Modeling transient edge plasma processes with dynamic wall recycling

M.V. Umansky[1], R.D. Smirnov[2], S.I. Krasheninnikov[2]
[1]LLNL, [2]UCSD

To be presented at IAEA TM meeting on Divertor Concepts
Vienna, Nov 7-10, 2022

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, and supported by the U.S. DOE Office of Science, Office of Fusion Energy Sciences, and Office of Advanced Scientific Computing Research through the Scientific Discovery through Advanced Computing (SciDAC) project on Plasma-Surface Interactions

LLNL-PRES-842102-DRAFT

Introduction and Outline

Why develop a self-consistent model for edge plasma with active wall?

- It may offer new insights on boundary plasma physics, for fusion devices and beyond
- It may help us understand better plasma-material interactions for transient phenomena
- It may help us find new approaches for solving the divertor problem

How is it implemented?

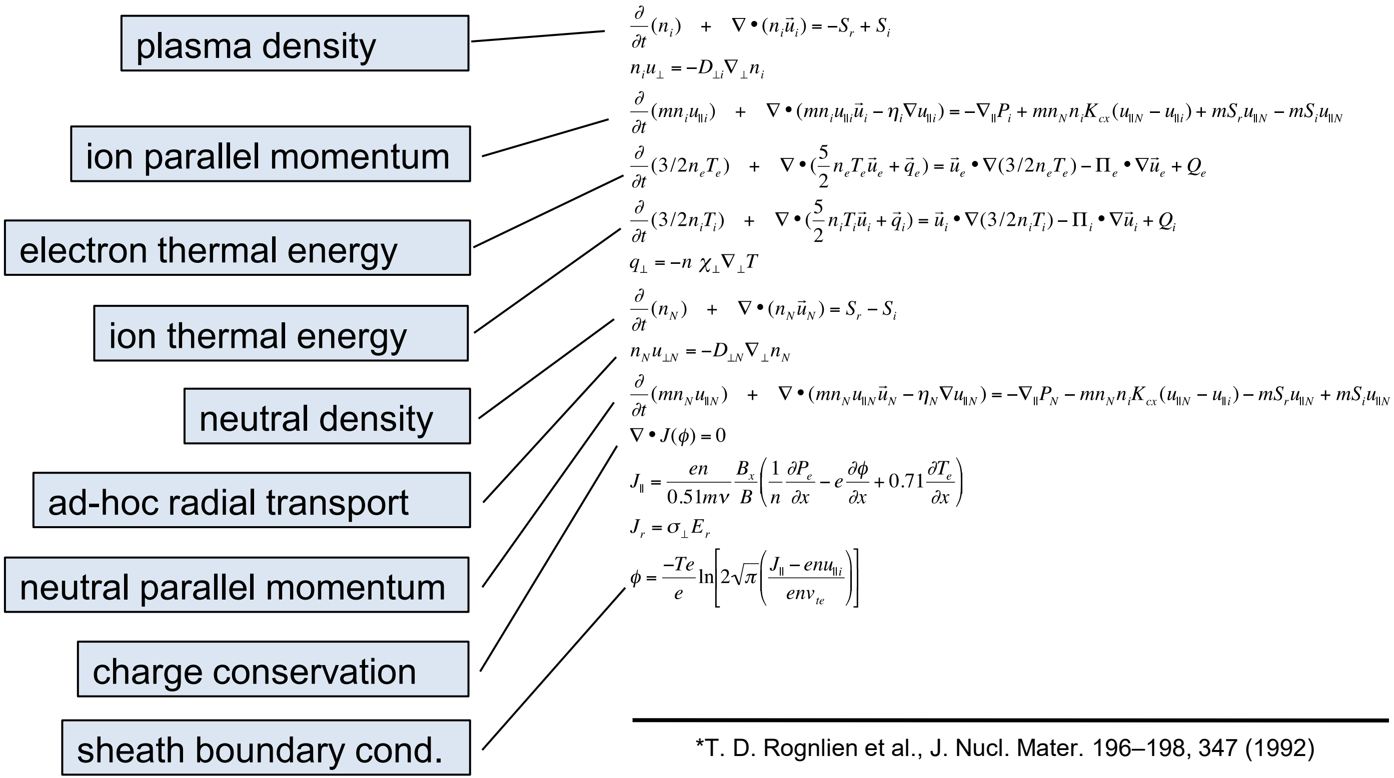
- Coupling of edge plasma code UEDGE with active wall code FACE
- Implemented with multi-physics framework IPS

What are the results?

- Coupled UEDGE and FACE provide a simulation model for transient PMI processes
- Modeling of tokamak strike point sweeping shows potential for dealing with divertor heat exhaust challenge
- Modeling of ELMs points to potential role of wall absorption/outgassing

Part I – Implementation of UEDGE and FACE coupling for self-consistent modeling of plasma dynamics with active wall

UEDGE is an established 2D fluid simulation model for boundary plasma transport



plasma density

ion parallel momentum

electron thermal energy

ion thermal energy

neutral density

ad-hoc radial transport

neutral parallel momentum

charge conservation

sheath boundary cond.

$$\frac{\partial}{\partial t}(n_i) \quad + \quad \nabla \bullet (n_i \vec{u}_i) = -S_r + S_i$$

$$n_i u_\perp = -D_{\perp i} \nabla_\perp n_i$$

$$\frac{\partial}{\partial t}(m n_i u_{\parallel i}) \quad + \quad \nabla \bullet (m n_i u_{\parallel i} \vec{u}_i - \eta_i \nabla u_{\parallel i}) = -\nabla_\parallel P_i + m n_N n_i K_{cx}(u_{\parallel N} - u_{\parallel i}) + m S_r u_{\parallel N} - m S_i u_{\parallel N}$$

$$\frac{\partial}{\partial t}(3/2 n_e T_e) \quad + \quad \nabla \bullet (\frac{5}{2} n_e T_e \vec{u}_e + \vec{q}_e) = \vec{u}_e \bullet \nabla (3/2 n_e T_e) - \Pi_e \bullet \nabla \vec{u}_e + Q_e$$

$$\frac{\partial}{\partial t}(3/2 n_i T_i) \quad + \quad \nabla \bullet (\frac{5}{2} n_i T_i \vec{u}_i + \vec{q}_i) = \vec{u}_i \bullet \nabla (3/2 n_i T_i) - \Pi_i \bullet \nabla \vec{u}_i + Q_i$$

$$q_\perp = -n \, \chi_\perp \nabla_\perp T$$

$$\frac{\partial}{\partial t}(n_N) \quad + \quad \nabla \bullet (n_N \vec{u}_N) = S_r - S_i$$

$$n_N u_{\perp N} = -D_{\perp N} \nabla_\perp n_N$$

$$\frac{\partial}{\partial t}(m n_N u_{\parallel N}) \quad + \quad \nabla \bullet (m n_N u_{\parallel N} \vec{u}_N - \eta_N \nabla u_{\parallel N}) = -\nabla_\parallel P_N - m n_N n_i K_{cx}(u_{\parallel N} - u_{\parallel i}) - m S_r u_{\parallel N} + m S_i u_{\parallel N}$$

$$\nabla \bullet J(\phi) = 0$$

$$J_\parallel = \frac{en}{0.51 m \nu} \frac{B_x}{B} \left(\frac{1}{n} \frac{\partial P_e}{\partial x} - e \frac{\partial \phi}{\partial x} + 0.71 \frac{\partial T_e}{\partial x} \right)$$

$$J_r = \sigma_\perp E_r$$

$$\phi = \frac{-Te}{e} \ln \left[2\sqrt{\pi} \left(\frac{J_\parallel - e n u_{\parallel i}}{e n v_{te}} \right) \right]$$

