PSI2 SciDAC — Integrating Codes to Model Plasma Surface Interactions: focus on Plasma Sheath Effects and Sputtering Near Surfaces

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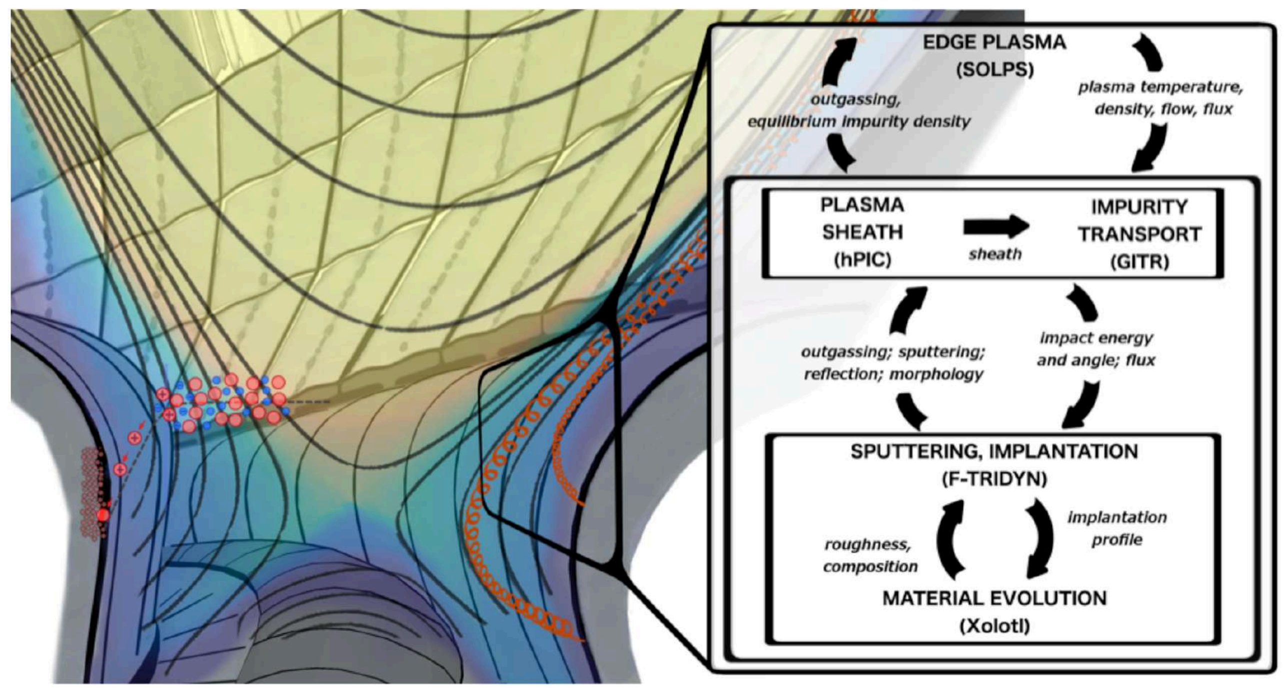
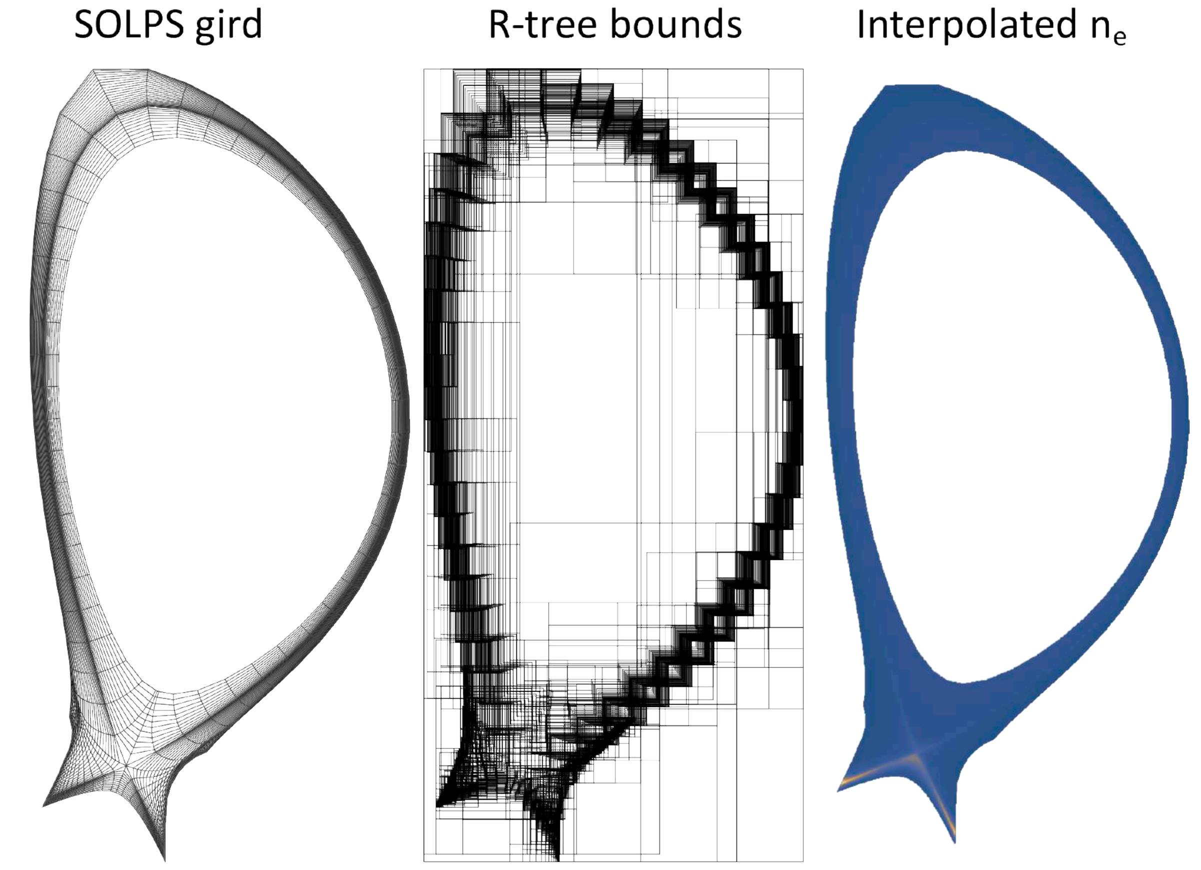
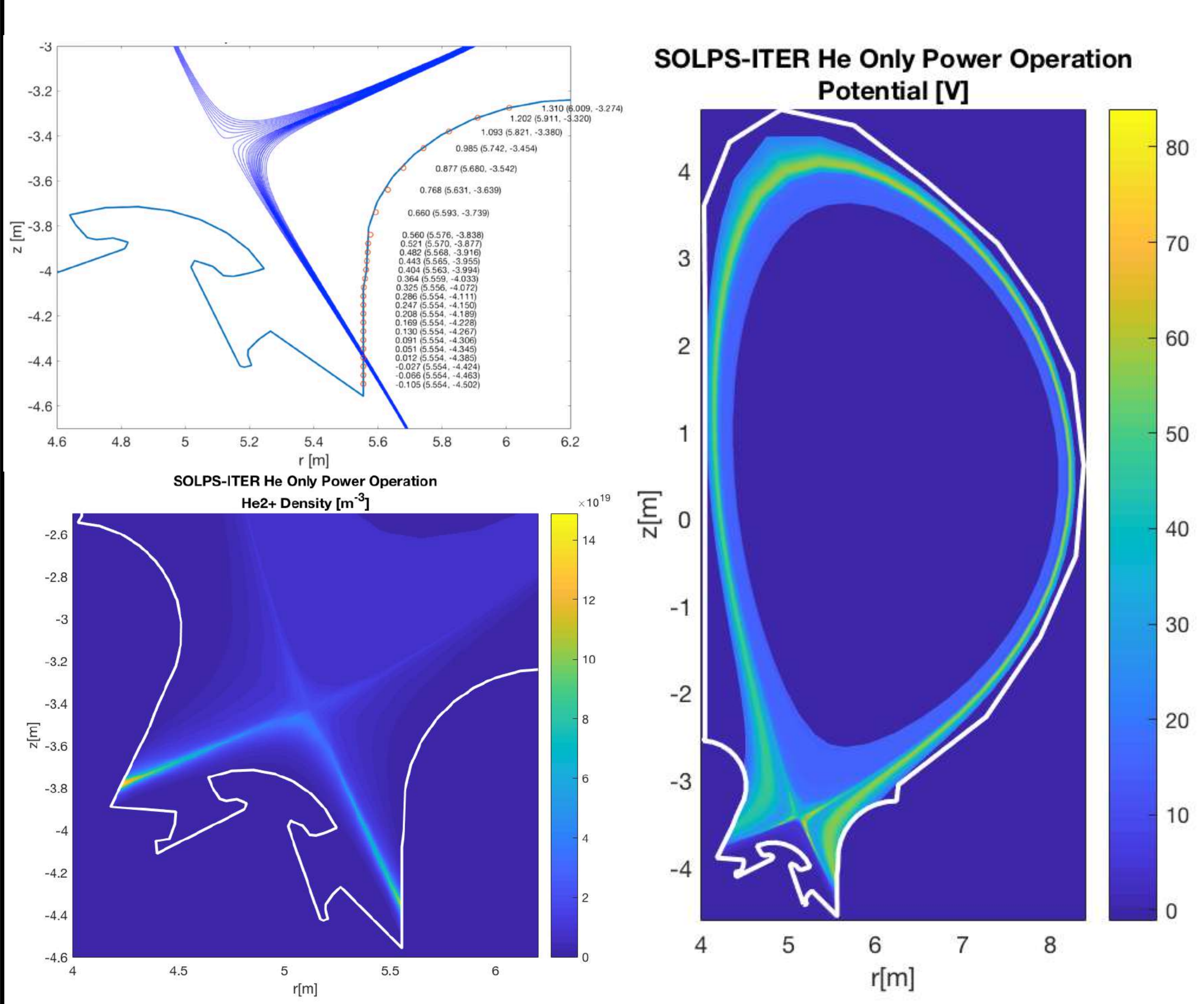


