FES-ASCR Partnership
Email: ksargsy@sandia.gov

Uncertainty Quantification and Propagation for Impurity Migration

Khachik Sargsyan[1], Timothy Younkin[2,3], Tiernan Casey[1], Habib Najm[1], Brian Wirth[2,3]

[1] Sandia National Laboratories, Livermore, CA [2] Oak Ridge National Laboratory, Oak Ridge, TN

[3] University of Tennessee, Knoxville, TN

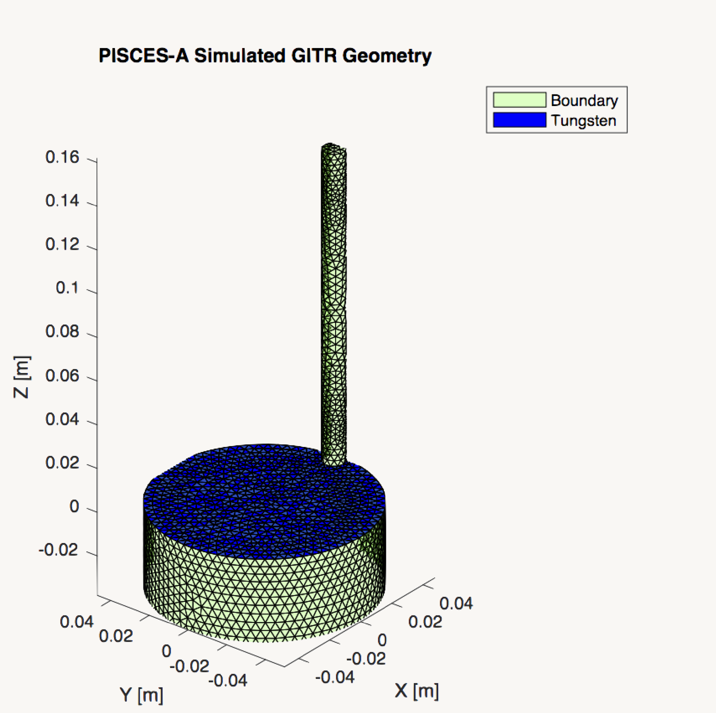
Partnership jointly funded by FES and ASCR

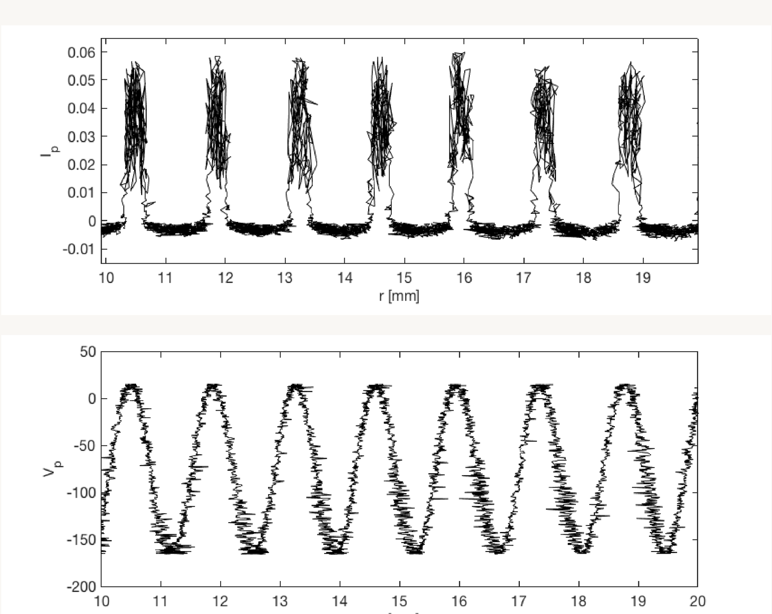
Plasma Surface Interactions 2: Predicting the Performance and Impact of Dynamic Plasma Facing Component Surfaces

Develop and integrate high-performance simulation tools capable of predicting plasma facing component (PFC) operating lifetime and the impact of the evolving surface morphology of tungsten-based PFCs on plasma contamination, including the dynamic recycling of fuel species and tritium retention, in future magnetic fusion devices.

