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EPFL

Bayesian Inference using microscopic and integral measurements to infer nuclear data parameters

International Workshop On Nuclear Data Evaluation for Reactor Applications (WONDER-2026)

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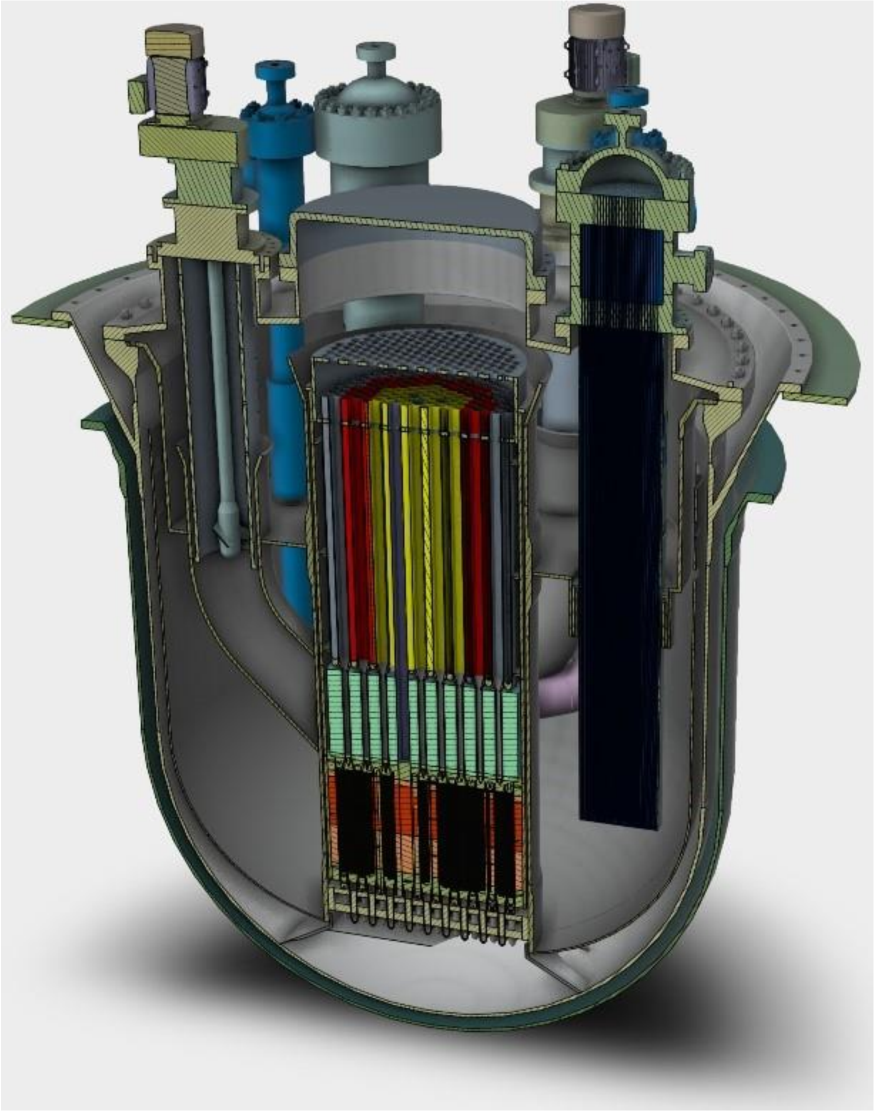
Date: 30/06/2026

Introduction

- SCK CEN is committed to building LFR SMR
  - EAGLES-300
  - Cooled with liquid lead
  - MOX fuel to close fuel cycle

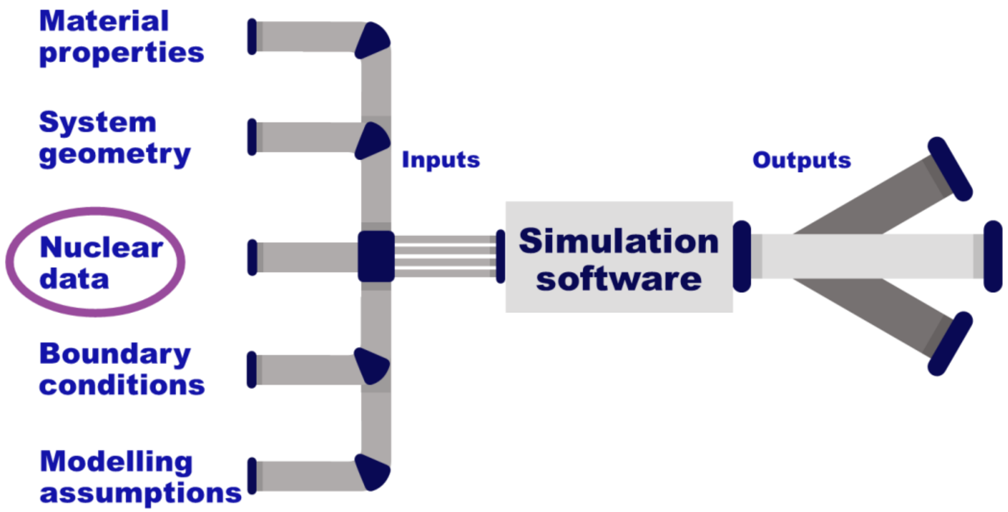
+	−
Enhanced safety	Corrosion
Efficient fuel use	Weight
HL waste reduction	Freezing risk
Passive cooling	Limited operating experience → **FOAK**
	…



EAGLES-300 conceptual design

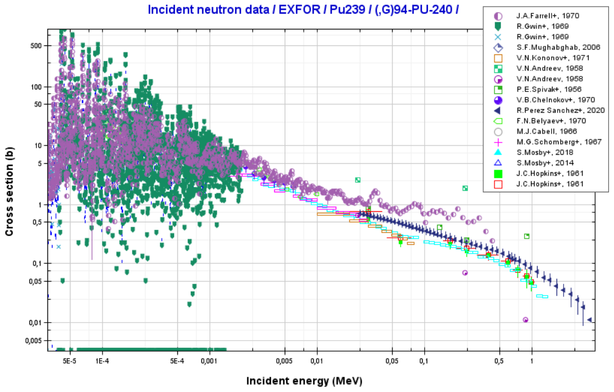
Introduction

- Design and safety studies of a FOAK
- Use of predictive simulations
- Algorithms well known
- Large uncertainty margins attributed to:
  - Input model parameters
  - **Nuclear data**
- Increased costs for design and safety studies



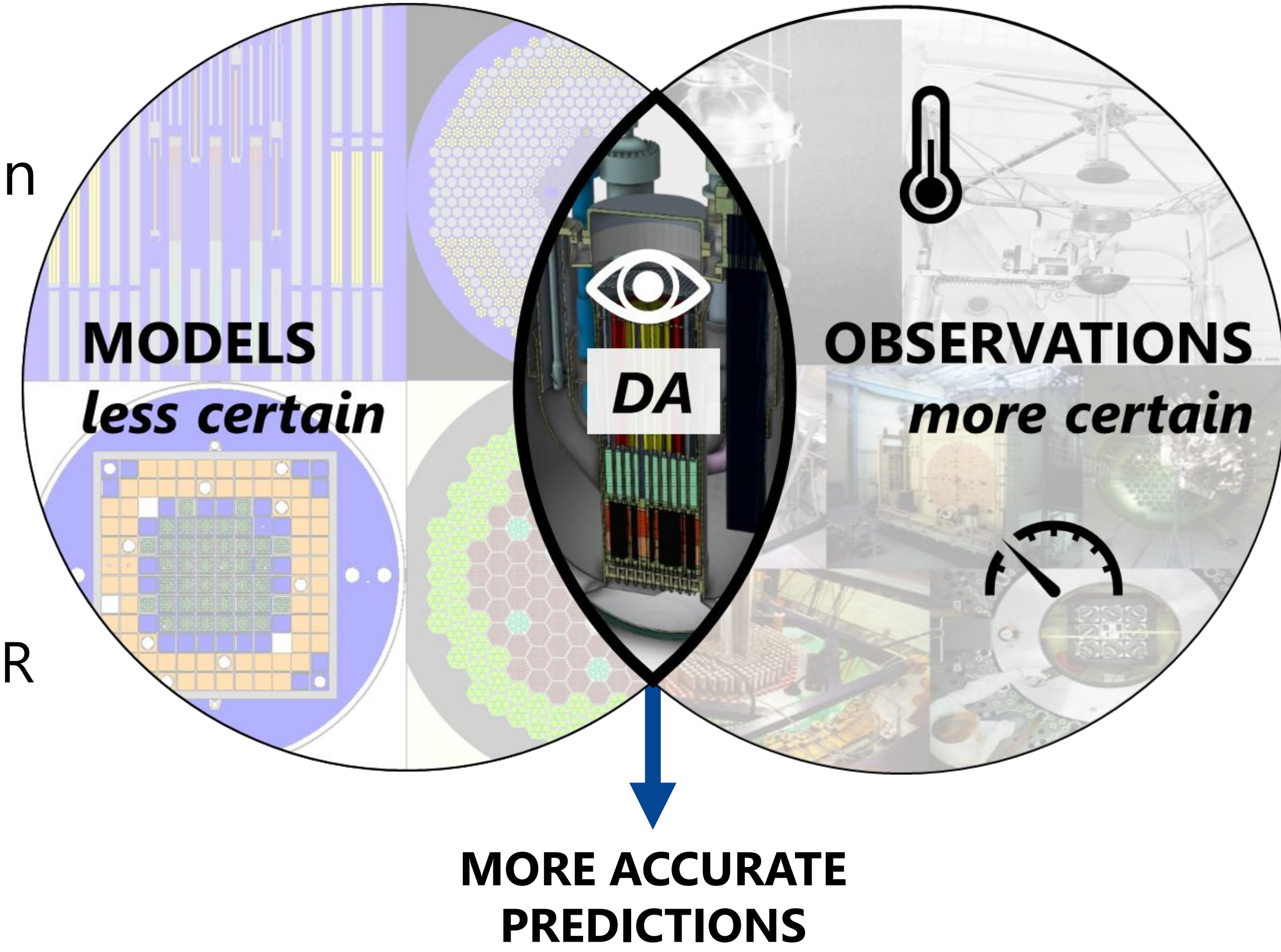
Major source of common uncertainty

→ Nuclear Data

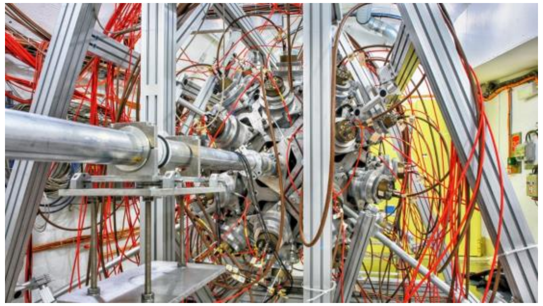


Introduction

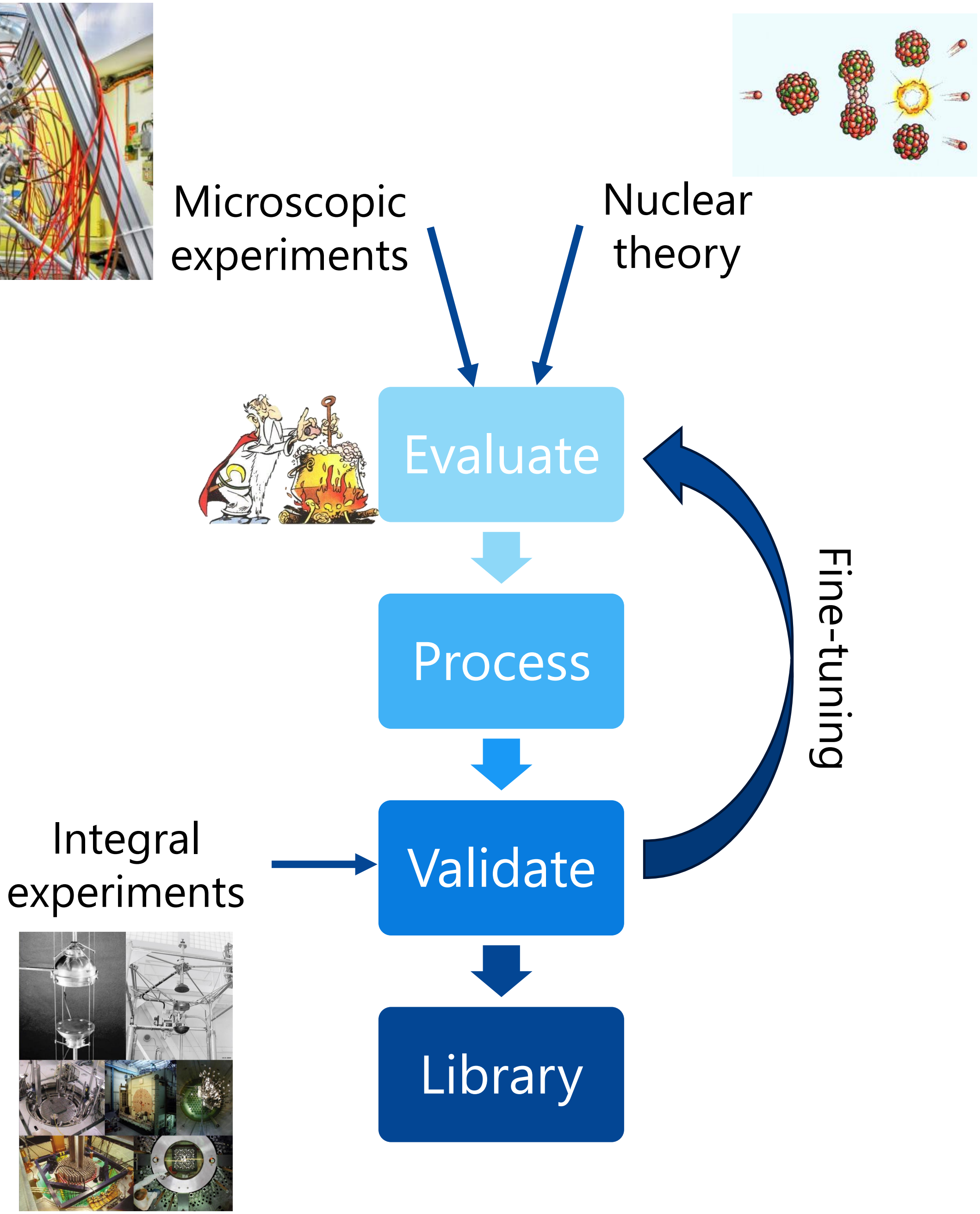
- Possible route to decrease prediction uncertainty:
  - Data assimilation leveraging past experiments
- For LFR highly similar experiments scarce
  - Use experiments not designed for LFR