---

*T. D. Rognlien et al., J. Nucl. Mater. 196–198, 347 (1992)

FACE is a 1D simulation model for particles and thermal energy transport in material wall

Thermal energy transport

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}(\lambda \frac{\partial T}{\partial x}) + \rho c_p u \frac{\partial T}{\partial x} + S_T$$

Particle species transport

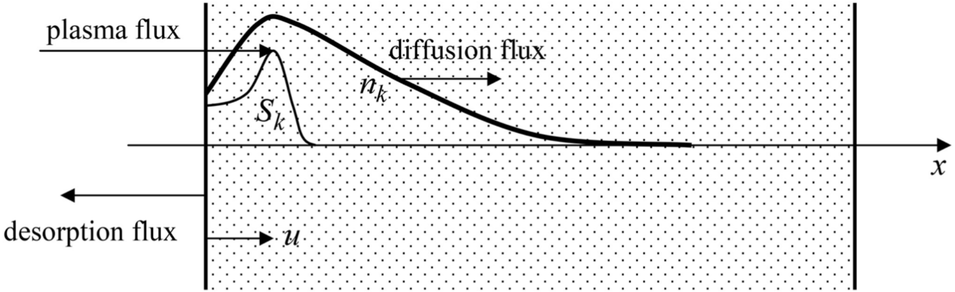
$$\frac{\partial n_k}{\partial t} = \frac{\partial}{\partial x}\left(D_k \frac{\partial n_k}{\partial x}\right) + u \frac{\partial n_k}{\partial x} + S_k + R_k$$

n_k = density of particles of sort k

D_k = temperature-dependent diffusion coefficient of k'th particles in the wall material

$u > 0$ = erosion speed of the wall surface due to sputtering

S_k, R_k = source and reaction terms describing volumetric rates of creation/destruction

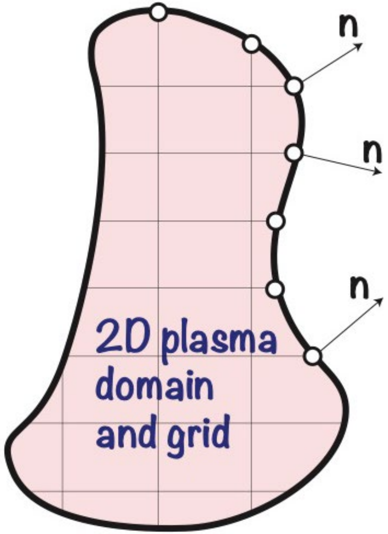


R.D. Smirnov et al.,
FUSION SCIENCE AND
TECHNOLOGY · v 71 (2017)

FACE implements an “active wall” model – a material wall model that accounts for accumulation and release of plasma particles and heat stored in the wall

UEDGE-FACE coupling implementation #1

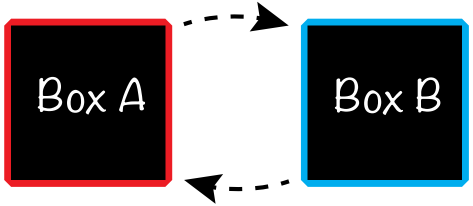
- A copy of FACE is set up at each grid point on wall boundary



- Using 2D plasma domain for UEDGE
- Using 1D wall domain for each copy of FACE
- Running multiple FACE processes in parallel
- Alternating time steps in UEDGE and FACE

UEDGE-FACE coupling implementation #2

- Two coupled “black boxes” A and B for “plasma” and “wall”
- Explicit time-stepping strategy:
    - Update box A w/ “frozen” box B
    - Next, update box B w/ “frozen” box A, etc.



- Closely related to “fractional step method”, “operator splitting method”, etc.
- Mathematical roots of it lie in the Zassenhaus formula for linear operators

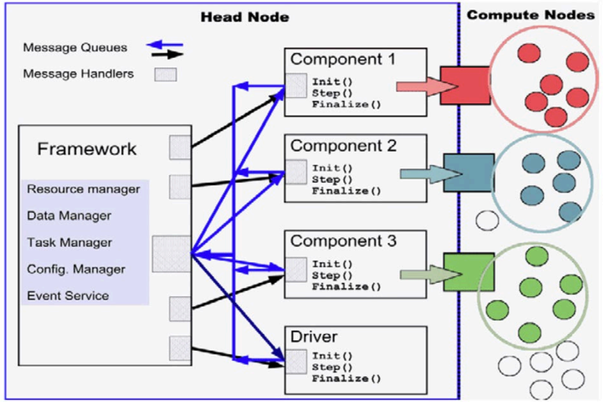
$$e^{t(X+Y)} = e^{tX}\; e^{tY}\; e^{-\frac{t^2}{2}[X,Y]}\; e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])} \quad \text{etc.}$$

- For our system of two coupled “black boxes”, linearized evolution operator is the sum of two operators: #1 acting on Box A, and #2 acting on Box B
- For convergence, need the splitting time step shorter than physics timescales

UEDGE-FACE coupling implementation #3

- Multi-physics code coupling framework IPS is used for implementation of UEDGE-FACE coupling

- IPS provides tools for managing complex workflows with multiple parallel processes



W.R. Elwasif et al., 18th Euromicro Conference on Parallel, Distributed and Network-based Processing, (2010), pp. 419-427.