Motivation

- Simulating PISCES-A linear device provides experimental benchmarking for impurity transport model and is a step towards modeling ITER tungsten components
- Comparison of impurity erosion, ionization, migration, and re-deposition model to experiment is essential before moving to more complicated cases
- Understanding sensitivity of impurity transport model to input parameters will enable quantification of uncertainty in net erosion, net deposition, and impurity density profiles
- Plasma profiles are measured by reciprocating probe 30cm upstream from the target and provide profiles for electron temperature, density, and ion flux



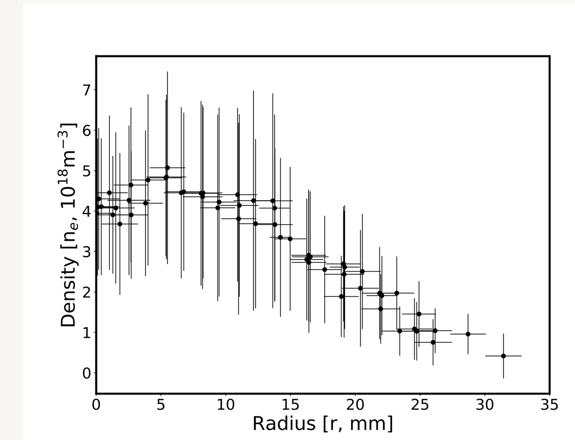


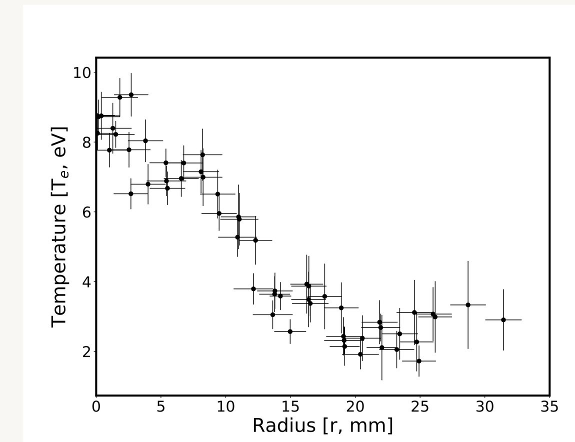
Reciprocating Langmuir probe raw data showing current and voltage traces used with fitting to produce temperature and density

- FASTMath/UQ target: represent and propagate uncertain input profiles of density and temperature fields

Bayesian Inference of Input Profiles

- Data on density and temperature
- Parameterize n_e and T_e profiles with uncertainty in order to propagate through impurity transport code, GITR
- Assume data is lognormal
- Assume the fit model is lognormal with polynomial log-mean $\mu(x)$ and log-stdev $\sigma(x)$
- Employ Bayesian inference with approximate likelihood set to symmetrized Kullback-Leibler (KL) divergence