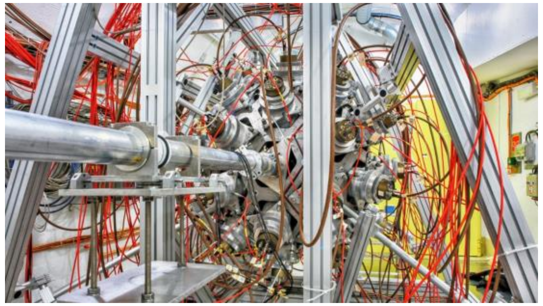
Introduction

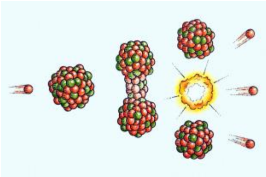


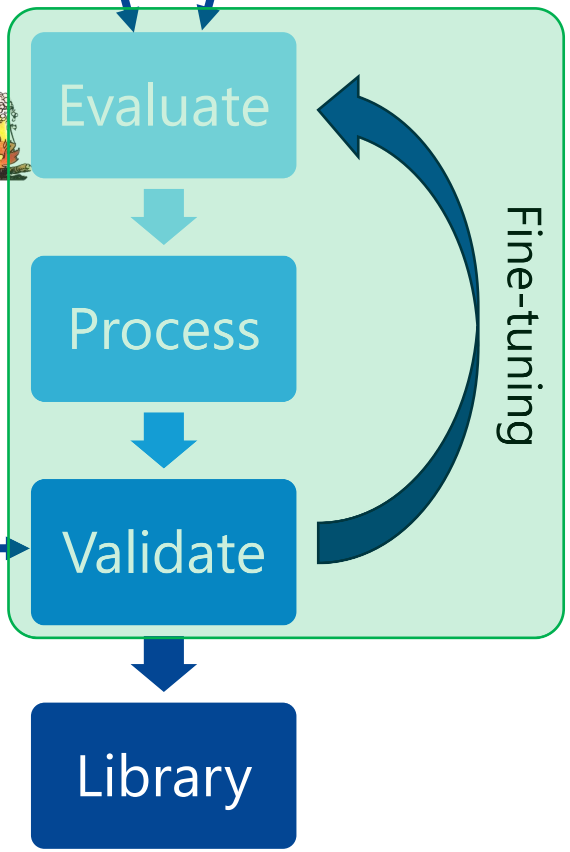
- Nuclear data evaluation process
  - Multi-step process
  - Evaluation ➔ Bayesian approach
  - Integral experiments used for validation

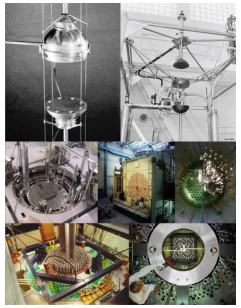


Objective





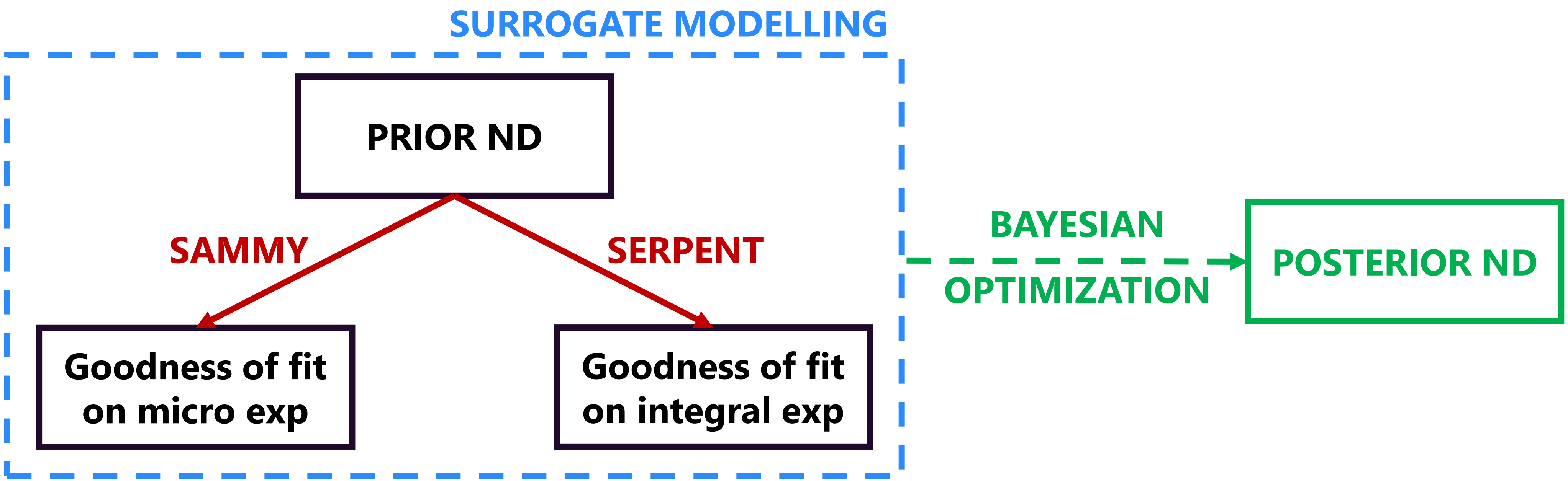




- Data Assimilation using both microscopic and integral measurement
- Identify limitations and challenges

Methodology

Overview



Methodology

$$\chi^2 = \frac{(C - E)^2}{\Sigma}$$

Formulation unnormalized posterior

$$\ln(p) =$$

PRIOR

$$-\frac{1}{2}\chi^2_{\mathrm{ND}}$$

MICROSCOPIC

$$-\frac{1}{2}\chi^2_{\mathrm{m}}$$

INTEGRAL

$$-\frac{1}{2}\chi^2_{\mathrm{i}}$$

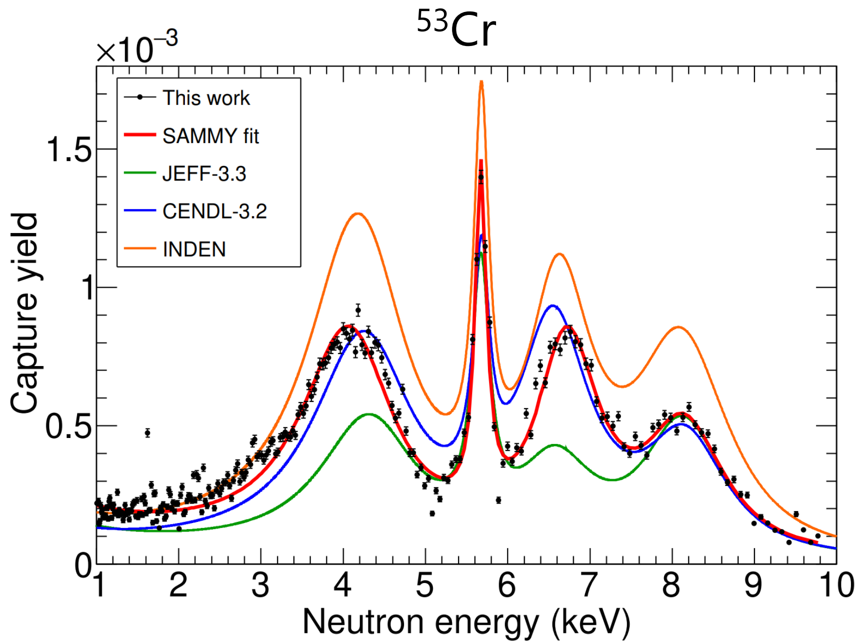
Case study: ^{53}Cr

Case study: ^{53}Cr

Why ^{53}Cr?

- Stainless steel (11-26% chromium)
- Structural materials of reactors → corrosion resistance
- ^{50,52,53}Cr important for k_{eff} in some nuclear systems (mostly (n,γ))
- ^{53}Cr was included in NEA High Priority Request List (1-100 keV)

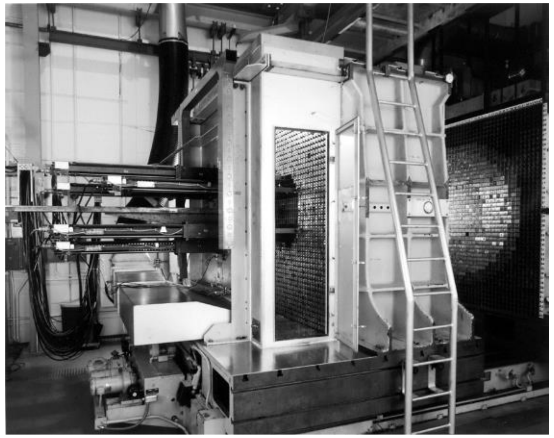
Isotope	Abundance (%)
Cr-50	4.34
Cr-52	83.8
Cr-53	9.50
Cr-54	2.37

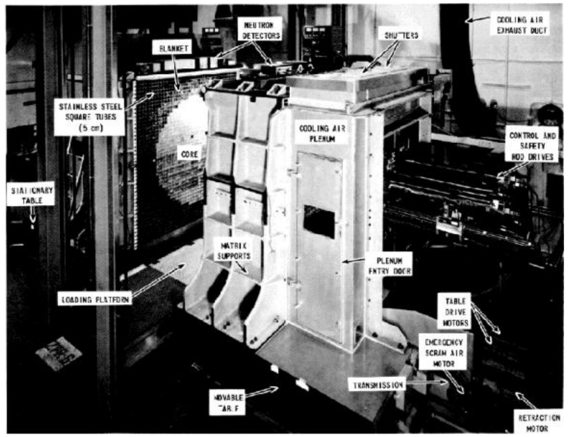


form P. Pérez-Maroto et al., "50Cr and 53Cr neutron capture cross sections measurement at the n_TOF facility at CERN," 2025

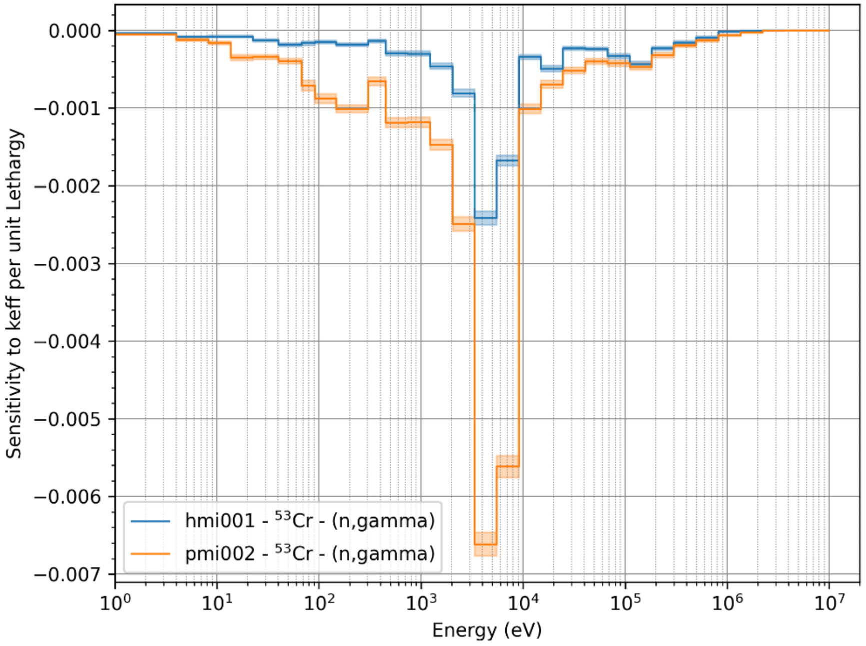
Case study: ^{53}Cr

Selection of integral experiments





- Requirements:
  - Sensitive to ^{53}Cr (n,γ) in 1-10 keV range
- Two most sensitive criticality experiments selected from ICSBEP [4]:
  - HMI-001
  - PMI-002



