NC STATE

Inverse Uncertainty Quantification with Machine Learning Models

Christopher L. Brady
clbrady@ncsu.edu

Department of Nuclear Engineering
North Carolina State University

2026 Workshop for Applied Nuclear Data Activities (WANDA-2026)
Arlington, VA

February 11, 2026

ARTISANS: ARTificial Intelligence for Simulation of Advance Nuclear Systems

ARTISANS: Artificial Intelligence for Simulation of Advanced Nuclear Systems

UQ of physical models with ML

- Forward and inverse UQ
- Sensitivity analysis
- Quantitative validation
- Bayesian calibration
- Integration of inverse UQ and quantitative validation
- Dimensionality reduction
- Reduced order modeling
- Model discrepancy
- Model averaging & selection
- Functional data analysis
- Multi-physics UQ

UQ of ML models

- Monte Carlo dropout
- Bayesian Neural Networks
- Deep ensembles
- Conformal prediction
- Probabilistic ML
- VVUQ framework of ML
- ML trustworthiness

Deep generative learning

- Data augmentation
- Generative Adversarial Nets
- Normalizing flows
- Variational autoencoders
- Diffusion models
- Physics-informed generation

Transfer learning

- Model fine-tuning
- Domain adaption
- Resource-constrained tasks
- Incremental learning
- Generalization across modalities

Nuclear forensics and non-proliferation

- Data assimilation of materials diagnostic measurement
- Nuclear data calibration for radiation transport and fallout formation simulations
- Bayesian inverse problems

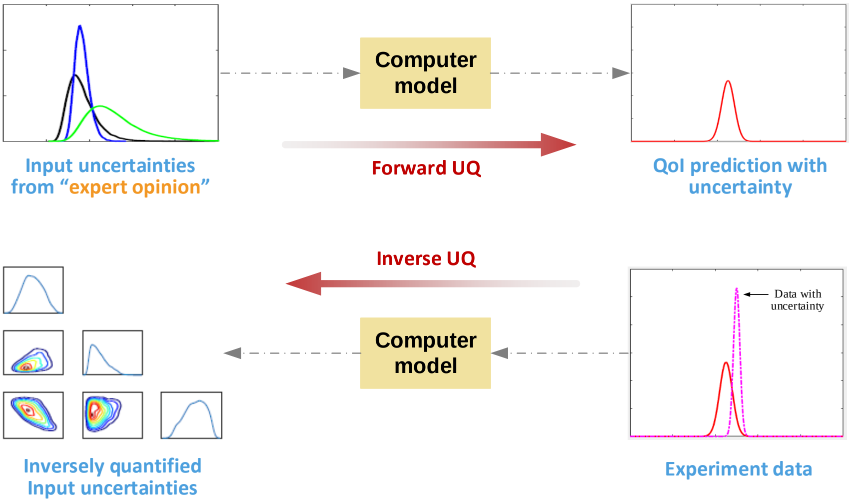
Anomaly detection

- Digital twins
- Continuous monitoring
- Multi-modal sensor fusion
- Material accounting to ensure nuclear safeguards
- Automated system analysis

LLM-based operator training

- AI-assisted nuclear workforce development using LLM
- Data from NRC GFE and NCSU PULSTAR training databases
- Implementation at NCSU NRP

Forward UQ vs. Inverse UQ[1]

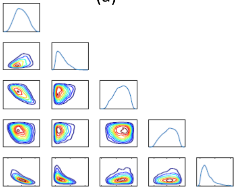


[1] Wu, X., Xie, Z., Alsafadi, F., and Kozlowski, T. (2021). A comprehensive survey of inverse uncertainty quantification of physical model parameters in nuclear system thermal–hydraulics codes. Nuclear Engineering and Design, 384:111460.

