic length h of each element $h = 1/2^m \; for \; m = 1, \ldots, 5$
- Analytical solution $\mathbf{U_a}$ considered for all the variables

$$n = 2 + sin(2\pi x) sin(2\pi y) \qquad u = cos(2\pi x) cos(2\pi y)$$

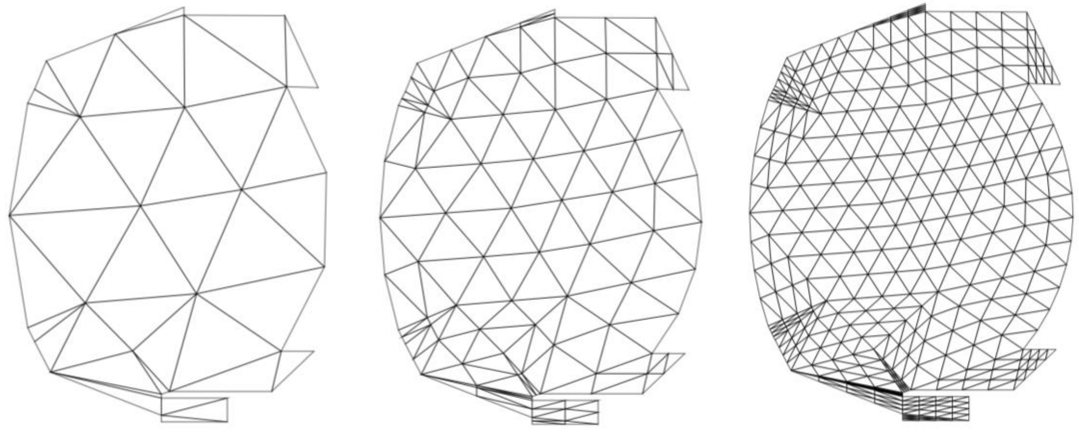
$$E_i = 20 + cos(2\pi x) sin(2\pi y) \qquad E_e = 10 - sin(2\pi x) cos(2\pi y)$$

- Cartesian magnetic field + Dirchlet BC

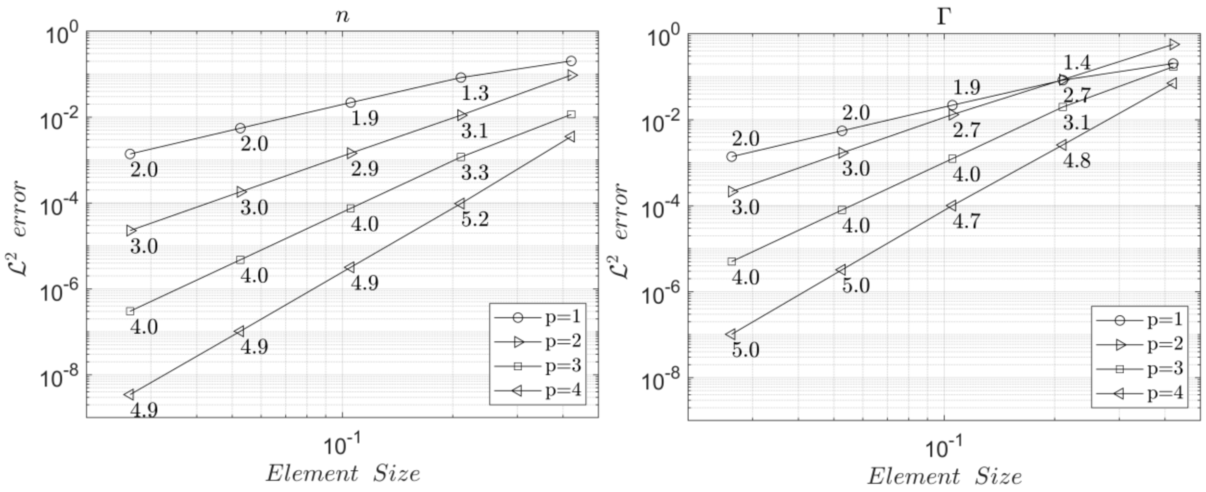
$$b_x = \frac{1}{30}(x - y^2 + 2) \qquad b_y = \frac{1}{30}(xy + y)$$

- $\mathcal{L}^2$error defined as the distance between the numerical solution $\boldsymbol{U}$ and the exact solution of the modified problem $\mathbf{U_a}$

$$\mathcal{L}^2 = \sqrt{\int_\Omega (\mathbf{U} - \mathbf{U_a})^2}$$



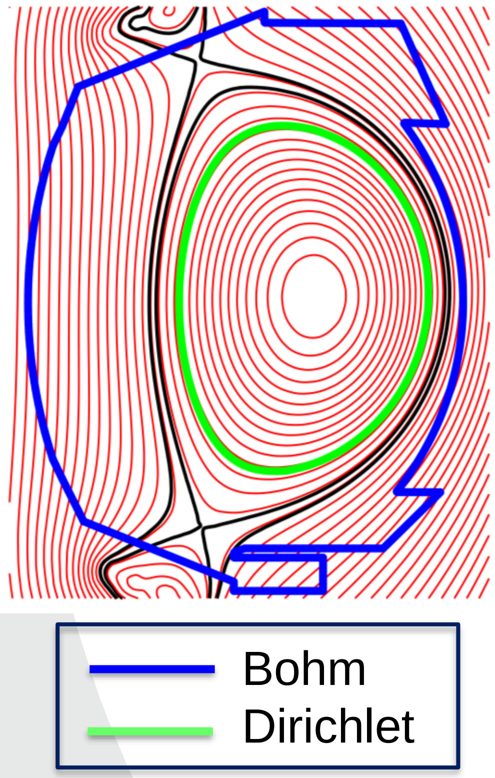
$h = 4 \times 10^{-2}$ $\qquad$ $h = 2 \times 10^{-2}$ $\qquad$ $h = 1 \times 10^{-2}$



→ recovered the expected theoretical rate of convergence p+1

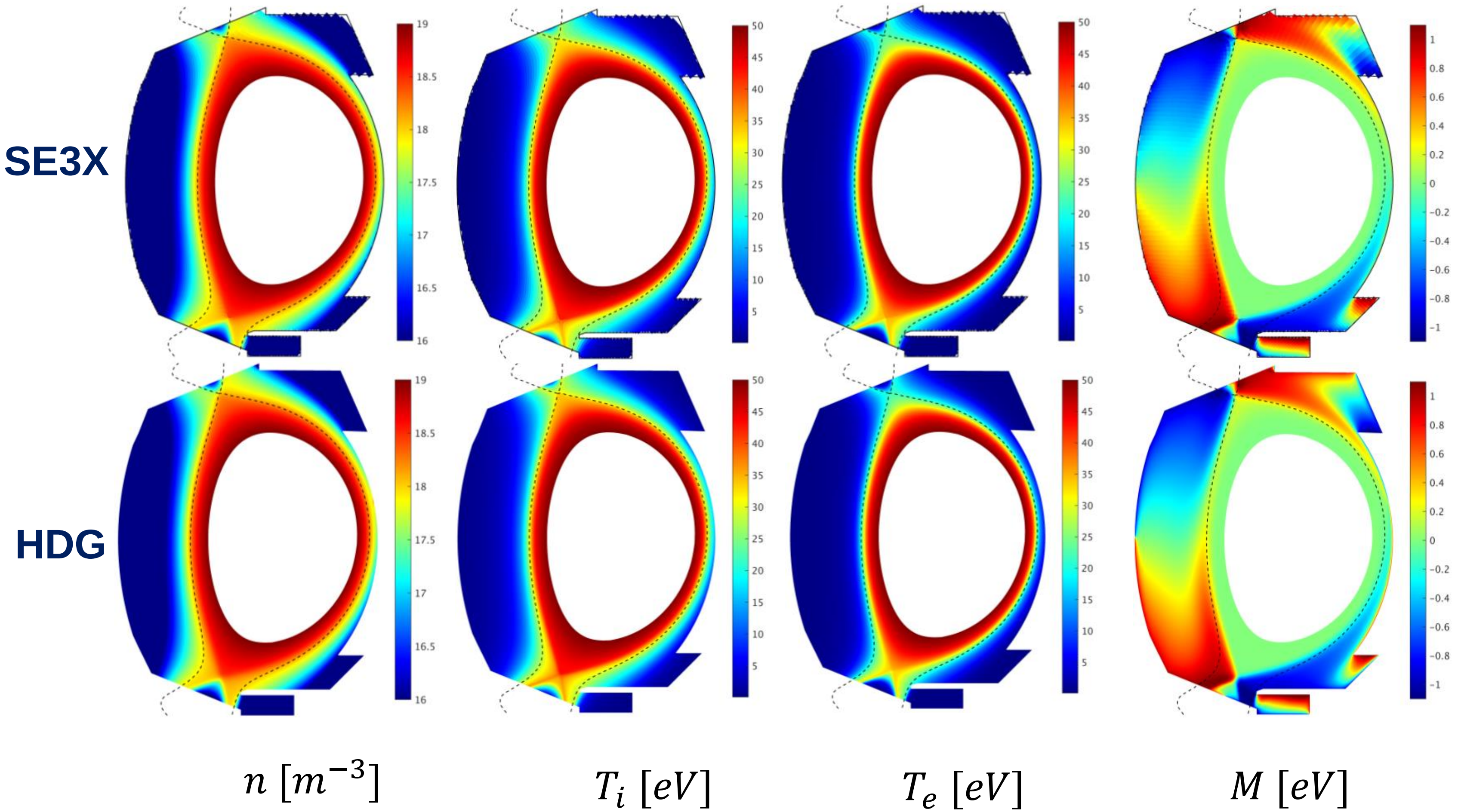
Benchmarking with SE3X (1/2)