Case study: ^{53}Cr

$$\chi^2 = \frac{(C - E)^2}{\Sigma}$$

Formulation unnormalized posterior

$$\ln(p) =$$

PRIOR	MICROSCOPIC	INTEGRAL
$-\frac{1}{2}\chi^2_{\mathrm{ND}}$	$-\frac{1}{2}\chi^2_{\mathrm{m}}$	$-\frac{1}{2}\chi^2_{\mathrm{i}}$

$$\chi^2 = \frac{(C-E)^2}{\Sigma}$$

Case study: ^{53}Cr

Formulation unnormalized posterior

$$\ln(p) = $$

PRIOR

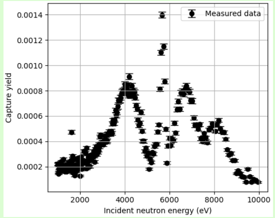
$$-\frac{1}{2}\chi^2_{\mathrm{ND}}$$

- 4 input parameters:
  - Γ_γ E=4.1 keV
  - Γ_γ E=5.7 keV
  - Γ_γ E=6.8 keV
  - Γ_γ E=8.2 keV
- 20% rel. unc. Γ_γ
- No correlation
- Multivariate normal

MICROSCOPIC

$$-\frac{1}{2}\chi^2_{\mathrm{m}}$$

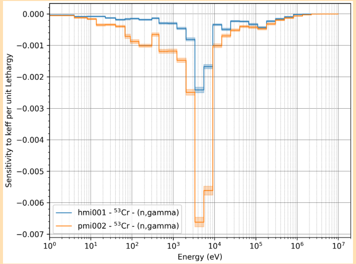
- 256 observations
- Treat normalization uncertainty as fitting parameter
- $\Sigma_{\mathrm{m}} = \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{norm}} + \Sigma_\alpha$



INTEGRAL

$$-\frac{1}{2}\chi^2_{\mathrm{i}}$$

$$\Sigma_i = \Sigma_{exp} + \Sigma_{GP} + \Sigma_\alpha$$



$$\chi^2 = \frac{(C-E)^2}{\Sigma}$$

Case study: ^{53}Cr

Formulation unnormalized posterior

MICROSCOPIC

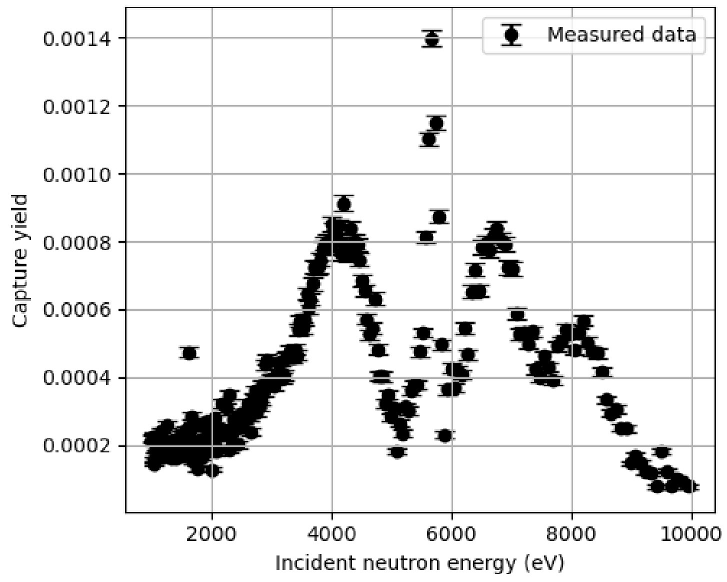
$$-\frac{1}{2}\chi^2_{\mathrm{m}}$$

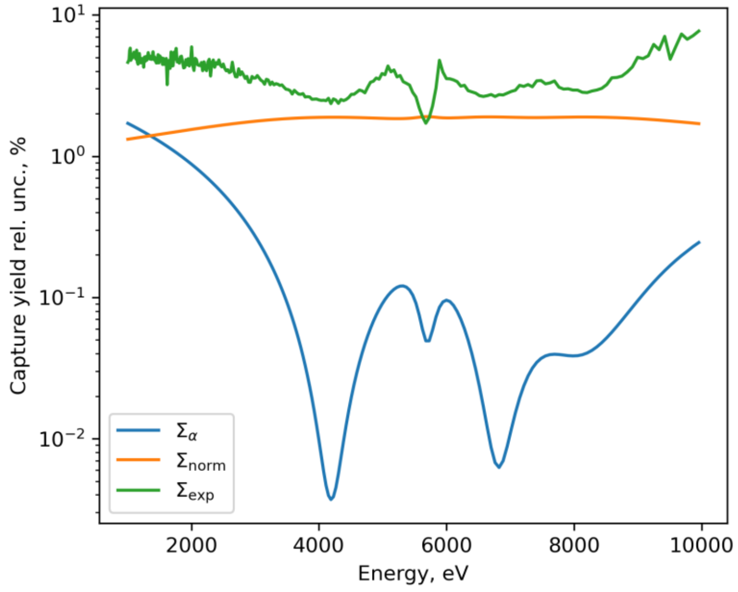
- 256 observations
- Treat normalization uncertainty as fitting parameter
- $\Sigma_{\mathrm{m}} = \Sigma_{\mathrm{exp}} + \Sigma_{\mathrm{norm}} + \Sigma_{\alpha}$

Σ_{exp}: Experimental setup

Σ_{norm}: Normalization factor

Σ_{α}: Other nuclear data





$$\chi^2 = \frac{(C-E)^2}{\Sigma}$$

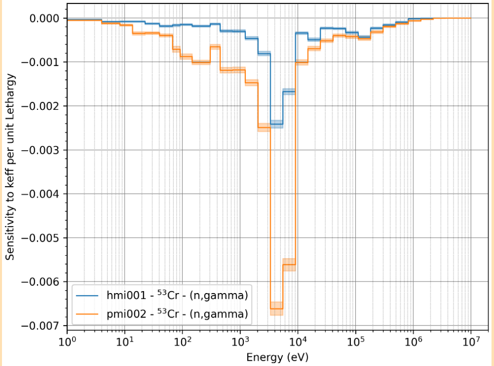
Case study: ^{53}Cr

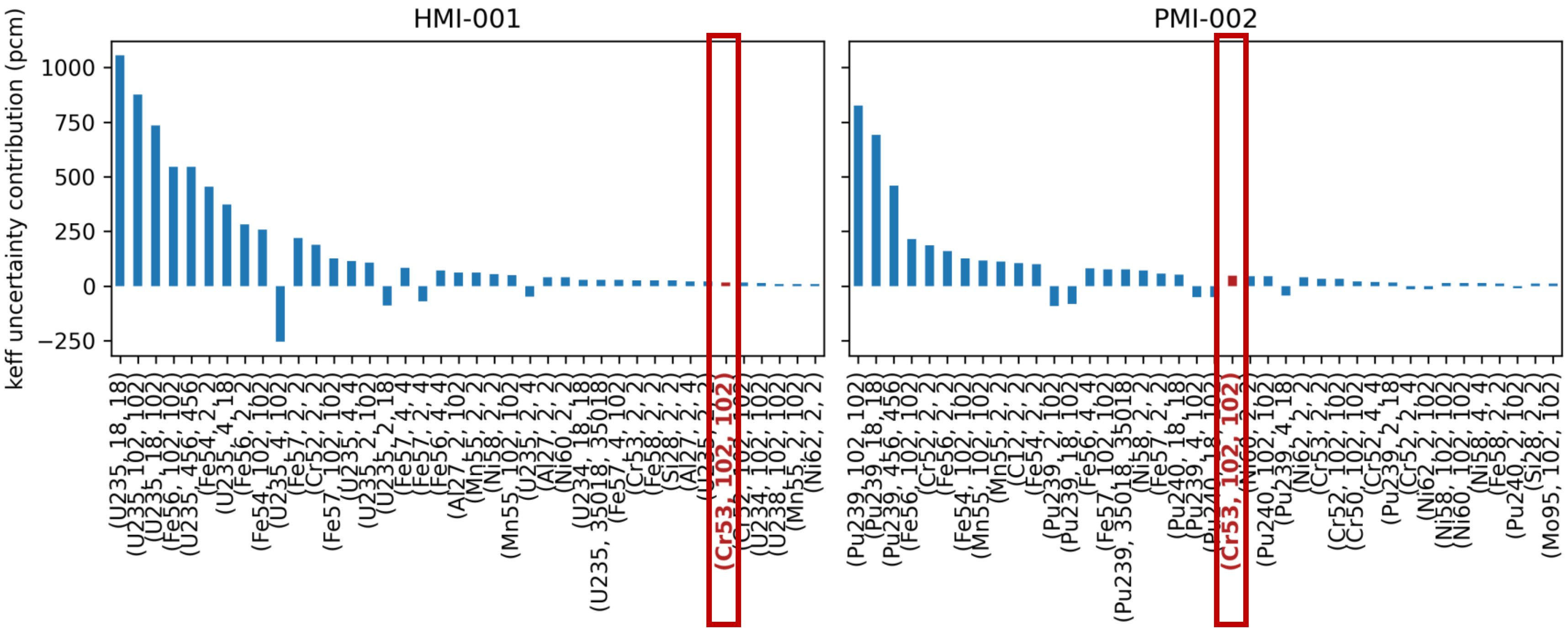
Formulation unnormalized posterior

INTEGRAL

$$-\frac{1}{2}\chi_{\mathrm{i}}^2$$

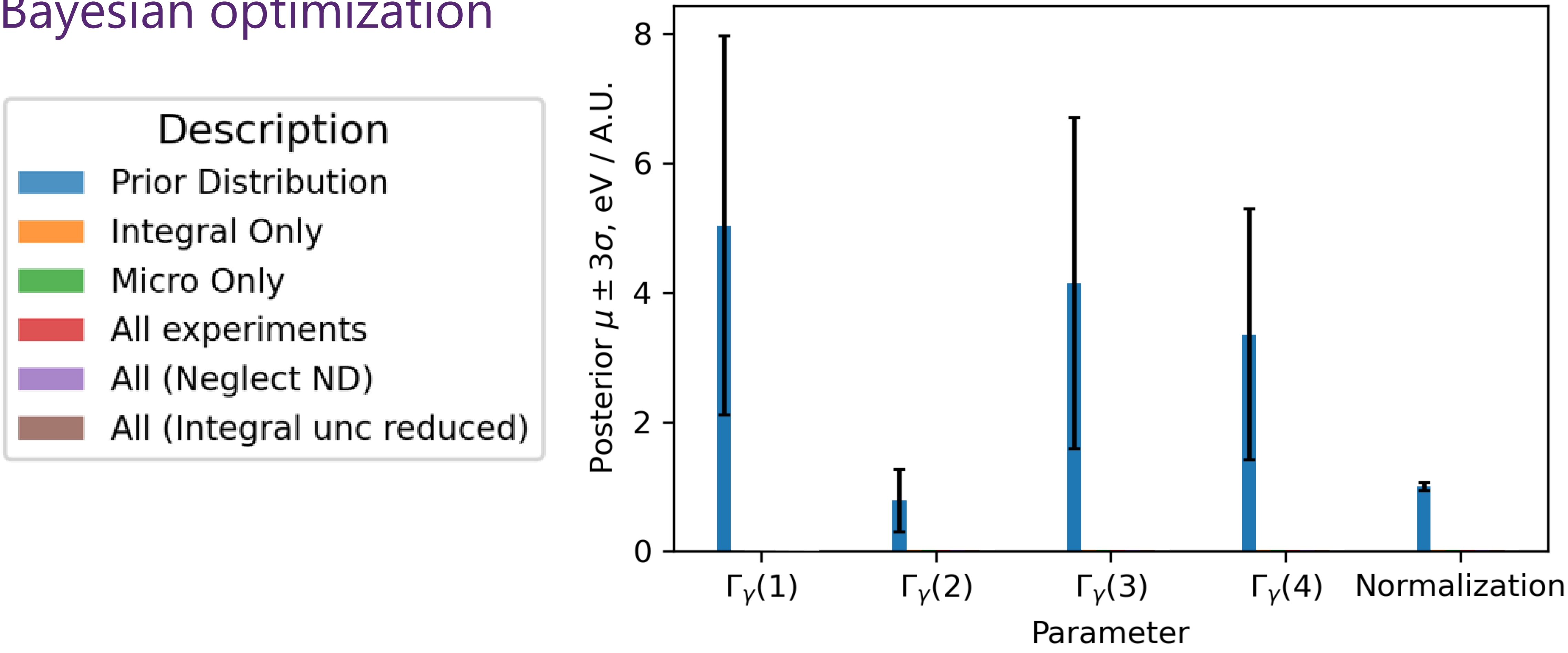
$$\Sigma_i = \Sigma_{\mathrm{exp.}} + \Sigma_{GP} + \Sigma_\alpha$$





