Time-dependent plasma surface interaction modeling to address dynamic recycling in a tungsten divertor

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with significant contributions from

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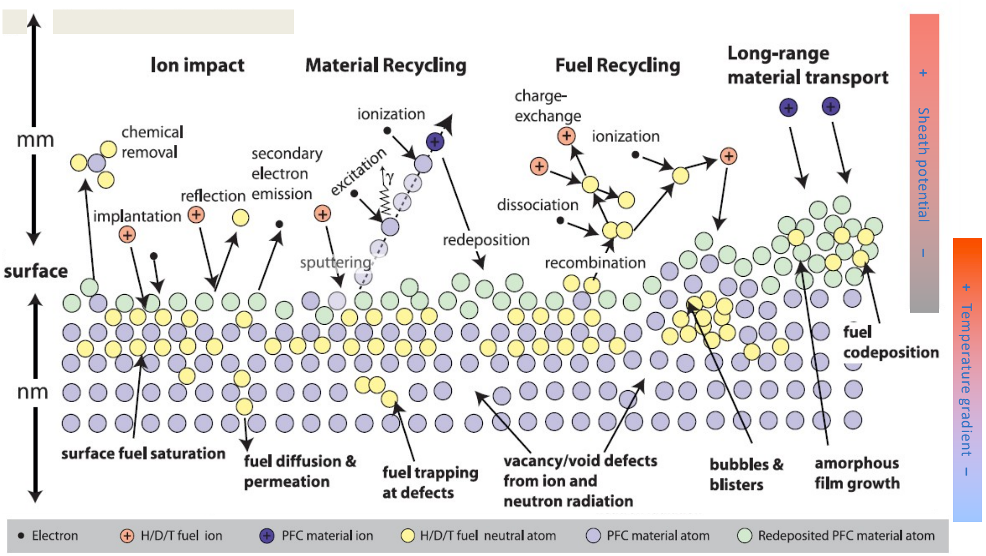
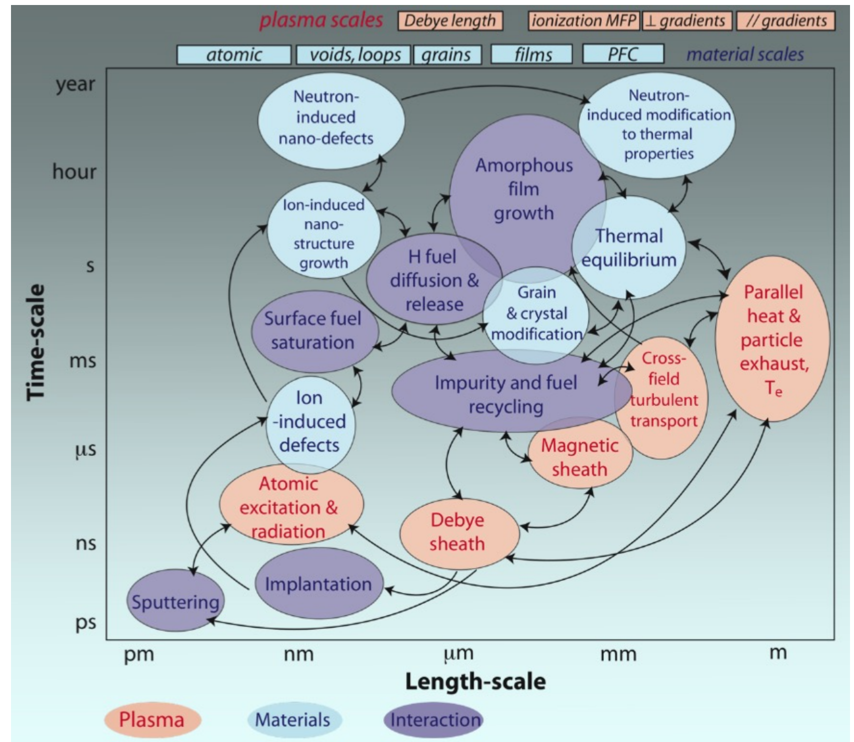
Physics governing plasma surface interactions is multiscale

- Large changes in plasma-facing surfaces driven by interactions with energetic ions and neutrals
  - Erosion, gas retention, sub-surface composition and morphology, etc.
- Material response can introduce impurities into the plasma, alter fuel recycling, etc.



Wirth, Nordlund, Whyte and Xu, *MRS Bulletin* **36** (2011) 216-222.
Wirth, Hammond, Krasheninnikov, and Maroudas, *J. Nucl. Mater.* ***463*** (2015) 30-38.



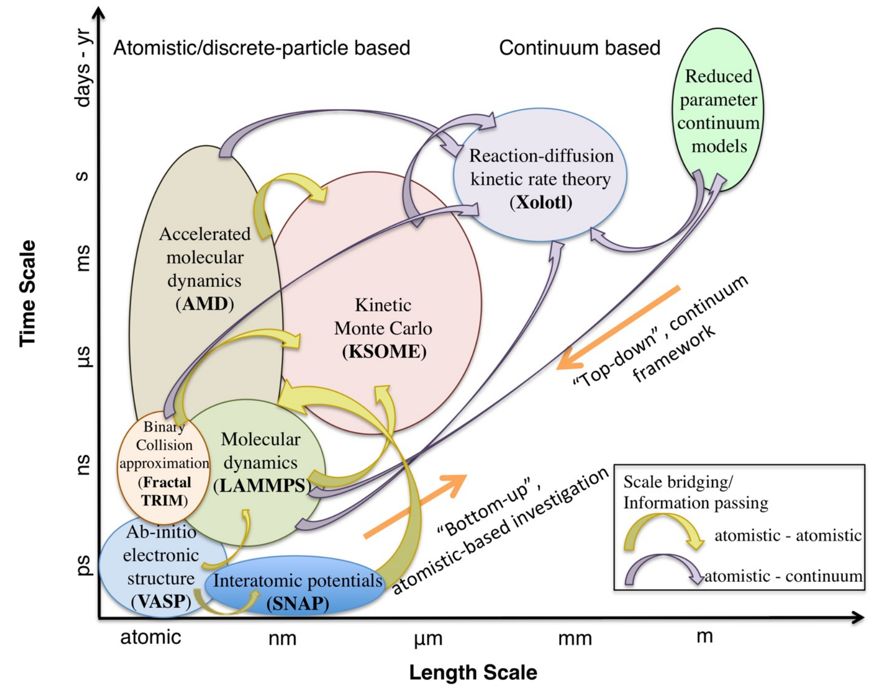
- PSI/PMI involve multiple physical processes from the atomic to macroscopic spatial and scales