- Comparison with the well established code SE3X in WEST geometry **[H. Bufferand, NF, 2015]**

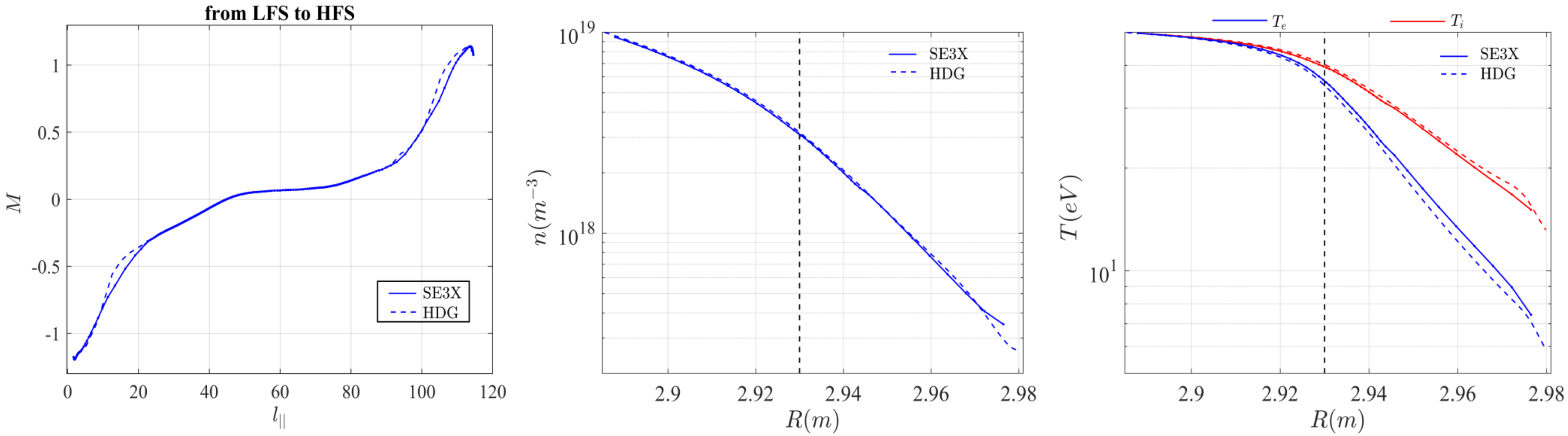


- $n_{Dir} = 1e19\ [m^{-3}]$
- $u_{Dir} = 0\ [m/s]$
- $T_{i,Dir} = T_{e,Dir} = 50\ [eV]$

$$D = \mu = \chi_i = \chi_e = 1\frac{m^2}{s}$$



Benchmarking with SE3X(2/2)



- Good agreement in between SE3X and SE3X-HDG profiles

- Small discrepancy in the far SOL especially in ion and electron mid-plane profiles

  → geometry discretization
  → different numerical method: Finite Volume for SE-3X vs Finite Element for SE-HDG
  → time of computation: 40 m SE3X-HDG, 12-14h SE3X

The benchmark test is satisfying making us confident on the non-aligned approach **!!**

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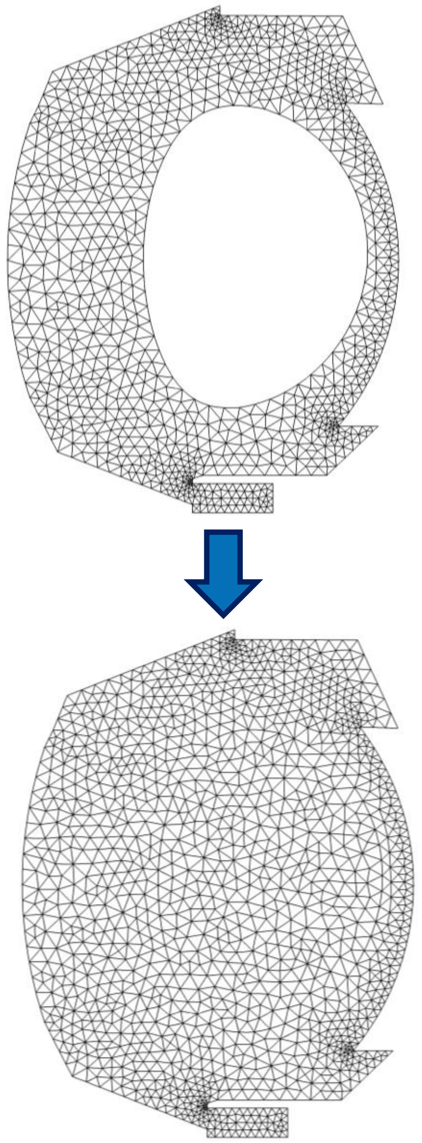
Core-edge coupling and sources

- Enrich core physics allowing to study
  - → Plasma heating
  - → Energy redistribution
  - → Transport of impurity
  - → Full experimental discharge simulation with variable magnetic equilibrium

- Source location is a critical point in plasma simulation **[D. Galassi, PoP, 2022]**
  - → Remove and replace the badly posed Dirichlet/ Neumann BC
  - → Extension of the domain of computation up to the core
  - → Investigation of the entire tokamak cross-section

- Need sources to get a stationary state in the whole domain
  - → Development of self-consistent sources of particle and energy
    - **Source of particle:** Neutral Model
    - **Source of energy:** Ohmic Heating



Neutral model

- Crucial role due to strong interaction with plasma
- Kinetic approach + Monte-Carlo solver: **EIRENE** **[D. Reiter et al., FSaT, 2005]**
  - → Rich and accurate in term of physics
  - → Slow convergence in high collisional regime
- Diffusive fluid neutral + plasma recycling at wall (charge exchange dominated regimes) **[Horsten et al., NF, 2017]**

$$\partial_t n_n - \nabla \cdot (D_{n_n} \nabla n_n) = S_{n_n,iz} + S_{n_n,rec} + S_{n_n}$$

$$- D_{n_n} \nabla n_n \cdot \mathbf{n} = -R\big(- D_{n_n} \nabla n \cdot \mathbf{n} + nu\mathbf{b} \cdot \mathbf{n}\big)$$

  → coupled to plasma with ionization-recombination-radiation terms $S_{n,iz}$, $S_{n,rec}$, $S_{\Gamma,cx}$, $S_{\Gamma,rec}$, $S_{E_i,iz}$, $S_{E_i,cx}$, $S_{E_i,rec}$, $S_{E_e,iz}$, $S_{E_e,rec}$: linear system for 5 Eqs. (4 for plasma + 1 for neutrals)

- **Source of particle** to fill up the core region
  - → Easly implementable in the HDG framework
  - → Allows to compute fast steady state solution (2h-6h in WEST geometry)
  - → More realistic description of plasma behaviour close to the target

