PSI SciDAC: Predicting the Performance and Impact of Dynamic PFC Surfaces

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In partnership with:

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DEPARTMENT OF NUCLEAR ENGINEERING

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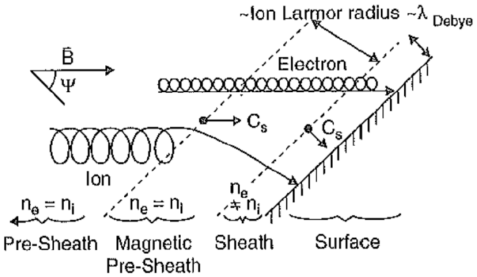
PSI Perspective

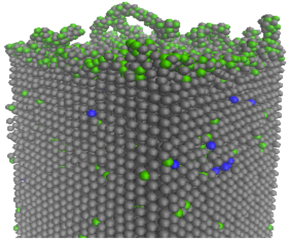
- Objective is to develop leadership-class modeling capability across coupled spatial regions:
  - **Edge/scrape-off-layer region of the plasma, with sheath effects**

  - **Near surface material response to plasma exhaust, with neutron damage and influenced/coupled to plasma sheath**



Plasma Edge
SOL
Sheath – heat & particle flux, recycling, etc.

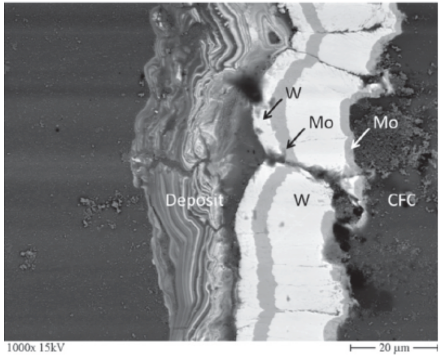
mm



Material surface - erosion (impurity & dust), T retention, surface evolution

10^2 – 10^3 nm

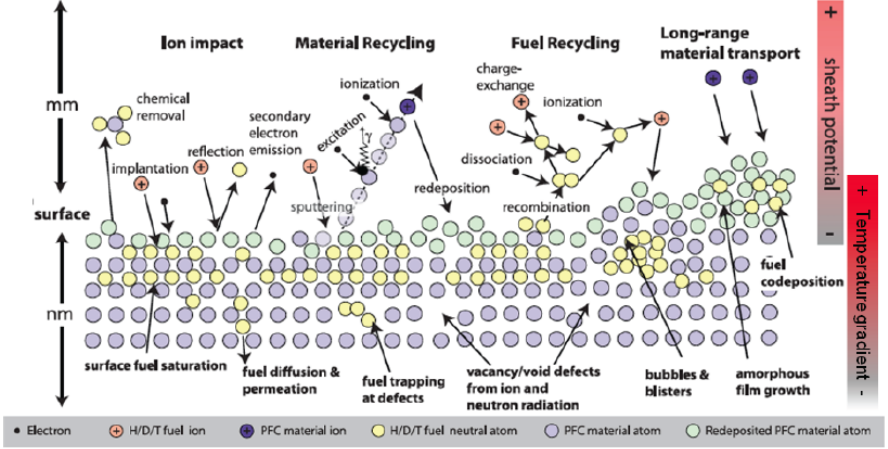
- Develop capability to understand mixed materials evolution & impact on properties, push towards transient conditions, and to dynamically couple the surface on the plasma boundary

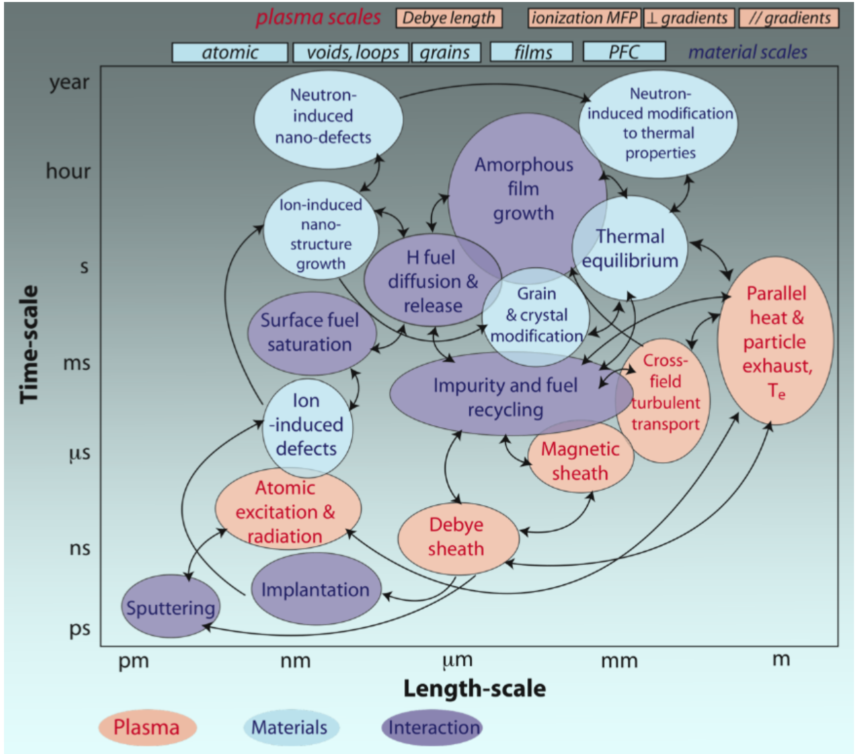


*Introduction to Plasma – Material Interactions**

Strong changes in surface are driven by interactions with plasma

- Erosion, gas retention, sub-surface morphology changes, etc.
- PSI compromise both material and plasma performance





* Wirth, Nordlund, Whyte, and Xu, *Materials Research Society Bulletin* **36** (2011) 216-222

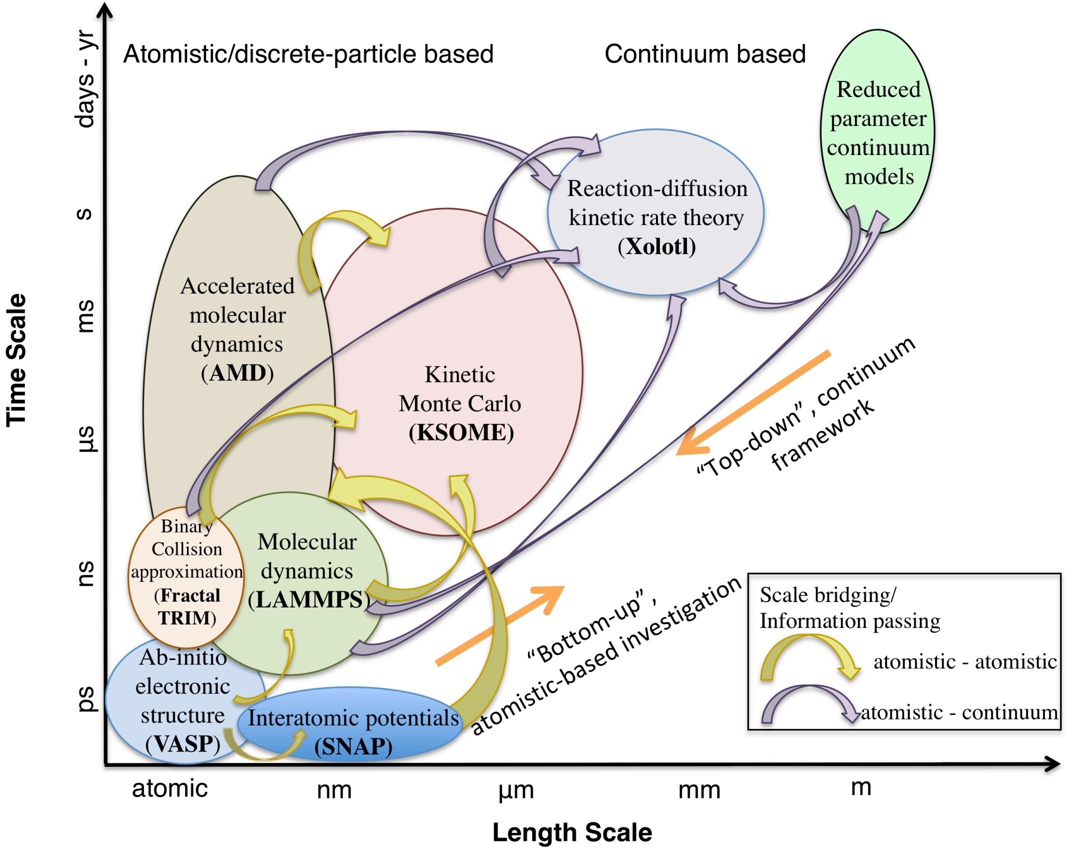
PSI Project Approach & Tasks

Task 1: Multiscale Modeling approach:

