Bayesian Uncertainty Quantification for Radiation Transport Calculations at FRIB

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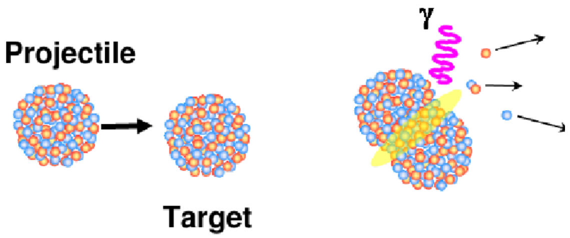
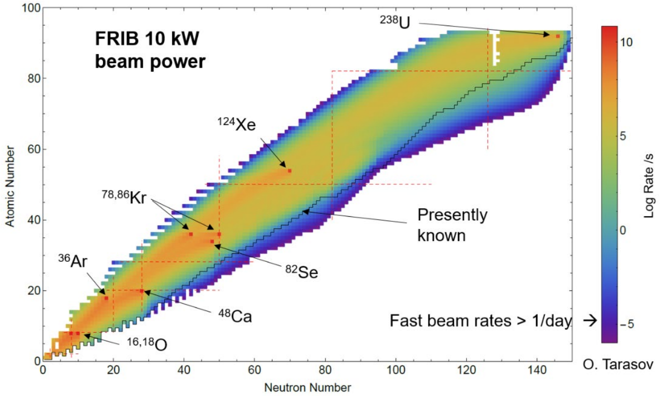
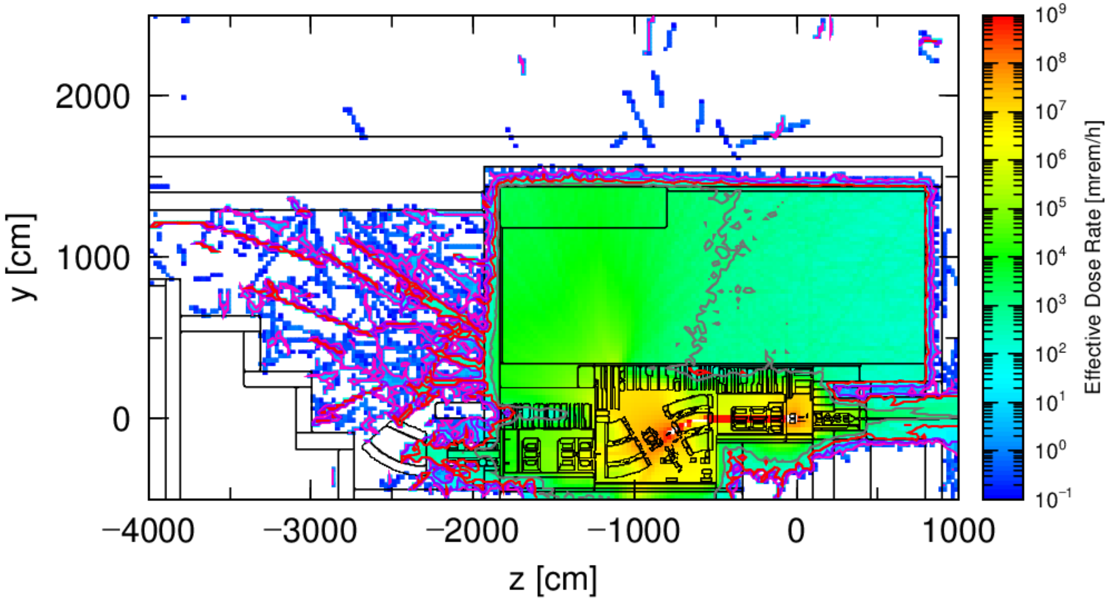
Secondary Radiation at FRIB