Atomistically-informed cluster dynamics models bridge scales from nanometers (ps) to experimental (sec to hours)

- Approach to multiscale modeling challenge bottom-up: DFT → MS, MD → CD
  - Use atomistic methods to understand gas dynamics in materials (He-H interactions, Ne/Xe-W interactions), material mixing (B-W and N-W), etc.
  - Continuum (spatial-dependent) cluster dynamics addresses the meso-scale

→ Workhorse to bridge scales from high-fidelity atomistics to experimental:

- Workflow for PSI (Xolotl) shown here; similar used for structural materials (whether discrete or stochastic cluster dynamics)
- Goal: Transition towards focus from interpretation to prediction of physical properties

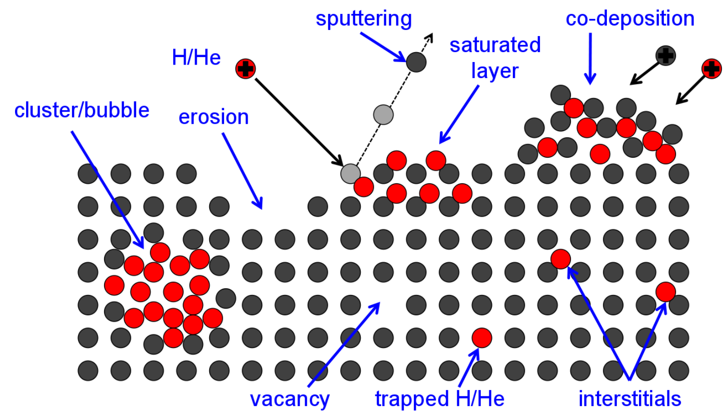


Our cluster dynamics code: Xolotl

- The tungsten is represented by the concentration of clusters at each spatial grid point:

Interstitials (I)
Vacancies (V)
Helium/Hydrogen (He/H)
Dilute plasma impurities (B/N)

Mixed: combination of He/H/B/N atoms trapped in tungsten vacancies



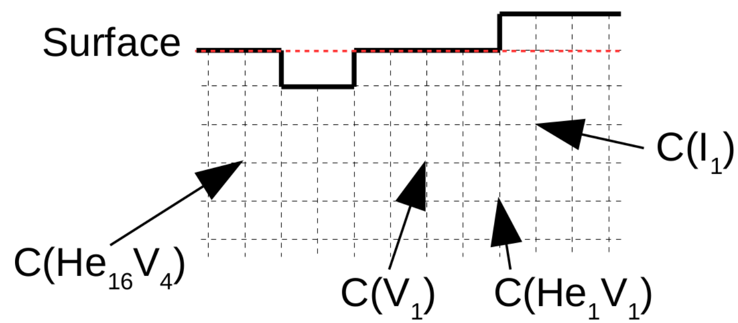
- The time evolution is given by the drift-diffusion-reaction equations:

$$\delta_t \bar{C} = \phi \cdot \rho - \nabla \bar{J} - \bar{Q}(\bar{C})$$

- $\bar{J} = -D\nabla\bar{C} + u\bar{C}$ is the Fickian diffusive and drift fluxes, with D_i following the Arrhenius equation

$$D_i = D_{0,i} e^{-E_m/k_B T}$$

with $D_{0,i}$ and E_m obtained from MD and DFT simulations



- Developed from scratch using C++, PETSc, MPI, Kokkos
- Open source code available at:
- https://github.com/ORNL-Fusion/xolotl

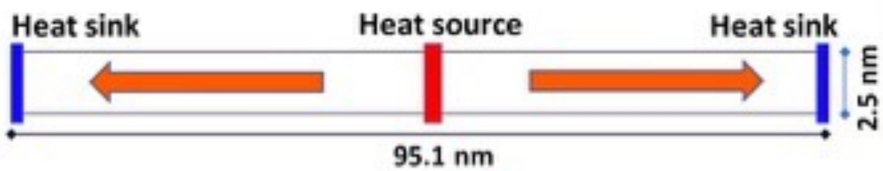
Today's discussion – 3 Case Studies

- Soret effect diffusion of SIA, He and H & impact on integrated modeling of Plasma Surface Interactions

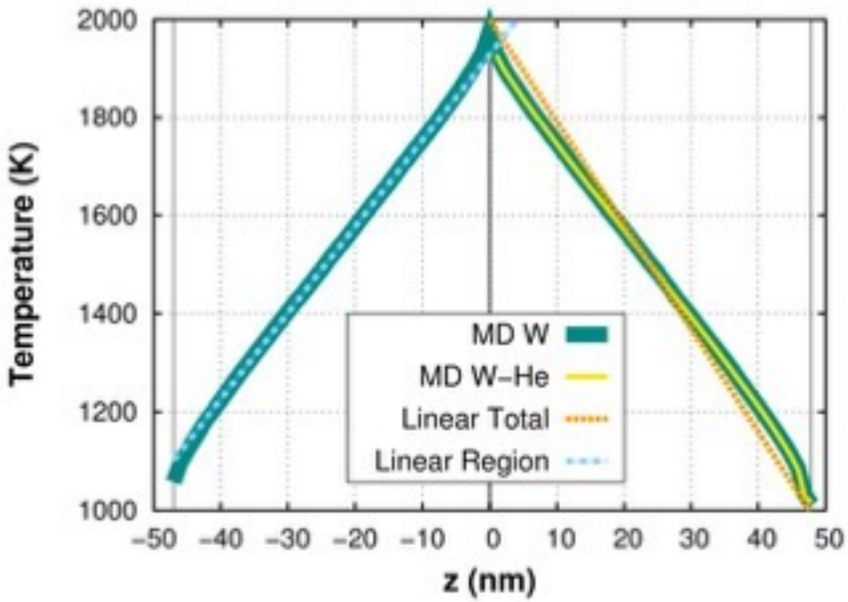
- First principles-based modeling of B impact on H behavior on W surfaces, and at W-B interfaces