Results

Bayesian optimization



Conclusions

- A methodology is presented to include both microscopic and integral measurements using surrogates
- Integral measurements can be included but uncertainties of other nuclear data should also be considered
- HMI-001 and PMI-002 are not sensitive enough to ^{53}Cr (n,γ) for DA
- Improvement mostly comes from microscopic measurement

References

- N. M. Larson, “Updated User’s Guide for Sammy: Multilevel R-Matrix Fits to Neutron Data Using Bayes’ Equations,” ORNL/TM-9179/R8, 941054, Oct. 2008. doi: 10.2172/941054.
- J. Leppänen, V. Valtavirta, A. Rintala, and R. Tuominen, “Status of Serpent Monte Carlo code in 2024,” *EPJ Nuclear Sci. Technol.*, vol. 11, p. 3, 2025, doi: 10.1051/epjn/2024031.
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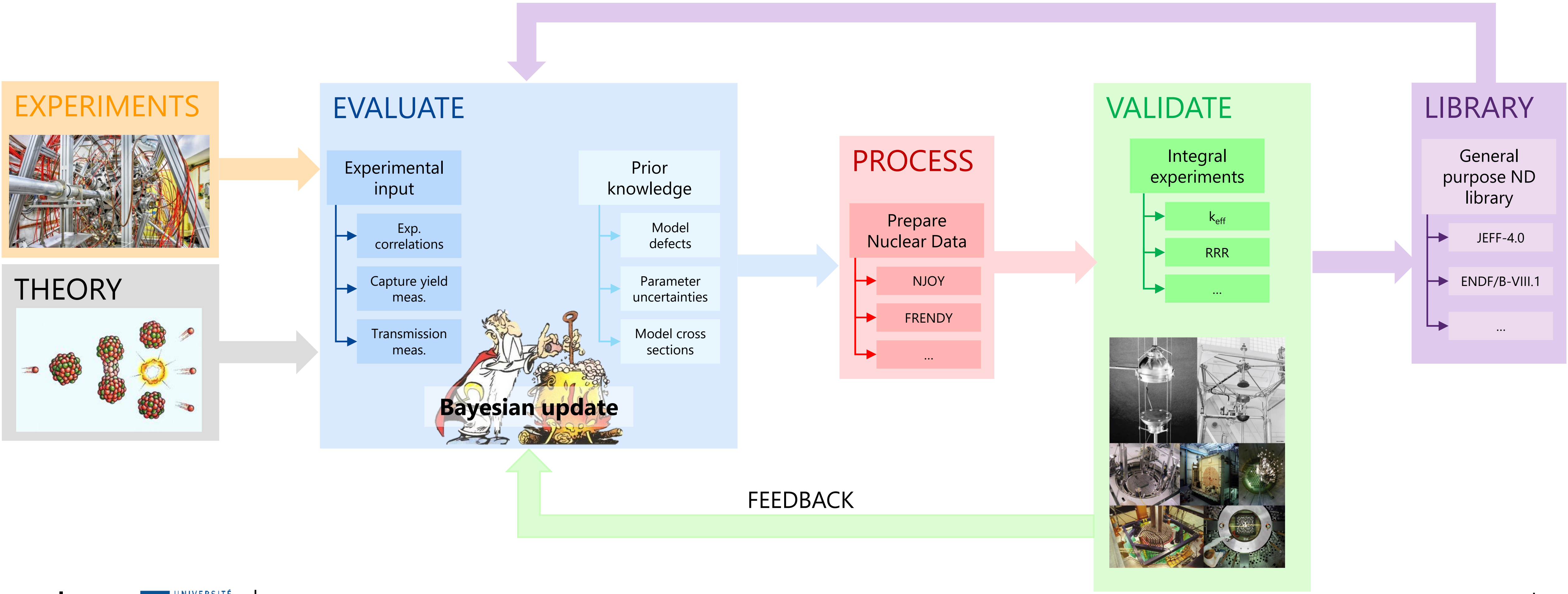
- J. D. Bess, T. Ivanova, J. Martin, I. Hill, and L. Scott, “The 2020 edition of the ICSBEP handbook,” *Nuclear Energy Agency, Organization for Economic Co-Operations and Development*, 2020.
- A. Trkov, O. Cabellos, and R. Capote, “Sensitivity of selected benchmarks to Cr-53 and Cr-50 capture”.
- G. P. A. Nobre et al., “Newly Evaluated Neutron Reaction Data on Chromium Isotopes,” Nuclear Data Sheets, vol. 173, pp. 1–41, Mar. 2021, doi: 10.1016/j.nds.2021.04.002.

Additional slides

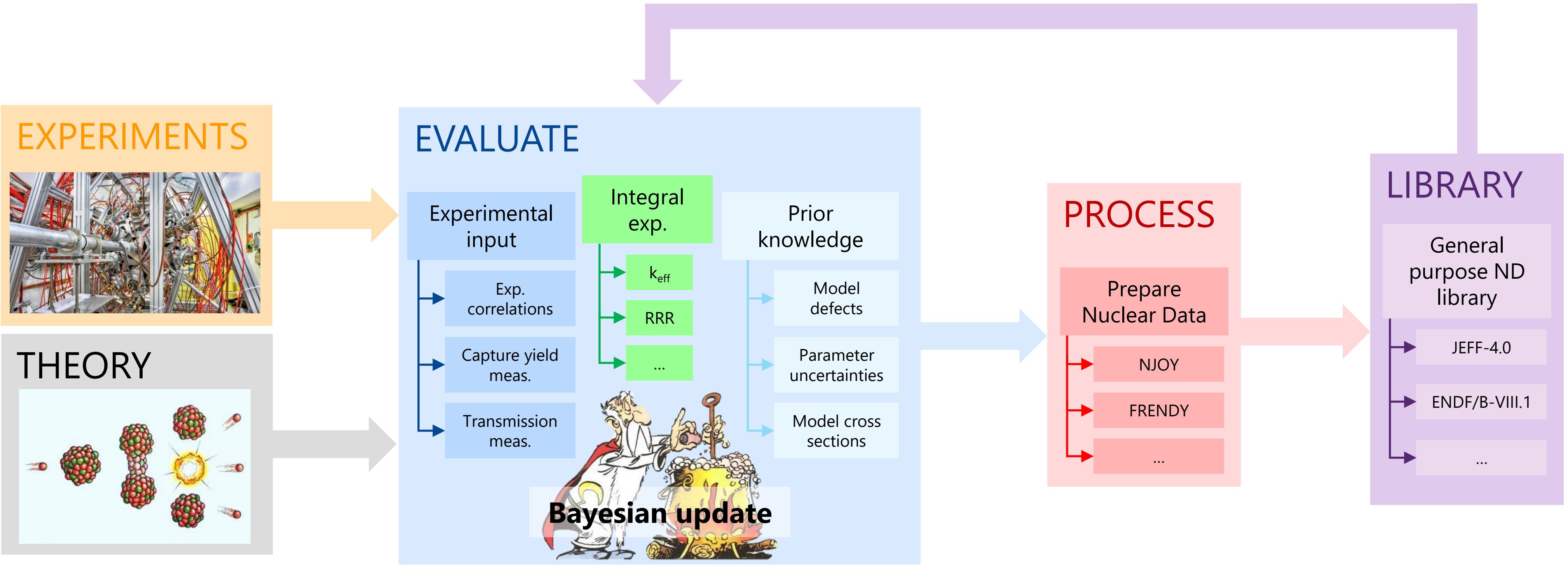
Introduction

Nuclear data evaluation process



Objective

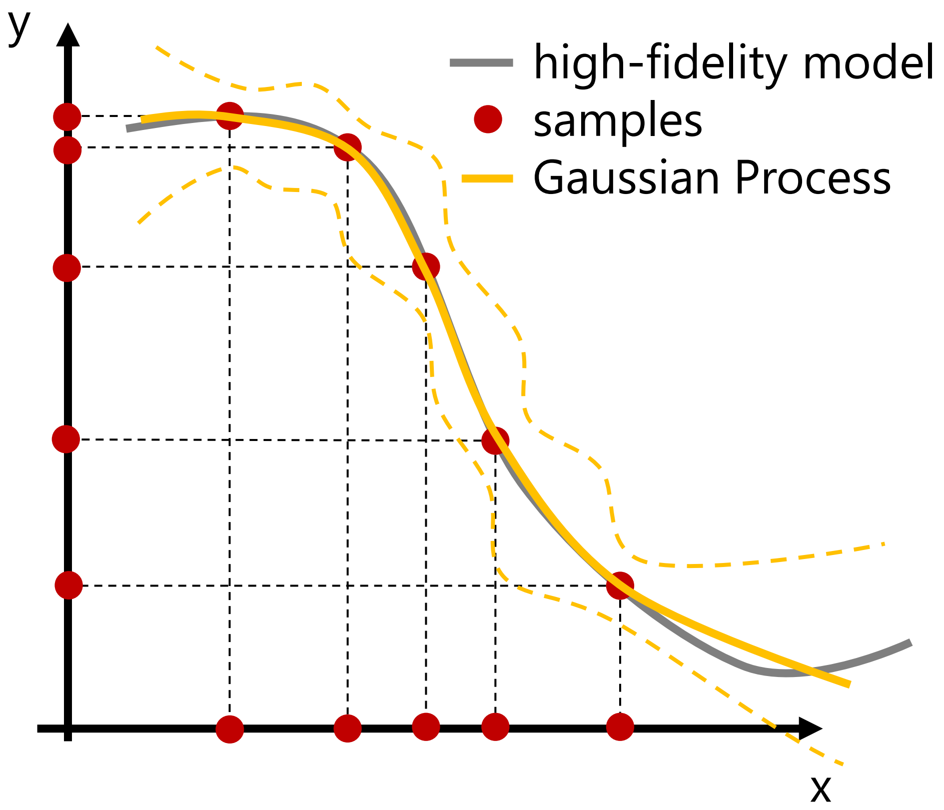
Combine integral and microscopic experiments in one step



Methodology

Surrogate modelling

- SAMMY and mostly SERPENT evaluations are expensive
- Train easy to evaluate surrogate model
  - Sample input parameters
  - Evaluate sample in high-fidelity code
  - Split in training and testing set (80/20)
  - Train a Gaussian Process with training set
  - Test GP on testing set

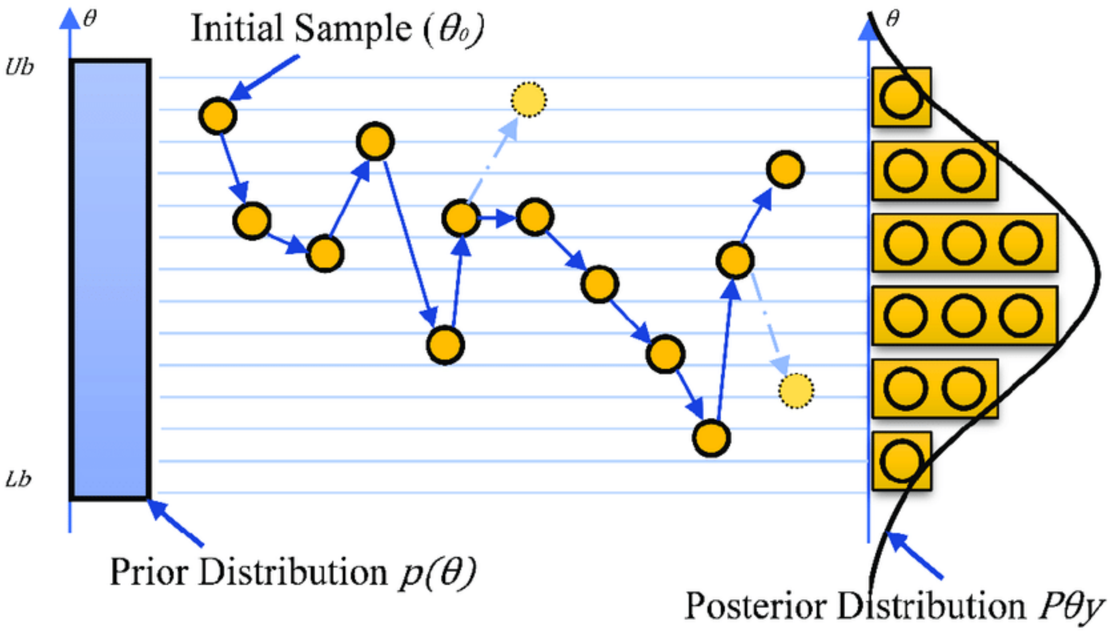


Hastings, W. Keith. "Monte Carlo sampling methods using Markov chains and their applications." (1970): 97-109.