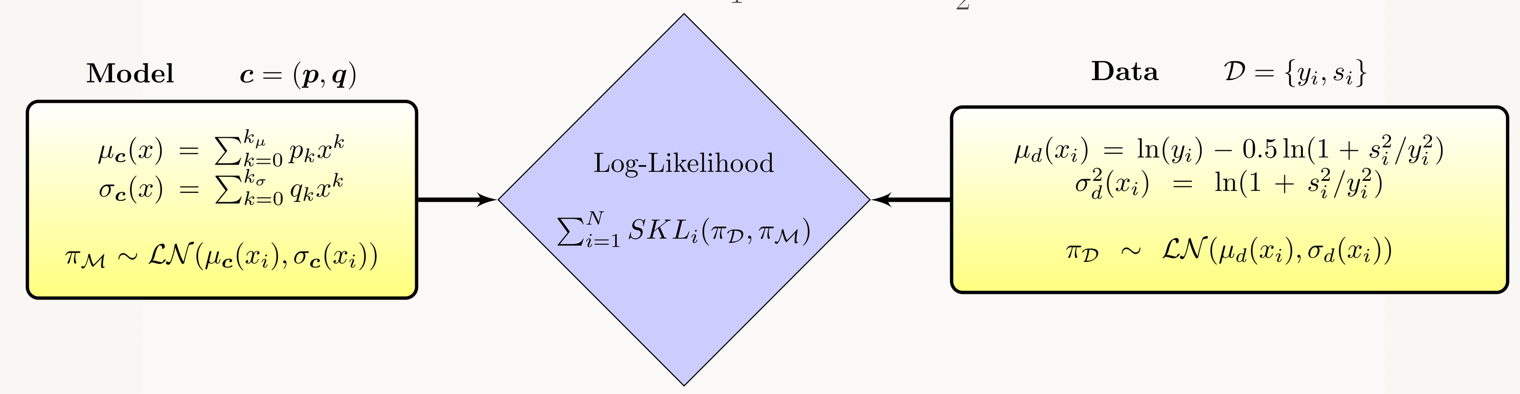




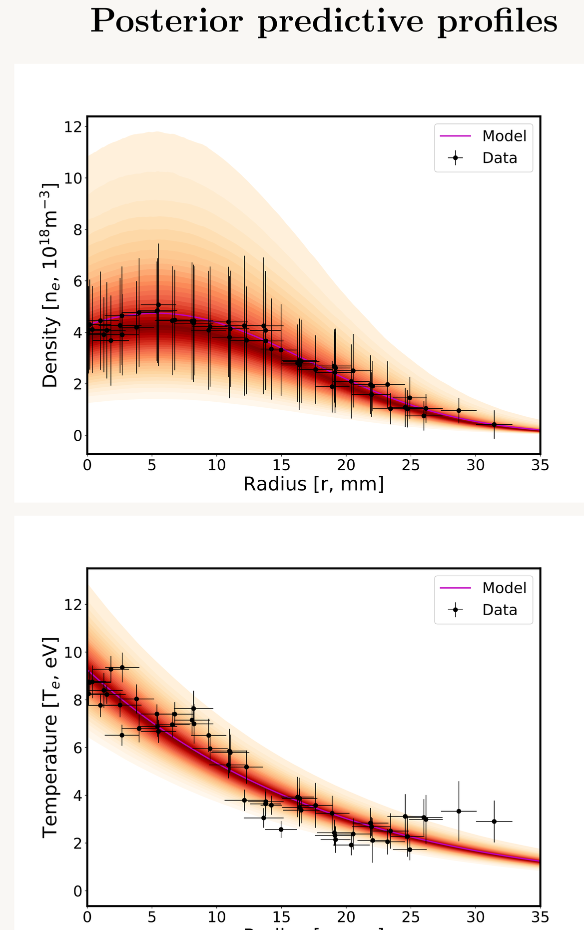
$$\log L_{\mathcal{D}}(\boldsymbol{c}) = -\sum_{i=1}^{N} \left[KL_i(\pi_{\mathcal{M}}||\pi_{\mathcal{D}}) + KL_i(\pi_{\mathcal{D}}||\pi_{\mathcal{M}})\right]$$

- (Log-)normal KL

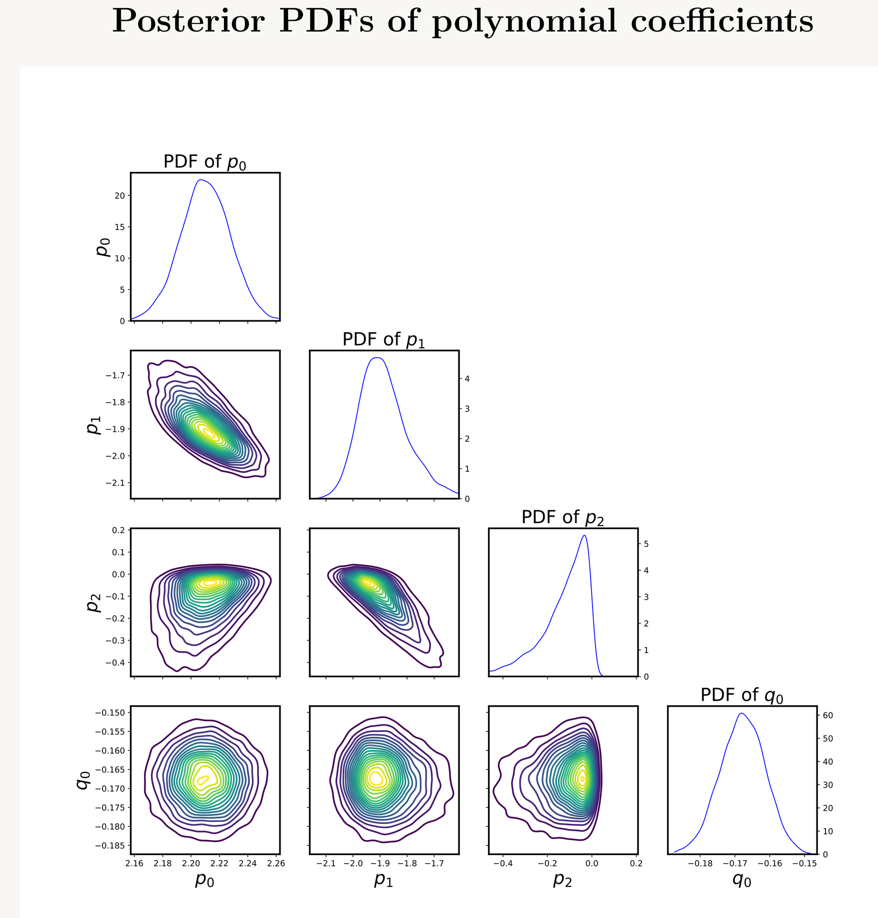
$$KL\left(\pi_1||\pi_2\right) = \log\frac{\sigma_2}{\sigma_1} + \frac{\sigma_1^2 + (\mu_1 - \mu_2)^2}{2\sigma_2^2} - \frac{1}{2}$$