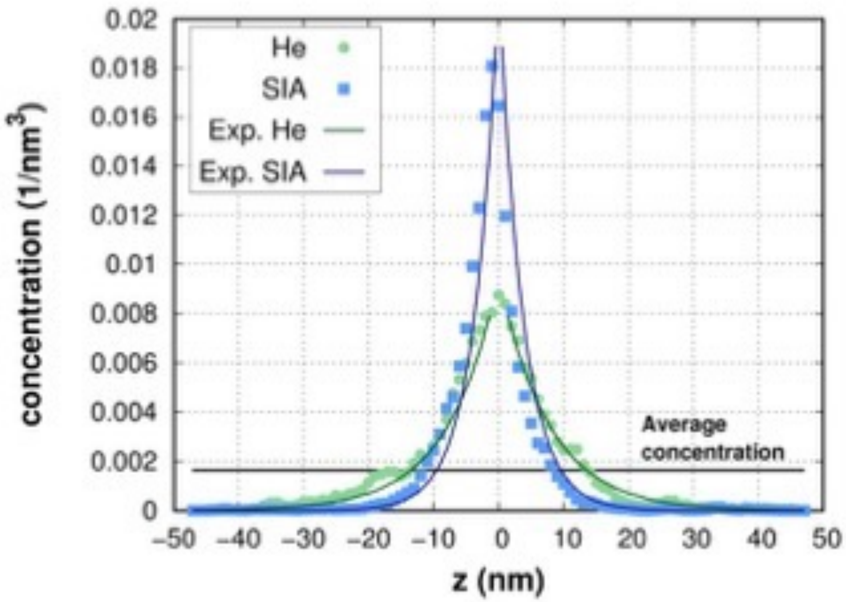
- Time-dependent (2-way coupled) PSI modeling of ELMs in ITER

Soret effect evaluation in W



Use non-equilibrium MD (NEMD) simulation with a fixed temperature gradient to study its effect on He and self-interstitial transport:





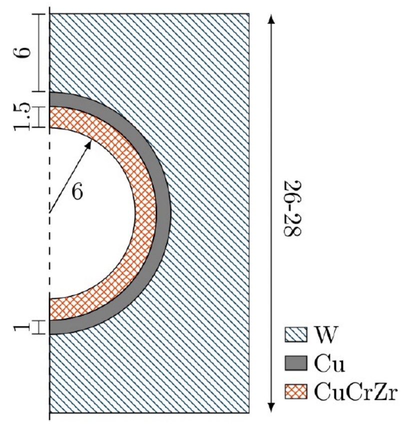
⇒ Both He and Self-Interstitials preferentially diffuse up the temperature gradient.

E. Martinez, N. Matthew, D. Perez, S. Blondel, D. Dasgupta, B.D. Wirth, and D. Maroudas, "Thermal gradient effect on helium and self-interstitial transport in tungsten", *Journal of Applied Physics* **130** (2021) 215904.

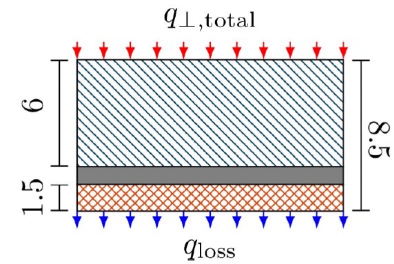
Atomistic-informed modeling of Soret effect (T-gradient diffusion)

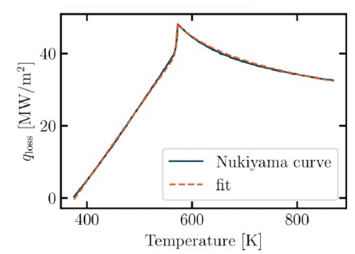
$$Q^*_{\mathrm{SIA}} = -0.0128 k_B T^2 \text{ eV}$$
$$Q^*_{\mathrm{He}} = -0.0065 k_B T^2 \text{ eV}$$
$$Q^*_{\mathrm{H}} \approx -0.0045 k_B T^2 \text{ eV}$$

Xolotl simulations of ITER W divertor geometry, with He-induced thermal conductivity degradation and ELMs



- 1 mm of copper plus 1.5 mm of CuCrZr
- Temperature dependent heat flux at the coolant side
- Temperature dependent specific heat capacity and heat conduction coefficient





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D. Dasgupta, S. Blondel, E. Martinez, D. Maroudas, and B.D. Wirth, "Impact of Soret effect on hydrogen and helium retention in PFC tungsten under ELM-like conditions", *Nuclear Fusion* **63** (2023) 076029

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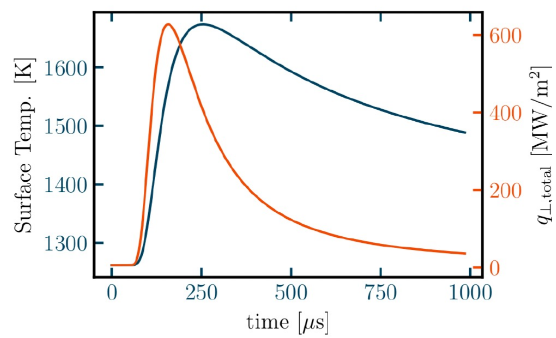