Scale bridging to Xolotl

Initiate modeling of mixed surface composition (e.g., Be-W + He/H and N-W) effects of interest to ITER

Transitioning focus to predicting physical properties



Tasks:

- Bridge the scales between atomistic/microstructural and continuum-based PFC simulations to predict evolving PFC surface response (Brian Wirth)

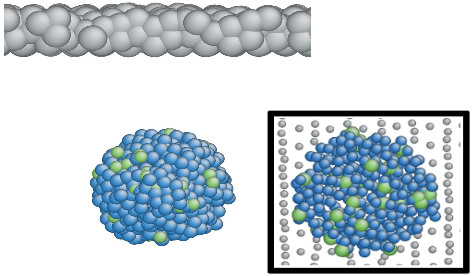
Atomistic modeling of He-H synergies

- MD simulations performed for 2 nm diameter bubble containing high pressure He (3 He/vac) and random distribution of H (0.5 H/vac) at 1800K

- H is observed to rapidly migrate to bubble periphery and remains ‘trapped’ at the bubble interface

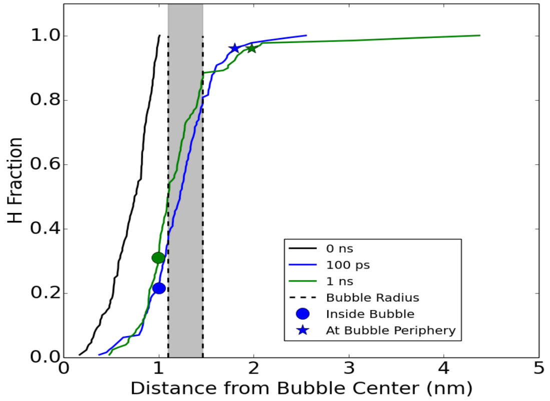
- Raises question about potential for tritium trapping/inventory
  - artifact of interatomic potential
  - short time MD simulations

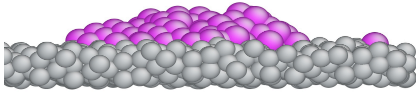
0 ps



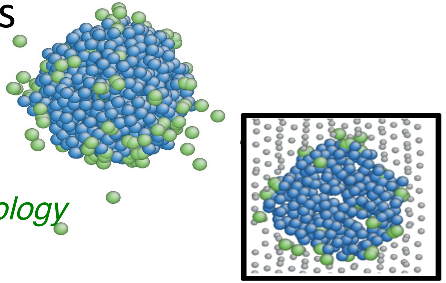
Green: Hydrogen
Blue: Helium
Grey: Surface Tungsten
Magenta: Adatoms

H Distribution for the (111) 1800 K with 3 He/V and 0.5 H/V

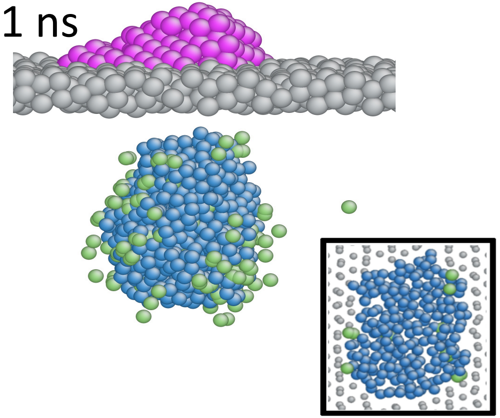




100 ps



1 ns

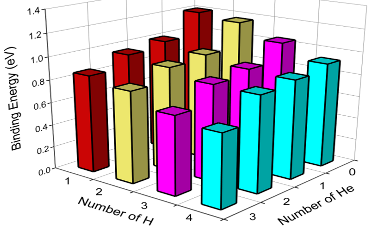


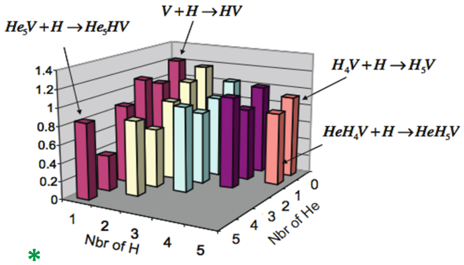
* Bergstrom, Cusentino and Wirth, *Fusion Science & Technology* ***71*** *(2016) 122-135.*

*Hydrogen interactions with He near W surfaces**

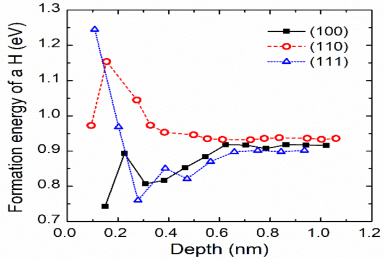
H-He in Bulk W

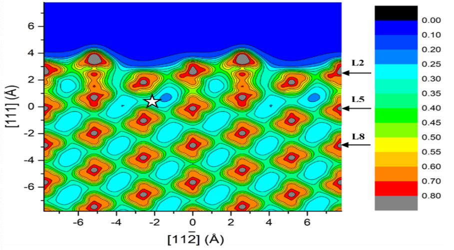
He_xH_yV





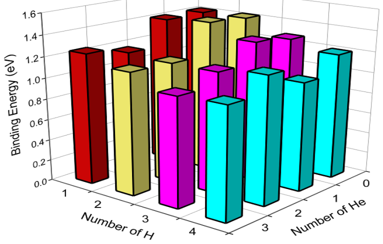
H-He near W (110) surface



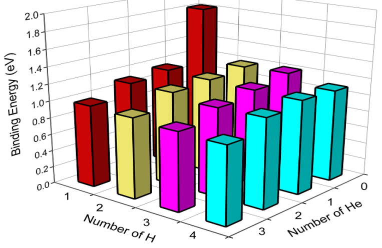


1st Nearest Neighbor

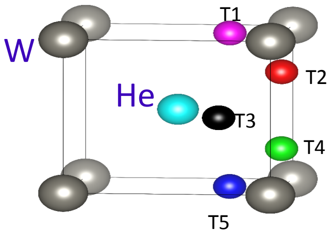
$He_xH_yV_2$

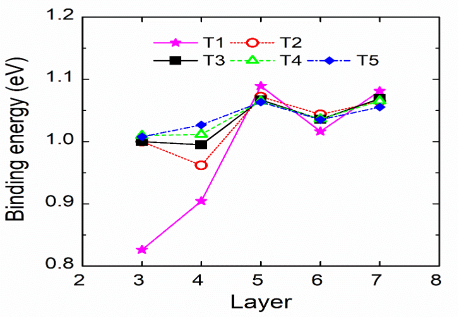


2nd Nearest Neighbor



H binding energy to a HeV below the W(100)





H-He interactions parameterized based on DFT and interatomic potential interactions

* Becquart and Domain, *Journal of Nuclear Materials* **386-388** (2010) 109.