Ohmic source

- Ohmic source of power given by

$$S_{Ohmic} = \eta j^2 = 0.51 \frac{m_e^{1/2} e^2 ln\Lambda}{3(2\pi)^{3/2}\epsilon_0^2}\frac{1}{T_e^{3/2}} j^2$$

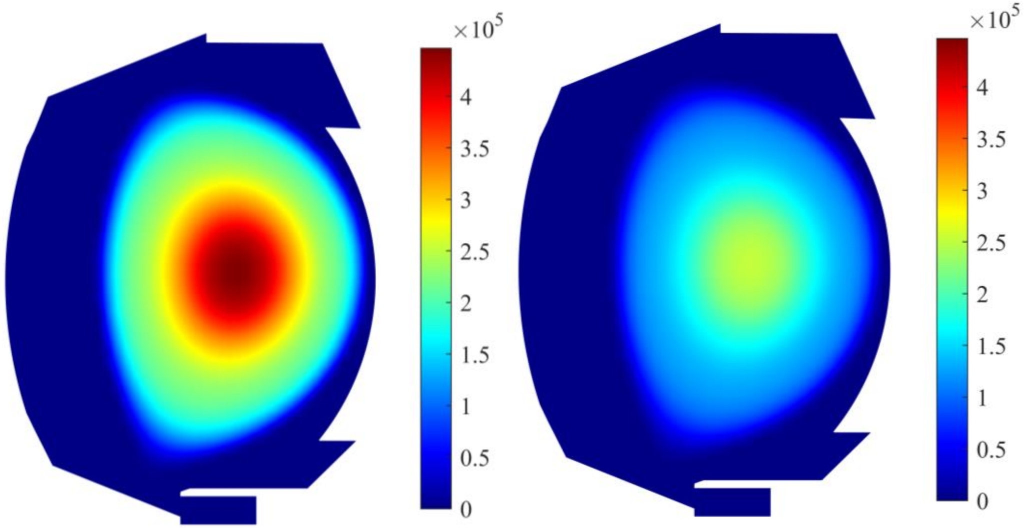
Spitzer Harm resistivity

→ Current density 2D distribution from equilibrium experimental reconstruction

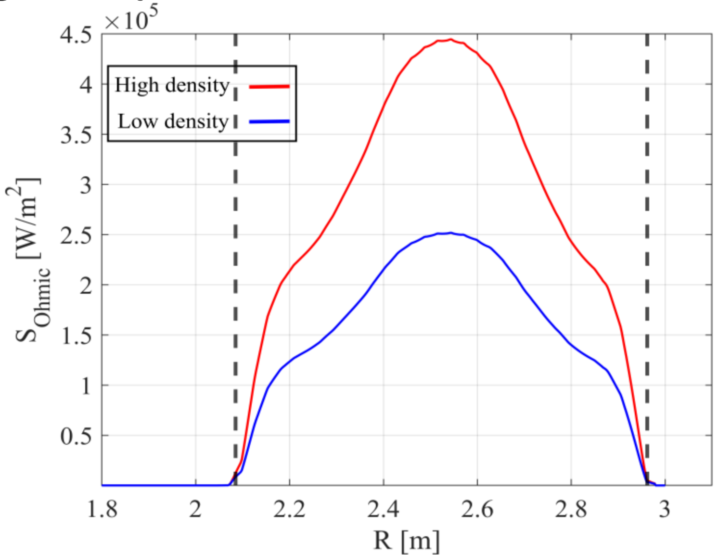
→ Non linear coupling with plasma temperature

- Easily implementable for other sources:
  → RF, ICRH, ECRH, LH …

S_{Ohmic} [W/m^3] Shot #54487 t = 4.5 [s]



High density **Low density**



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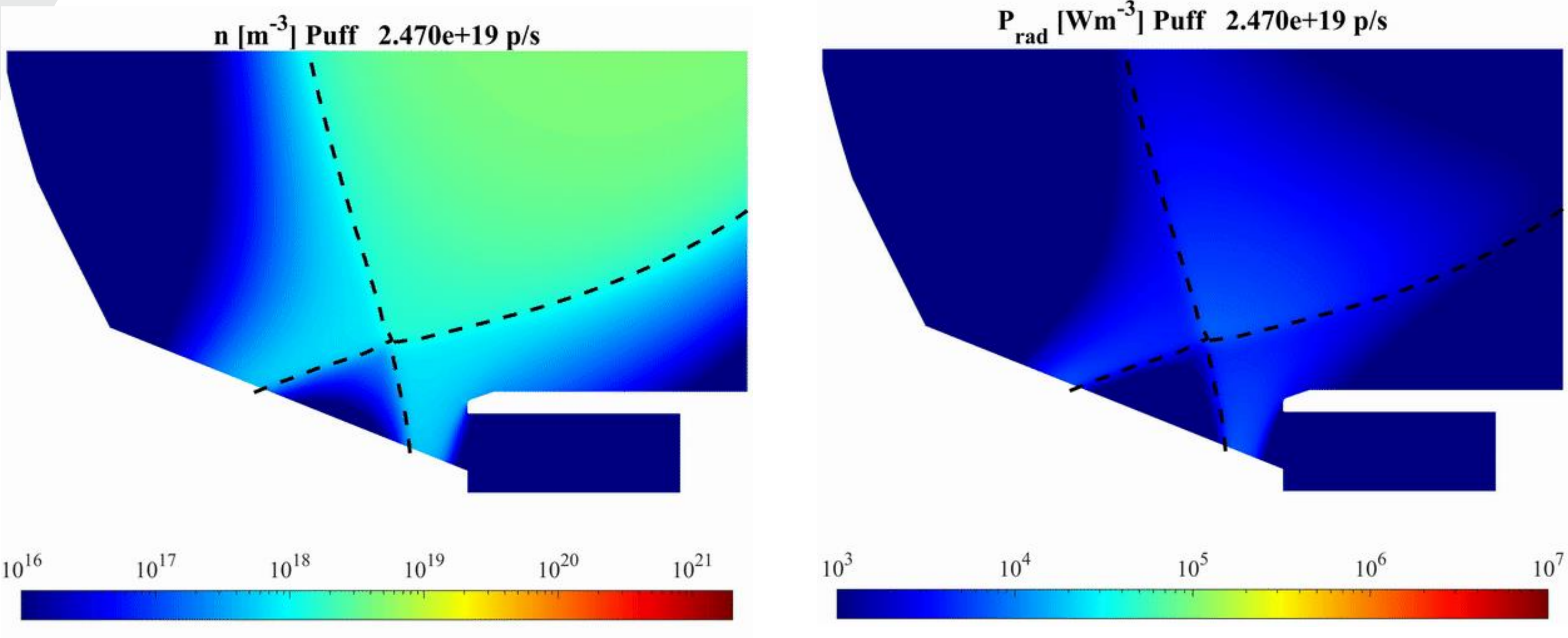
Density scan toward plasma detachment