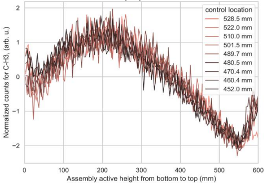
Sources of uncertainties in physical modeling & simulation

Parameter Uncertainty	Experimental/Data Uncertainty	Numerical Uncertainty	Model Uncertainty (Bias, Discrepancy)	Code/Interpolation Uncertainty
unknown exact values of the model input parameters, and/or randomness	noise or error in the measurement and/or data processing process	numerical approximation errors due to e.g., insufficient convergence, mesh	missing, inaccurate and/or incomplete underlying physics in the computer model	emulation of expensive computer codes using data-driven surrogate model

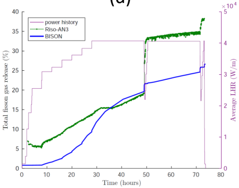
(a)



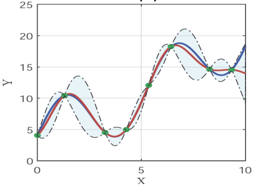
(b)



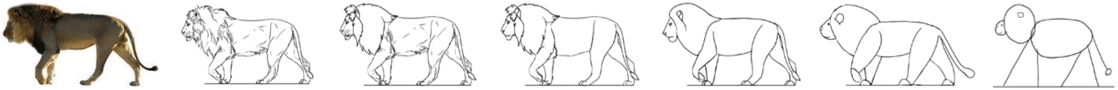
(d)



(e)



(c)

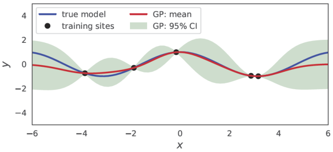


Observation | Good model | Model 1 | Model 2 | Model 3 | Model 4 | Model 5

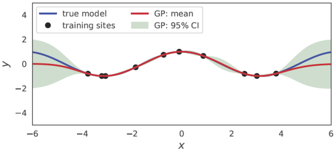
Sources of uncertainties in data-driven machine learning models

Data Noise	Data Coverage	Extrapolation	Imperfect Model	Training
noises in training data from either physical simulation models or experiments	few and/or gappy data that has incomplete coverage of training domain	generalization to the extrapolated domains outside of the training domain	ML model architecture is not properly defined, e.g., model is too simple or too complex	random initialization, convergence to local minima, hyper-parameter tuning, etc

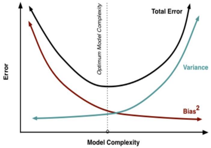
(a)



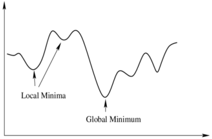
(b)



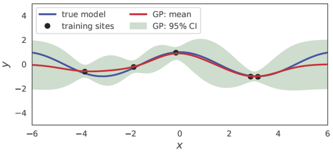
(e)



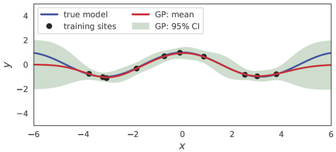
(f)



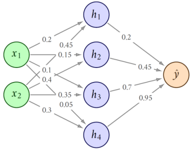
(c)



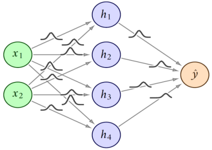
(d)



(g)

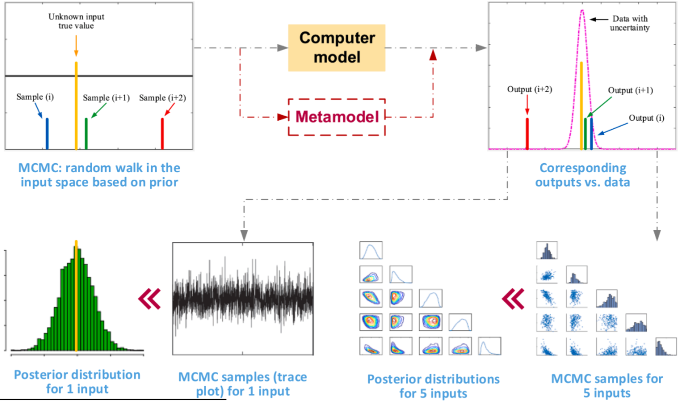


(h)



Modular Bayesian Approach for Inverse UQ

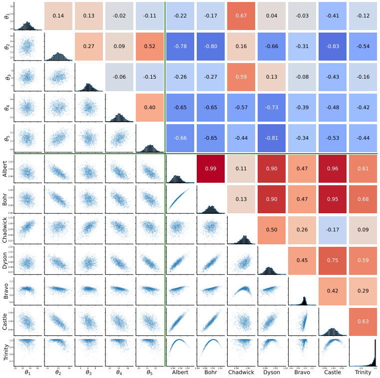
- Provides statistical descriptions of the uncertain input parameters that produce model predictions consistent with experimental data.
- Employs Markov Chain Monte Carlo (MCMC) to sample posterior parameter distributions.
- Employs ML surrogate models to reduce MCMC computational cost.