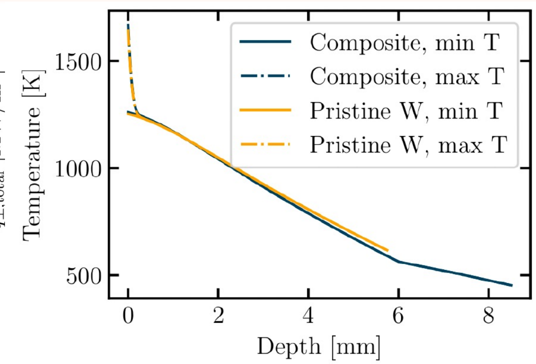

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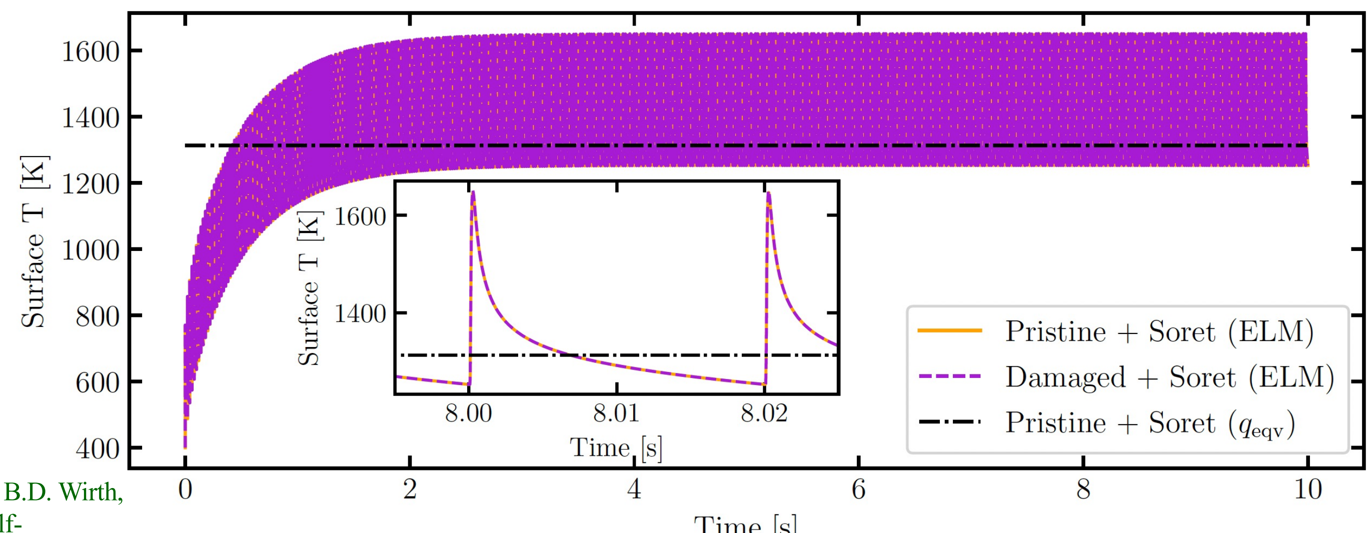

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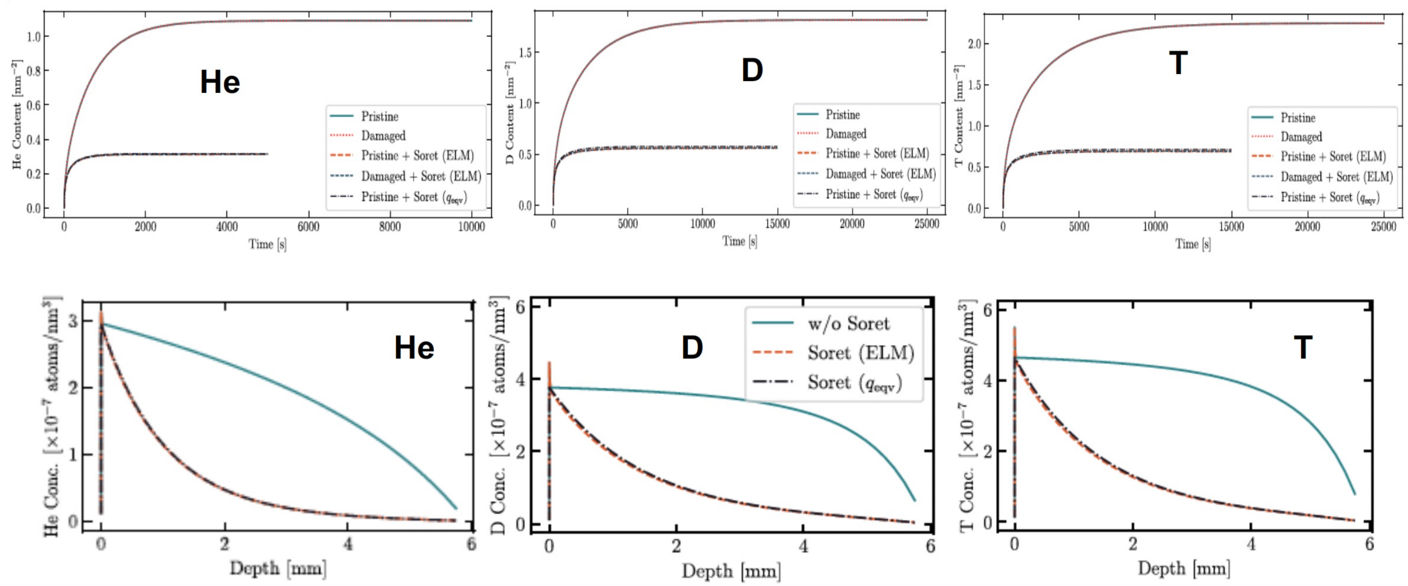


Thermal gradients help recycling of D, T but also He

E. Martinez, N. Matthew, D. Perez, S. Blondel, D. Dasgupta, B.D. Wirth, and D. Maroudas, "Thermal gradient effect on helium and self-interstitial transport in tungsten", *Journal of Applied Physics* **130** (2021) 215904.

D. Dasgupta, S. Blondel, E. Martinez, D. Maroudas, and B.D. Wirth, "Impact of Soret effect on hydrogen and helium retention in PFC tungsten under ELM-like conditions", *Nuclear Fusion* **63** (2023) 076029

First-principles (DFT) assessment of B effect of H on W

Multiple recent publications, and ongoing activities, to evaluate B influence on the H behavior on W surfaces, H and He behavior in W-borides, and H trapping and diffusion behavior at WB – W interfaces

L. Yang and B.D. Wirth, "First-principles study of diffusion of intrinsic defects in tungsten borides", *Journal of Nuclear Materials* **591** (2024) 154931.

L. Yang and B.D. Wirth, "Surface stability and H adsorption and diffusion near surfaces of W borides: A first-principles study", *Nuclear Fusion* **63** (2023) 066002.