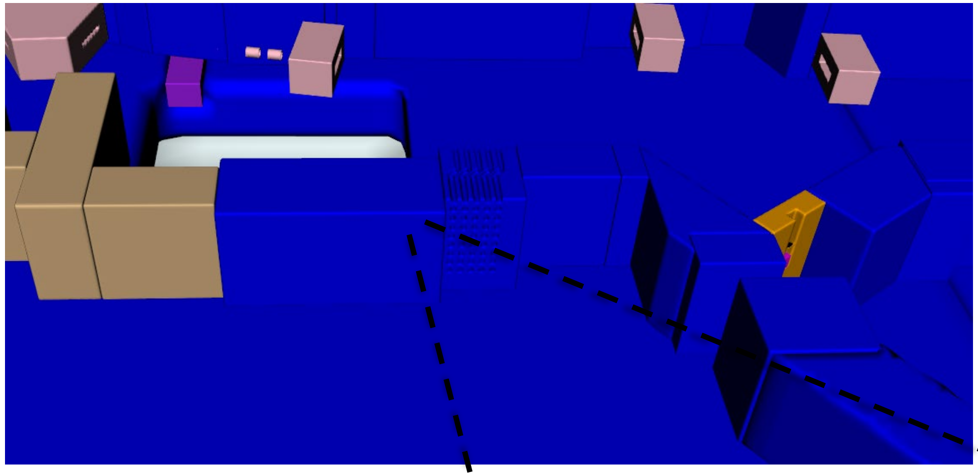
FRIB: Facility for Rare Isotope Beams

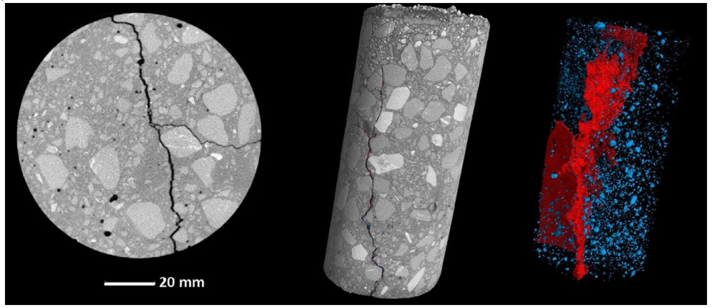
- Multiple radiation scenarios (T. Ginter’s talk)
- Accelerator facility: primary beams from ^{1}H to ^{238}U
- Max. Energy: ~ 200 MeV/u (upgrade 400 MeV/u)
- Beam power up to 400 kW
- Strong neutron fields

Systematic Uncertainties in Transport Models

Simulation ⟷ Reality

Geometry
- Overlapping, gaps, shape
- Material composition, density
- Non-uniformities, shield cracks

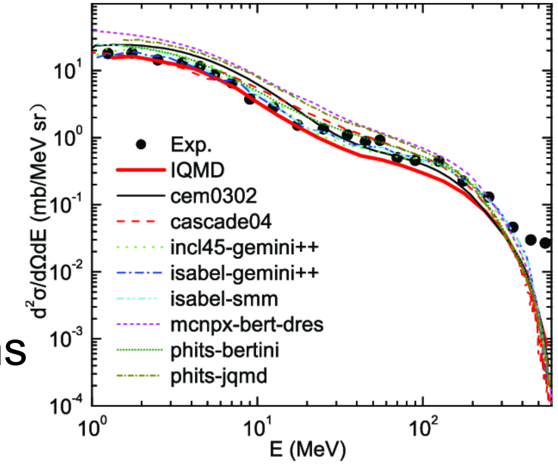




Plessis, Constr. Build. Mat.,**199**, 637 (2019)

Nuclear Data
- Cross sections
- Systematics
- Reaction probes

Models
- Physics assumptions
- Approximations



Xu, Phys. Rev. C.,**101**, 024609 (2020)

Bayesian Inference

A consistent approach that makes use of a prior probability (hypothesis) and data (evidence) to estimate a posterior probability