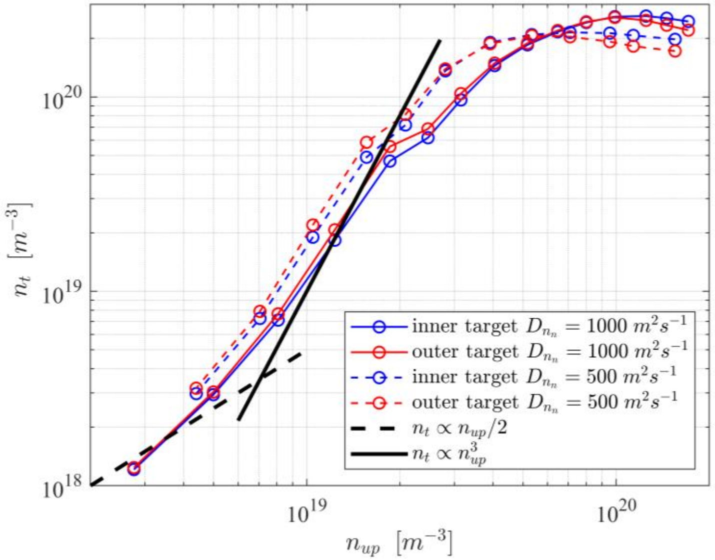


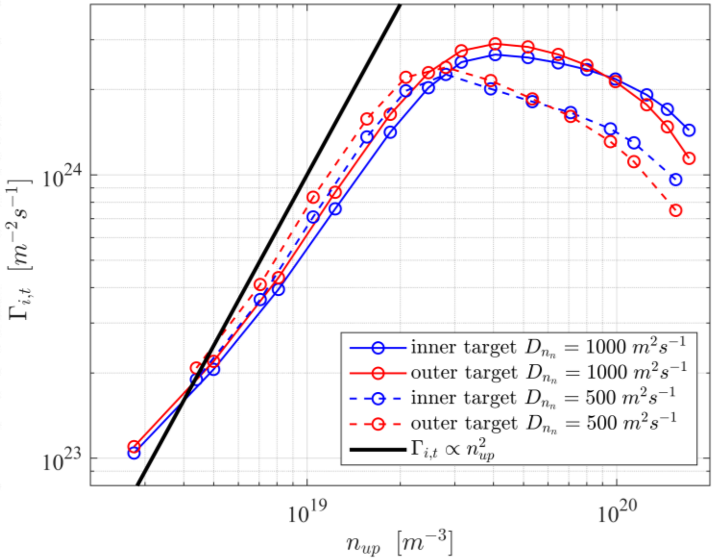
- Analysis of plasma detachment achievement
  → Double single null magnetic configuration as in benchmark test with SE3X
  → $D = \mu = \chi_i = \chi_e = 1\ m^2/s$
  → Ohmic source of power in the core
  → Neutral model + plasma recycling with R = 0.99
  → Prescribed puff with $D_{n_n} = 1000\ m^2/s.$

Analysis with the 2 point model (2PM)

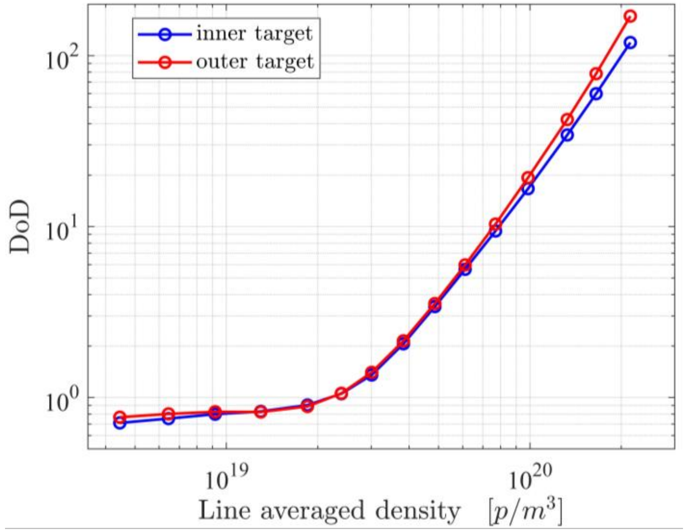
- Clear evidences of plasma detachement
  - → Comparison with 2PM predicted slopes for $n_t, \Gamma_t, T_{e,t}$ in function of n_{up} indicates a transition from sheath limited to high recycling regime
  - → Saturation and decrease of n_t
  - → Rollover of the flux of particle at the target contrary to 2PM which prescribes

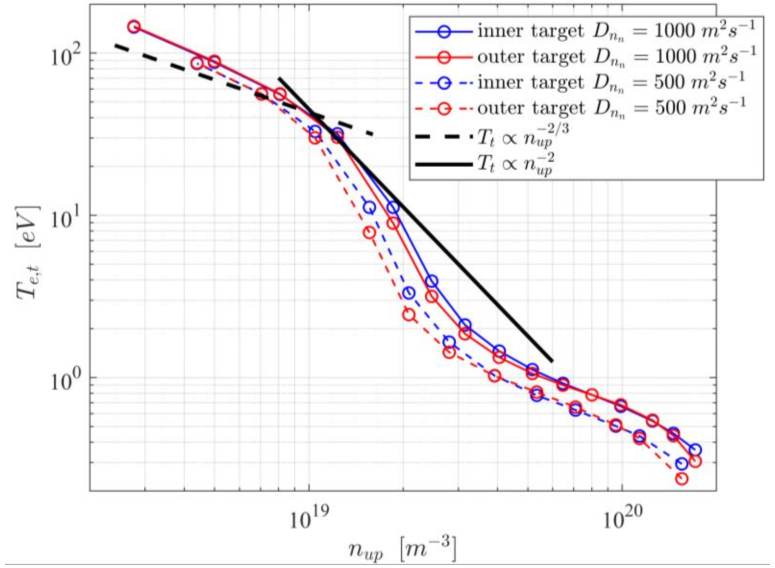
$$\Gamma_t = n_t c_s = \left(\frac{7\gamma L_c}{8k_0 m_i}\right)^2 \frac{n_{up}^2}{T_{up}^{3/2}}$$





- → DoD ≥ 2 **[A. Loarte, et al., NF, 1998]**





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Full WEST disharge: shot #54487

- 2D transport simulation of an entire experimental discharge

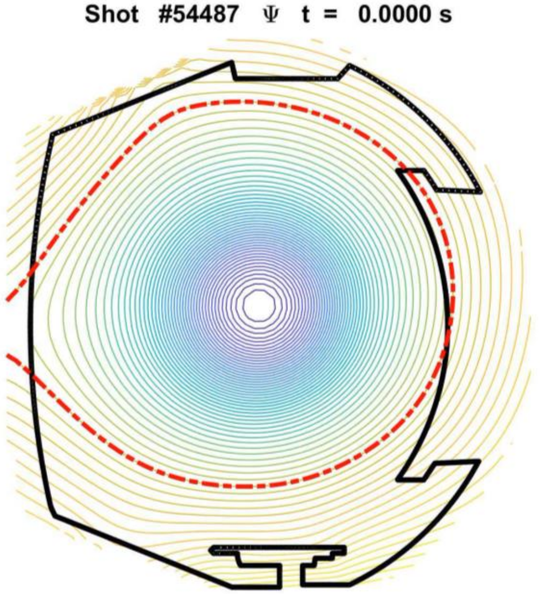
  → impact of the transient phase: limiter-divertor(L-D)
  → comparison with experimental data
  → analysis of fluxes at the PFCs
  → impurity contamination (W)

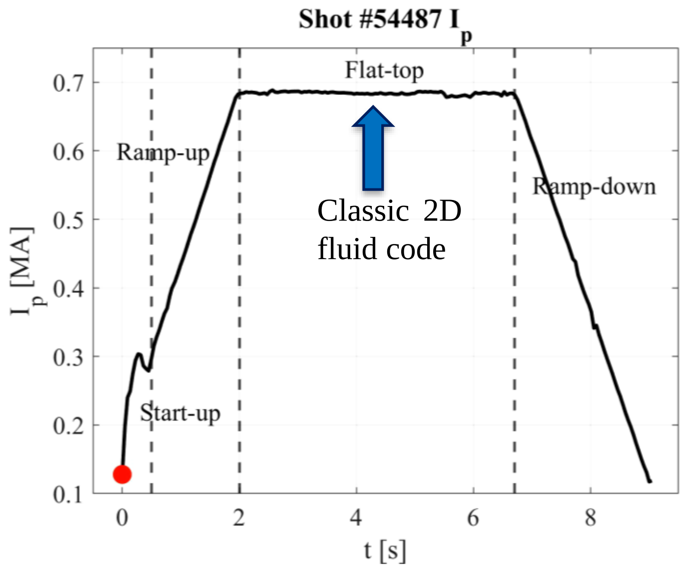
- Magnetic equilibrium and current 2D distribution from experimental reconstructuion

  → WEST shot #54487 (pure Ohmic discharge)