SOLPS ITER

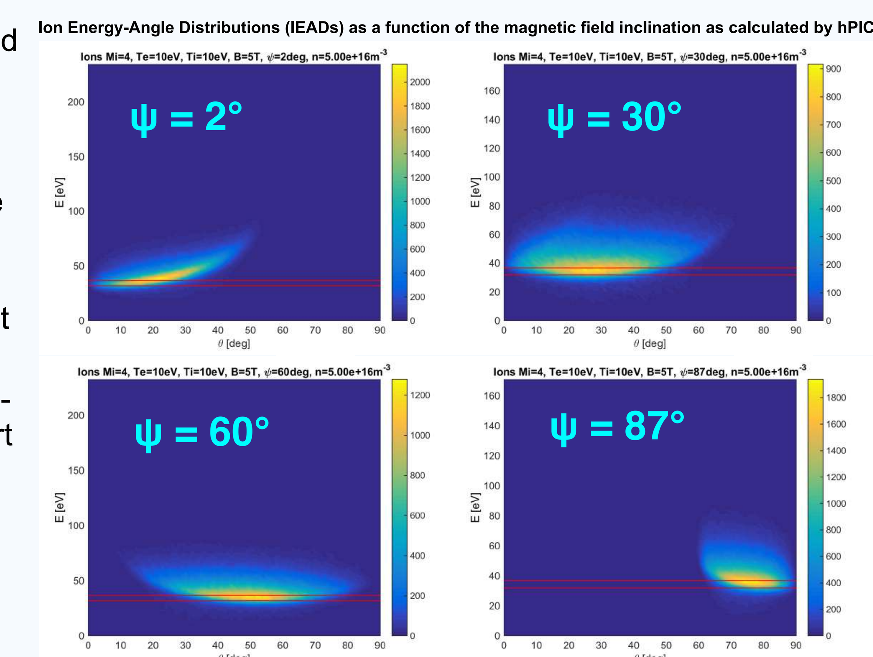


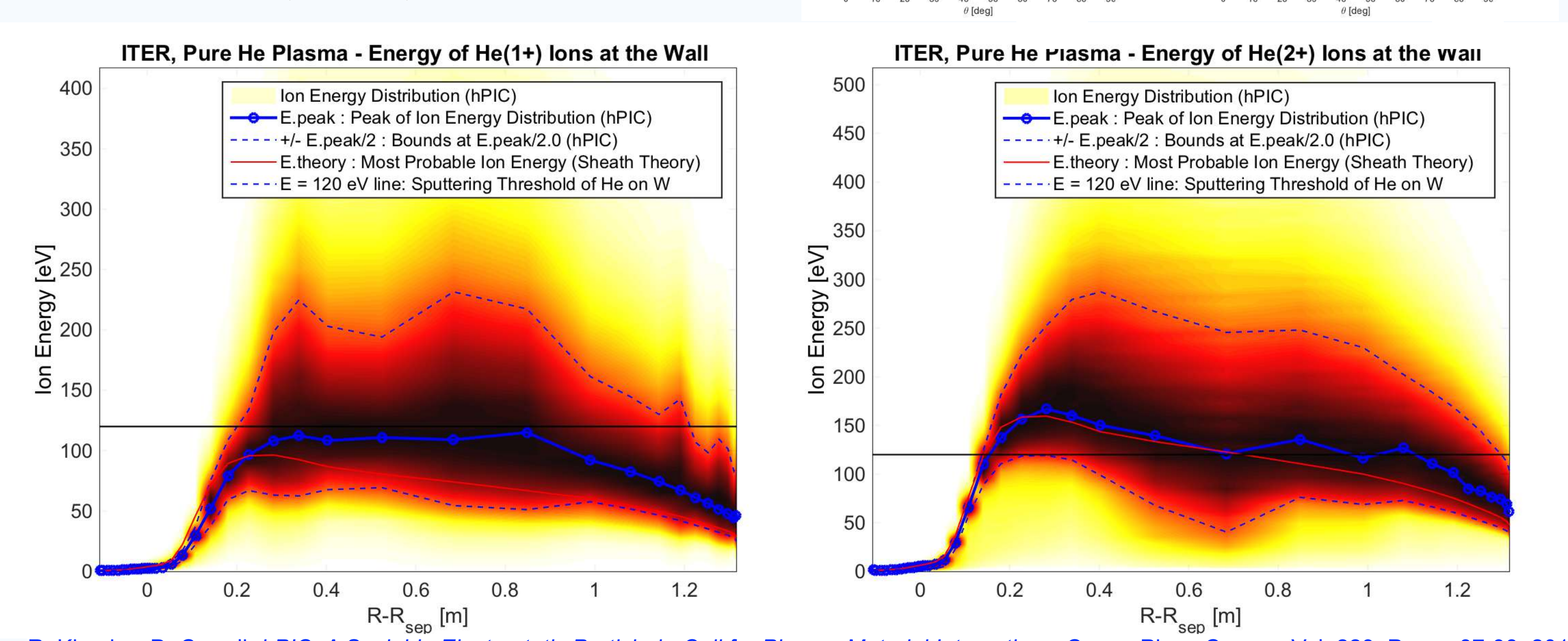


hPIC - Plasma Sheath

- Plasma Sheath: establishes the link between "Edge" and "Wall"
- UIUC's full-f full-orbit plasma sheath code hPIC is used to analyze the near-surface ion kinetics
- hPIC accurately captures finite-orbits effects near to the wall, which are responsible for the generation of the magnetic presheath in oblique magnetic fields
- hPIC produces Ion Energy-Angle Distributions (IEAD) at the wall for plasmas made of multiple ion species
- IEADs are a necessary input to surface models (Fractal-TRIDYN & XOLOTL) and to the global impurity transport model (GITR)
- hPIC accepts inputs from plasma edge codes (SOLPS, XGC, etc.) and produces outputs which can be easily coupled to Material Codes
- hPIC libs: PETSc, CMAKE, ADIOS