$P(\theta)$: prior probability

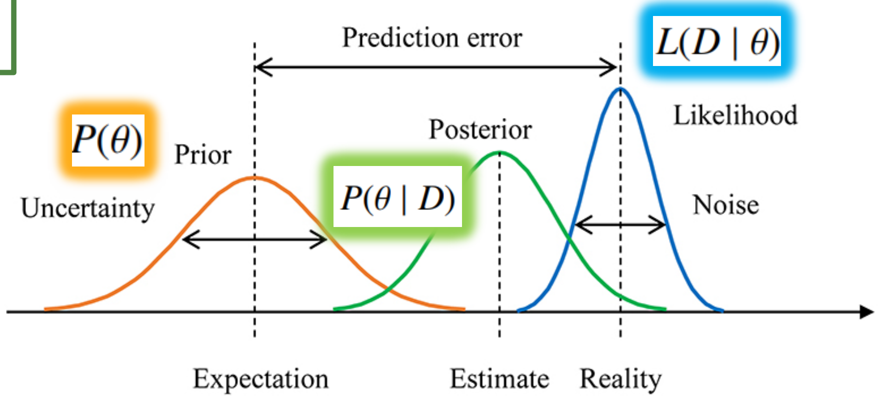
$P(\theta \mid D)$: posterior probability

$L(D \mid \theta)$: likelihood function

θ : parameters

D : data

Z : normalization

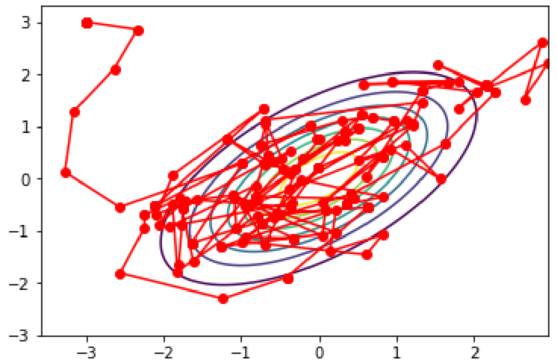


Bayes' Rule

$$P(\theta \mid D) = \frac{L(D \mid \theta)P(\theta)}{Z}.$$

Markov chain Monte Carlo

Stochastic sampling the posterior probability using a random walk



Drawback: requires a large number of evaluations

Yanagisawa, Front. Comput. Neurosci., **13** (2019)

Surrogate Modeling:
Machine Learning

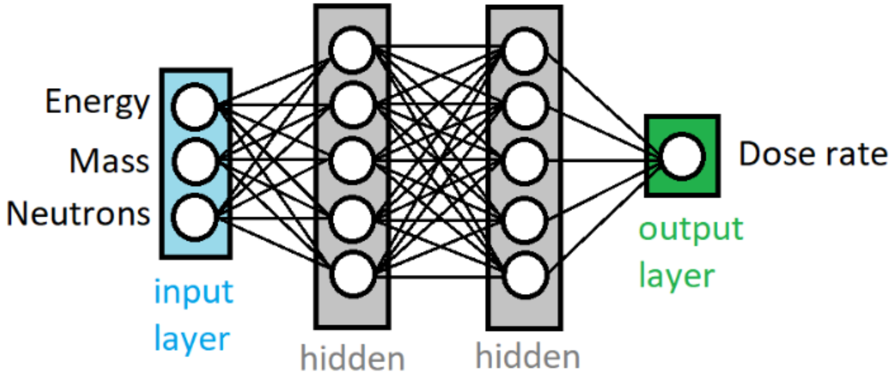
It is necessary to use a surrogate model that emulates or mimics the radiation transport results while significantly reducing the computational time required for each sampling evaluation.

MC Radiation Transport (~ hours)

ML Surrogate Model (~ seconds)