Methodology

Markov Chain Monte Carlo

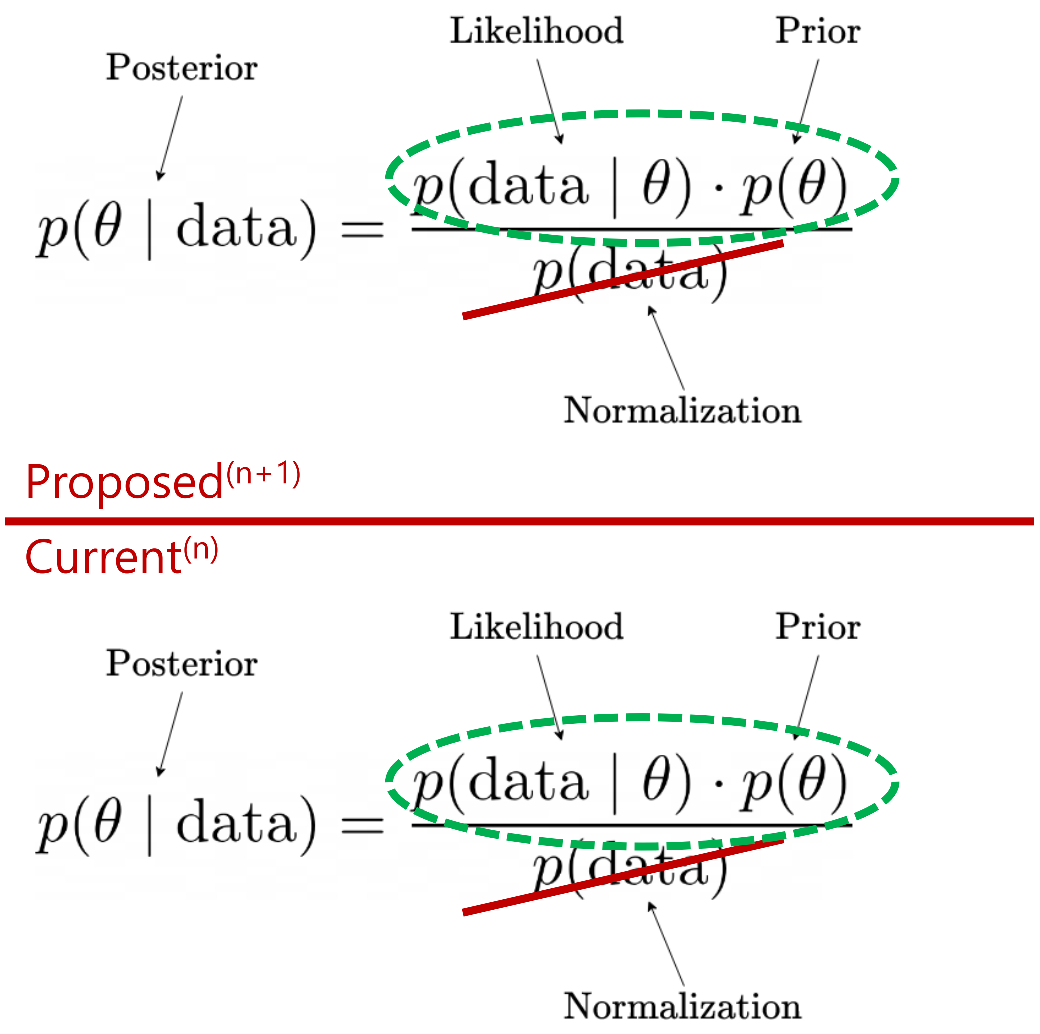
- Instead of randomly sampling the input space
- Carefully select next sample based on likelihood
- Propose new position:
  - If position is more likely → Accept
  - If not → sample to Accept / Reject
- If Accepted → go there
- Rejected → propose new position
- Eventually we sample from stationary distribution = target distribution



Methodology

Markov Chain Monte Carlo

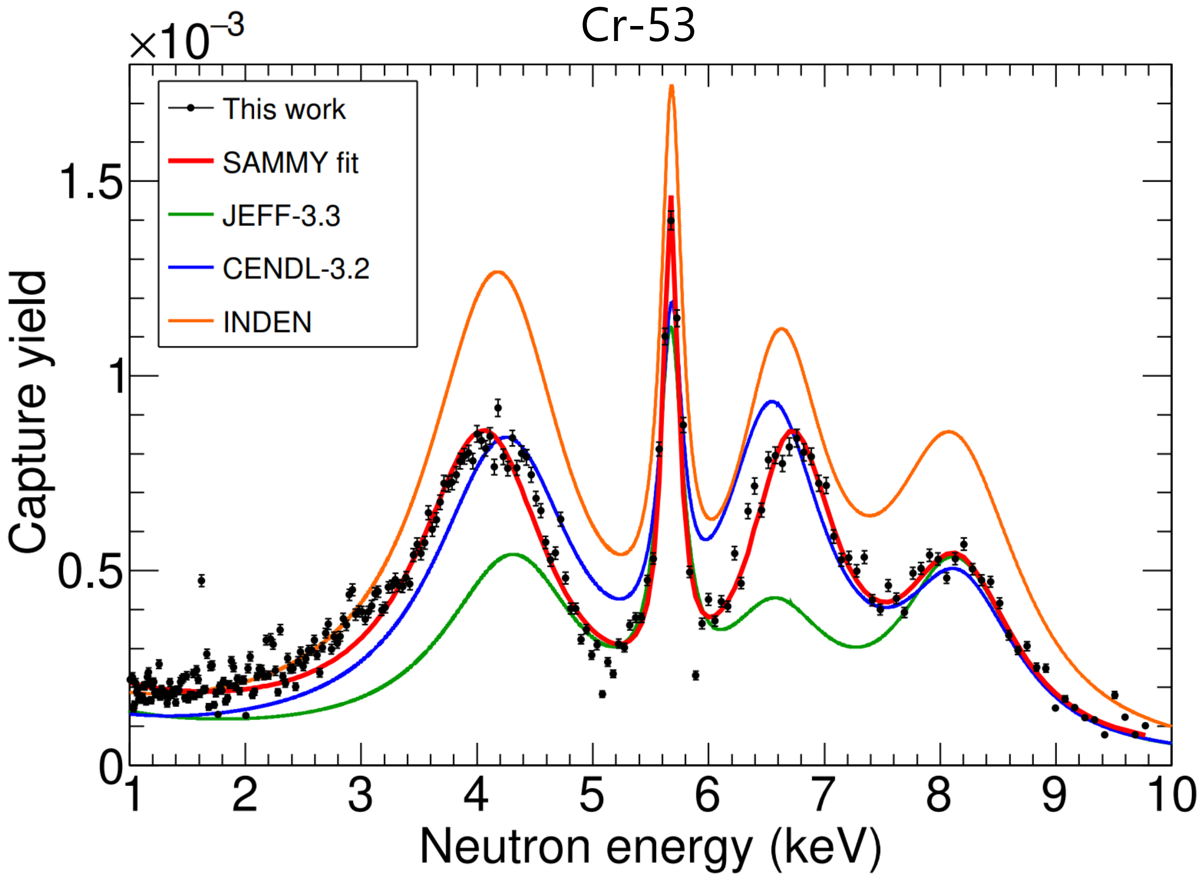
- Accept proposed state based on ratio of unnormalized posterior:
  - Probability of observing proposed state in prior distribution
  - Probability of observing experiments given proposed state
- Probabilities can be small!
  - Take log for numerical stability



Case study: ^{53}Cr

New capture yield measurement

- Neutron time-of-flight
- Using thin target
- Not yet included in evaluation
- Focus on 1-10 keV range
  - **Infer Γ_γ-widths**

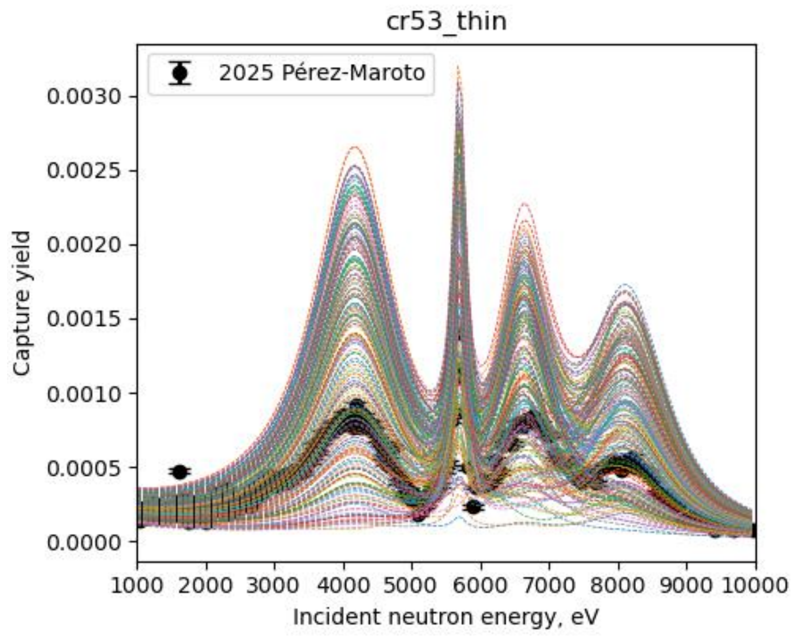


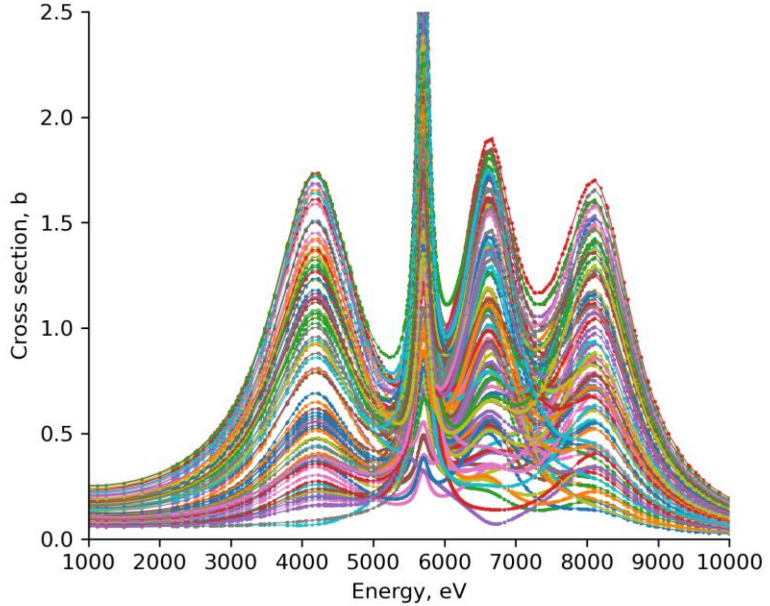
form P. Pérez-Maroto et al., "50Cr and 53Cr neutron capture cross sections measurement at the n_TOF facility at CERN," 2025