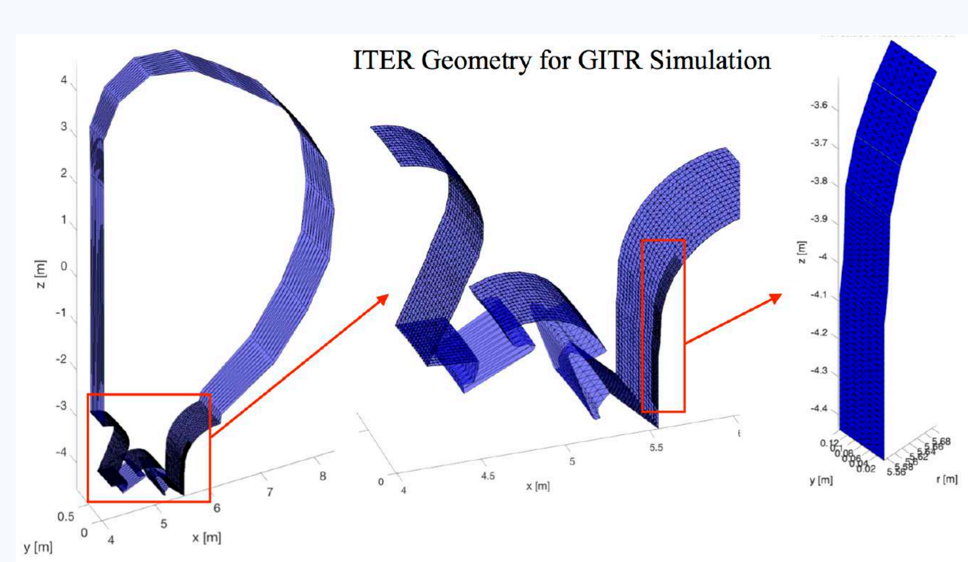
Ion Energy-Angle Distributions (IEADs) as a function of the magnetic field inclination as calculated by hPIC