[2] Wu, X., Kozlowski, T., Meidani, H., and Shirvan, K. (2018). Inverse uncertainty quantification using the modular Bayesian approach based on Gaussian process, part 1: theory. Nuclear Engineering and Design, 335:339–355

Extending Inverse UQ to Nuclear Data Adjustments

- Inverse UQ has been demonstrated in Thermal Hydraulics and Fuel Performance applications.
- Working to extend Inverse UQ to Nuclear Data Adjustment applications.
- Demonstrated in OECD NEA WPNCS international benchmark exercise for data adjustments.[3]



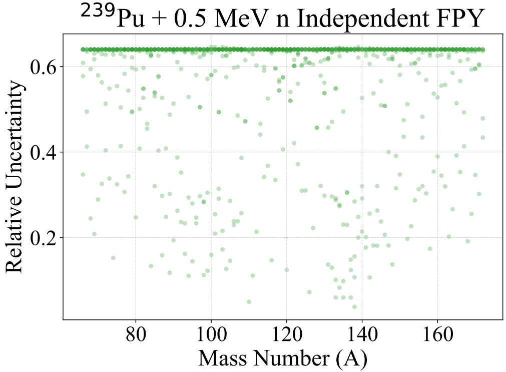
Prior

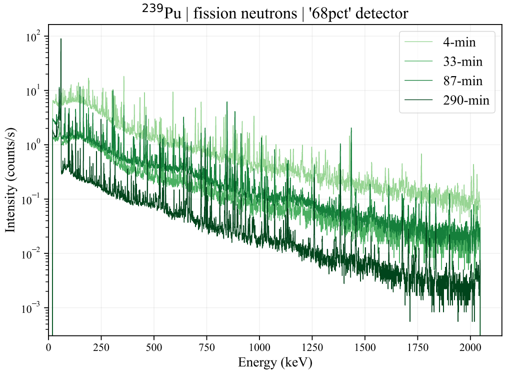
Posterior

[3] Brady, C. and Wu, X. (2025). Nuclear Data Adjustment for Nonlinear Applications in the OECD/NEA WPNCS SG14 Benchmark – A Bayesian Inverse UQ-based Approach for Data Assimilation. (in press at Nuclear Science and Engineering)

Estimating Independent Fission Product Yield Uncertainties

- Large relative uncertainties in current independent fission product yields.
- Use Serpent burnup models alongside experimental gamma spectra data of irradiated specimens.
- Use SANDY to perturb nuclear data passed to Serpent.





[4] Brady, C. and Wu, X. (2026). Estimation of Neutron-Induced Fission Product Yield Uncertainties from Gamma Spectra Data with Bayesian Inverse UQ. In Proceedings of the International Conference on Physics of Reactors (PHYSOR 2026). Turin, Italy, April 19-23, 2026

Challenges of AI/ML applications in Nuclear Engineering

- Application-agnostic algorithms, or those designed for more traditional ML applications such as computer vision and natural language processing, cannot be directly applied to scientific data in high-consequence NE problems without non-trivial, task-specific modifications.
- There are significant gaps in the predictive credibility assessment of AI/ML before deployment in nuclear systems. Rigorous verification, validation and uncertainty quantification (VVUQ) of AI/ML is needed that matches the quality standards for VVUQ of traditional nuclear M&S models.
- The data scarcity issue also significantly limits the AI trustworthiness for nuclear engineering.

Questions or Comments?

This material is based upon work supported by the Consortium for Nuclear Forensics under Department of Energy, National Nuclear Security Administration award number DE-NA0004142. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.