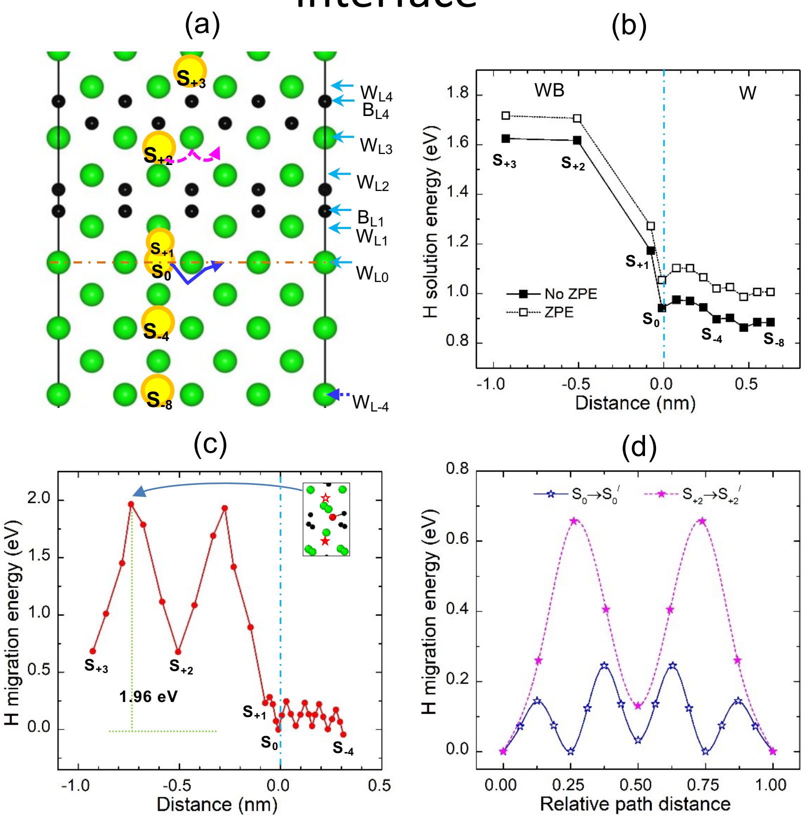
L. Yang and B.D. Wirth, "Energetics of intrinsic point defects and hydrogen in tungsten borides: a first-principles study", *Nuclear Fusion* **62** (2022) 086013.

L. Yang and B.D. Wirth, "Boron segregation and effect on hydrogen energetics near tungsten surfaces: A first-principles study", *Surface Science* **717** (2022) 121983.

L. Yang and B.D. Wirth, "Energetics of boron near tungsten surfaces: A first-principles study", *Journal of Applied Physics* **130** (2021) 015101.

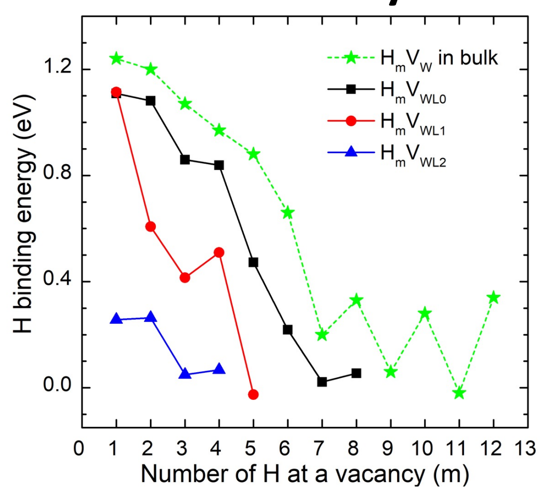
First-principles (DFT) assessment of H at WB-W(001) interface

Solution and diffusion of H interstitial near WB – W(001) interface

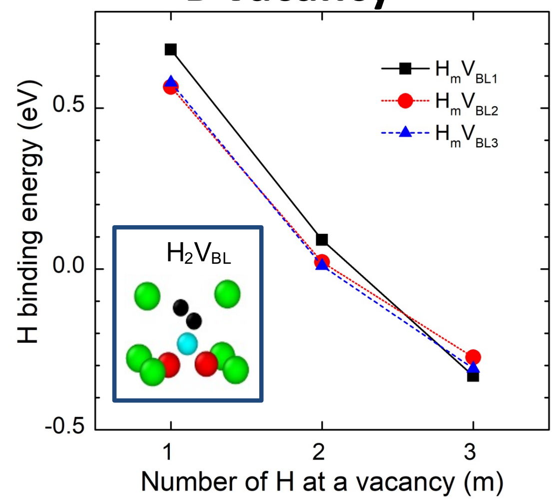


H clustering at vacancy near WB – W(001) interface

W vacancy



B vacancy



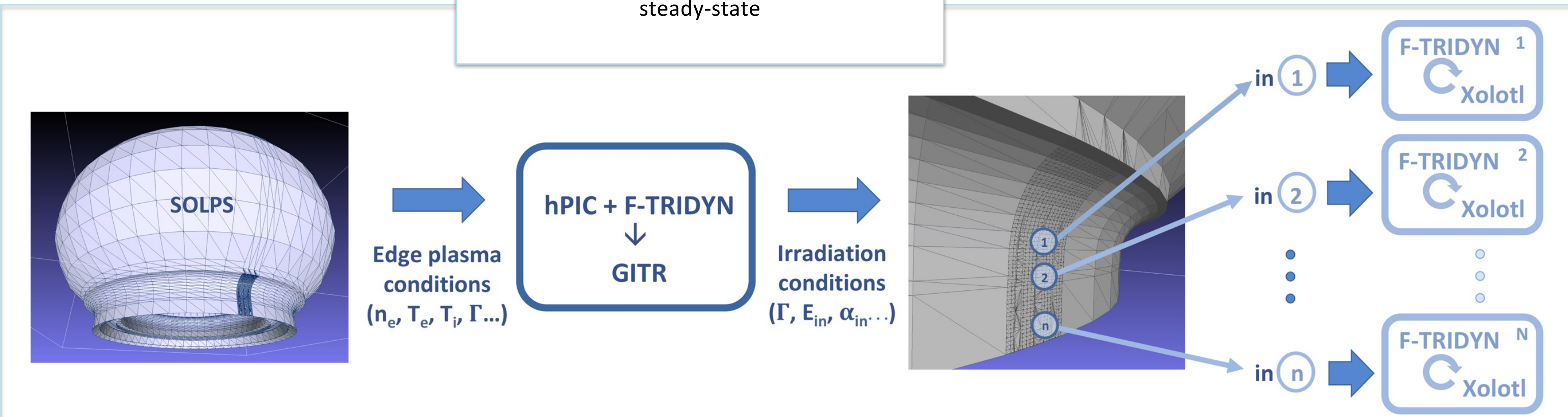
- H interstitials at the WB/W interface prefer to diffuse into bulk W or move along the interface
- H trapping capacity of a vacancy at the W/WB interface decreased relative to bulk W

L. Yang and B.D. Wirth, "First principles study of H solution, diffusion and clustering at the W/WB interface", *manuscript pending submission (2024).*

Integrated PSI modeling approach

- This technique has been successfully applied to interpret and predict PSI experiments in current and future tokamaks