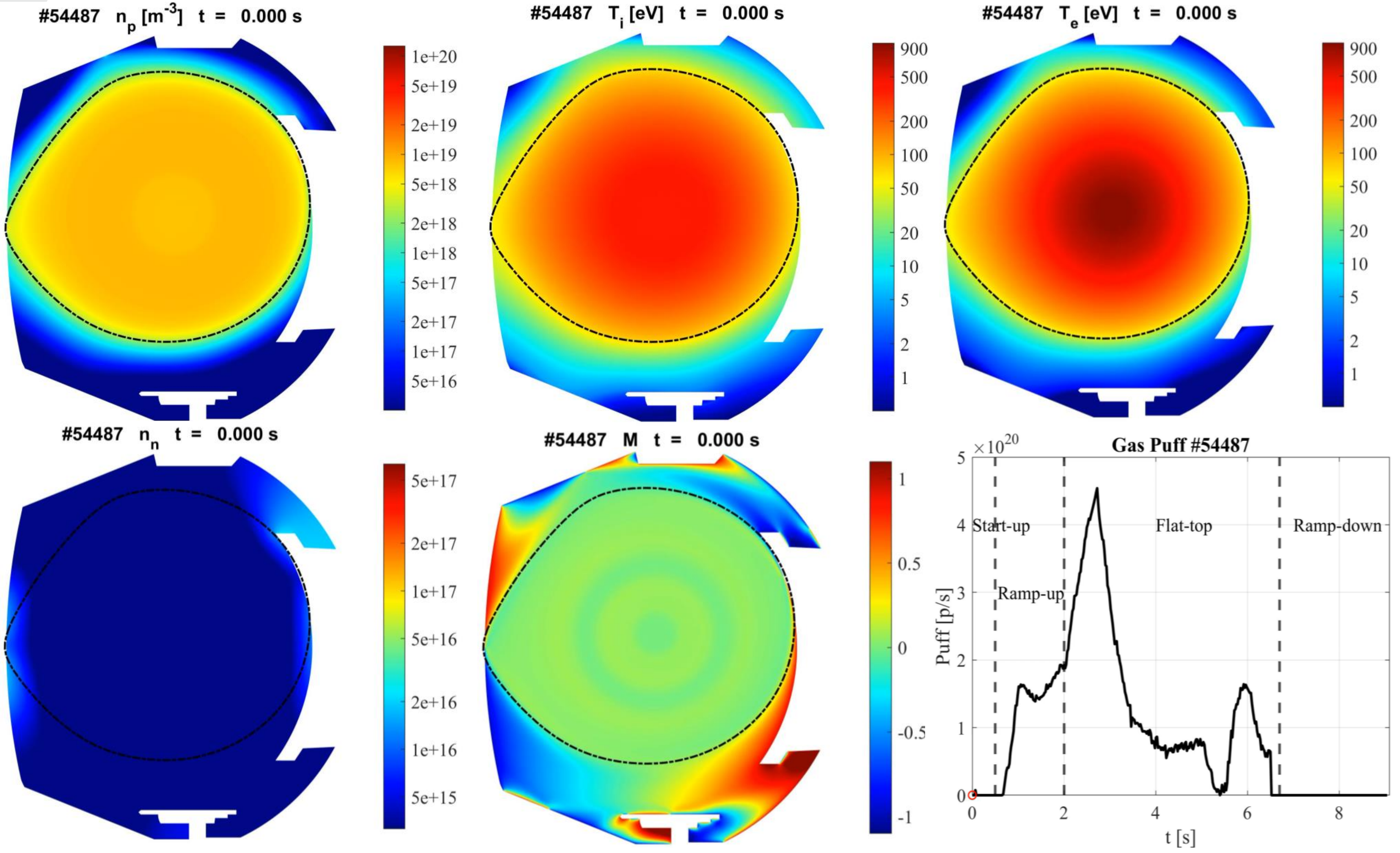
- Numerical and physical parameters

  → $D = \mu = \chi_i = \chi_e = 0.5\ m^2/s \quad D_{n_n} = 2000\ m^2/s$
  → dt = 0.02 s
  → R = 0.998 + experimental puff rate
  → 403 different equilibriums for a total time of integration of 10 s
  → Real time of computation: 240 h, 1 node 32 cpus, OMP

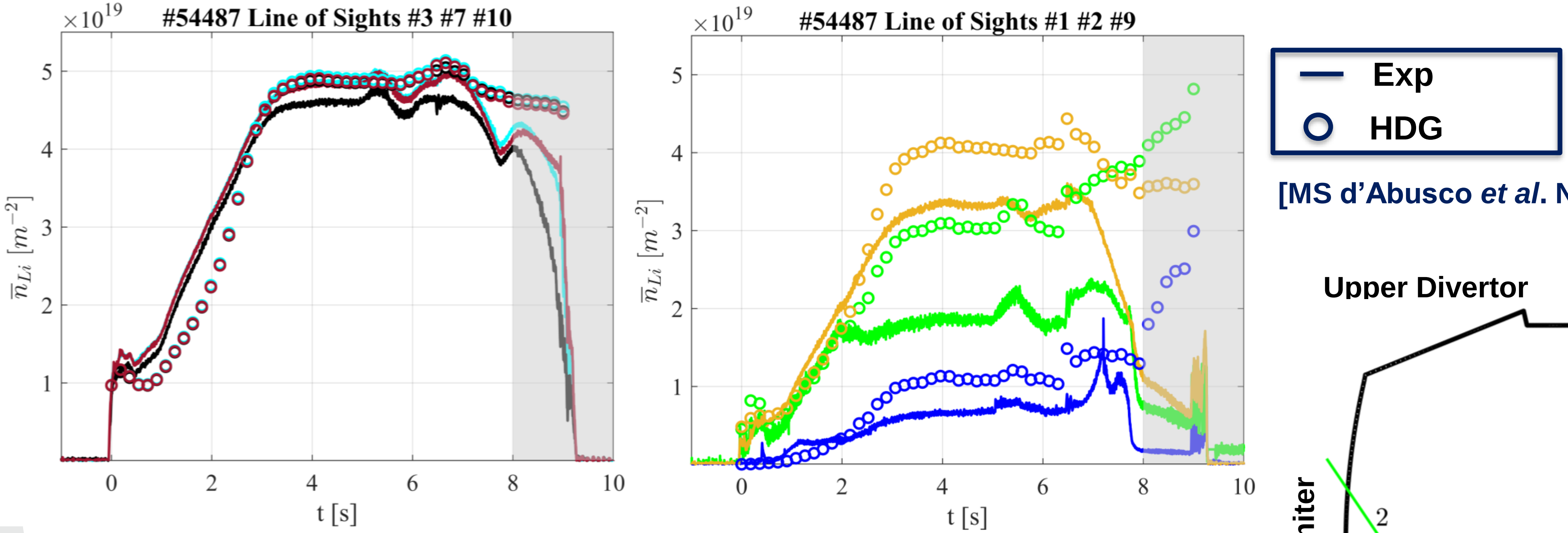




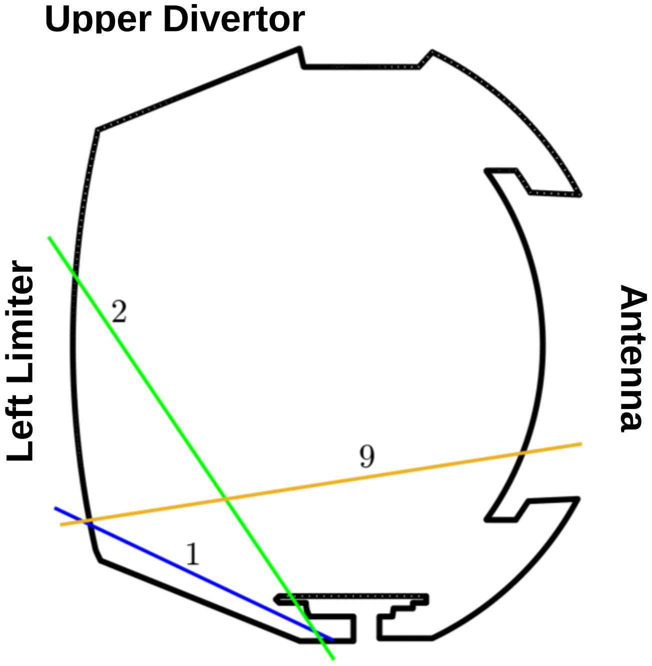
WEST Shot #54487: 2D map of the fluid quantities



WEST Shot #54487: comparison with experiments



[MS d'Abusco *et al*. N. Fus. 2022]