- Our IPS based application developed for this project is called IPSUF (**IPS**+**U**EDGE+**F**ACE), and it is hosted on GitHub

Part II – Using coupled UEDGE and FACE for modeling of strike point sweeping in tokamak divertor

Strike point sweeping has been proposed for mitigation of divertor heat loads in a tokamak

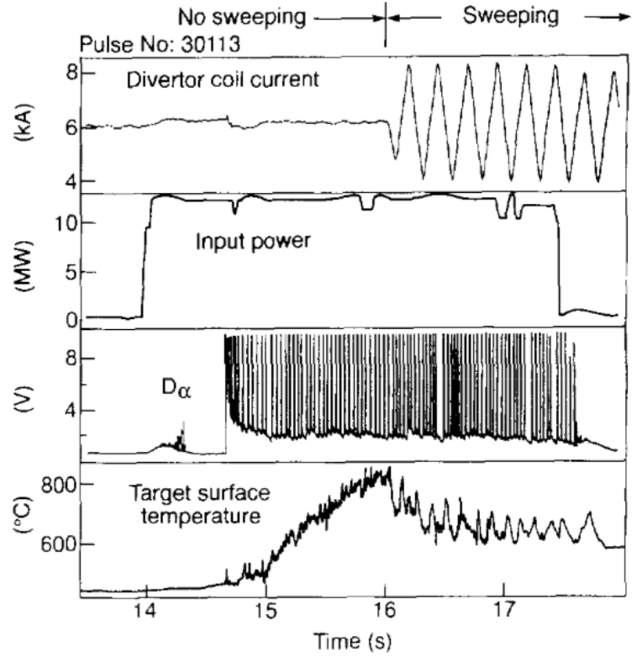


Fig. 4. Time traces showing the effect of divertor X-point sweeping on the tile temperature in high power ELM-free and ELMy discharge.

Figure from Ref. [1]

- Strike point sweeping was studied experimentally since 1990s [1-3]
- Proposed for future experiments [4-5]

[1] Jacyuinot et al., Fusion Eng. Design 30 67-84 (1995)

[2] Ambrosino et al., IEEE Trans. Plasma Science, v. 36, n. 3, (2008)

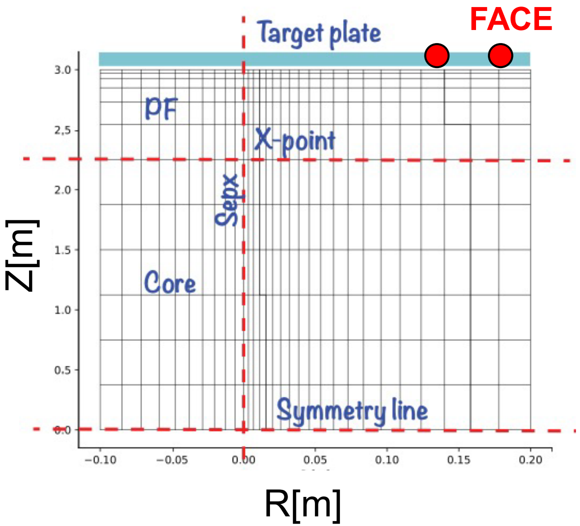
[2] Silburn et al., Phys. Scr. T170, 014040 (2017)

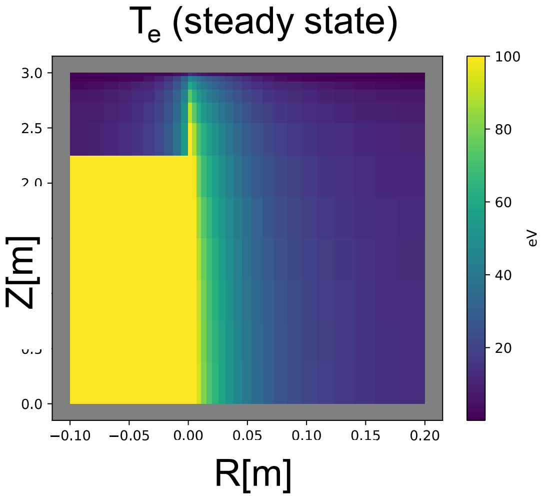
[4] Kuang et al., J. Plasma Phys., vol. 86, 865860505 (2020)

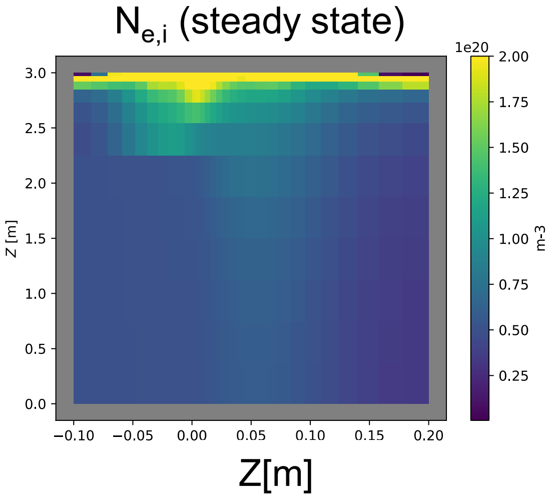
[5] Soukhanovskii – private communication (2021)

UEDGE rectified edge plasma setup used for strike point sweeping study

- Simplified geometry but captures main features of X-point divertor
- Boundary conditions set to mimic divertor in a high-power tokamak
- Peak power flux on target plate ~50 MW/m^2
- Power flux profile width on the plate~1 cm




T_e (steady state)

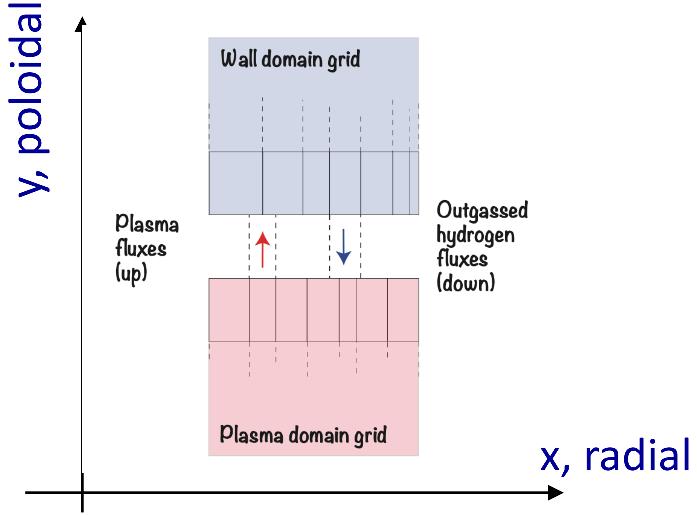

$N_{e,i}$ (steady state)

FACE model setup is focused on hydrogen transport

- Material: tungsten-like properties, 1 cm thick
- Species included: hydrogen (“free”, i.e., interstitial, and “trapped”)

- Reactions included: trapping and thermally activated de-trapping of hydrogen in/from the traps; at the surface molecular desorption of hydrogen
- Trapping: 3 kinds of traps for hydrogen in material with de-trapping energies 0.9 eV, 1.35 eV and 1.95 eV and uniform concentrations of 0.1 at.%, 0.025 at.%, and 0.0125 at.%
- Thermal transport: 1D heat conduction equations solved on separate grid
- Boundary conditions: on back side of plate, T=500 K, zero hydrogen flux Γ=0