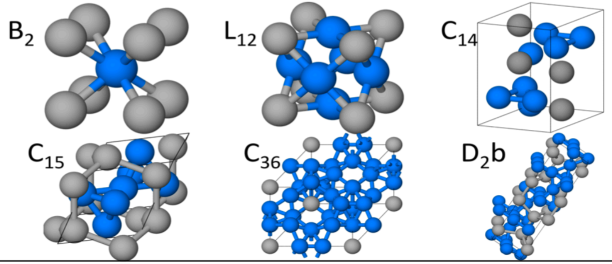
Yang and Wirth, *Journal of Applied Physics* **123** (2018) 2152104; Yang, Bergstrom and Wirth, *Journal of Applied Physics* **123** (2018) 205108; Yang, Bergstrom and Wirth, *Journal of Nuclear Materials* ***512*** *(2018) 357-370.*

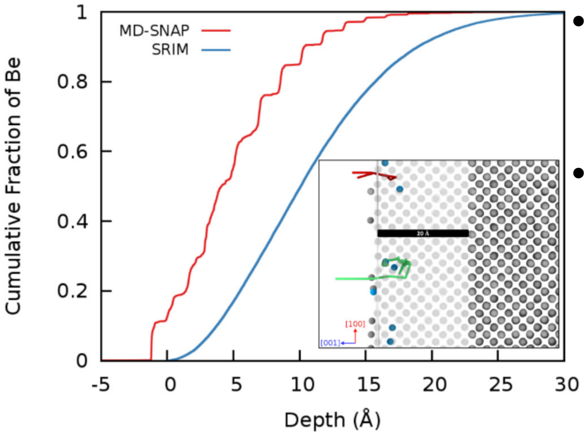
Task 1 – Developing machine learning potentials for W-Be

- SNAP potential of W-Be
- Training data includes DFT for W, Be and mixed W-Be configurations
- Reproduces material properties like cohesive energies and elastic constants

Description	N_E	N_F	σ_E	σ_F
W-Be:				
Elastic Deform†	3946	68040	$\mathbf{3 \cdot 10^5}$	$2 \cdot 10^3$
Equation of State†	1113	39627	$2 \cdot 10^5$	$4 \cdot 10^4$
DFT-MD†	3360	497124	$7 \cdot 10^4$	$6 \cdot 10^2$
Surface Adhesion	381	112527	$2 \cdot 10^4$	$\mathbf{9 \cdot 10^4}$

† Multiple crystal phases included in this group:



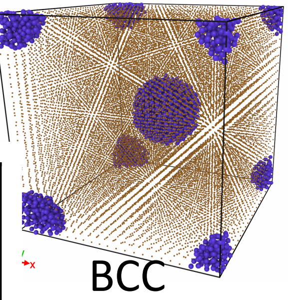


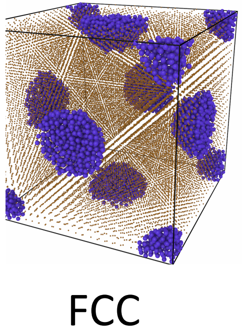
Defect type	Implanted Be Percent	Formation Energy (eV) DFT	SNAP	BOP
[111] Dumbbell	41.2	4.30	3.66	0.67
Substitution	22.2	3.11	3.29	−2.00
Surf. hollow Site	12.3	−1.05	−1.39	−3.52
Tetrahedral inter.	10.4	4.13	4.20	−0.28
[110] Dumbbell	8.4	4.86	4.29	−0.03
Octahedral Inter.	5.3	3.00	5.11	0.34
Surf. Bridge Site	0.03	1.01	0.44	−1.30

- Potential tested for scenarios outside of training data
- SNAP predicts 75 eV Be to implant within 2 nm of surface and reside at <111> dumbbell and substitutional sites or at surface
- DFT formation energies calculated and compared to SNAP
- Overall SNAP reproduces DFT values fairly well and is substantial improvement on existing BOP potential

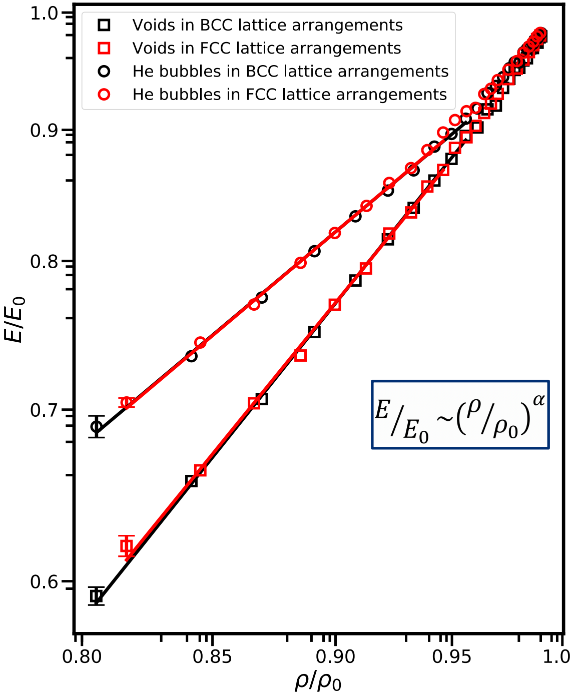
Task 1 – Utilizing atomistic modeling to predict W properties

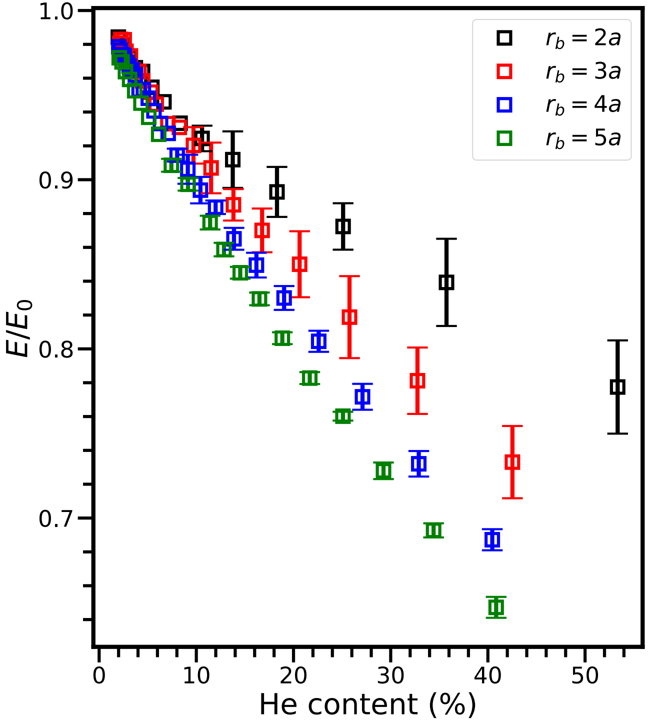
- Molecular-dynamics (MD) simulations with regular He nanobubble arrangements to investigate the effects of plasma exposure on the elastic modulus (stiffness) of PFC tungsten





- Power-law modulus-density scaling relations in PFC tungsten throughout the range of parameters examined
- Stiffness reduction of PFC tungsten with increasing He content, with further reduction with increasing nanobubble size

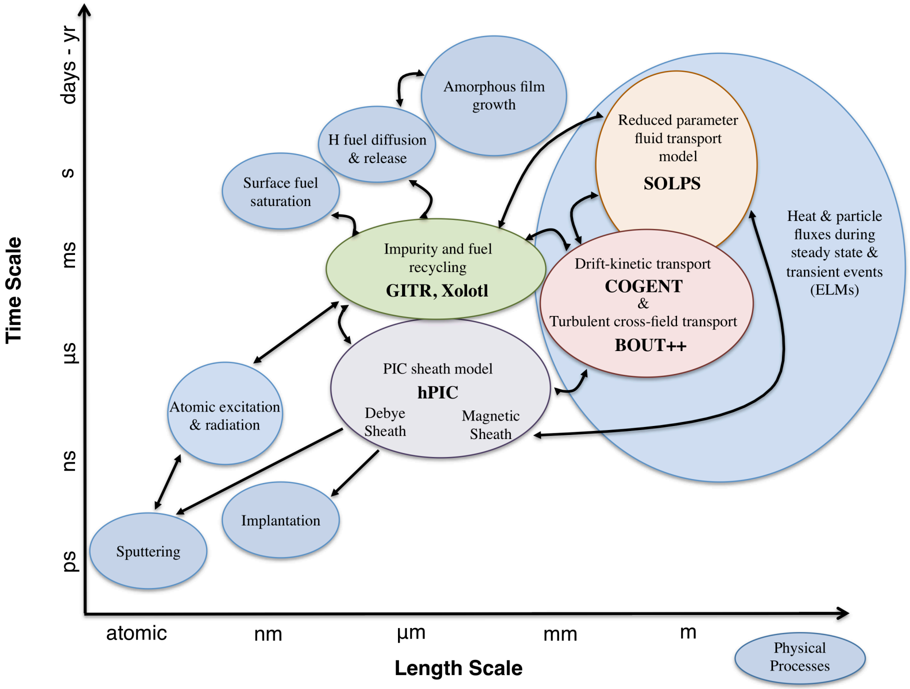




PSI Project Approach & Tasks

Task 2-3: PMI & Boundary Physics Integration –
Physical processes, codes and scale integration