Results

Input data

- Draw 100 uniform samples of:
  - Γ_γ's
  - Normalization for capture yield

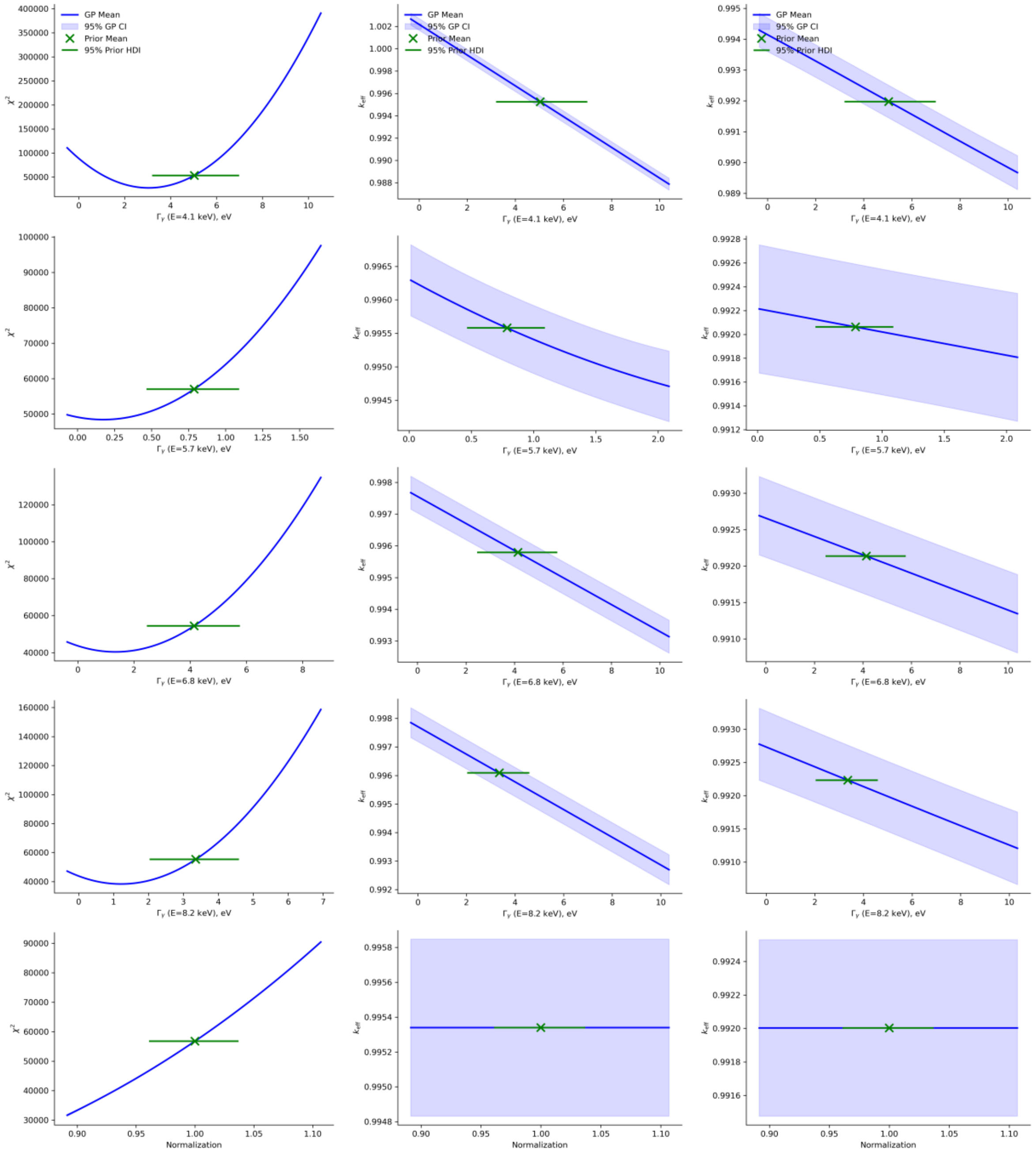




Results

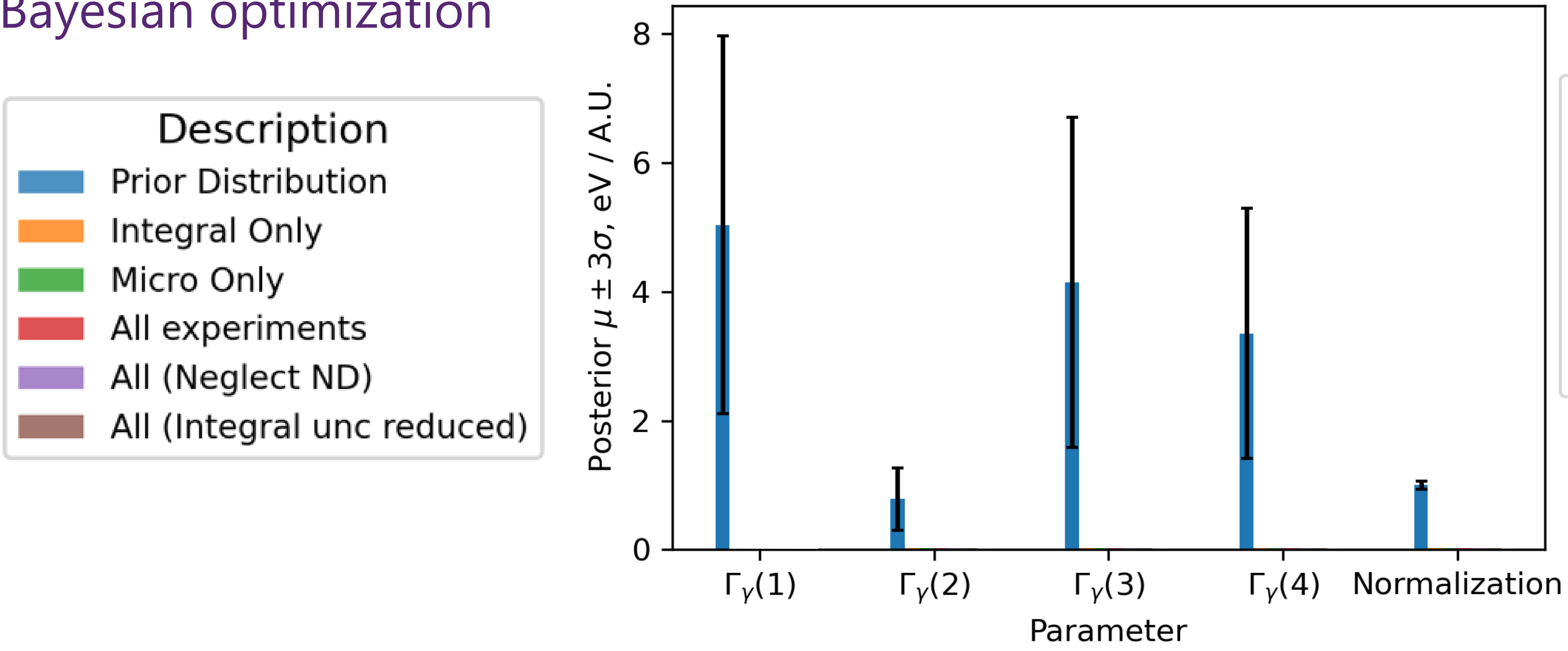
Surrogate behavior

- Learn behavior of experiment
- GP performance on testing set
- SAMMY
- SERPENT



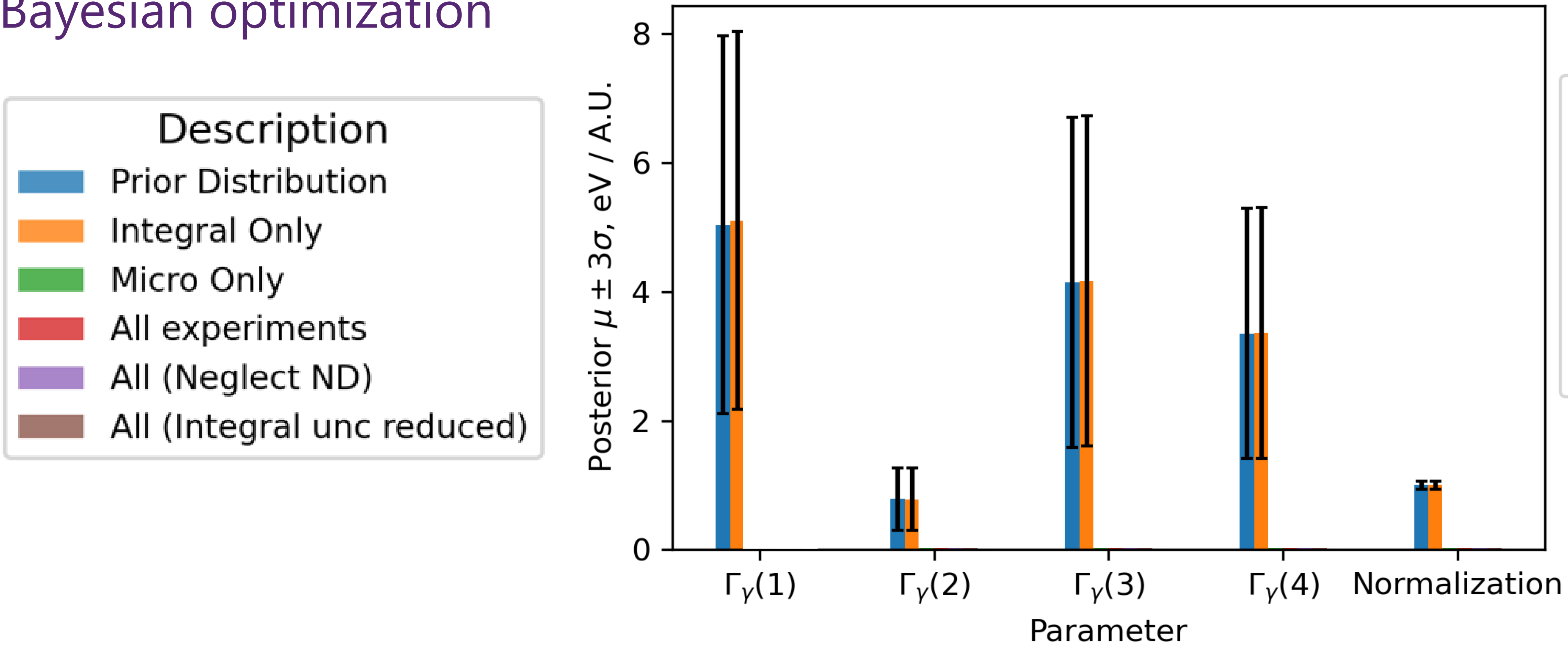
Results

Bayesian optimization



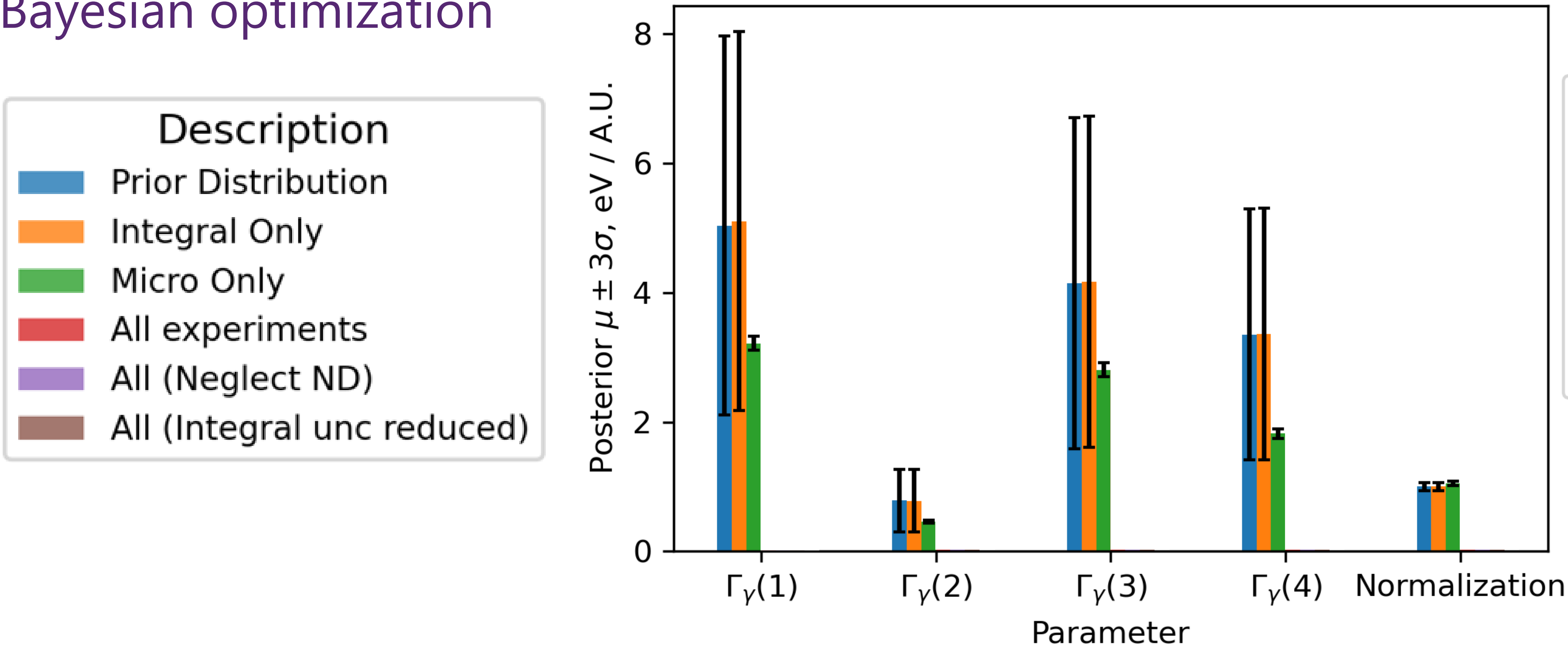
Results

Bayesian optimization



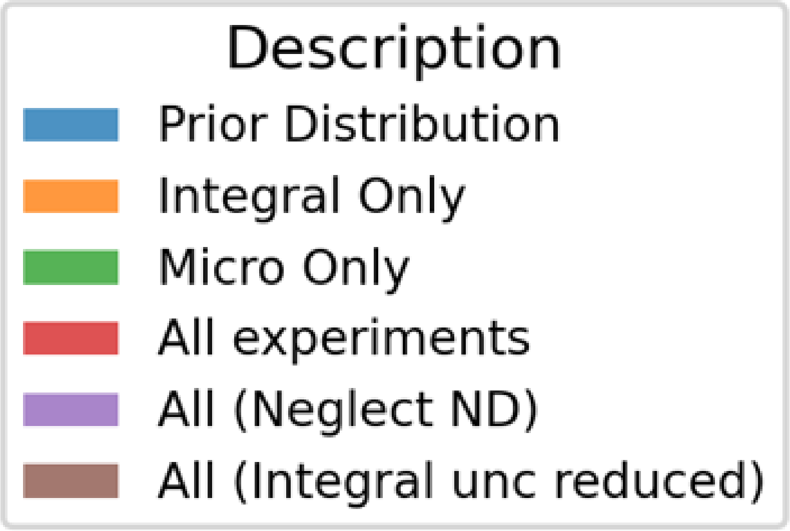
Results

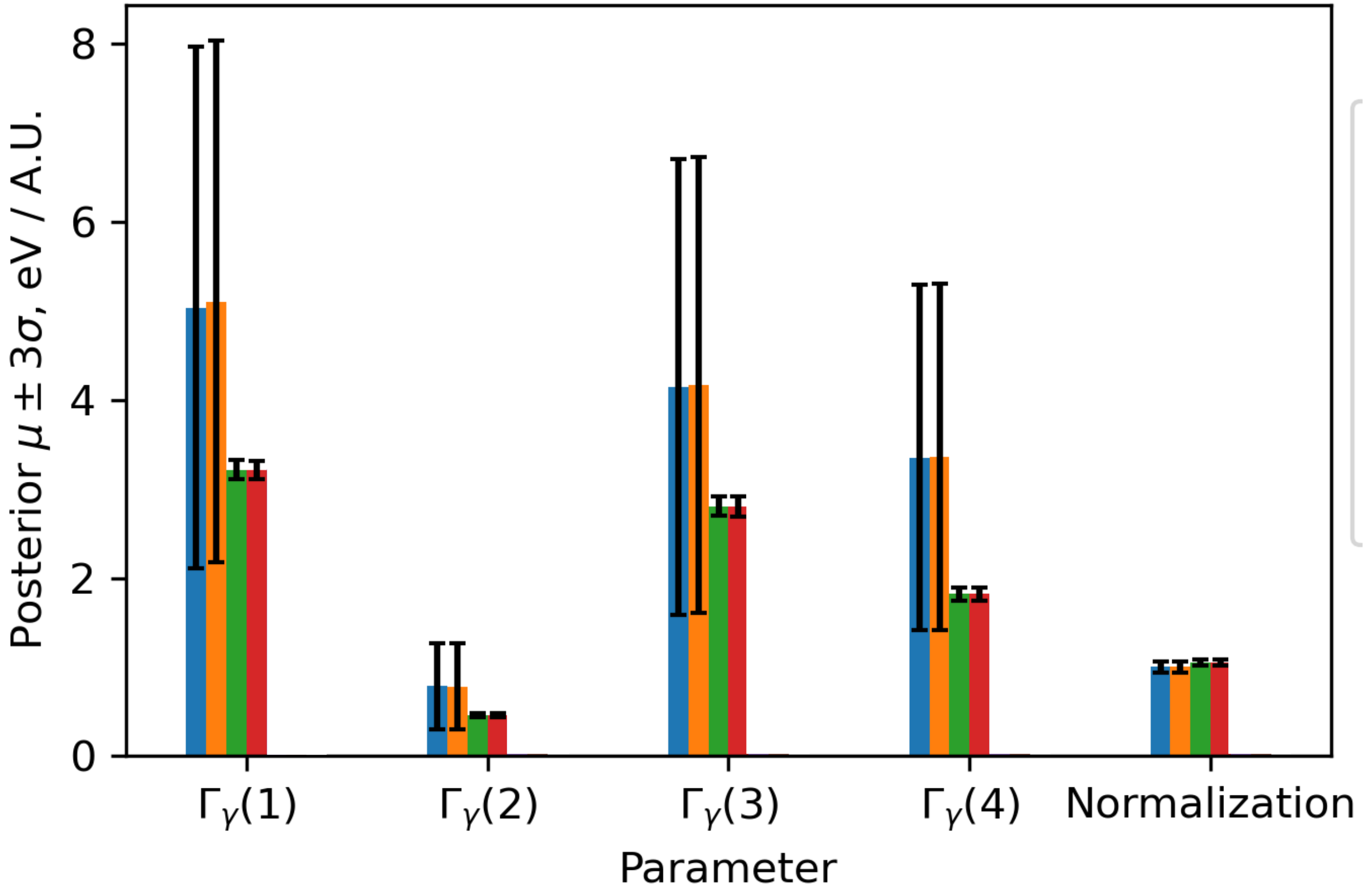
Bayesian optimization