Implementation of divertor strike point sweeping, using coupled UEDGE & FACE



- Plasma and wall domains communicate via fluxes of particles and energy
- Γ_{ij} is the flux between ith cell on plasma side and jth cell on wall side
- Relative radial displacement of plasma and wall domains changes distribution of fluxes Γ_{ij}

- Our wall model is 1D, it neglects fluxes along the wall surface
- That's appropriate if perturbations of parameters in the wall domain are confined to a narrow layer on the target plate surface: $L_x << L_y$

"Temperature waves" analysis justifies quasi-1D treatment

- Consider a 1D diffusion equation with sinusoidally driven BC

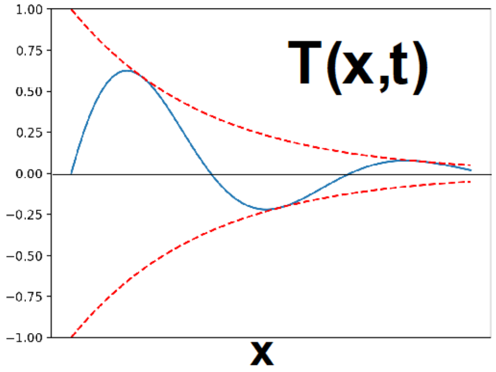
$$\frac{\partial}{\partial t}T = \chi \frac{\partial^2}{\partial x^2} T$$

$$x \in [0, \infty);\ T(x=0) = T_0 e^{-i\omega t};\ T(x=\infty) = 0$$

- Once the transients die out, solution is

$$T(x,t) = T_0 e^{-i\omega t + ikx}, \text{where } k = \sqrt{i\omega/\chi}$$

Decaying wave



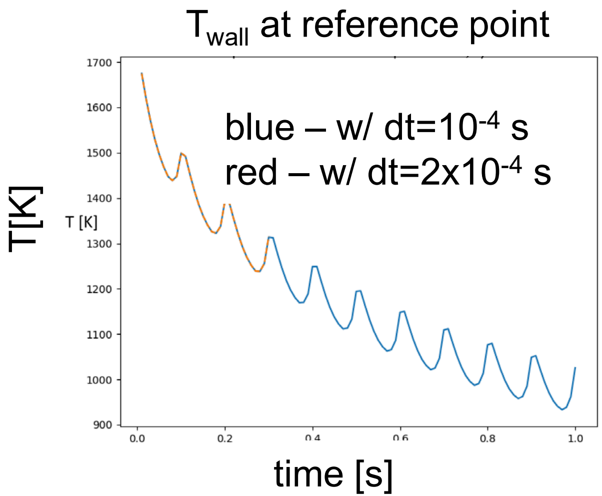
- For tungsten (χ~50 mm^2/s at T=300 K)
  - ν=10 s^{-1} => L_x ~ 5 mm
  - ν=1 s^{-1} => L_x ~ 15 mm

- Assuming realistic sweep parameters: ν~1-10 Hz, amplitude L_y ~ 10 cm
  - Plate temperature perturbations are confined to ~1 cm layer on the surface
  - Transport processes in the plate can be treated as a quasi-1D problem

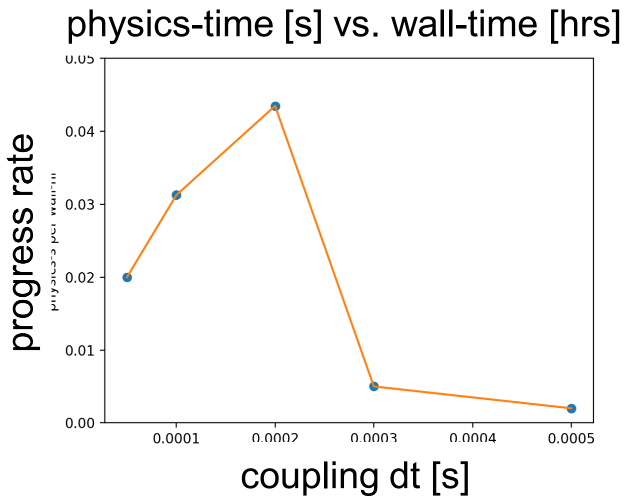
Time evolution with coupled UEDGE & FACE uses optimal time step

- Case Box2g
  - Sweep parameters: frequency 10 Hz; amplitude 10 cm
  - Coupling run parameters: dt=2e-4s, N_t=1e4, total time=2s