Initiating PSI feedback to boundary plasma and modeling of transient events



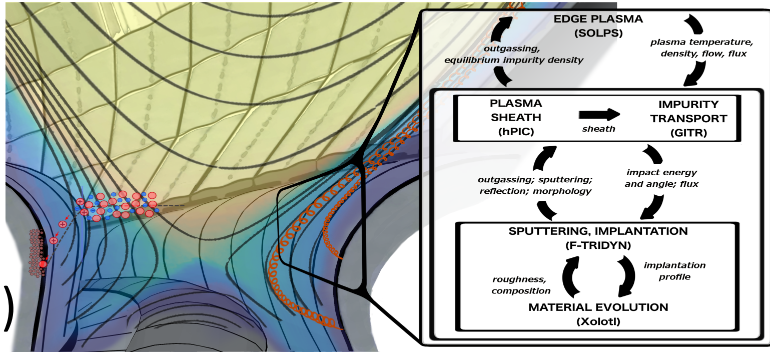
Tasks:

- Integrate boundary plasma and surface evolution models, specifically investigating effects of plasma sheath and evolving surfaces (John Canik)
- Study the dynamic response of the surface to transient events, and exploring synergistic phenomena between the near-surface plasma and wall response emphasizing dynamic recycling processes (Ilon Joseph and Sergei Krasheninnikov)

Developing an integrated PSI modeling capability

Includes models for

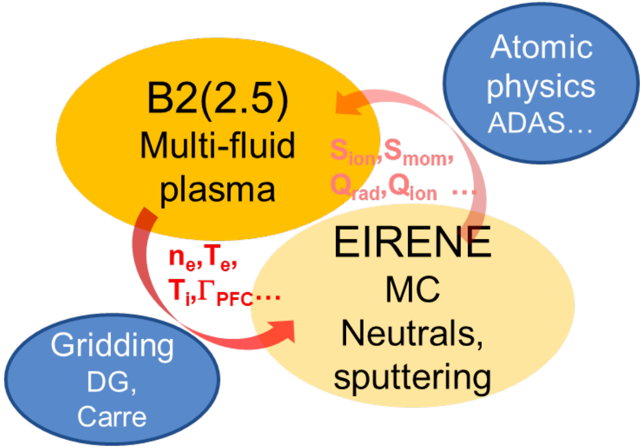
- Background plasma transport (SOLPS)
- Near-surface sheath (hPIC)
- Erosion and transport of wall material (GITR)
- Implantation of ions into the material (F-TRIDYN)
- Dynamics of the subsurface (Xolotl)



- Workflow implemented with one-way coupling from plasma to material modeling steady-state conditions

*Subject of 2018 DOE-FES Theory & Simulation Performance Target: full report can be found at https://science.energy.gov/fes/community-resources/

Edge plasma modeled with fluid (SOLPS-ITER) and kinetic (hPIC) simulations



B2(2.5)
Multi-fluid
plasma

Atomic
physics
ADAS…

$S_{ion}, S_{mom}, Q_{rad}, Q_{ion}$ …

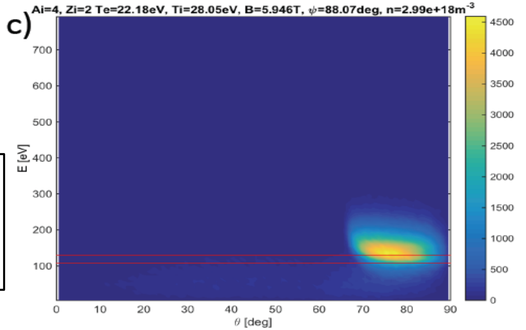
EIRENE
MC
Neutrals,
sputtering

$n_e, T_e, T_i, \Gamma_{PFC}$…

Gridding
DG,
Carre

- **SOLPS-ITER** models coupled plasma/neutral transport
  - Classical transport assumed parallel to magnetic field (+kinetic corrections)
  - Ad-hoc transport coefficients in the cross-field direction
- 2D: radial+poloidal
- Monte Carlo code EIRENE simulates neutral transport
- Comprehensive atomic and PMI models

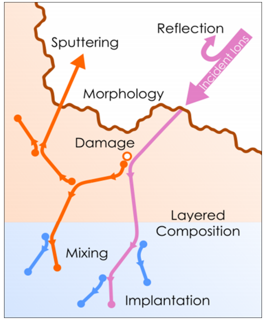
IEAD for ITER-like condition



- **hPIC**: Full-f, full-orbit particle-in-cell code
- Inputs
  - Local plasma parameters near surface from SOLPS
  - Magnetic field strength and angle
- Outputs
  - Ion energy-angle distribution (IEAD) of particles striking the wall

See poster by
D. Curreli

Wall impurity erosion, transport and re-deposition are modeled using Fractal TRIDYN and GITR



Fractal (F)-TRIDYN: Ion-solid interactions calculated using binary collision approximation

Version of TRIDYN** that includes effect of surface morphology

Fractal surface models either explicitly or statistically to account for surface roughness on sputtering etc

Input: IEAD; outputs reflection, erosion, implantation rates for mixed surface compositions

*Drobny, J, et al, J. Nucl. Mat. **494** (2017) 278
Miller, W., Comp. Phys. Comm. **51 (1988) 355

Global Impurity Transport (GITR) code uses trace impurity approximation

- Full-orbit Monte Carlo with operators for Lorentz force, Coulomb collisions, diffusion, and atomic physics
- Background plasma profiles, geometry, sheath and surface characteristics as input (SOLPS, hPIC, F-TRIDYN)

$$m_a \frac{\Delta \bar{U}}{\Delta t} = \underbrace{q_a(\bar{E} + \bar{U}\times\bar{B})}_{\text{Lorentz Force}} + \underbrace{m_a\left[\overbrace{\hat{U}_\parallel \frac{U}{\tau_s} \pm \hat{U}_\parallel\sqrt{\frac{U^2}{\tau_W \Delta t}} \pm \hat{U}_{\perp,1}\sqrt{\frac{U^2}{2\tau_D\Delta t}} \pm \hat{U}_{\perp,2}\sqrt{\frac{U^2}{2\tau_D\Delta t}}}^{\text{Classical velocity change moments (Fokker-Planck)}}\right] + \overbrace{(\alpha\nabla_\parallel T_e + \beta\nabla_\parallel T_i)}^{\text{Thermal gradient force correction}}}_{\text{Collisional Terms}}$$

$$\Delta\bar{x} = \bar{v} * \Delta t + \underbrace{\sqrt{D_\perp \Delta t}\cdot \hat{e_\perp}}_{\text{Anomalous perp. Diffusion}}$$

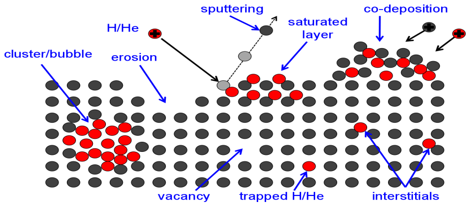
Xolotl models surface evolution*

- Solves the Drift-Diffusion-Reaction equations in one or more dimensions

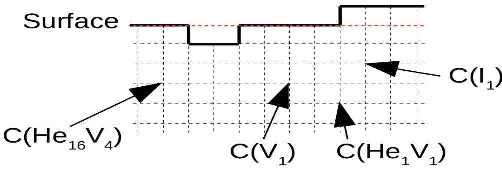
$$\partial_t C_i(z,t) = -\nabla \cdot u_i(z) C_i(z,t) + D_i(T)\nabla^2 C_i(z,t) - Q_i(\bar{C}(z,t)) + \Gamma \cdot \rho_i(z,t) \ ,$$

- 2D/3D implemented
- Tungsten material is represented by the concentration of clusters at each spatial grid point
  - Interstitials, Vacancies, Helium, Deuterium, and Tritium, and Mixed He-D-T-V clusters
  - Includes models for bubble bursting and motion of surface
- Parameters for equations obtained from atomistic simulations, geometric considerations
  - Successfully benchmarked against molecular dynamics simulations
- Open source, available at: https://github.com/ORNL-Fusion/xolotl/