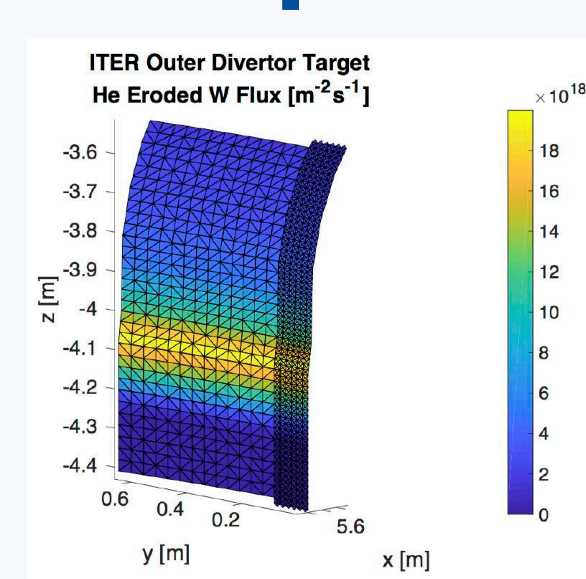


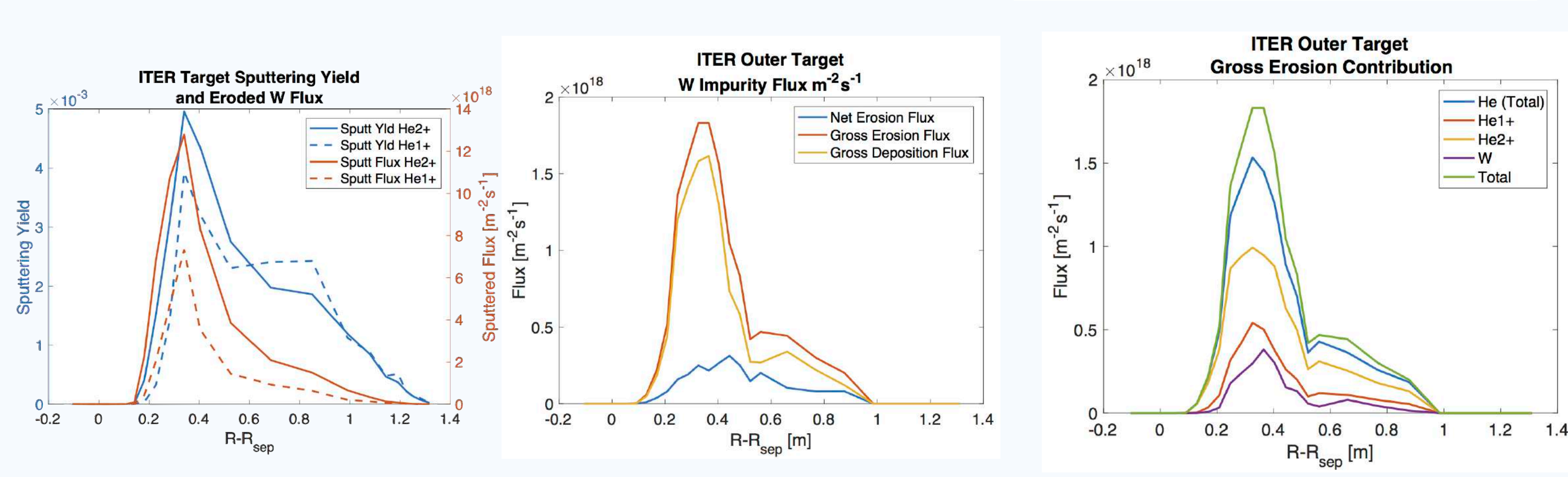


- R. Khaziev, D. Curreli, *hPIC: A Scalable Electrostatic Particle-in-Cell for Plasma-Material Interactions*, Comp. Phys. Comm., Vol. 229, Pages 87-98, 2018
- R. Khaziev, D. Curreli, *Ion energy-angle distribution functions at the plasma-material interface in oblique magnetic fields*, Phys. Plasmas 22(4):043503