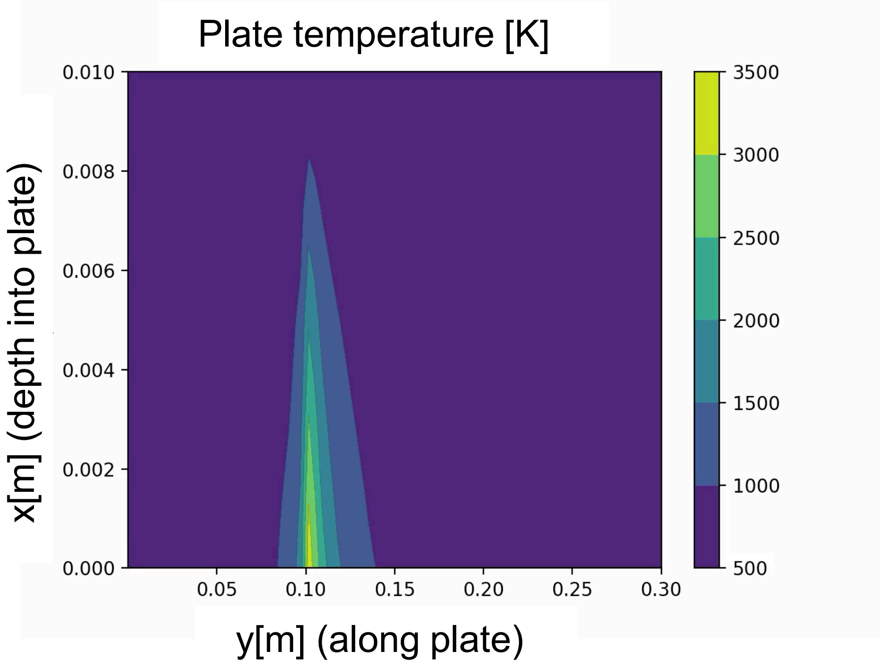
- Convergence in dt to ~1e-2%

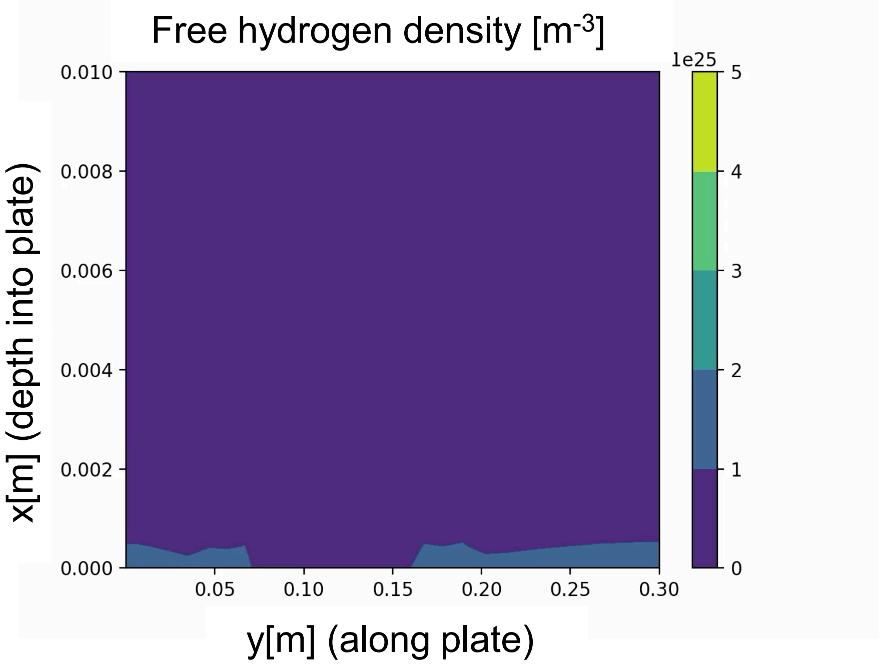


- There is sweet spot for coupling step dt



Oscillatory regime is established in target plate; temperature and free hydrogen density follow sweeping

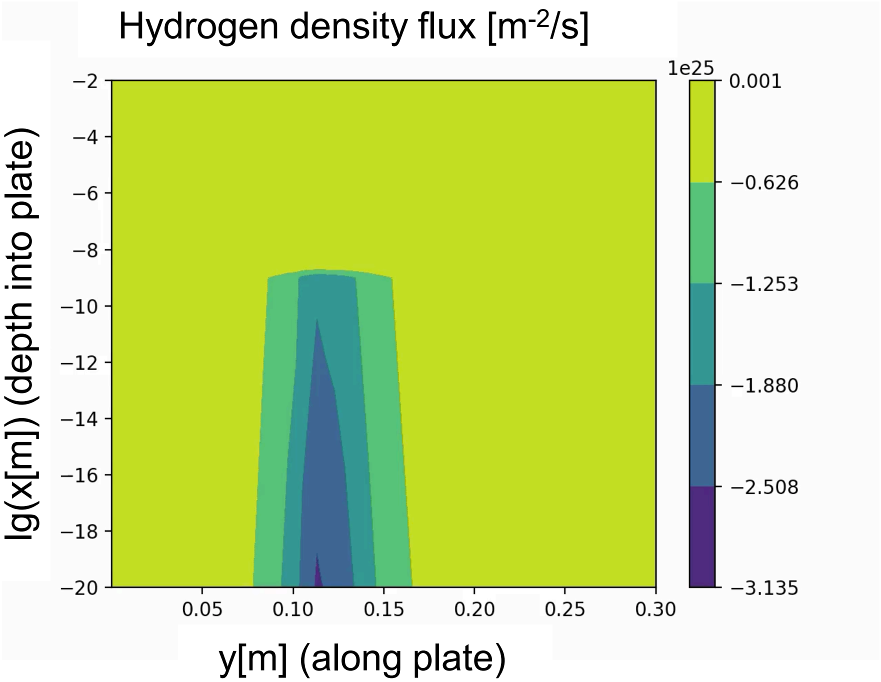




- Without sweeping => close to W melting point
- With sweeping => under 1500 K – problem solved?

- Variation due to hydrogen flow?
- Or de-trapping of trapped hydrogen?

Escaping flux of hydrogen (outgassing) exists only in the first 1-2 nm of target plate surface, at ion implantation depth



- Temporal variation of free hydrogen density in the plate volume is not caused by hydrogen ions/atoms entering/exiting the plate

- It is caused by trapping and de-trapping of hydrogen

- Beyond the first 1-2 nm, hydrogen transport in the plate is too slow to play a role on considered time scales

Part III – Using coupled UEDGE and FACE for modeling of ELM cycle in tokamak

Experimental evidence points to importance of hydrogen absorption/outgassing by the wall in ELM crash/recovery

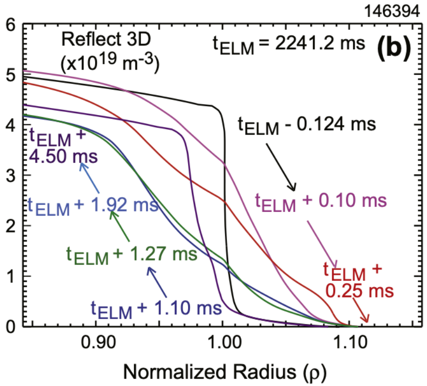


Fig. 3. Evolution of edge electron density profiles during the ELM with (a) temporal evolution from D_α emission in the outer divertor leg, and (b) multiple n_e profiles at times during the ELM evolution marked by vertical dashed lines in (a).

Figures w/ DIII-D data from Fenstermacher et al.
JNM 438 (2013) S346–S350

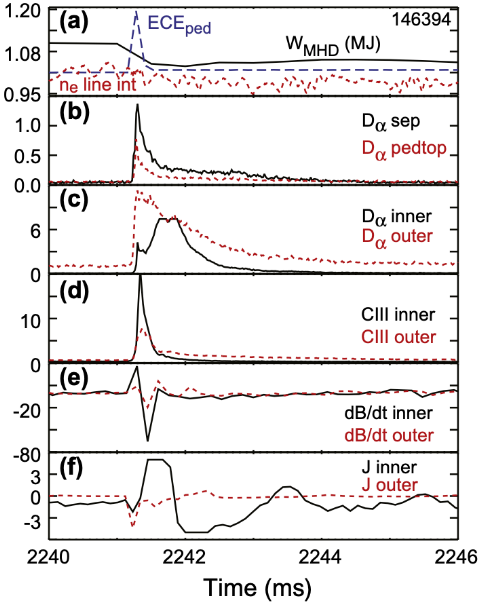


Fig. 2. Evolution of multiple local measurements during the Type-I ELM at 2241.15 ms including (a) total stored energy (MJ), line-integrated density along a horizontal midplane chord (1.4 × 10^{20} m^{-2}) and ECE emission near the top of the pedestal (au), (b) D_α emission from the top of the pedestal and near the separatrix at the LFS midplane (au), (c) D_α, and (d) CIII (465 nm) emission from the ISP and LFS X-point (au), (e) dB/dt (T/s), and (f) ion saturation current [j_{sat} (au)] from the ISP and OSP.