Atomistic picture

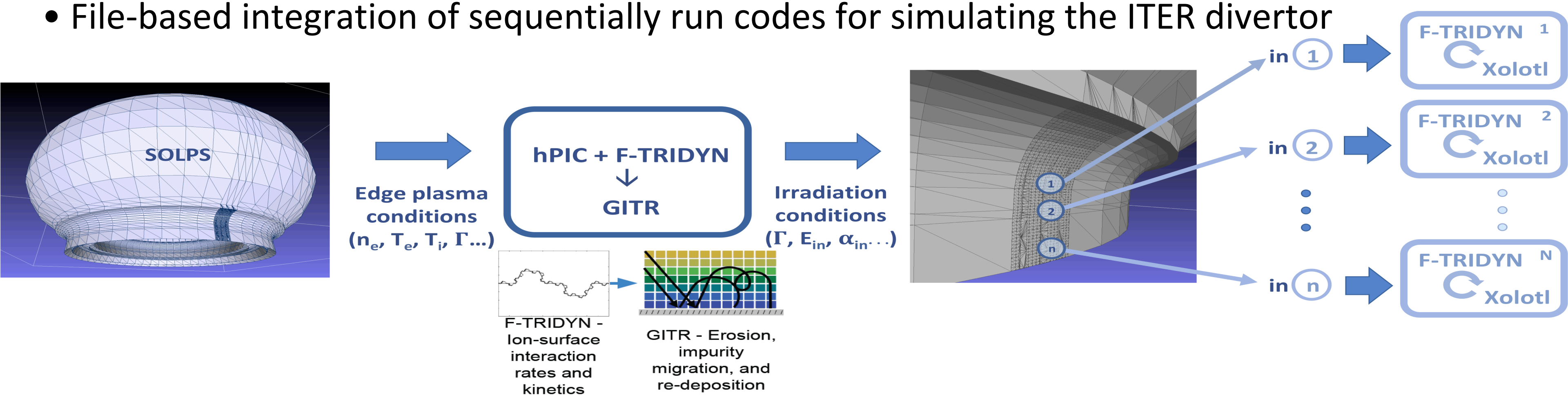


Continuum picture



Code Integration Framework

- IPS HPC interface framework, developed by FES AToM SciDAC used to integrate plasma edge and materials modeling codes
- File-based integration of sequentially run codes for simulating the ITER divertor



SOLPS

Edge plasma conditions (n_e, T_e, T_i, Γ...)

hPIC + F-TRIDYN
↓
GITR

F-TRIDYN - Ion-surface interaction rates and kinetics

GITR - Erosion, impurity migration, and re-deposition

Irradiation conditions (Γ, E_{in}, α_{in}...)

in 1 → **F-TRIDYN 1 Xolotl**

in 2 → **F-TRIDYN 2 Xolotl**

in n → **F-TRIDYN N Xolotl**

SOLPS provides background (edge) plasma conditions to hPIC (sheath effects), which provides incident particle flux to F-TRIDYN (sputtering yields, implantation profiles) & to GITR (impurity transport and re-deposition) & Xolotl (sub-surface gas dynamics)

− Recently demonstrated predictions of a 10-second helium plasma discharge & burning plasma operation in ITER & benchmarked against linear plasma device PISCES (shown last year)

Workflow involved performing 25-36 independent, 1-dimensional coupled F-TRIDYN − Xolotl simulations as a function of spatial location to sample varying plasma conditions − using 160-200 nodes on NERSC Edison

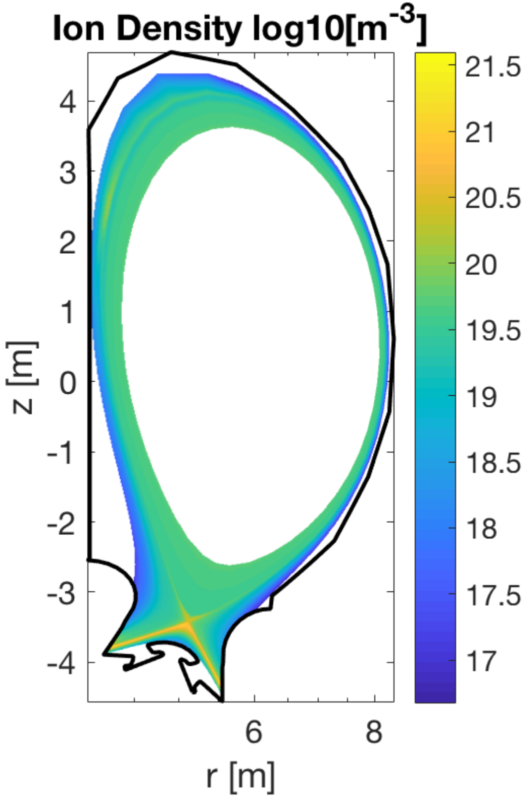
Sol-PS provides edge plasma conditions at the divertor

ITER Burning Plasma

SOLPS

- P_{in}=100MW, D plasma + He, Ne, Be (CX-only)
- P_{rad}=73 MW, mainly by Ne, in the divertor

→ ~7 MW/m2 at the target



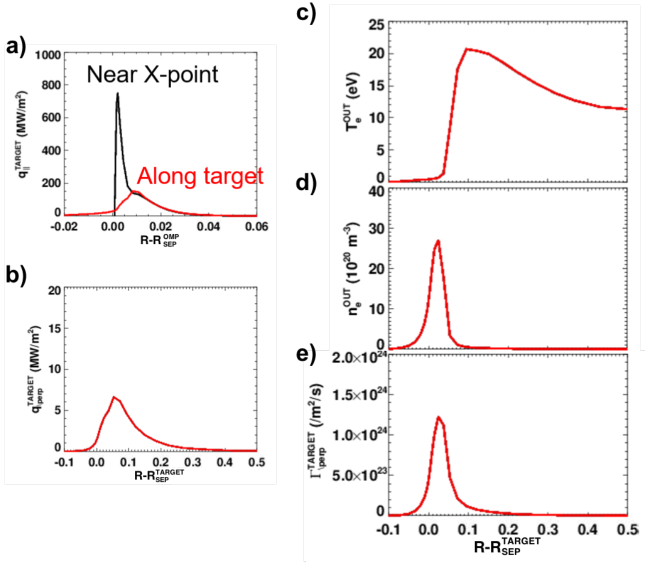
Sol-PS provides edge plasma conditions at the divertor

Predicted plasma profiles are representative of a partially detached divertor

SOLPS

- P_{in}=100MW, D plasma + He, Ne, Be (CX-only)
- P_{rad}=73 MW, mainly by Ne, in the divertor

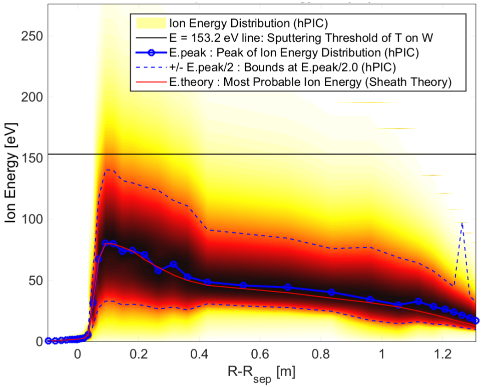
  → ~7 MWm^{-2} at the target
- The calculated plasma profiles are consistent with a partially detached divertor



hPIC calculates the impact energy-angle distributions

hPIC

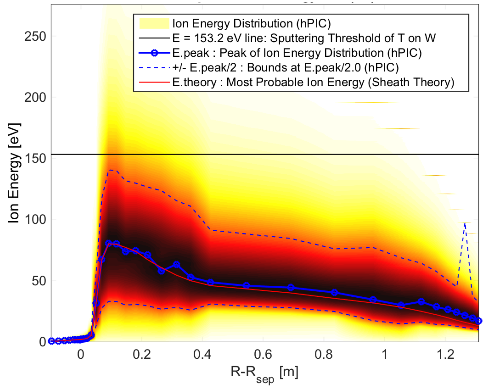
- 1D3V, Multi-species (D, T, He, Ne), 36 locations



hPIC calculates the impact energy-angle distributions

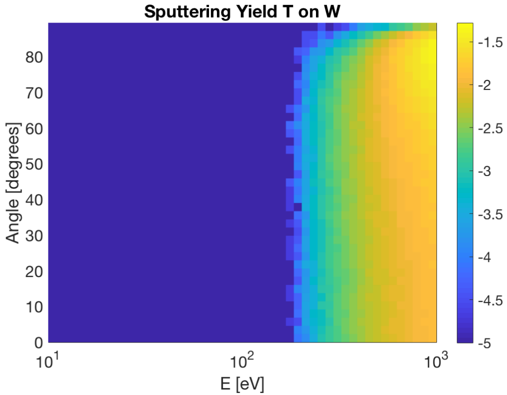
hPIC

- 1D3V, Multi-species (D, T, He, Ne), 36 locations
- hPIC calculated peak of distribution is consistent with the most probable energy expected from classical sheath theory
- Particles with E_{in} in the high-energy tail, as predicted by hPIC, can contribute to sputtering of W by light species