Posterior predictive profiles



Posterior PDFs of polynomial coefficients



Uncertainty Propagation via PC

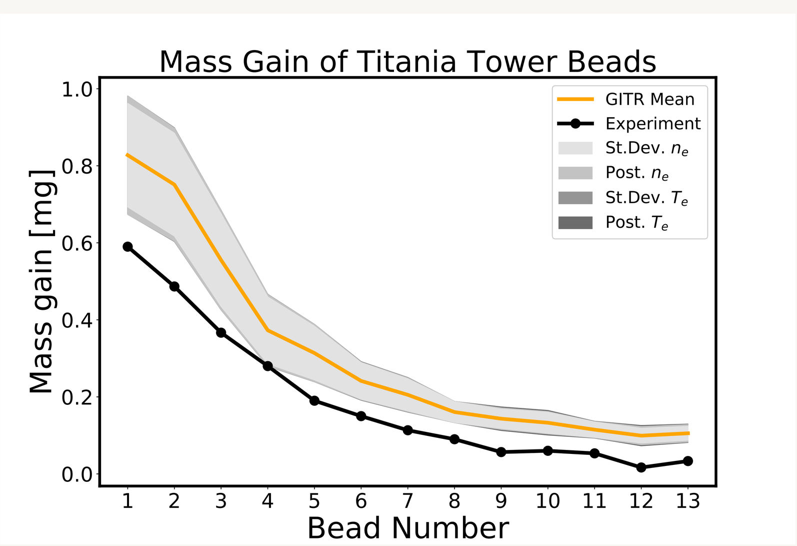
- Parameterize posterior PDF of polynomial coefficients with Polynomial Chaos (PC) expansion $\boldsymbol{c} = \boldsymbol{c}(\boldsymbol{\xi})$
- Augment $\boldsymbol{\xi} = (\xi_1, \dots, \xi_K)$ with the input profiles stochasticity ξ_{K+1} to get $\tilde{\boldsymbol{\xi}} = (\boldsymbol{\xi}, \xi_{K+1})$
- Propagate input profiles...