Non-intrusive approach

Multidimensional regression problem

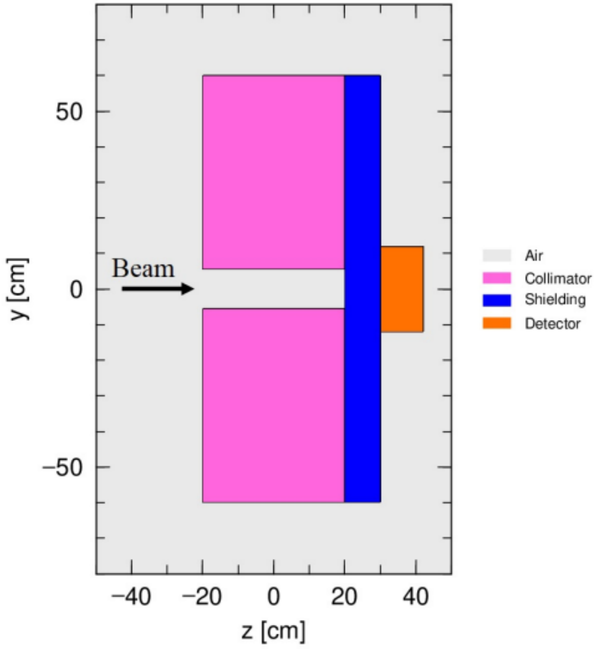


See R. Pal Chowdhury's poster

Zamora et. al., Proceedings SATIF-15, (2021)

Application 1
Neutron Shield

Radiation Transport Simulation Using PHITS



Convolutional Neural Network

Nakao et al., Nucl. Sci. Eng. ,**124**, 228 (1996)

Transmission Through Shields of Quasi-Monoenergetic Neutrons Generated by 43- and 68-MeV Protons—I: Concrete Shielding Experiment and Calculation for Practical Application

Noriaki Nakao*

Tohoku University, Cyclotron and Radioisotope Center, Aramaki, Aoba-ku, Sendai 980, Japan

Predicted Neutron Fluence

Zamora et. al., in preparation

Uncertainty Quantification for Neutron Shield

Posterior Probability Density Functions

Neutron Fluence

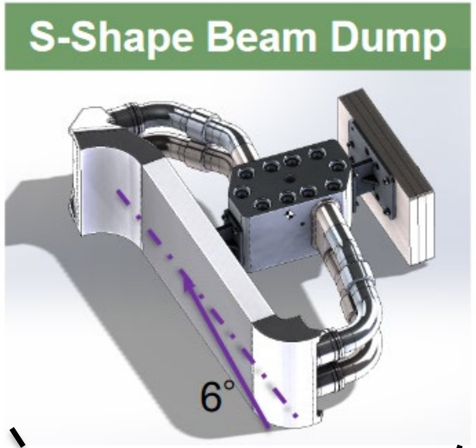
Data: Nakao et al., Nucl. Sci. Eng. ,**124**, 228 (1996)

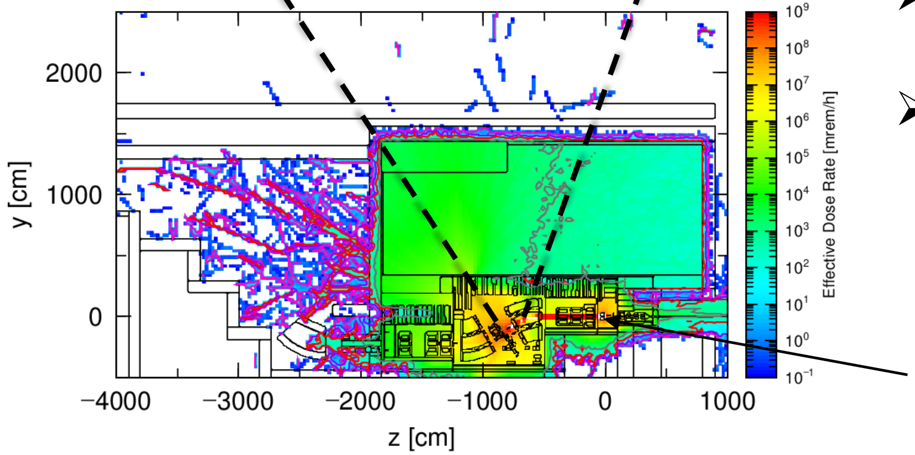
Cumulative Probability

Nominal Thickness	3%	16%	50%	84%	97%
25	23.1	24.0	25.1	26.2	27.2
50	49.2	49.8	50.7	51.5	52.4
100	98.1	98.8	99.8	100.7	101.6
150	148.4	149.3	150.4	151.5	152.4