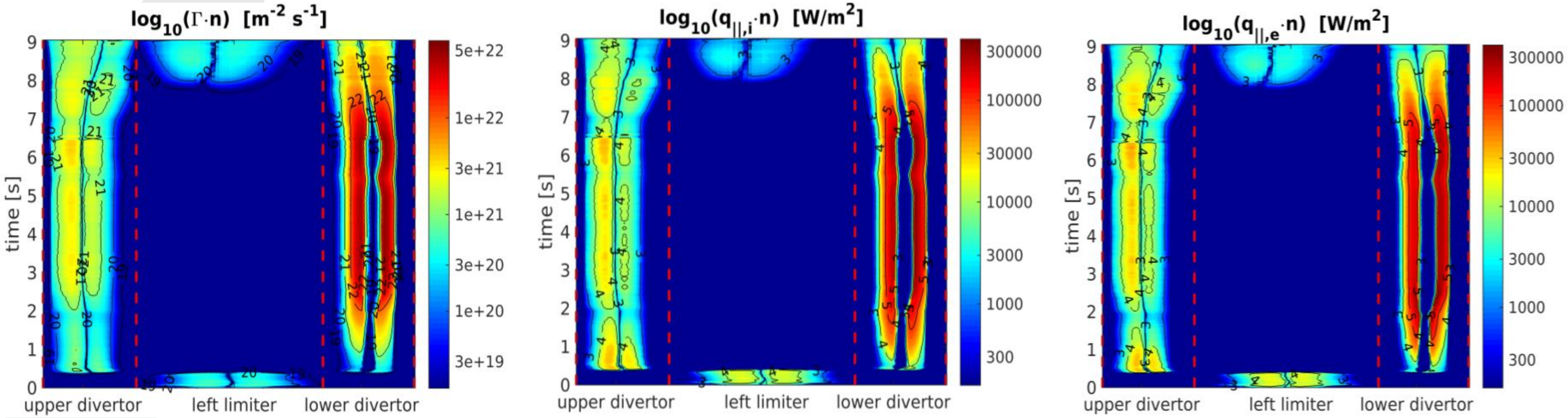


- **Interferometry data analysis:**

  → Qualitatively agreement with experimental data (ram-up, flat-top)
  → Good reproductuon of central line integrated density (LoS 3,7,10)
  → Imperfect agrrement with line integrated density close to X-point (LoS 1, 2, 9)
  → Inability to reproduce the last second of the discharge (8-9 s MHD events, instabilities ecc …)

WEST Shot #54487: quantities at PFCs vs Time (1/2)

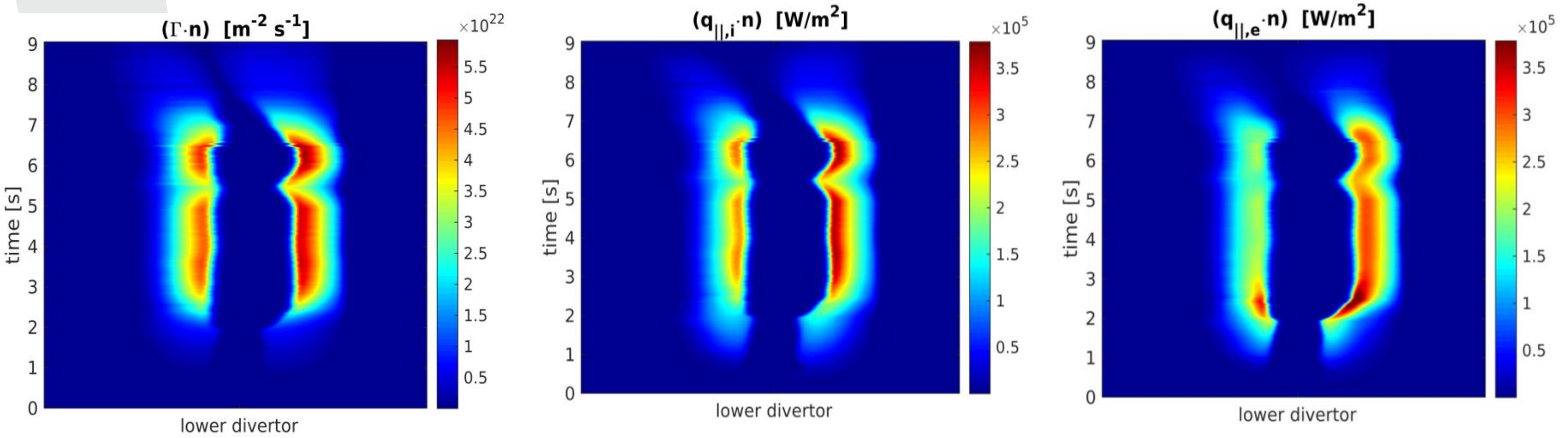
- $\Gamma, q_{\parallel,i}, q_{\parallel,e}$ in function of wall coordinates **(Log Scale):**



→ Fluxes cocentrated on the HFS limiter for t < 1 s

→ Peaks reached at the L. Div. with maximum located at the outer target (LFS)

- $\Gamma, q_{\parallel,i}, q_{\parallel,e}$ at lower divertor **(Linear Scale):**

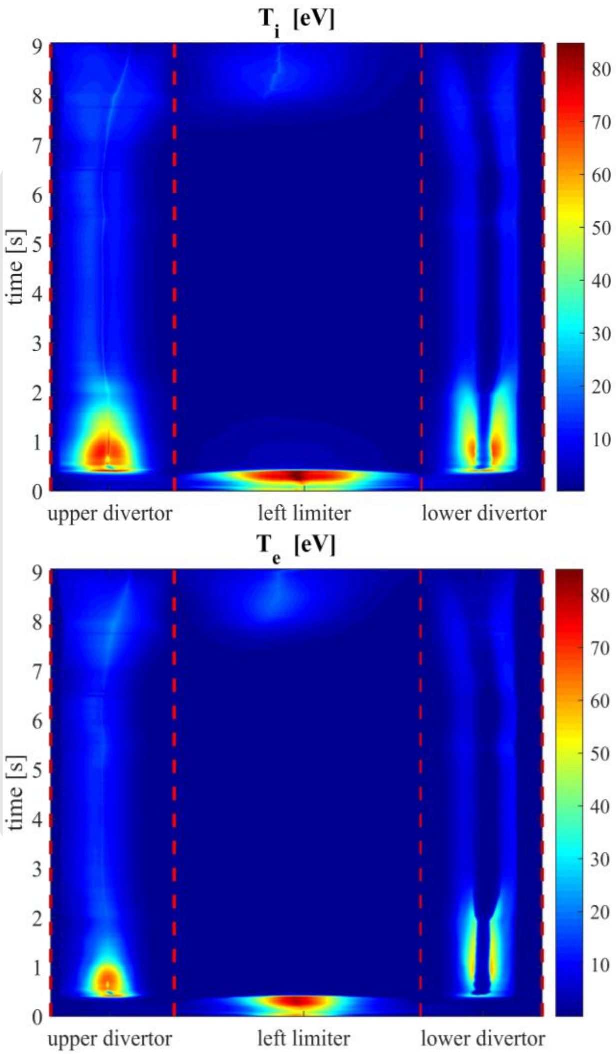


→ $(q_{\parallel,i} \cdot n) > (q_{\parallel,e} \cdot n)$ in the stationary phase contrary to transient phase

→ Location of the peaks spreads in time along L. Div. coordinates

[MS d'Abusco *et al*. N. Fus. 2022]

WEST Shot #54487: quantities at PFCs vs Time (2/2)



Temperatures 2D map:

→ erosion Map

$\propto \Gamma \cdot \boldsymbol{n} Y(T_{i,e}, Zeff)$

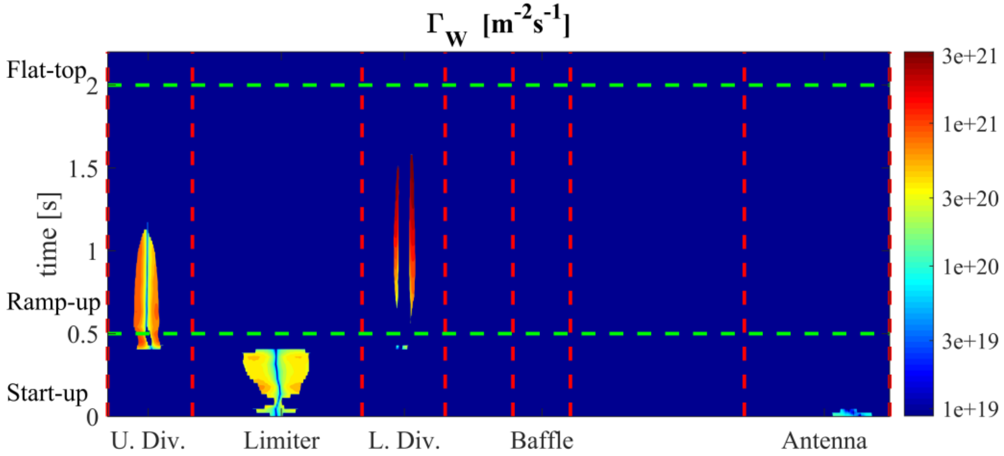
→ E_{impact} = energy to release a W atom in a D-W head collision

$$E_{impact} = 2k_bT_i + Z3k_bT_e$$

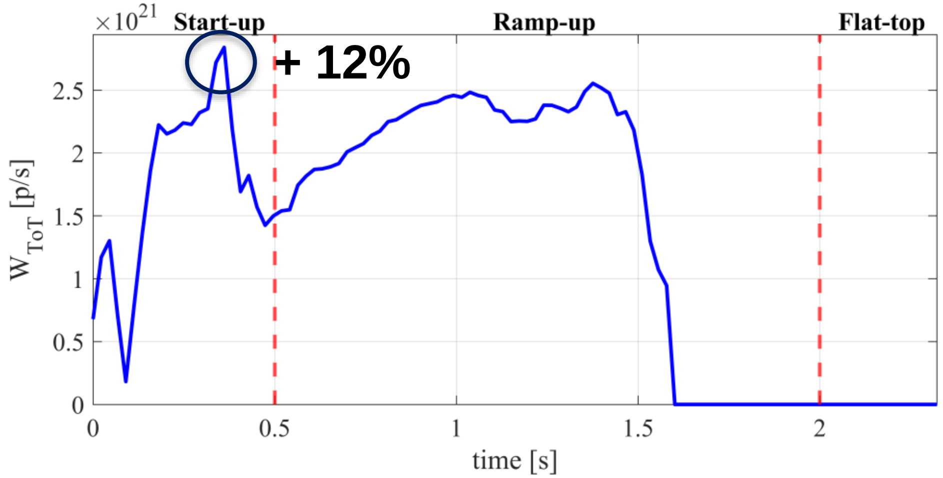
[P. C. Stangeby, The Plasma Boundary of Magnetic Fusion Devices, 2000]

[MS d'Abusco *et al*. N. Fus. 2022]

$(a)\ \Gamma_W(\boldsymbol{x},t) = \mathcal{H}(E_{impact} > E_{th})\Gamma_{D^+}$ **Tungsten Influx**



$(b)\ W_{ToT}(t) = \int_{\partial\Omega} \mathcal{H}(E_{impact} > E_{th})\Gamma_{D^+} ds$ **Tungsten Total Contamination**



WEST Shot #54487: Tungsten evolution using ERO

- SOLEDGE3X-HDG plasma backgrounds post processed by ERO 2.0 to compute the evolution of tungsten density

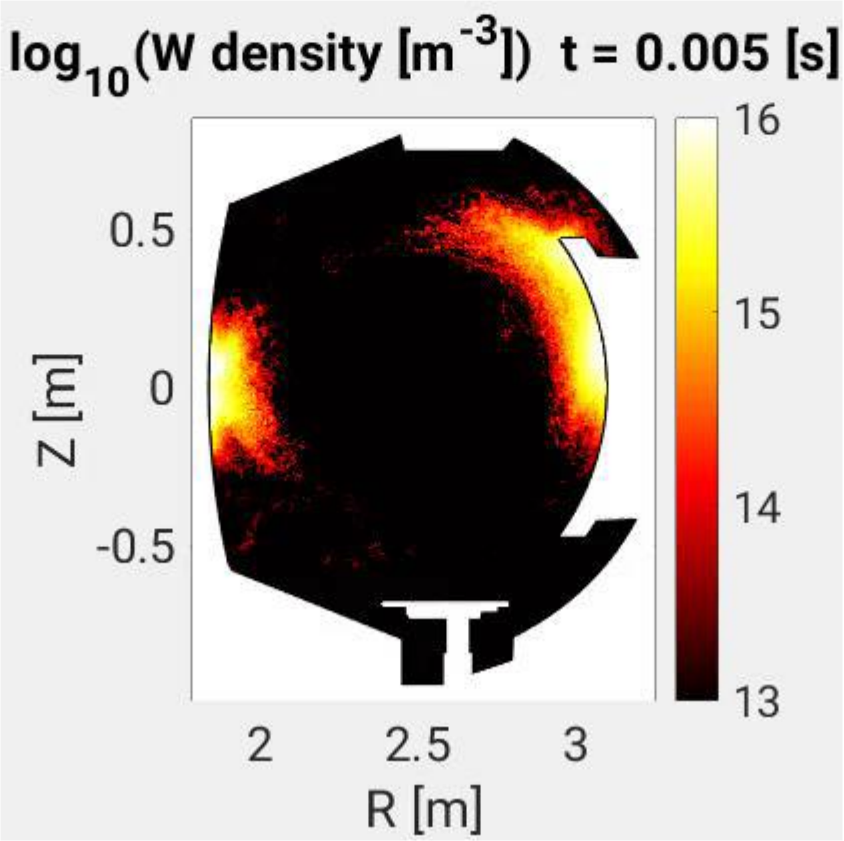
  → **Start-up phase:**
  sputternig mainly concentrated on the high field left limiter and antenna and high core contamination

  → **X-point onset:**
  sputtering mainly concentrated on the diverotr target (Upper and Lower)

- Good qualitative agreement with the crude cinematic model

  → Reproduction of the sputtering peak approximately at the same time t = 0.4 s

Tungsten Contamination



HDG #54487 background → **ERO 2.0**
[Montecarlo 3D code J. Romazanov et al., NME, 2019]

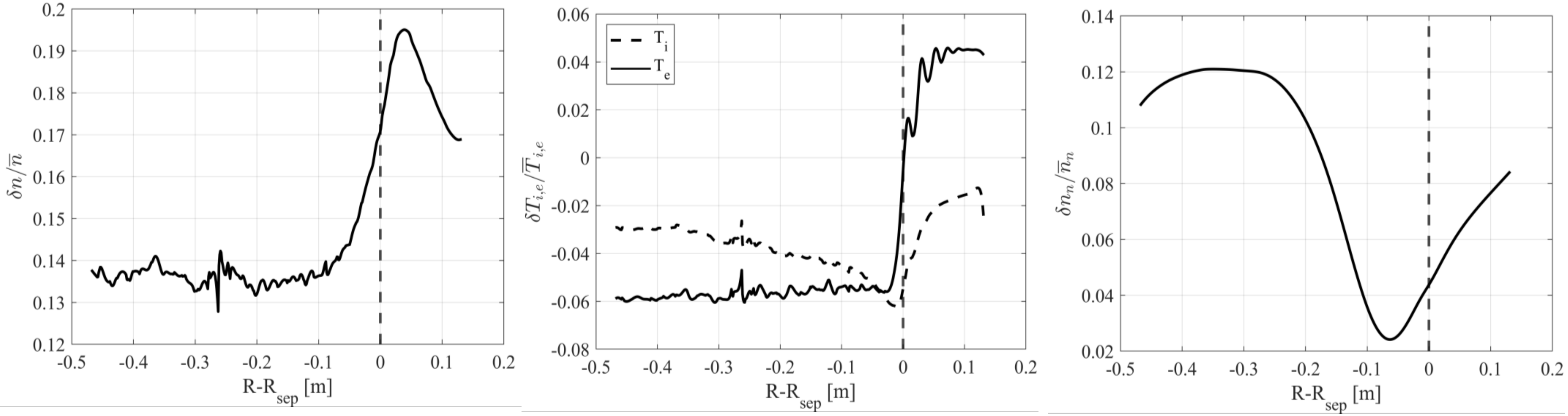
Outlines

- Mathematical and numerical model
- Verification and validation
- Core-edge coupling and sources
- Preliminary investigation of a detached plasma
- Full 2D transport simulations of an entire experimental discharge
- **Steady vs transient**

WEST Shot #54487: Steady vs transient

- Comparison with steady simulation performed at the flat top phase t = 4.510 s

  → higher value of plasma density in the unsteady computation than in the steady one