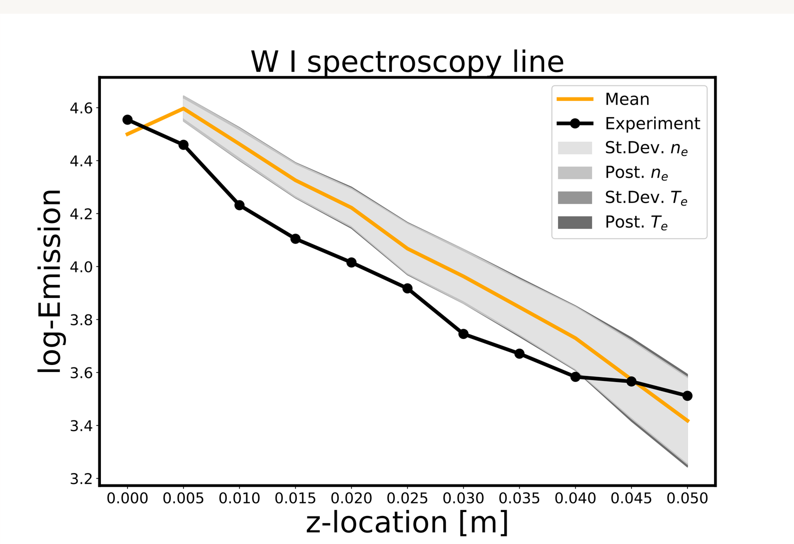
$$f(x;\tilde{\boldsymbol{\xi}}) = \exp\left(\mu_{\boldsymbol{c}(\boldsymbol{\xi})}(x) + \sigma_{\boldsymbol{c}(\boldsymbol{\xi})}(x)\xi_{K+1}\right)$$

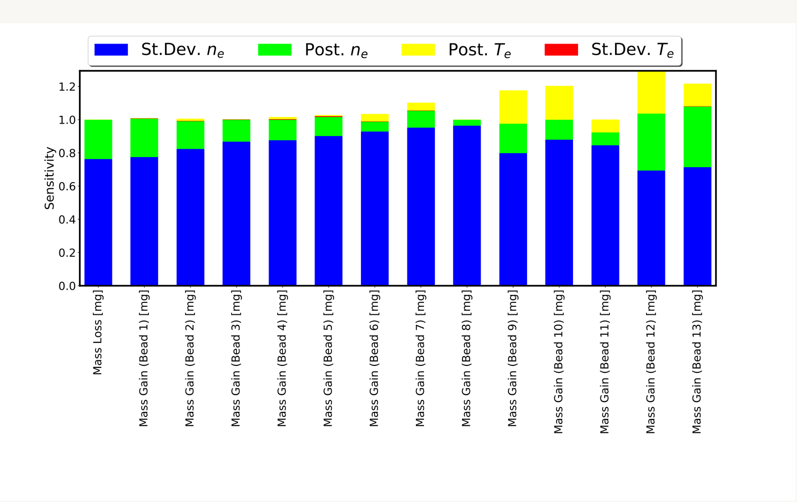
- ... through any model G (GITR in this case)

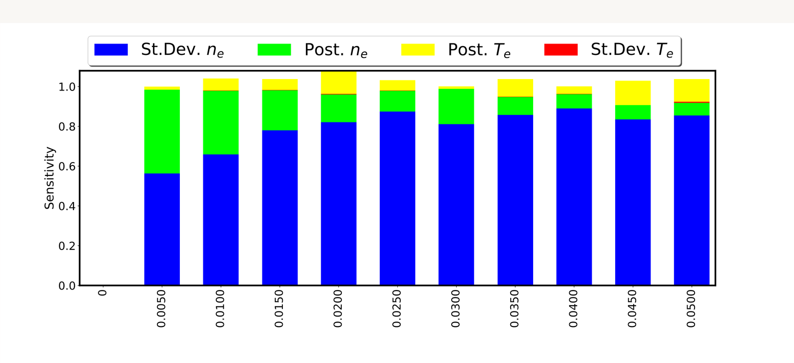
$$G(f(x;\tilde{\boldsymbol{\xi}})) = g(\tilde{\boldsymbol{\xi}}) = \sum_{j=0}^{J} g_j \Psi_j(\tilde{\boldsymbol{\xi}})$$

GITR Prediction and Uncertainty Attribution









Uncertainty in density profile n_e is the main contributor to output variance

Summary

- Formal UQ for representing uncertain input profiles
- Uncertainty propagation through GITR, the impurity migration module of an integrated simulation for plasma surface interactions
- UQ Toolkit has been employed for both Bayesian inference and PC representations (*www.sandia.gov/uqtooolkit*)
- Next, augment the input profiles with the rest of the uncertain inputs, deal with the high-dimensionality

This research is supported by the U.S. Department of Energy, Office of Science, Fusion Energy Sciences (FES) and Advanced Scientific Computing Research (ASCR), Scientific Discovery through Advanced Computing (SciDAC) program through the FASTMath Institute.