Zamora et. al., in preparation

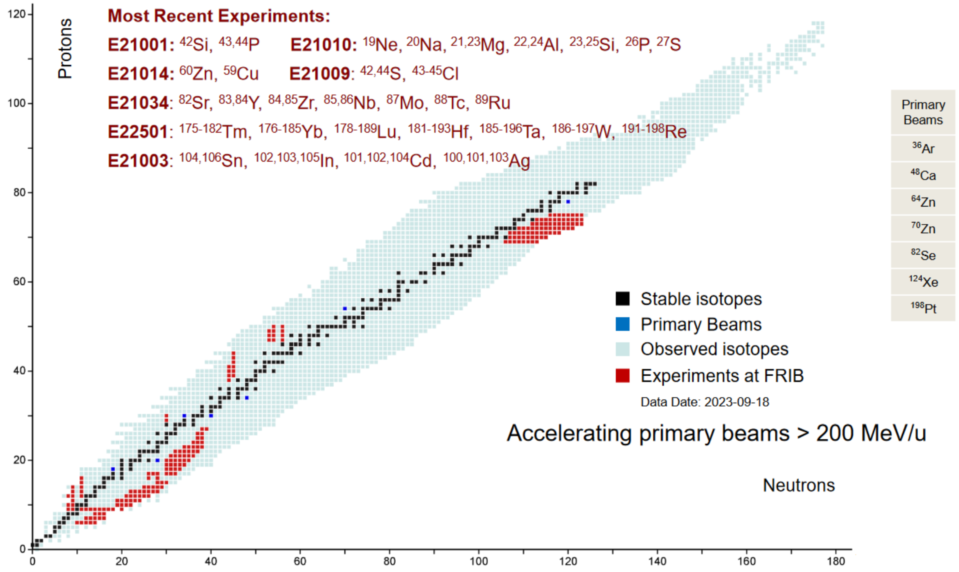
Application 2
Beam Dump Activation





PHITS + DCHAIN Calculations

- 19 primary beams for PAC1: energy, power, element
- Uncertainty propagation
- Activation
- Isotope inventory
- Residual dose rate