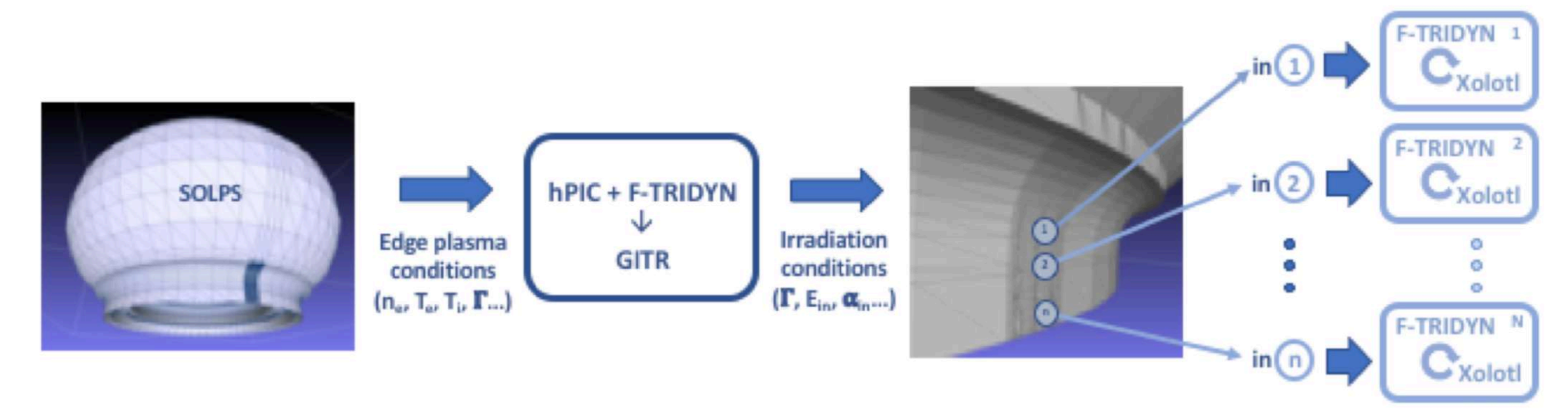
GITR - Impurity Transport





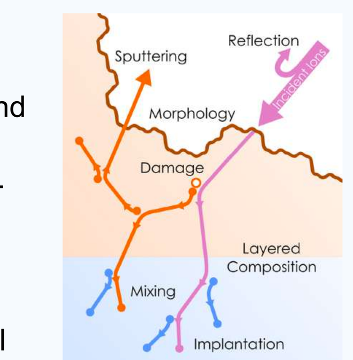


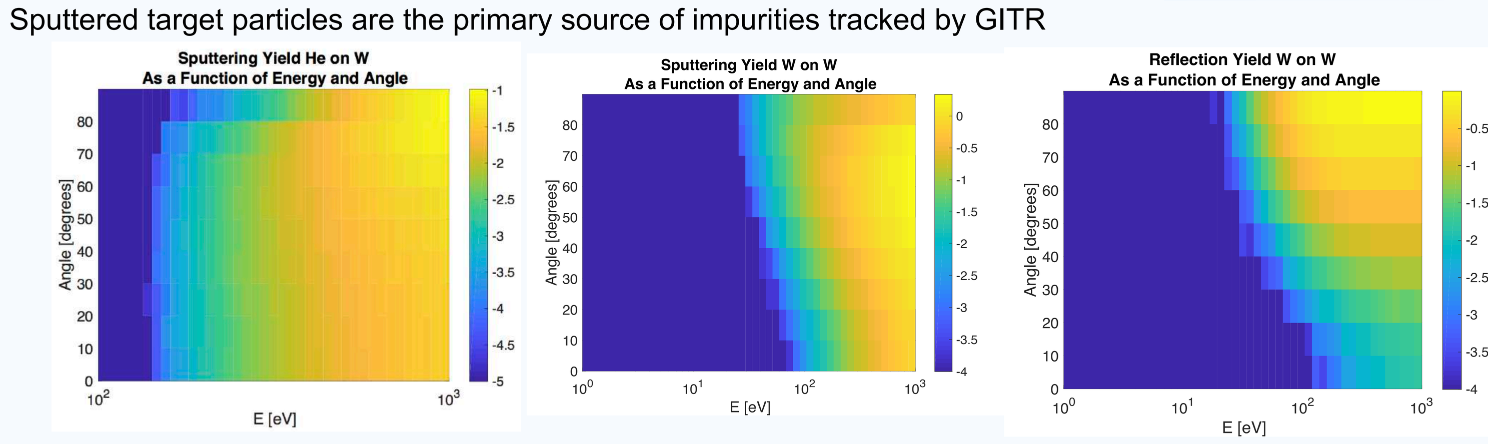
https://github.com/ORNL-Fusion/GITR

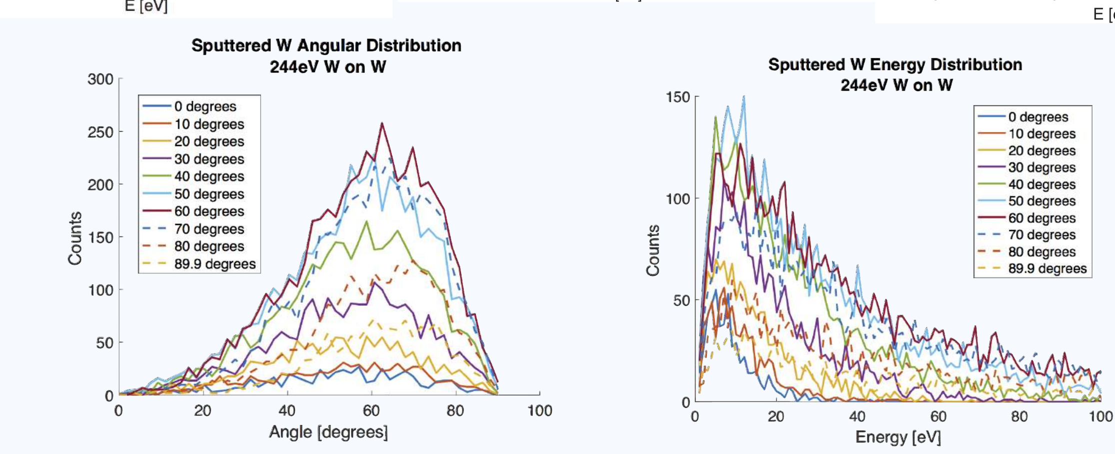


F-TRIDYN - Ion/Matter Interaction

- Surface Sputtering: the mechanism driving particle exchange between the plasma edge and wall
- F-TRIDYN is a Monte Carlo, Binary Collision Approximation code that handles atomic-scale ion-material interactions including reflection, implantation, damage, and sputtering
- Surface morphology is modeled in F-TRIDYN, which has a significant effect on ion-material interactions
- F-TRIDYN produces depth profiles of implanted plasma species and energy-angle distributions of reflected plasma and sputtered target species
- Accurate implantation profiles are necessary to model material evolution with Xolotl
- Sputtered target particles are the primary source of impurities tracked by GITR