- During ELM crash 5% of plasma density is lost
- That amounts to ~0.5e20 ions
- Volume outside LCFS ~1 m^3
- Average gas density outside LCFS << 1e20 m^{-3}
- Not enough neutrals to rebuild core density?

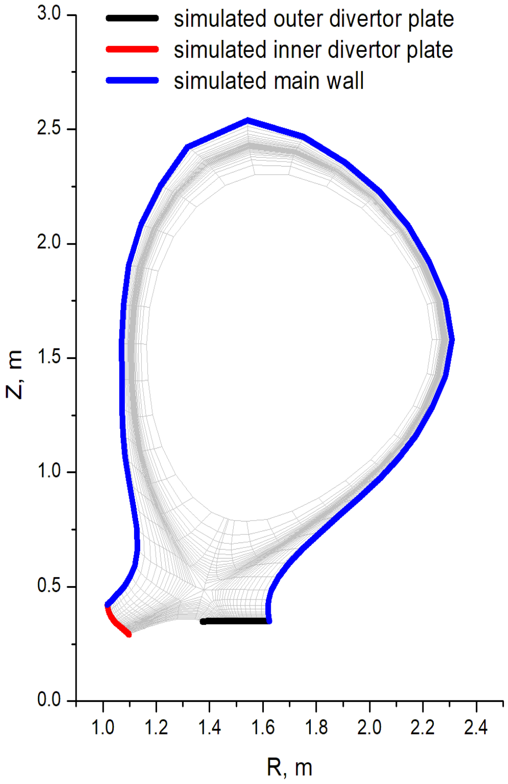
Model setup for ELM simulations uses periodic bursts of heat and particles into SOL

- FACE is coupled w/ UEDGE on outer wall & target plates, in realistic X-point geometry

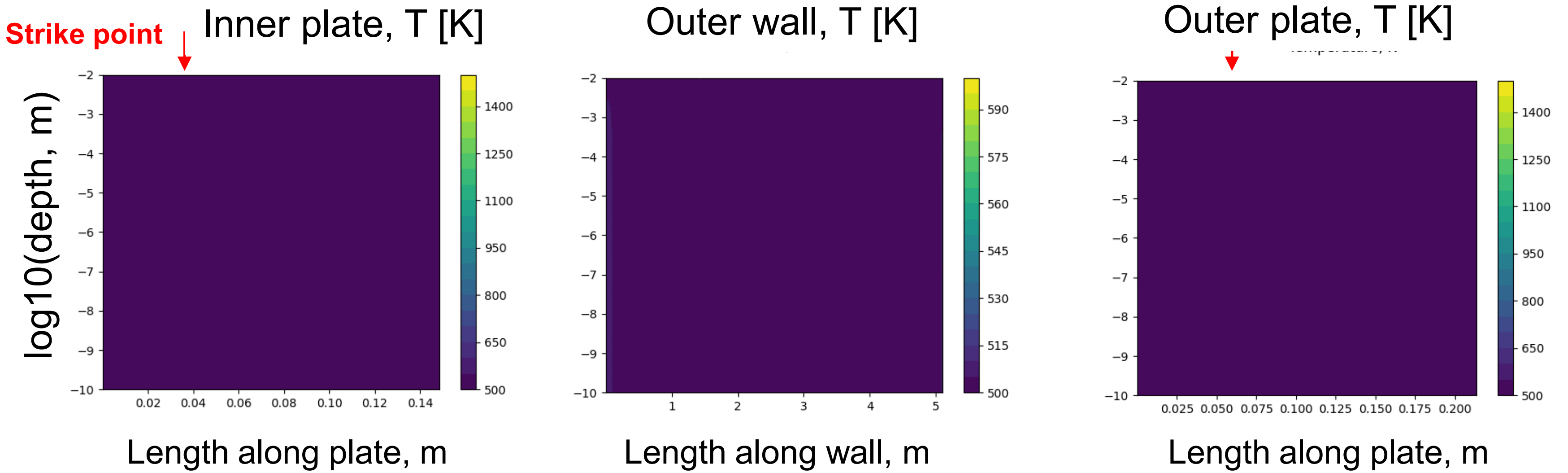
- ELMs modeled in UEDGE as short 3 ms bursts of heat and density flux into SOL, repeating every 30 ms

- UEDGE setup
  - Mid-size high-power tokamak parameters
  - Core boundary: n=2e20 m-3
  - At ELM crash: P=1 GW, χ,D=15 m^2/s; otherwise
  - P=2 MW, core χ,D=0.1 m^2/s, SOL χ,D=1.0 m^2/s,

- FACE setup
  - Tungsten-like material properties, 1 cm thick



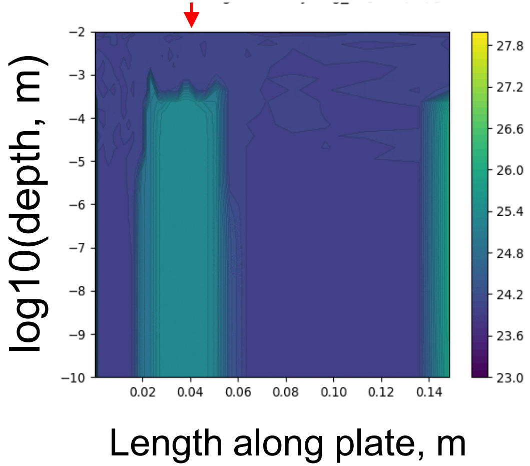
Temperature in material surfaces is affected by ELM within ~100 µm depth



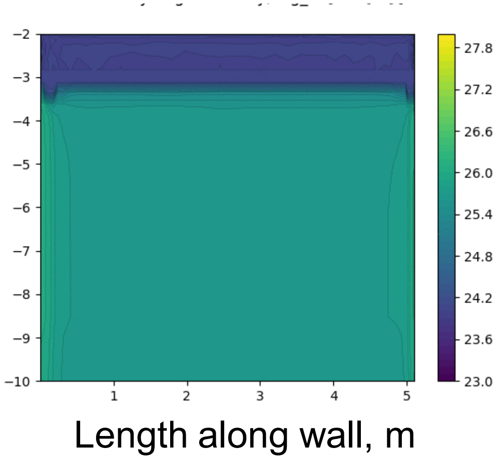
- On target plates, material temperature spikes within ~1 cm from strike points
- Main wall heating is comparatively low and uniform