- The system doesn't reach the steady state over the time step of computation

[MS d'Abusco *et al.* N. Fus. 2022]

$$\frac{1}{\tau_c} = \frac{\int_\Omega \partial_t n \mathbf{dx}}{\int_\Omega n \mathbf{dx}}\Big|_{t=4.51} = -3.15 \times 10^{-4} s^{-1} \Rightarrow \tau_c = 3 \times 10^4 \ s$$ time scale to reach stationary state

$$\frac{\partial N}{\partial t} = \frac{N}{\tau_c} + Q_{puff} \Rightarrow N(t) = Q_{puff}\tau(1 - e^{-t/\tau_c}) + N_0 e^{-t/\tau_c}$$

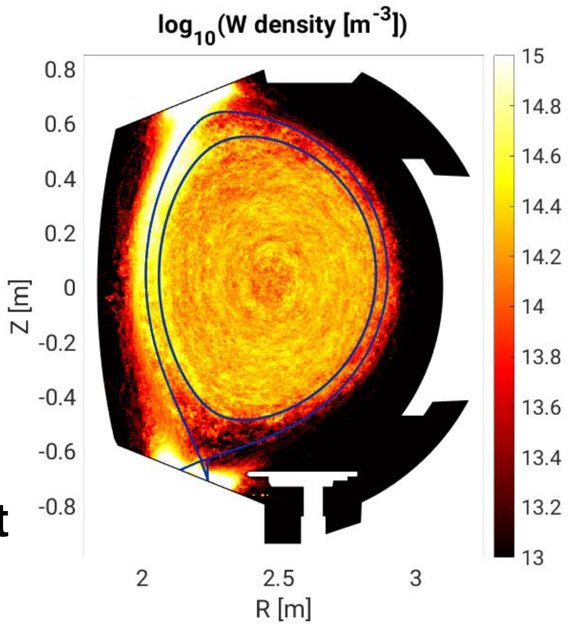
→ total number of particle relaxes to $Q_{puff} \times \tau_c$ over a time scale τ_c much grater than $dt = 0.02 \ s$

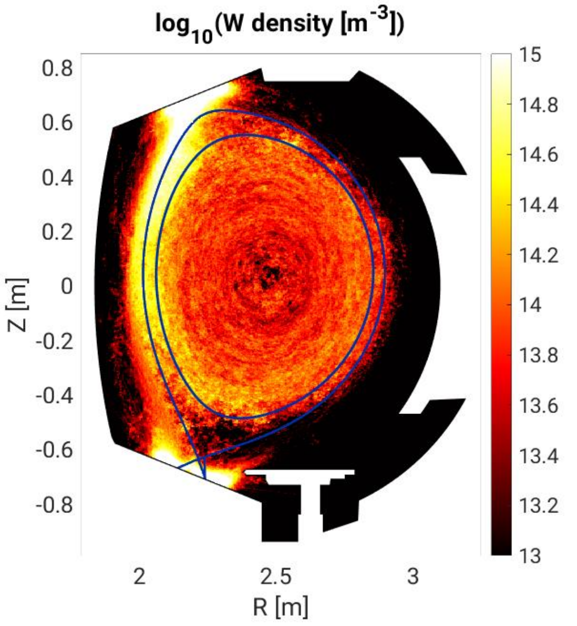
Steady vs transient in ERO

- **Calculation with transient phase:**
  → Evolution of the SE3X-HDG plasma backgrounds since the beginning of the discharge up to t = 1.02 s: **Left plot**

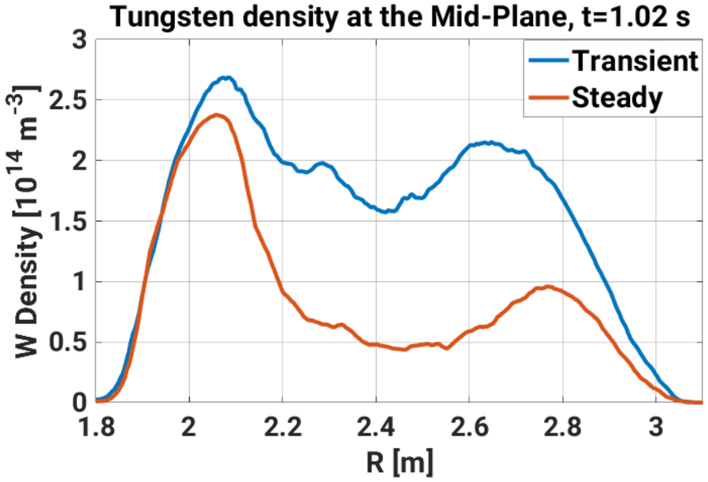
- **Steady:**
  → Fixed plasma bakground at t = 1.02 s: **Right plot**

- Higher core tungsten contamination when the transient phase is accounted
  → Tungsten density in the core 3 times greater for transient simulation vs steady case





Transient vs Steady at t = 1.02 s



Concluding remarks

- Core-edge transport fluid simulations have been performed in realistic tokamak geometry including transient phases: from start-up to shut-down

- Thanks to the new capabilities of the SOLEDGE3X-HDG: non-aligned grid + efficient time integration scheme + «self-consistent» sources

Physics highlights

- Heat fluxes estimation
  → Switch in the dominant power heat flux from electrons to ions in different phases of the discharge
  → Spreading in time of the power heat flux peaks along the divertor coordinates

- W sputtering and concentration:
  → Impact of the limiter-divertor transition: strong W contamination

This work confirms the interest on developing magnetic equilibrium free solver to support experimental data analysis and to target predictive capabilities in the future.

Future works and developments

- **Physics investigation**:
  → Investigation of **energy equipartition** problem by simple linear model: $\boldsymbol{\tau} = \frac{\boldsymbol{T_i}}{\boldsymbol{T_e}}$

- **Two-short terms physical model improvements**:
  → Reduced model for cross-field transport**: k-epsilon**
  → Neutral sources: **Advanced fluid model** then **EIRENE** coupling

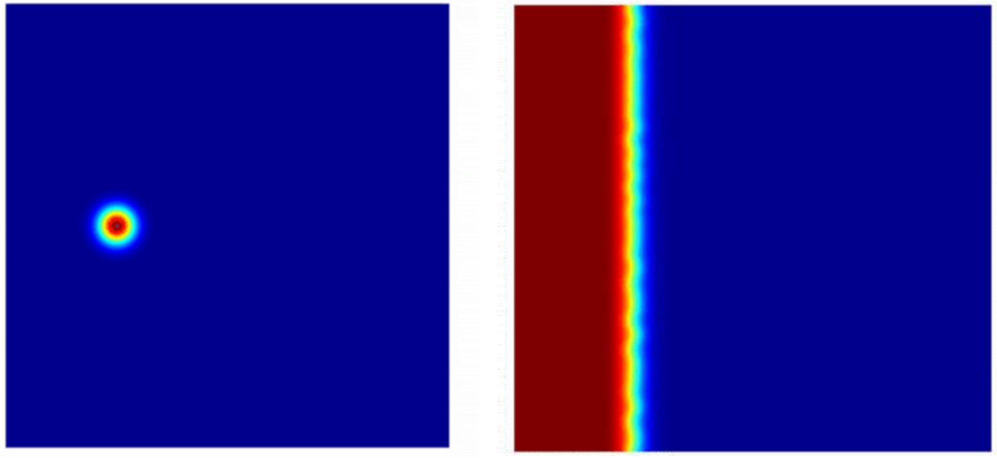
- **Numerical improvments increasing the DoF**:
  → **2D**
    - Bigger size Tokamak simulations→ **ITER** plasma volume ≈ 30 times **WEST**
    - **Multi-species** problem

  → **3D**
    - Transport simulation in **non-axisymmetric** geometries or with **3D magnetic perturbation**
    - Impact of **3D** plasma facing components on **transport proprieties** and **impurities**
    - **3D turbulent** simulation at **ITER** scale

Preliminary results for future works

- **2D turbulent fluid model in SLAB geometry:**
  → SLAB geometry

Courtesy of **G. Giorgiani**



- **First ITER real size simulation:**
  → SOLPS-ITER like wall geometry
  → 2D non-isothermal model + fluid neutrals

MS. d'Abusco