Results

Bayesian optimization



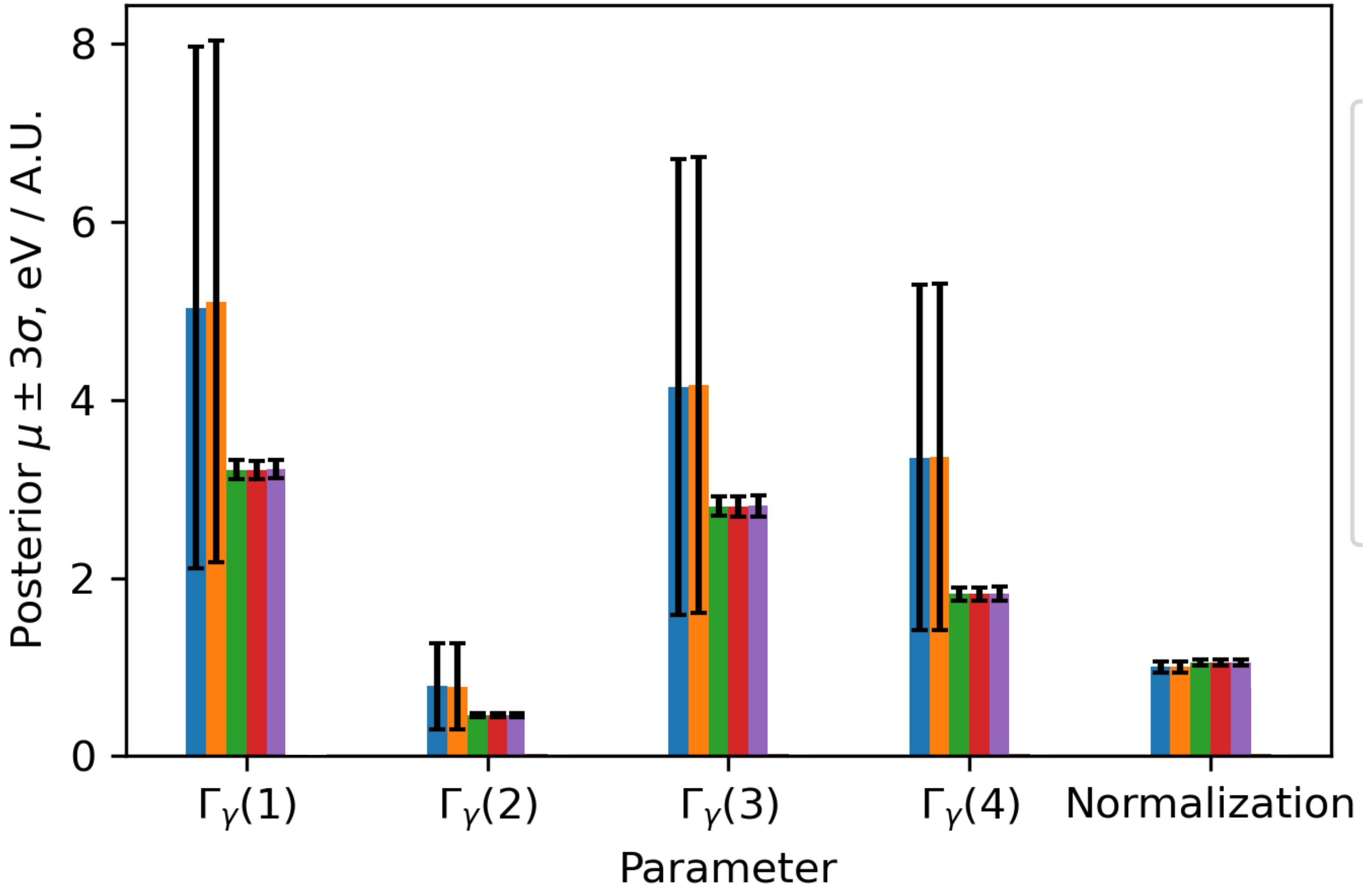


Results

Bayesian optimization

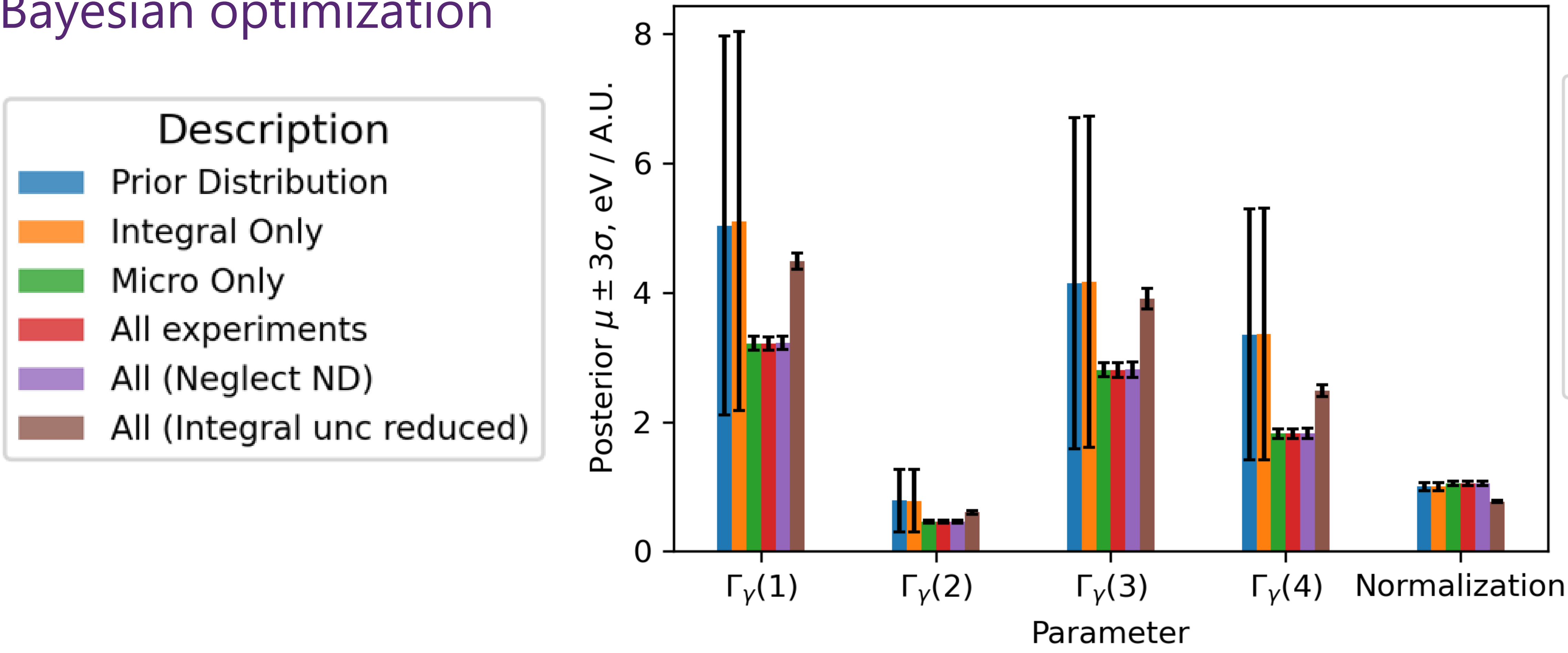
Description

- Prior Distribution
- Integral Only
- Micro Only
- All experiments
- All (Neglect ND)
- All (Integral unc reduced)



Results

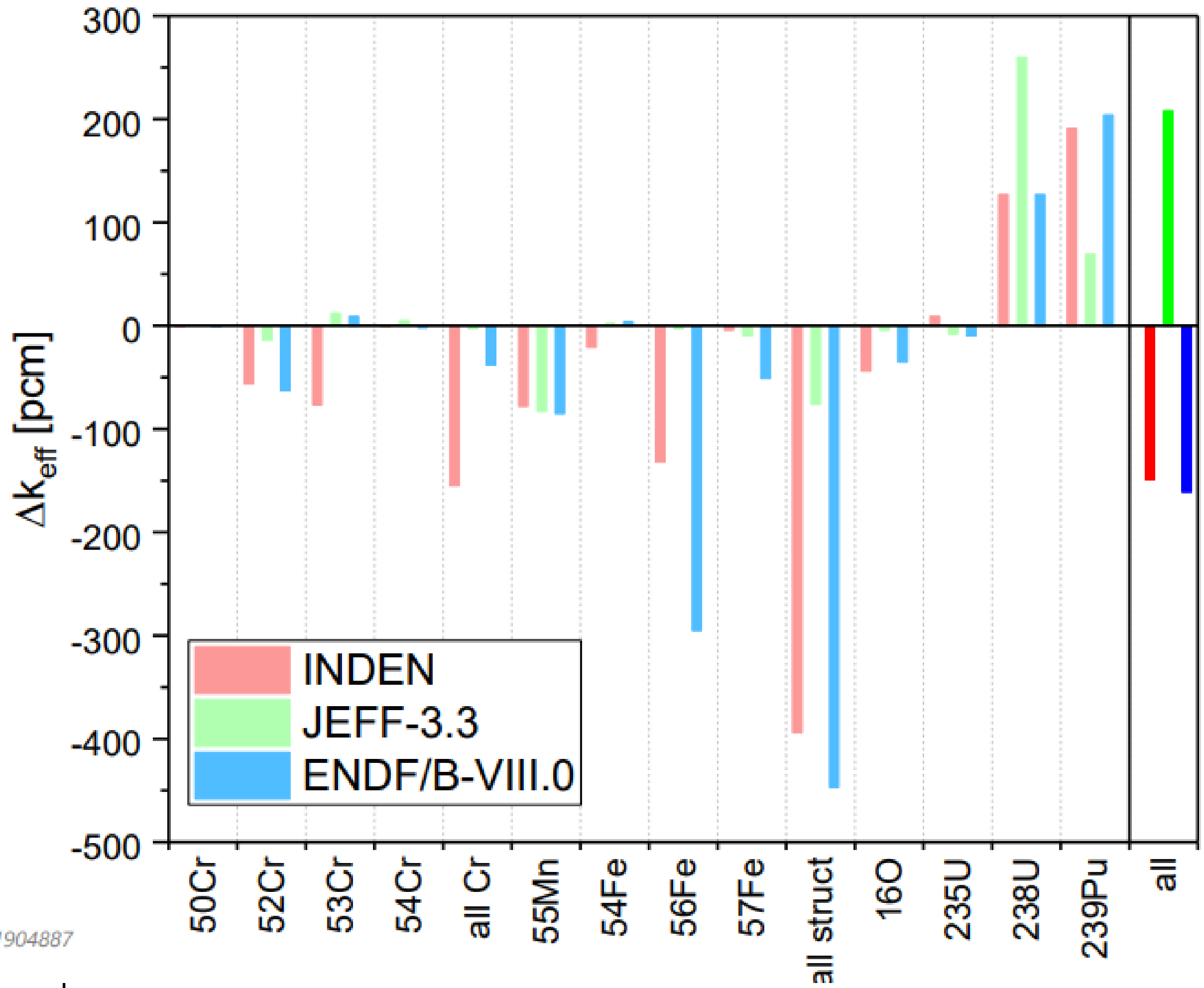
Bayesian optimization



Keff sensitivity to ND library

Nuclear data fles were processed at relevant temperatures (1300 K for fuel, 650 K structural materials)
Reference library JEFF-3.1.2. Replacement per isotope or whole data set