Hydrogen retention in material surfaces is affected by ELM within ~1 μm depth

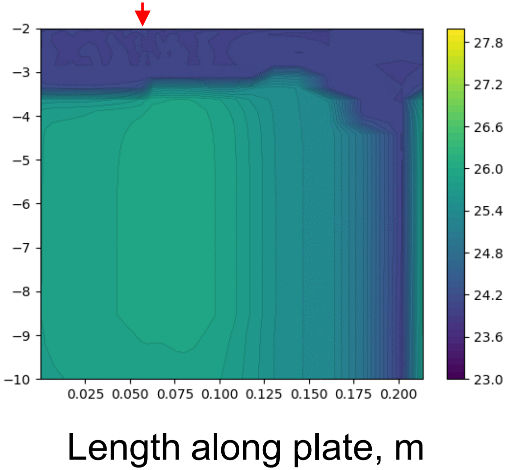
Inner plate lg(n_H [m-3])



Outer wall lg(n_H [m-3])



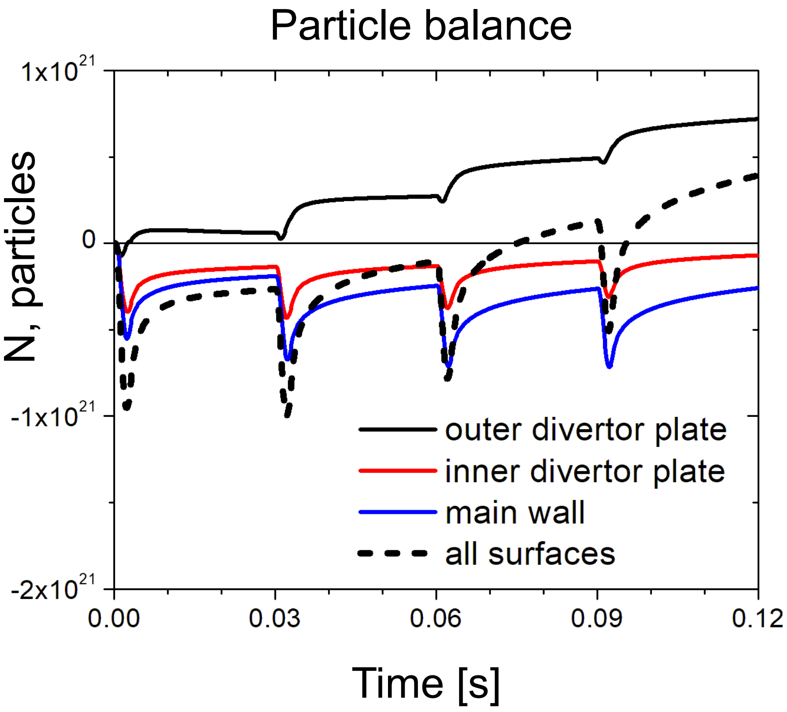
Outer plate lg(n_H [m-3])



- At ELM start, retained deuterium amount increases along all surface
- Near strike points, hydrogen is faster depleted due to material heating

Variation of hydrogen retention in material surfaces throughout ELM cycle comparable to edge plasma contents

- Stationary oscillation have not been achieved yet (long simulations)
- Extrapolating from several ELM cycles so far, variation of hydrogen inventory in the walls ~1e21 particles throughout ELM cycle
- Number of hydrogen particles in edge simulation domain ~1e21
- Points to potentially important role that wall storage & outgassing play in mass balance

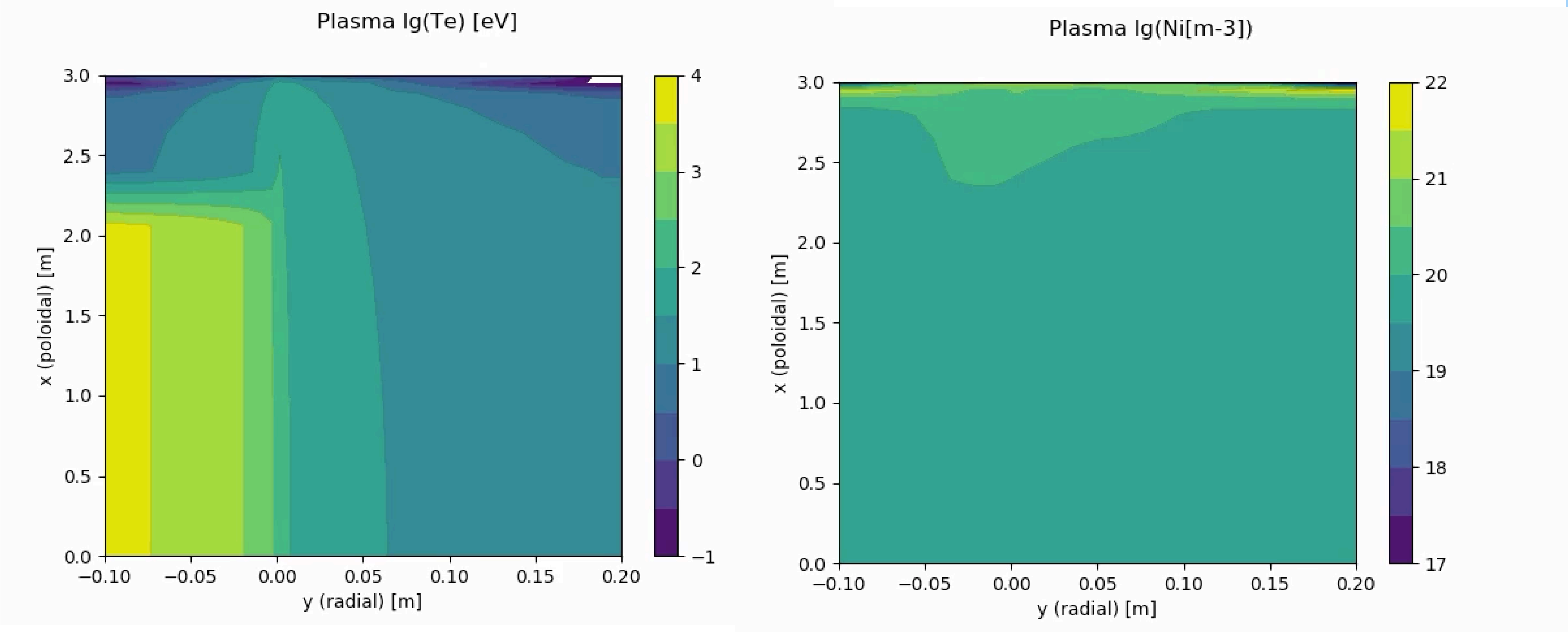


Summary & Conclusions

- UEDGE and FACE codes coupled using IPS framework enable 2D plasma modeling with dynamic recycling on all wall surfaces
- Application of the coupled model to strike point sweeping, in a high-power tokamak, shows that for realistic sweep parameters the temperature on the tungsten target plate can be maintained below 1500 K
- Modeling of large ELM pulses for high-power mid-size tokamak conditions shows that hydrogen density profiles in material are affected up to depth ~1 μm, while temperature profiles are affected up to ~100 μm.
- Simulations results point to significant potential role played by wall hydrogen storage & outgassing in mass balance during ELMs