F-TRIDYN

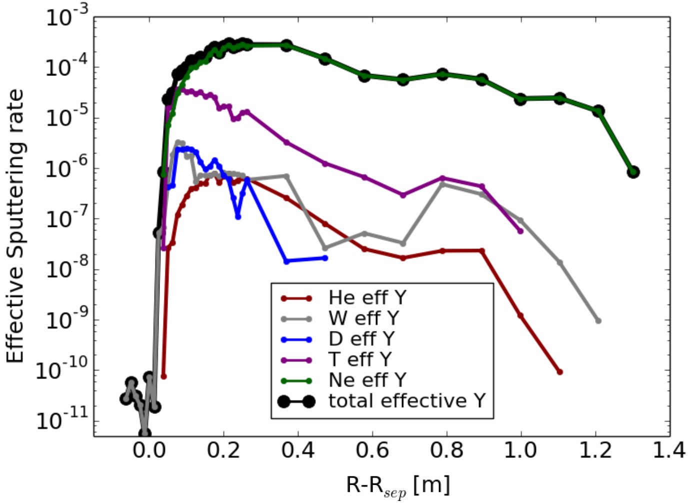
- A reduced binary collision approximation model calculates the W sputtering & gas implantation source, based on the hPIC input fluxes and
- Based on $O(10^4)$ combinations of impact species, energy and angle



GITR models W impurity transport in ITER

GITR

- models W migration across the divertor target
    - In 3D, 2.5M particles, *O*(10^6) time-steps

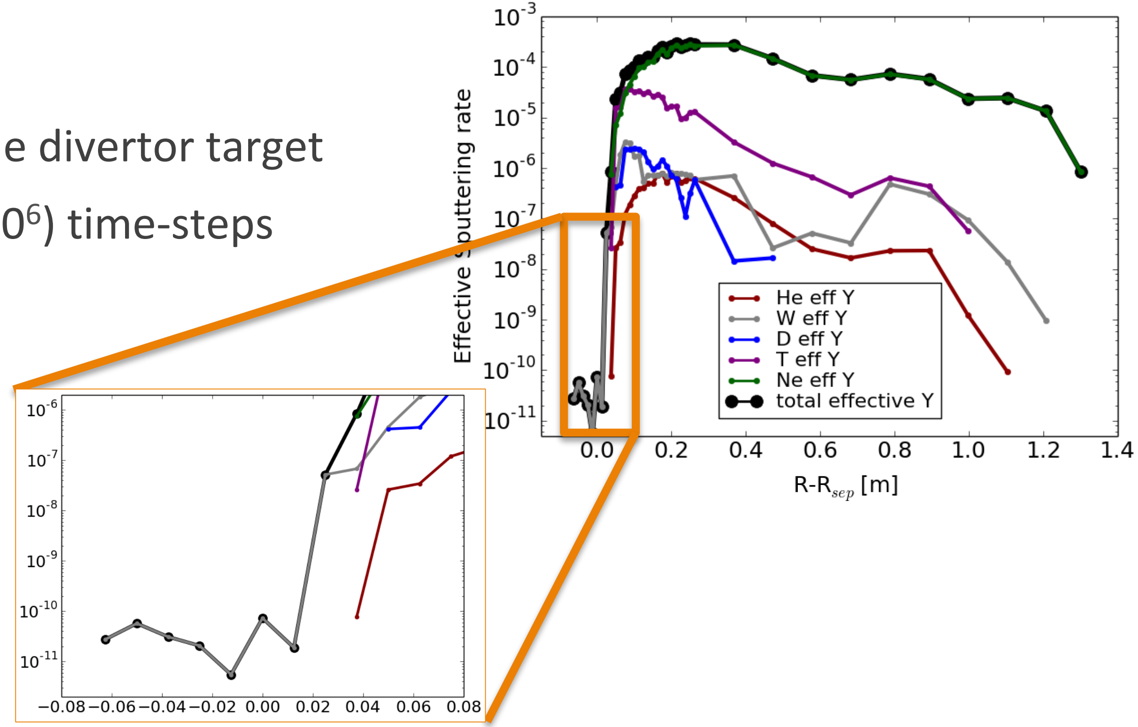


GITR models W impurity transport in ITER

<u>GITR</u>

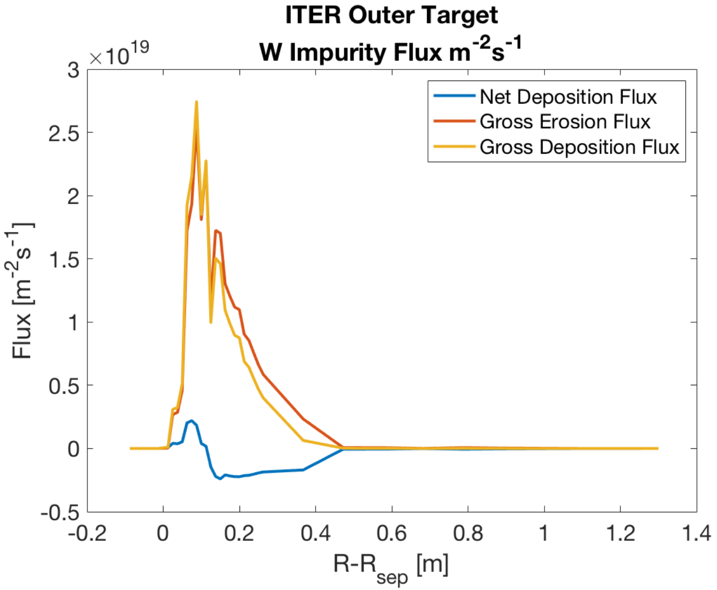
- models W migration across the divertor target
  - In 3D, 2.5M particles, *O*(10^6) time-steps

- Neon dominates surface sputtering
  - except around strike point



GITR predicts strong local re-deposition, with net deposition near strike point & erosion along the target

- 10^4 instances of F-TRIDYN each with 10^5 particles build the reduced model for sputtering and reflection yields
- Simulations of GITR with 2.5×10^6 particles for 10^6 time-steps model W migration across the divertor
- W erosion and re-deposition are strongly correlated
  - Due to 93% of prompt and local re- sdeposition
  - Net deposition around the strike point results from transport by local E fields and more effective deposition with lower T_i

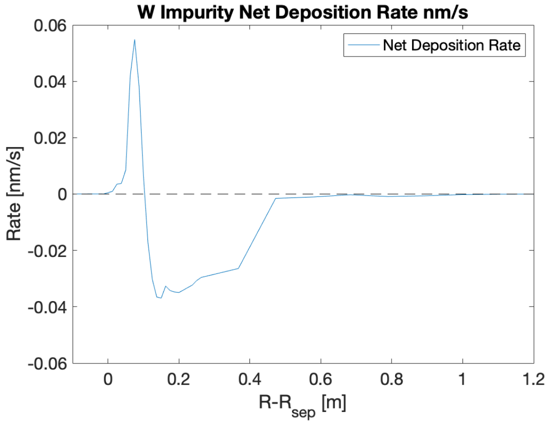


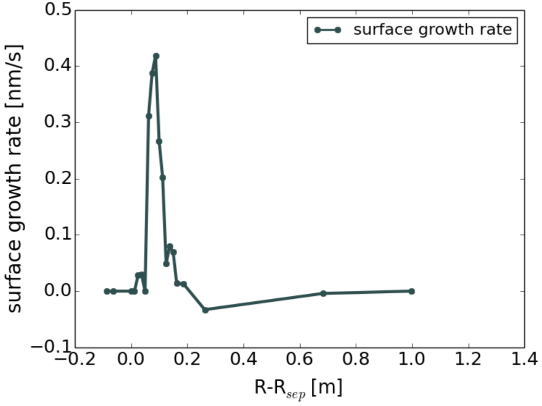
Surface erosion predicted by Xolotl resembles that predicted by GITR, mediated by sub-surface gas dynamics

F-TRIDYN / Xolotl

- General characteristic of surface erosion look the same in GITR and Xolotl
- Differences around the strike point arise from trap mutation and surface growth induced by He clusters

- Higher growth in Xolotl around the strike point, caused by trap mutation (T_i~eV, shallow He implantation)
- Surface height in Xolotl resembles that of GITR further along the target, as trap mutation is less likely (Ti~40eV, deep He implantation)