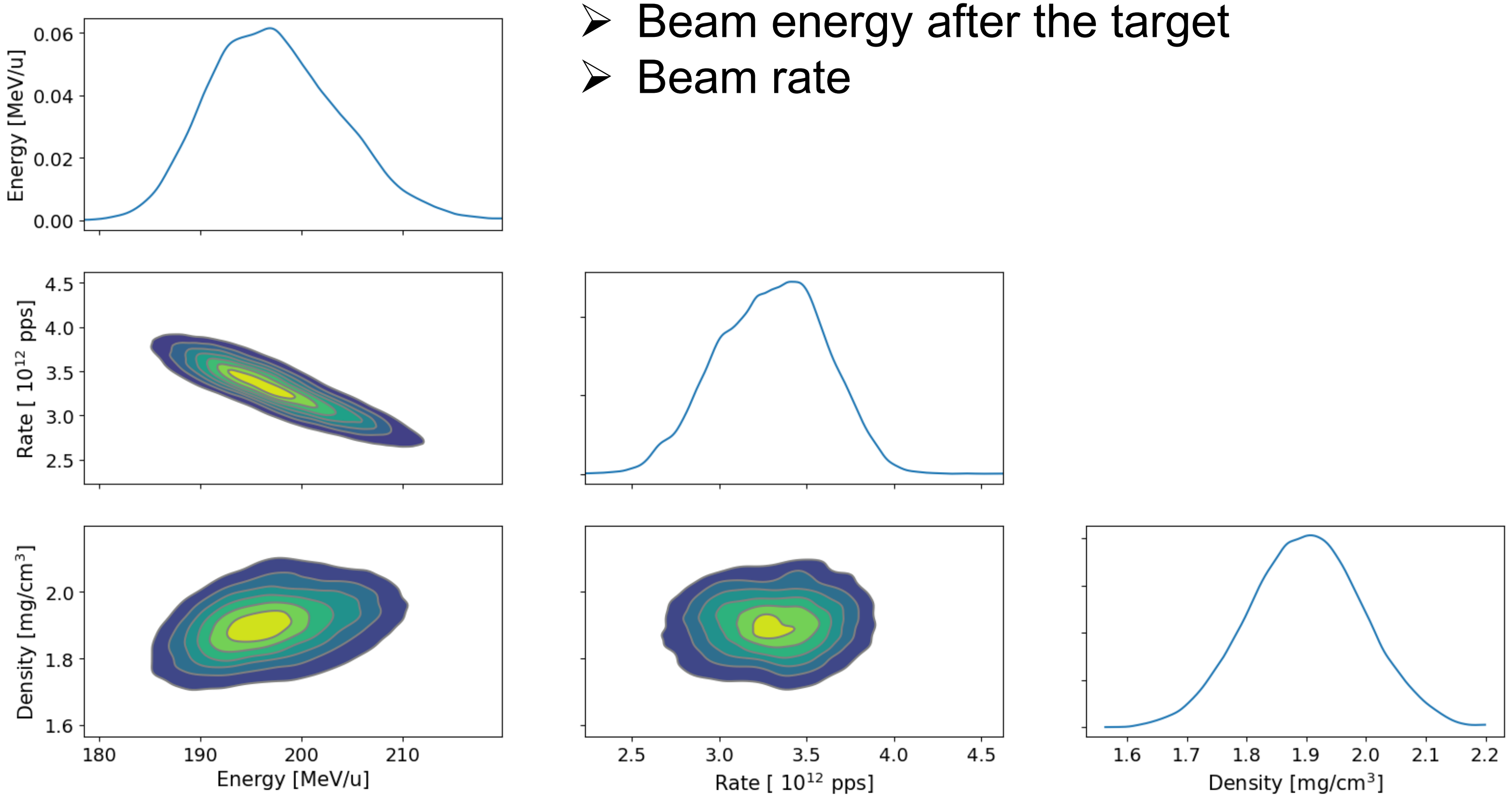


Accelerating primary beams > 200 MeV/u

Application 2
Posterior Probability Distributions

Parameters:

- Density of the production target
- Beam energy after the target
- Beam rate

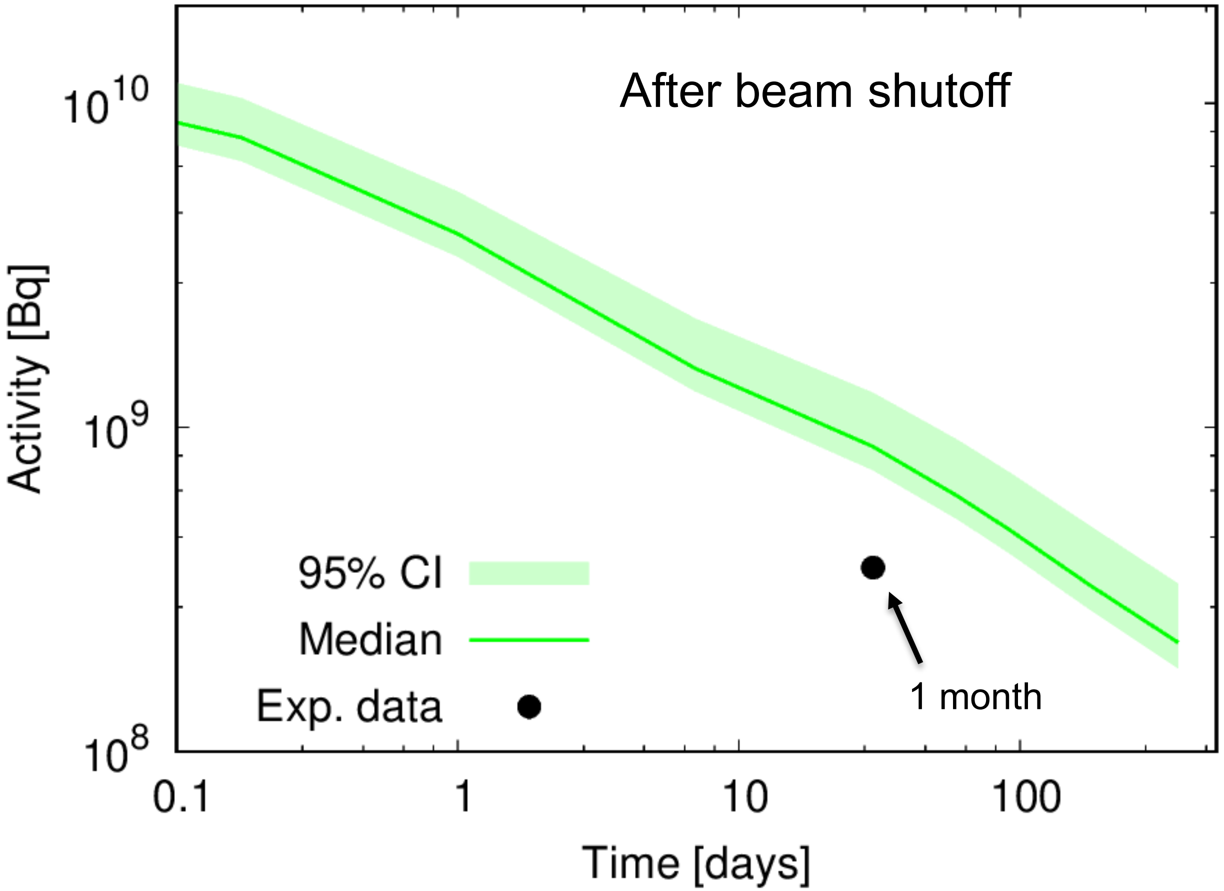


Propagation of systematic uncertainty through DCHAIN (burnup code). UQ tested with synthetic data (std = 10%)

It is possible to study correlations and parameter sensitivity

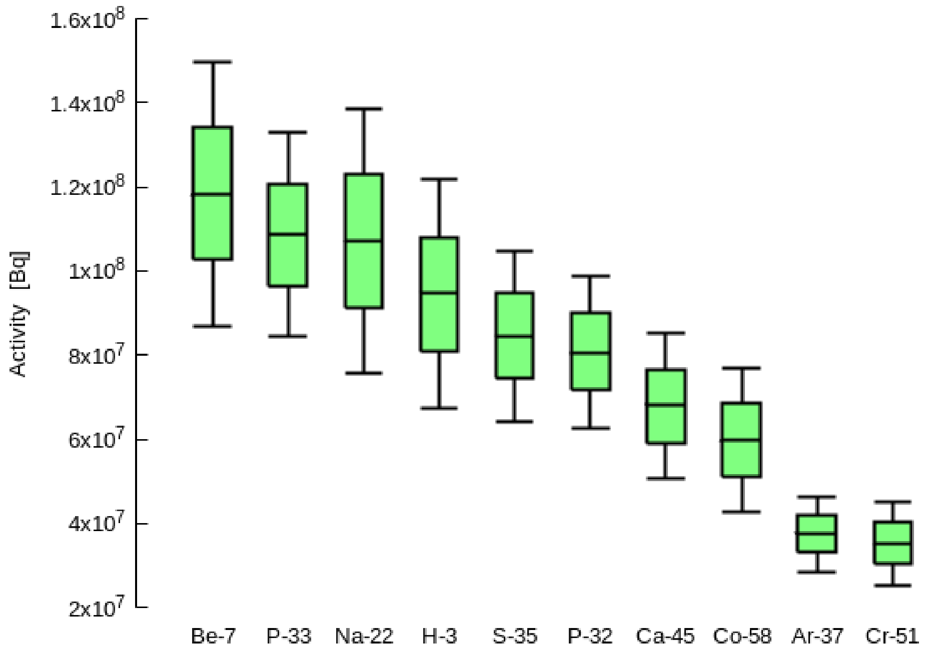
Application 2
Activation After One-Year of FRIB Operation

1 year operation (19 experiments) ~ 5 kW



Uncertainty in the nuclide inventory.
Isotope by isotope basis

Top 10 isotopes after 1 month cooling



Summary

- A Bayesian inference framework was developed to quantify uncertainties arising from radiation transport calculations. The approach is non-intrusive and can be utilized for various codes.
- Machine learning application is employed for surrogate modeling. The model emulates the radiation transport results while significantly reducing the computational time required for each sampling evaluation.
- The method can be used to study systematic uncertainty propagation and parameter sensitivity involving coupling to burnup codes.

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Thanks for your attention!