Backups

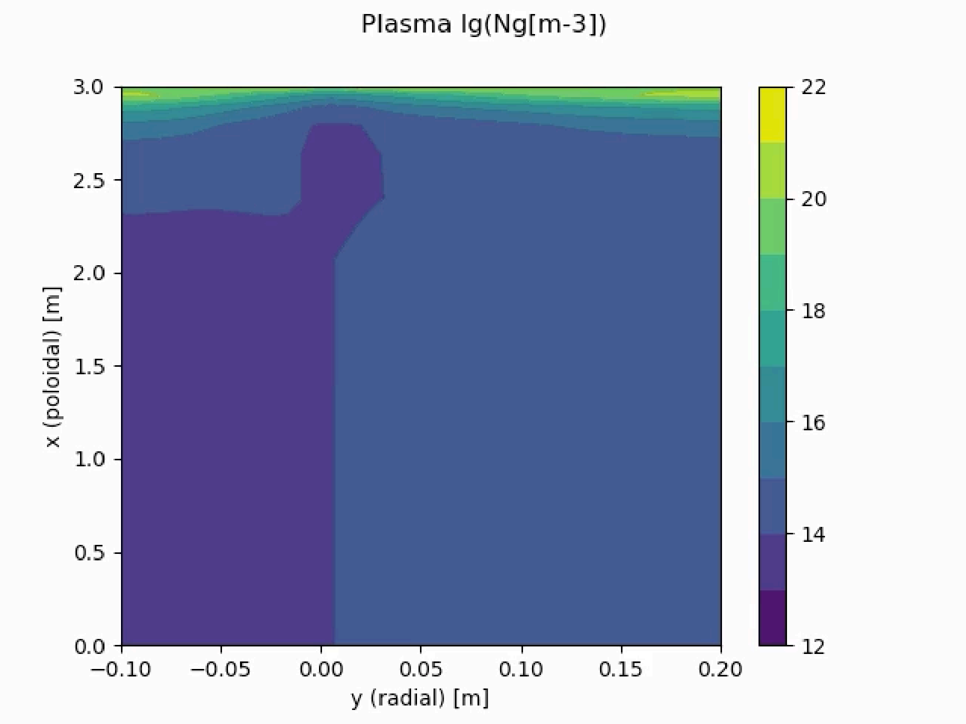
Strike point sweeping leads to modest changes on the plasma side



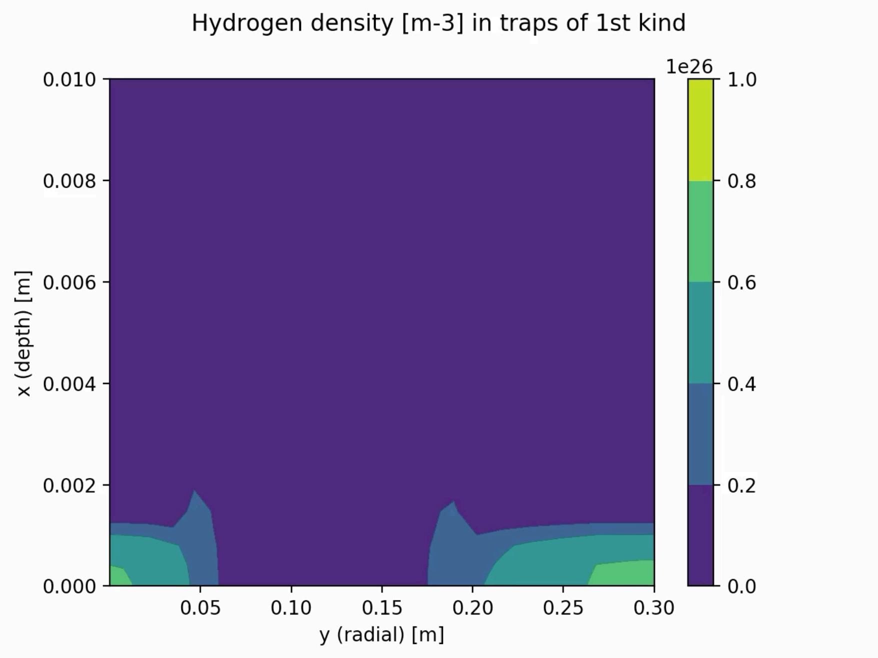
From plasma point of view, strike point sweeping ⇔ target plate moves periodically

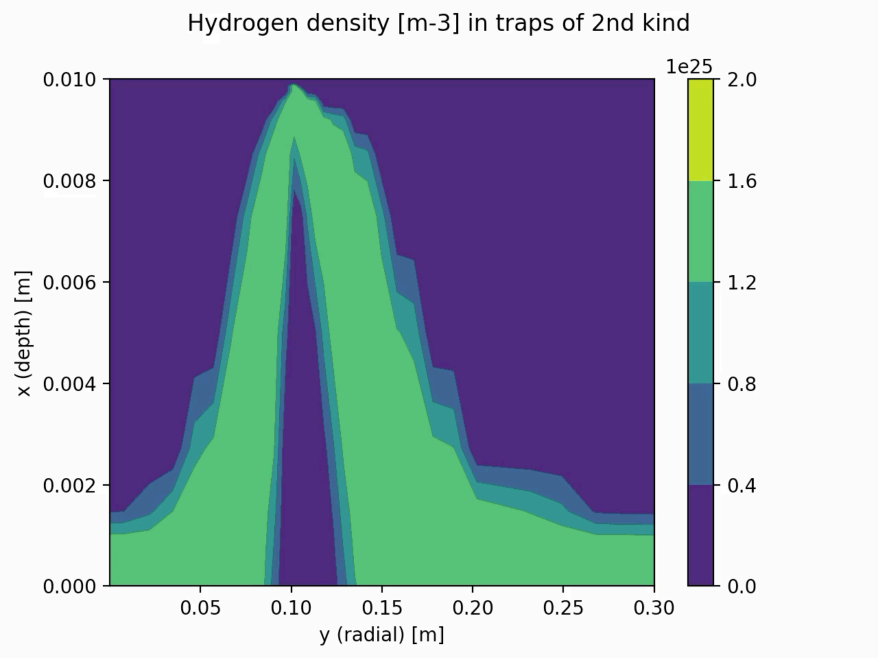
From the plasma point of view, in our model strike point sweeping means that target plate is moving radially

- There is some variation of plasma parameters, caused by strike point sweeping (outgassing) – but not very dramatic



Density of trapped hydrogen is weakly affected


Hydrogen density [m-3] in traps of 1st kind


Hydrogen density [m-3] in traps of 2nd kind