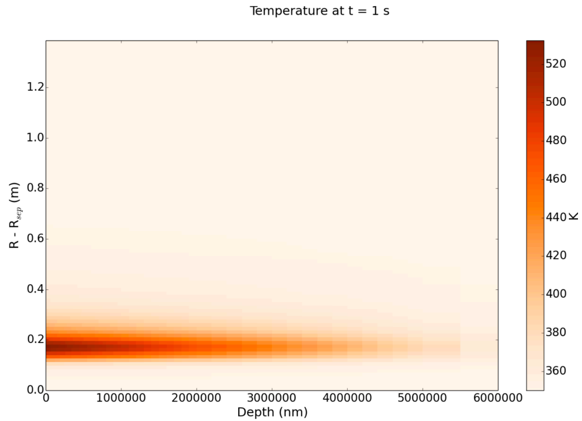


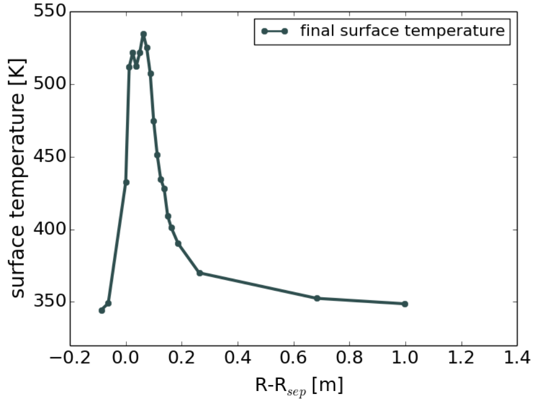


Heat flux increases surface temperature by ~200K

Xolotl

- The thermal coupling between locations is small
    - We run multiple, independent 1D locations & temperatures agree well with 2-D calculations
    - This may change in the full power operation of 500 MW
- We predict changes in T_{surf} of up to ~200K
    - No threat of melting or recrystallization (no transients included)
    - It does affect gas dynamics



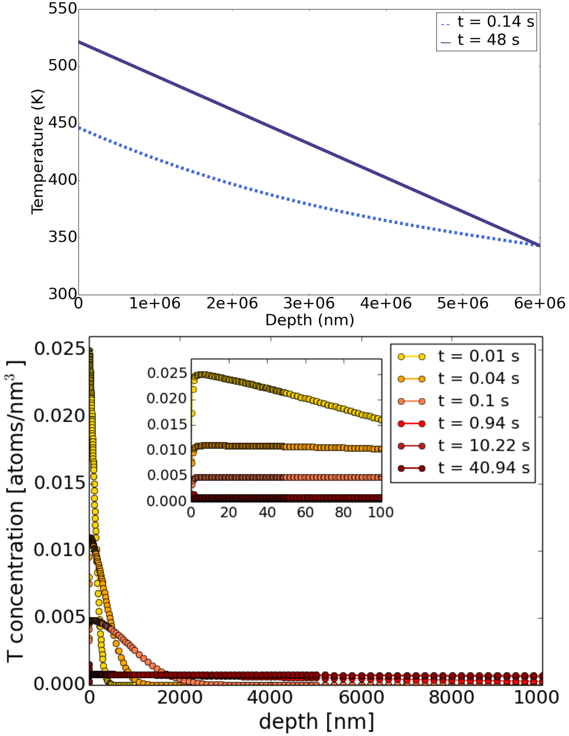


D & T diffuse faster with increasing surface temperature

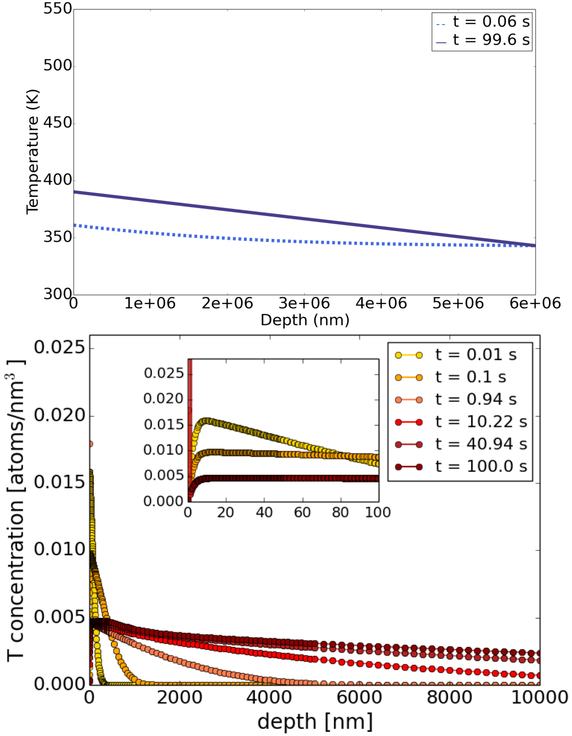
Xolotl predictions:

- The peak in concentration takes the value expected for $T=T_{surf}(t)$
- Gases diffuse faster, mainly outgassing
- Results for D follow the trends of T, and thus are not shown here