Workflow for integrated modeling PSI in steady-state



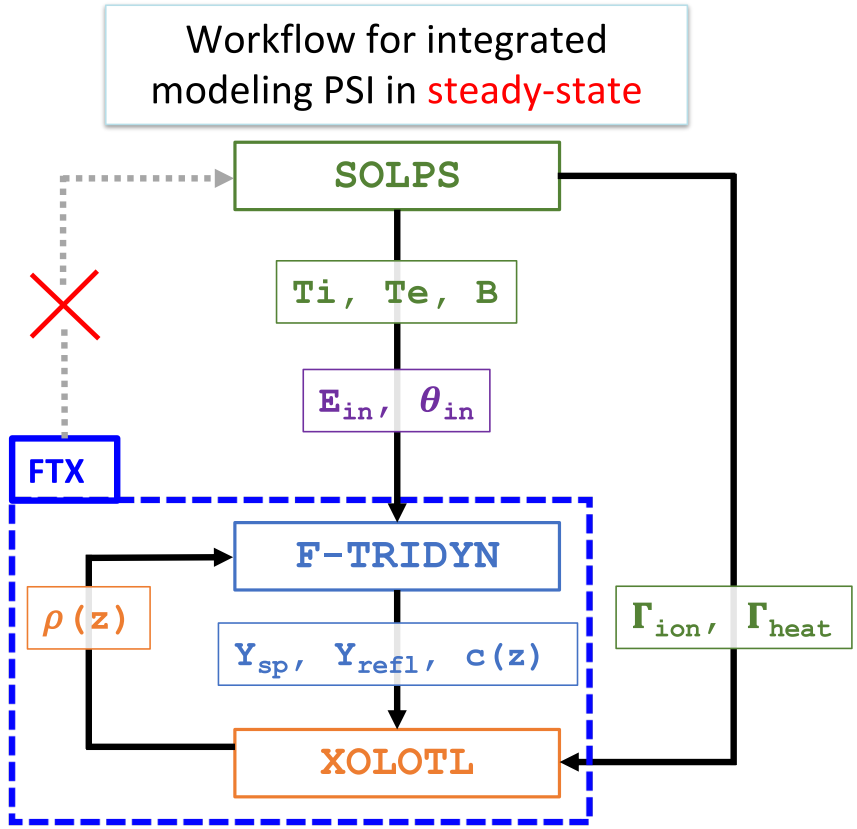
- We have previously applied this framework to model multiple locations in the ITER divertor, during steady-state, full-power burning plasma operations, for pristine W as well as W pre-damaged by He plasma
  - Includes He clustering and bursting, H/He interaction, solving the heat equation, Soret effect diffusion , and global sensitivity analysis

A. Lasa et al, *Nucl. Fusion* **61** (2021) 116051
A. Lasa et al., *Phys. Scripta* **T171** (2020) 014041
D. Dasgupta et al., *Nuclear Fusion* **63** (2023) 076029
P. Robbe et al., *Comp. Mater. Science* **226** (2023) 112229

One-way coupling: SOLPS -> FTX (F-TRIDYN & Xolotl)

- Here we re-develop the high-fidelity one-way workflow used in [1,2]

- Main components:
  1) **SOLPS**: Fluid plasma + MC neutrals
  2) **F-TRIDYN**: Binary-collision approximation code
  3) **Xolotl**: Continuum cluster dynamics code



Y_{sp} = sputtering yield
c(z) = implantation profile
Y_{refl} = reflection coefficient
Y_{rec} = total recycling coefficient
ρ(z) = material composition
E_{in} = impact energy
θ_{in} = incident angle

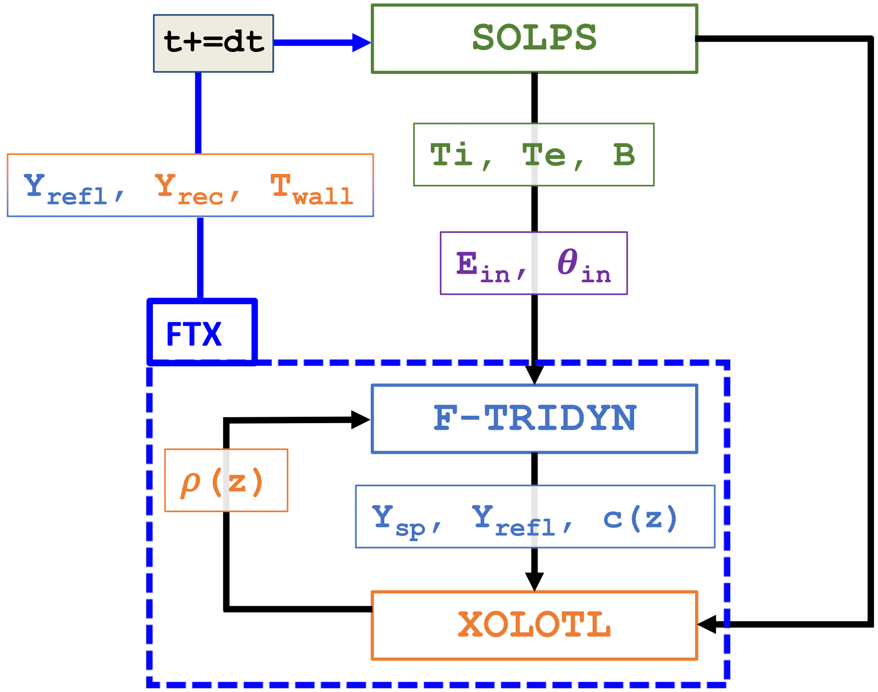
[1] J.M. Canik et al., *27th IAEA, FEC,* 2018
[2] A. Lasa et al, *Nucl. Fusion* **61** (2021) 116051

Two-way coupling workflow can address transient scenarios

- New **two-way** workflow using IPS allows modeling of transient scenarios

  → applied this model to simulate W sample in DIII-D DIMES probe subject ELMy plasmas (not covered here in interest in brevity, but successful proof of concept – presented at PSI-2024 by J.-S. Park)*