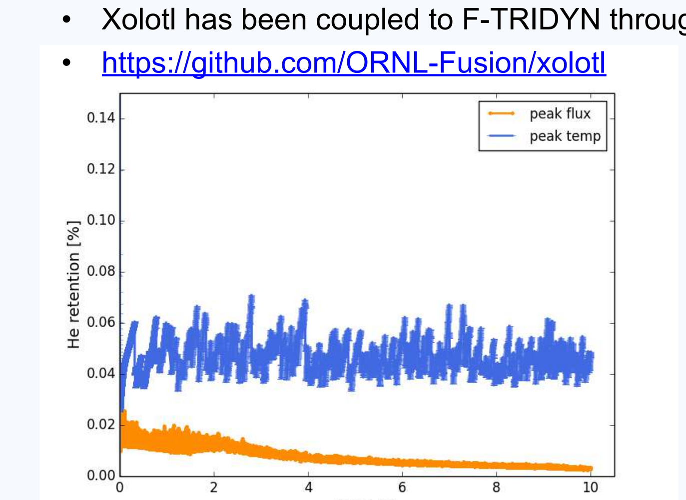




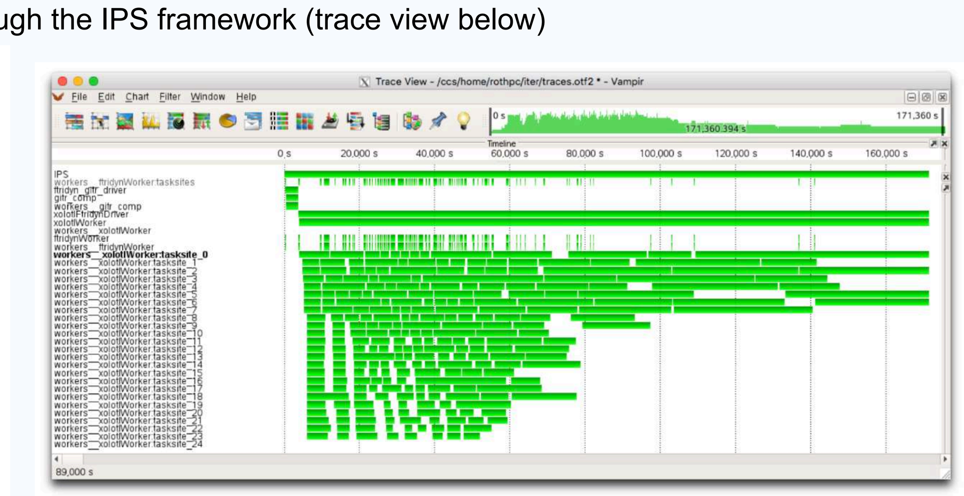
- J. Drobny, D. Curreli, *F-TRIDYN Simulations of Tungsten Self-Sputtering and Applications to Coupling Plasma and Material Codes*, Computational Materials Science, Volume 149, 15, Pages 301–306 (2018)
- J. Drobny, A. Hayes, D. Curreli, D. N. Ruzic, *F-TRIDYN: A Binary Collision Approximation Code for Simulating Ion Interactions with Rough Surfaces*, Journal of Nuclear Materials, Volume 494, Pages 278-283 (2017)

XOLOTL - Material Evolution

- XOLOTL: Diffusion Advection Reaction model of cluster dynamics
- Xolotl solves the helium cluster evolution (cluster concentration, cluster size) and predicts quantities such as the percentage of implanted ions that is retained below the surface, fuel retention, etc.
- The code captures retention oscillations as a function of time due to bubble bursting at the surface (fig below)
- Xolotl has been coupled to F-TRIDYN through the IPS framework (trace view below)
- https://github.com/ORNL-Fusion/xolotl



Percentage of implanted helium that is retained below the W surface during the first 10 seconds of ITER He discharge, at two W divertor positions of peak plasma flux (R – Rsep = 0.051 m) and peak temperature



Timeline visualization focusing on the 25 concurrent Xolotl simulation tasks running within a 25-wide IPS task pool

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