$R\text{-}R_{sep}$=0.025m: q~5MW/m^2



$R\text{-}R_{sep}$=0.19m: q~1MW/m^2

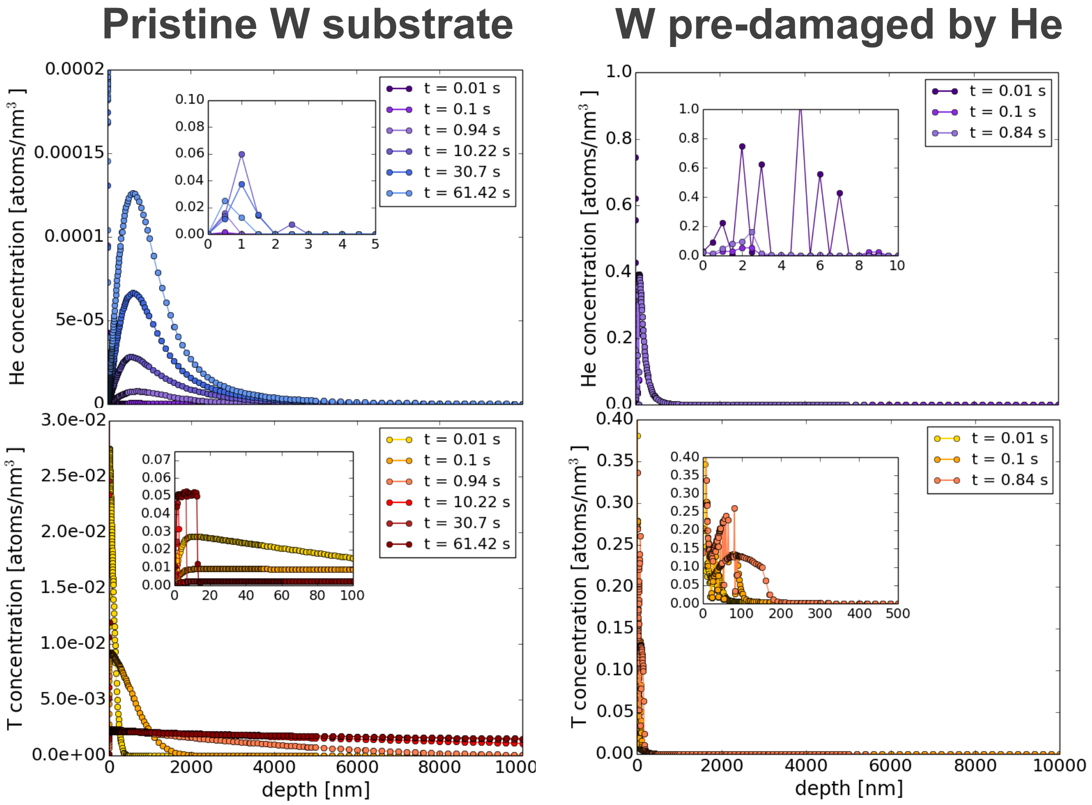


He pre-exposure provides a barrier to deeper T permeation

At $R\text{-}R_{sep}$=0.11m,

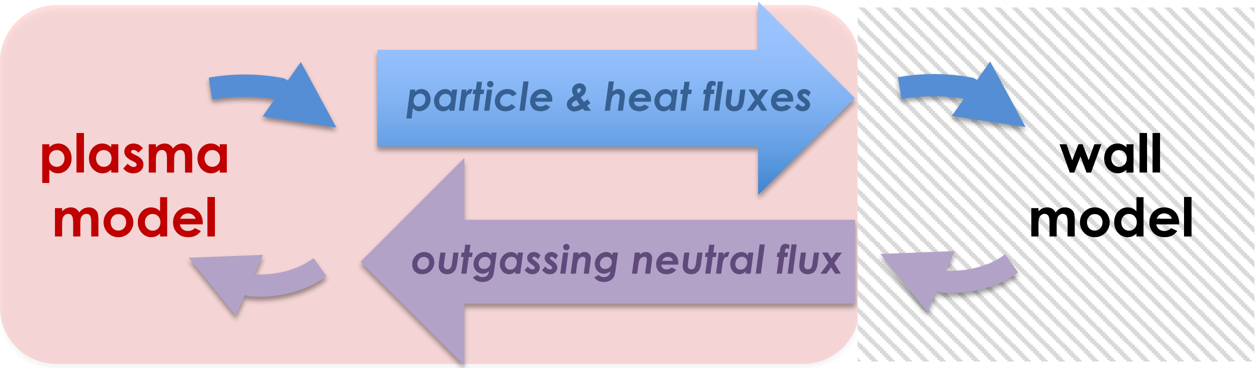
q~3 MW/m^2

- The pre-implanted He clusters burst as T_{surf} increases, leaving V-clusters and voids that trap T (D) as well as refill with He
- V and He clusters (which trap T in the near surface) form a permeation barrier and limit the T_{surf} dependence of the near-surface T concentration (in this T_{surf} and *q* ranges)



Task 3: Dynamics of coupled PSI

- **High-fidelity models for both the edge plasma and material PFCs must be coupled to develop predictive capability**
  - Perform the first studies of dynamic recycling and material erosion caused by transient events from the SOL plasma to the sheath to the material surface



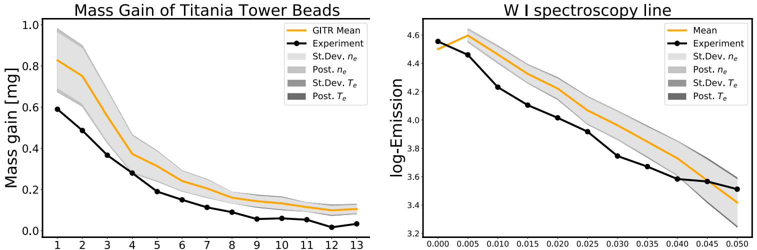
See poster by
M. Umansky

- **Dynamic coupling of plasma and materials models will be used to understand main ion recycling, material erosion, & impurity production**
  - Do these interactions cause new types of coupled plasma-wall oscillations and instabilities? Will plasma-wall interactions change the character of turbulence near material surfaces?

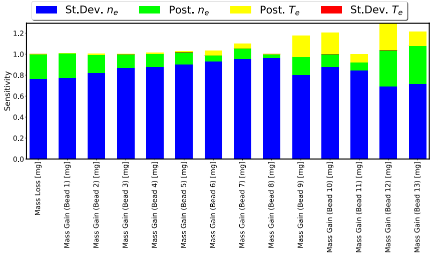
Uncertainty Quantification for Impurity Migration

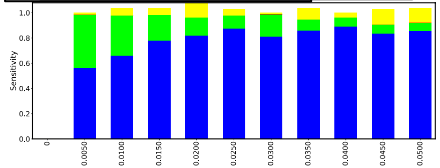
- Bayesian inference of input profiles of plasma density and temperature using processed data from Langmuir probe measurement
- Polynomial chaos (PC) representation of Bayesian posterior probability density functions, augmented with the intrinsic stochasticity of the input profiles
- Propagation of PC through GITR using regression to build GITR output PC expansions
- Variance decomposition of output PCs and attribution of uncertainties

Output profiles from GITR:
predictive uncertainty decomposition



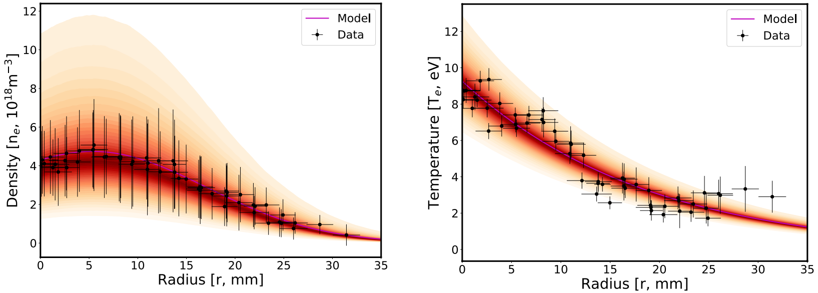
See poster by
K. Sargsyan





Sensitivity via variance decomposition: uncertainty in density profile is the main contributor to output variance

Input profiles: processed data and uncertain model fits



Bayesian inference, PC representation, propagation and variance decomposition employed UQTk (www.sandia.gov/uqtoolkit), an uncertainty quantification library supported by FASTMath SciDAC Institute.

Anisotropic mesh development for hPIC & GITR

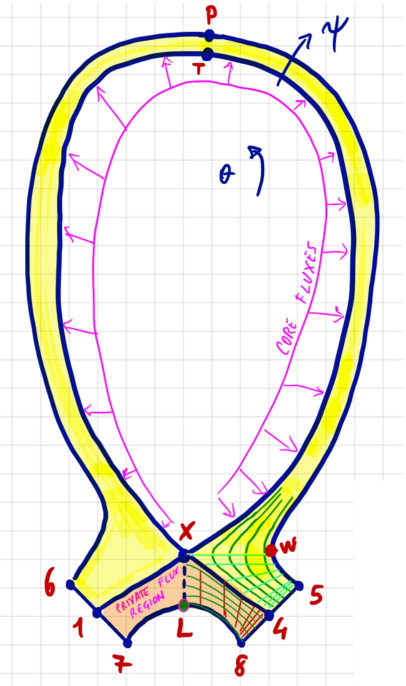
hPIC meshing is driven by three use cases

- 1D radial
- 1D toroidal/poloidal
- 2D SOL

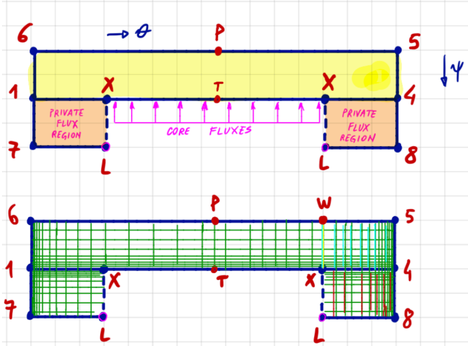
Developed anisotropic boundary layer (BL) mesh capability for hPIC in the following form

- One-sided BL
- Two-sided BL
- Multi-block 2D BL

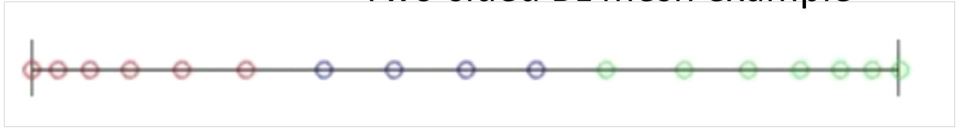
Mesh is represented in an implicit/logical form and mesh operations are supported using interfaces (APIs). Preliminary integration performed at the kernel level (e.g., charge density). Parallelism is under discussion.



See talk by
M. Shephard



Two-sided BL mesh example



Summary & Future Efforts

- Strong interactions within team & with SciDAC Institutes – involving performance/optimization of Xolotl (RAPIDS), strong engagement of PETSc team for solver optimization (FASTMath), engagement on visualization (RAPIDS) and UQ/experimental validation (FASTMath)
- Significant ongoing effort to utilize IPS (ATOMS) for coupling boundary plasma & surface evolution codes to predict tungsten divertor performance in ITER for He discharges (not shown) and burning D-T plasma conditions (ongoing)
- Substantial effort and opportunity to improve individual code performance (e.g., Xolotl, KSOME, hPIC, GITR) and code integration
- Efforts underway to model dynamic PSIs (e.g., feedback of the surface on boundary plasma physics) and develop capability to assess transient (ELM) effects
- Successful completion of the project (2022) will provide simulation tools to evaluate tungsten-based plasma facing divertor component performance and feedback of surface/plasma boundary on the burning plasma