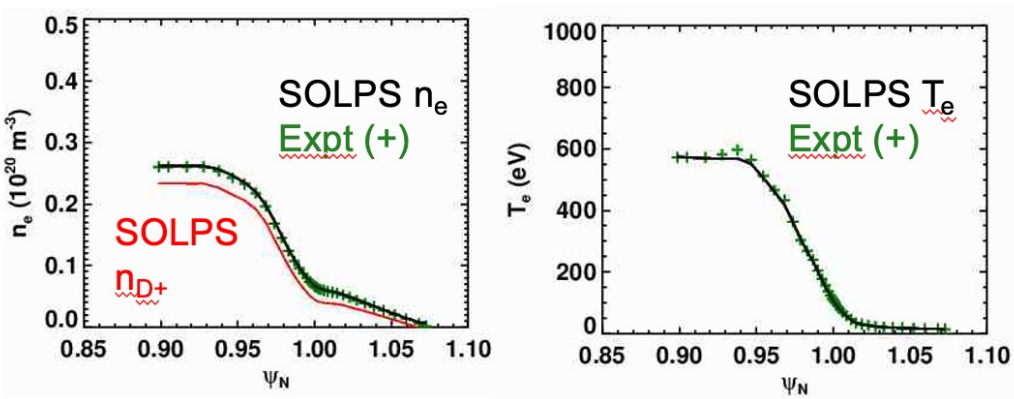
Workflow for integrated modeling PSI in two-way

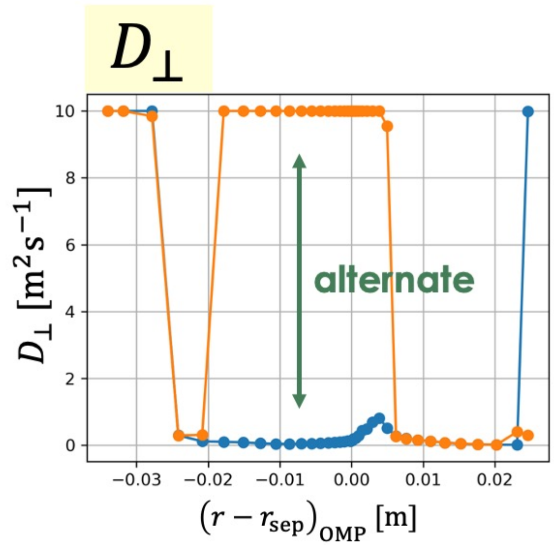


* A. Lasa, J.-S. Park, J. Lore, et al., "Exploring the effect of ELM and Code-Coupling Frequencies on Plasma and Material Modeling of Dynamic Recycling in Divertors", *Nuclear Fusion (2024) manuscript under review*

DIII-D Example of time-dependent SOLPS for ELMy plasma

Constrain the simulation using inter-ELM DIII-D experimental upstream profiles to get $D_\perp$ and $\chi_{i,e}$ → Enhance $D_\perp$ & $\chi_\perp^{i,e}$ to increase cross-field transport, simulating ELMing conditions → Periodically **alternate** the transport profiles between those with and without the transport enhancement

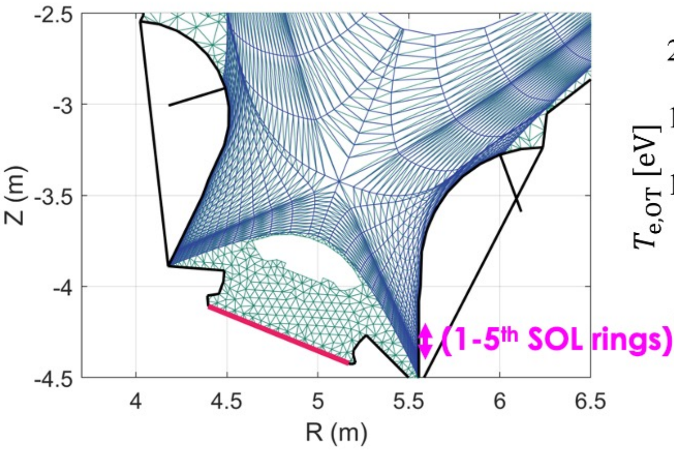


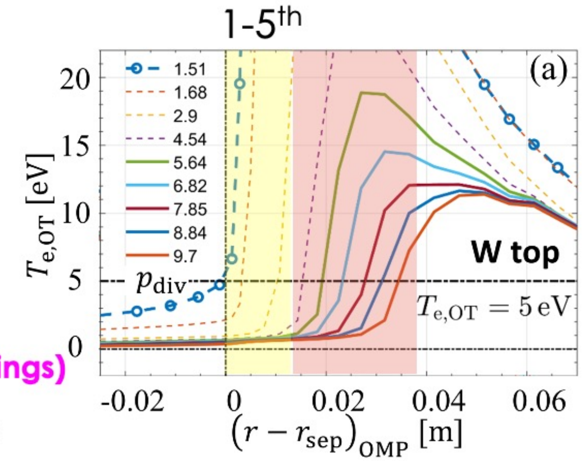


DIII-D discharge condition

- 1.8 T, 0.9 MA
- T_{et}~30 eV
- $q_\perp$~0.54 MW/m^2
- ELM freq.: 50-110 Hz
- $\Delta W_{MHD}/W_{MHD} < 6\%$

Coupled workflow applied to ELMy ITER plasma





Preliminary result – ITER

Coupling at 5 locations: (1-5th SOL rings)

- Attached condition from ITER PFPO-1 SOLPS-ITER simulation database (IDS#: 103045)*
- [1ms inter-ELM + 1-5 ms intra-ELM]

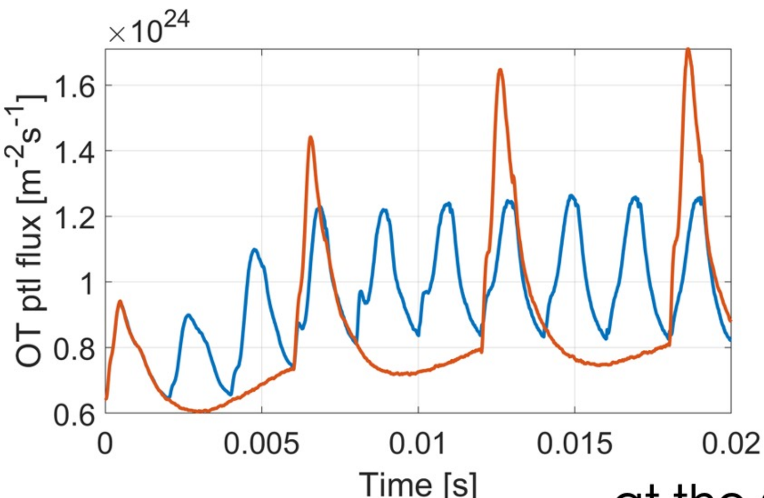
* J.-S. Park et al. *Nuclear Fusion* (2021)

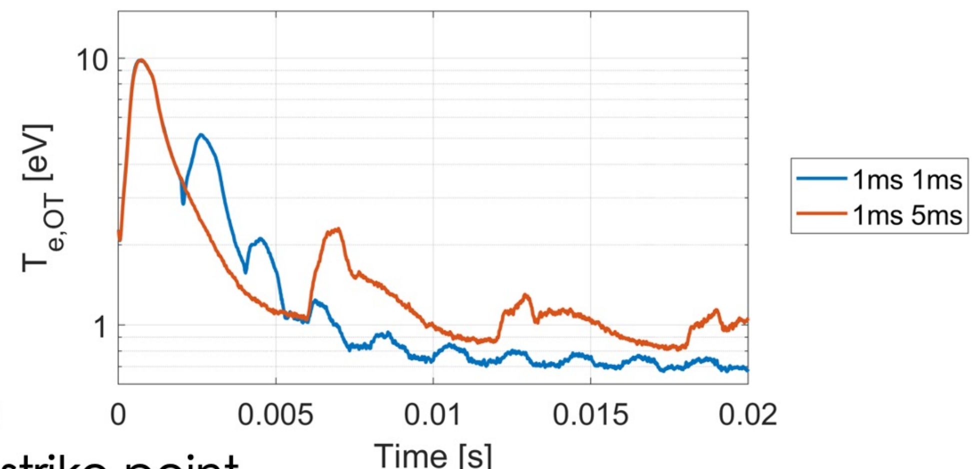
ITER cyclic heat & particle fluxes from time-varying transport profile

Cyclic heat and particle fluxes are introduced through a time-varying transport profile for ITER, like that of DIII-D

- Longer cycle: higher peaks in particle flux and Tet

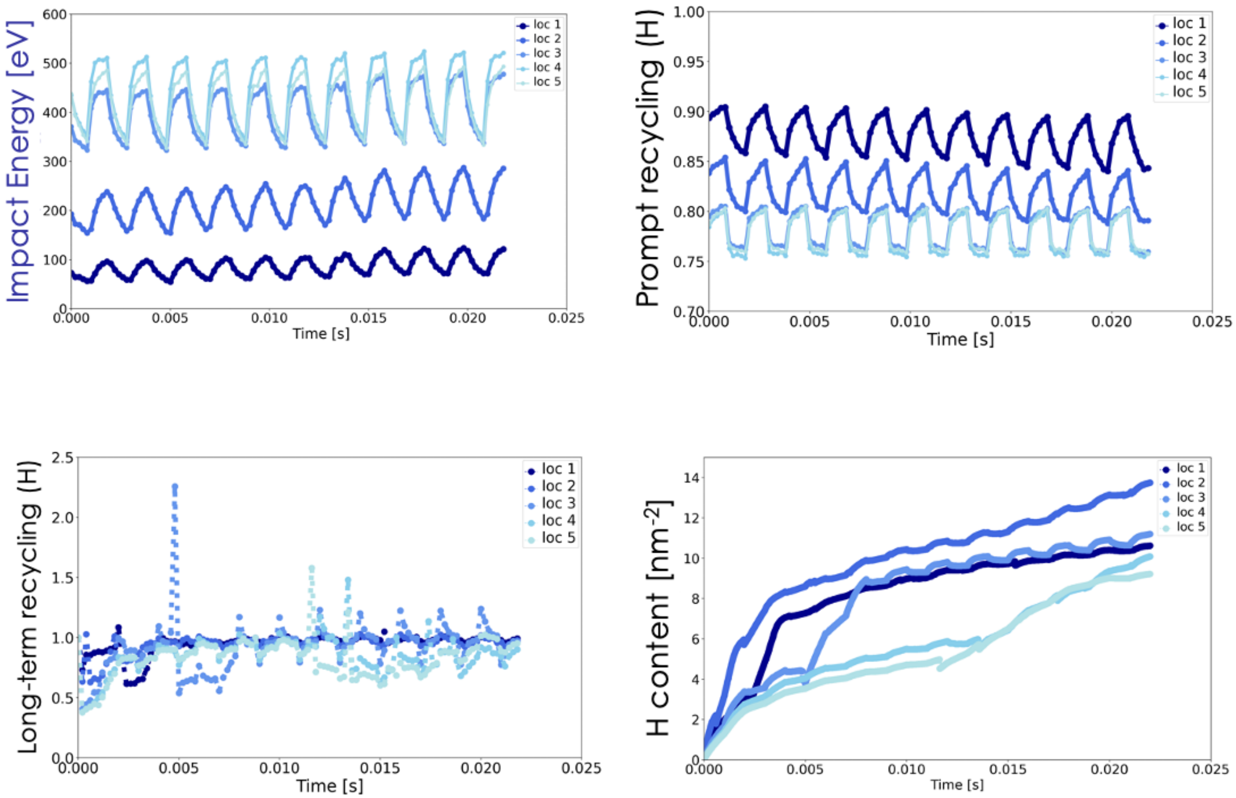
Preliminary result – ITER





at the strike point

ELM cycling



Preliminary result – ITER

- E_{in} varies significantly by locations due to steep target $T_{e,i}$ profiles
- E_{in} significantly affect recycling and implantation characteristics like DIII-D (not shown)*

* A. Lasa and J.-S. Park et al. *Nuclear Fusion* (2024) under review.

Summary & Future Work

- We have discussed a multi-scale & multiphysics modeling approach to addressing plasma-surface interactions
- Atomistically-informed meso-scale model – continuum cluster dynamics (Xolotl) – is the workhorse to integrate the different scales & species at the surface and sub-surface
- Demonstrated time-dependent, coupled PSI model (to be improved for ITER ELM modeling in future using SOLPS-ITER)

- We have shown examples of recent modeling:
  - T-gradient diffusion of SIA, He and H with driving force to reduce
  - H trapping and diffusion at WB-W interface
  - Preliminary results of H isotope recycling (prompt & long-term) and H sub-surface inventory with dynamically coupled PSI model of multiple ELMS

- Remaining challenges are still efficiently dealing with dilute impurities & bridging timescales from 10^{-6} to 10^{5} seconds