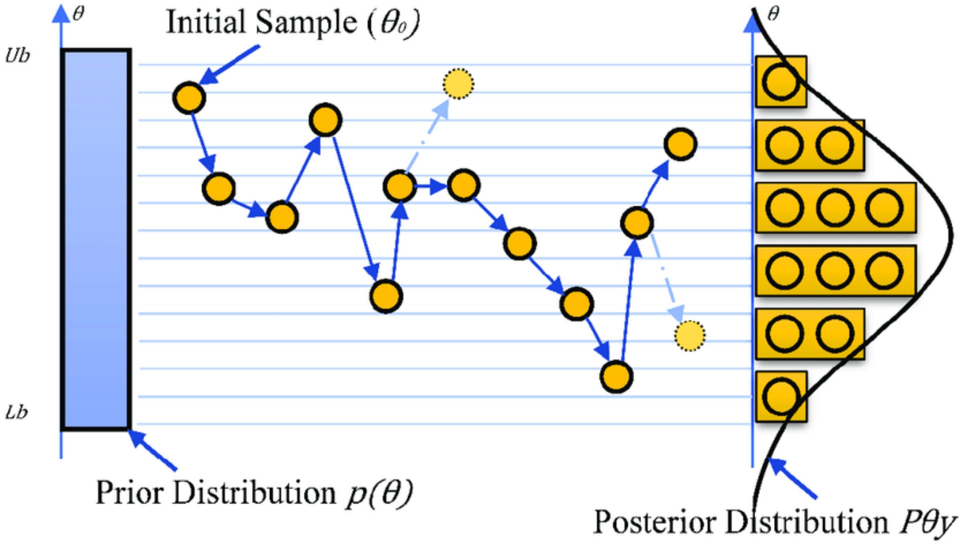
Update of INDEN (higher statistics) + JEFF-3.3 and ENDF/B-VIII.0



- Results of Cr (all isotopes) are confirmed
- Individual Cr isotopes became consistent, so that sensitivity to all is linear combination of individual
- Negative effect of all structural materials is even more pronounced in case of ENDF/B-VIII.0
- Overall, INDEN and ENDF/B-VIII.0 provide lower k_{eff} that reference JEFF-3.1.2 while JEFF-3.3 results in highest k_{eff}

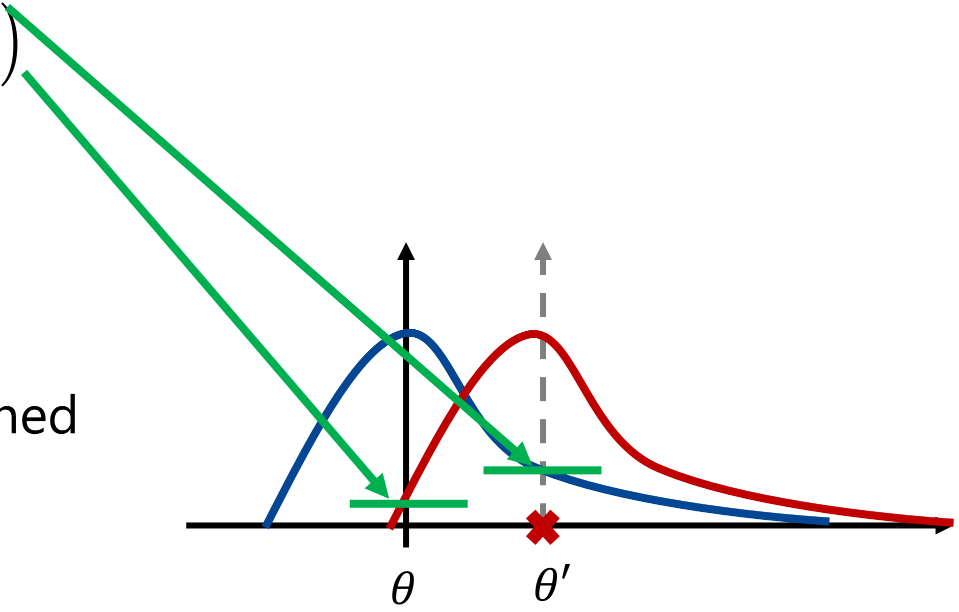
Methodology

Metropolis-Hastings algorithm



1. Start from a random starting position θ
2. Propose new position θ' by sampling from lognormal distribution centered in θ
3. Accept or reject new position: $\alpha(\theta'|\theta) = \min\left(1, \frac{\pi(\theta')}{\pi(\theta)} \cdot \frac{Q(\theta|\theta')}{Q(\theta'|\theta)}\right)$
   - $\frac{\pi(\theta')}{\pi(\theta)}$ is ratio of unnormalized posterior distributions
     - Likelihood x prior (normalizing constant cancels in ratio)
   - If reject → propose another position
4. Sample many times until stationary distribution is reached

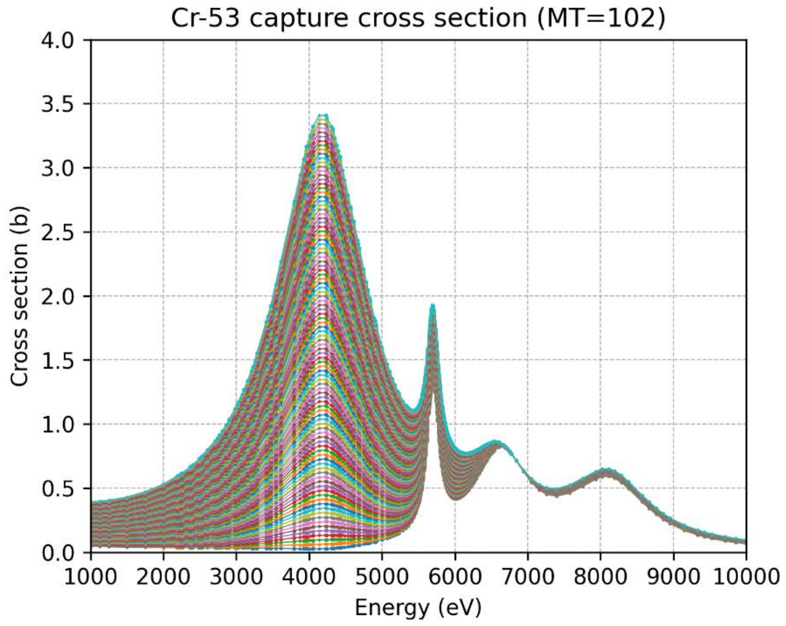
   Stationary distribution = target distribution

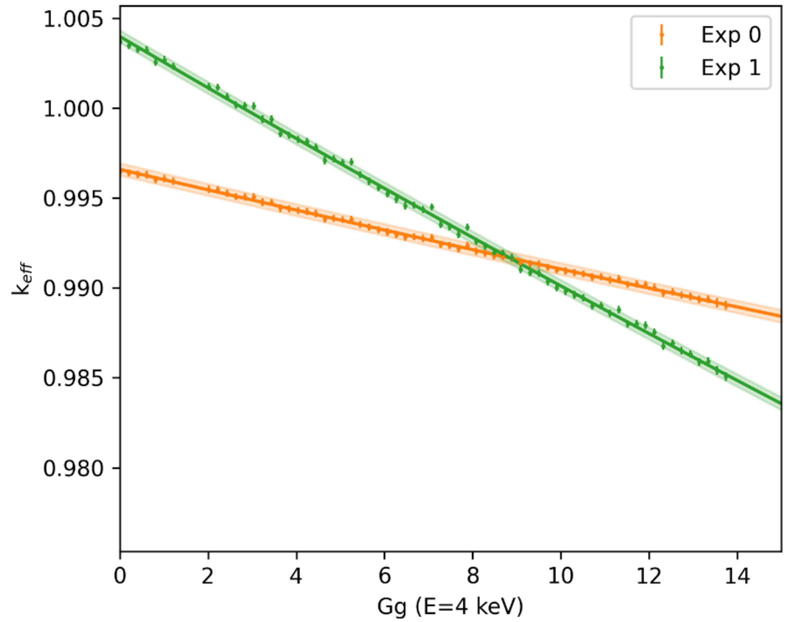


PRELIMINARY

Results

- Surrogate integral measurement
- Vary the first Γ_γ width (4 keV)
- For 2 criticality experiments:
  - Sensitive to Cr-53

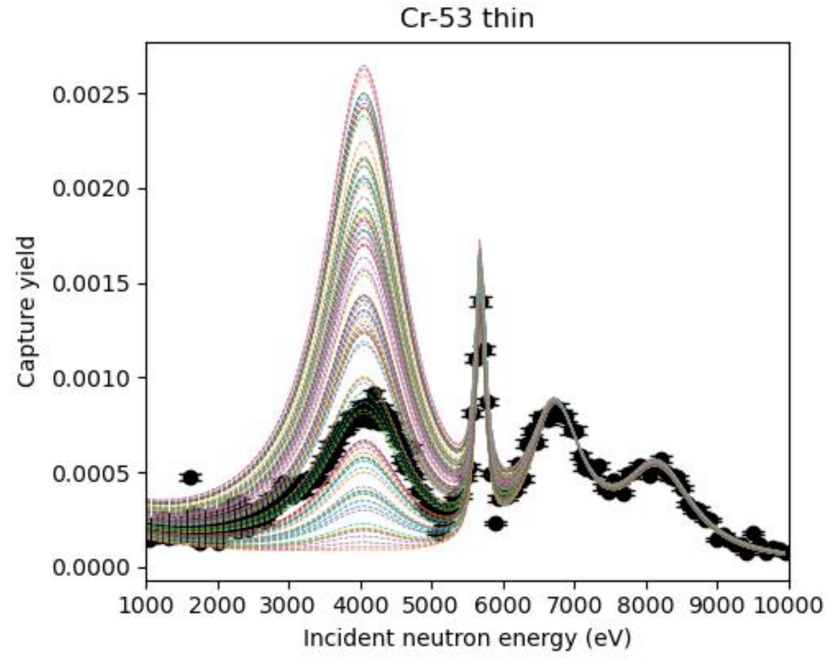


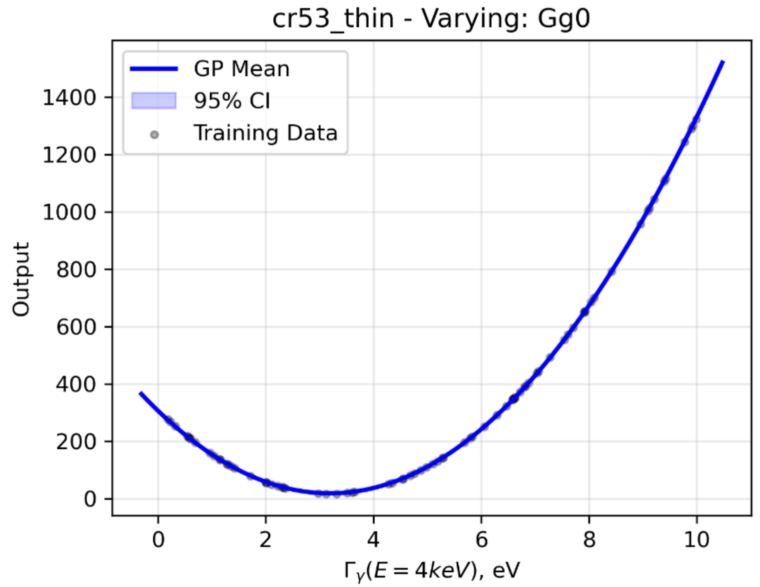


PRELIMINARY

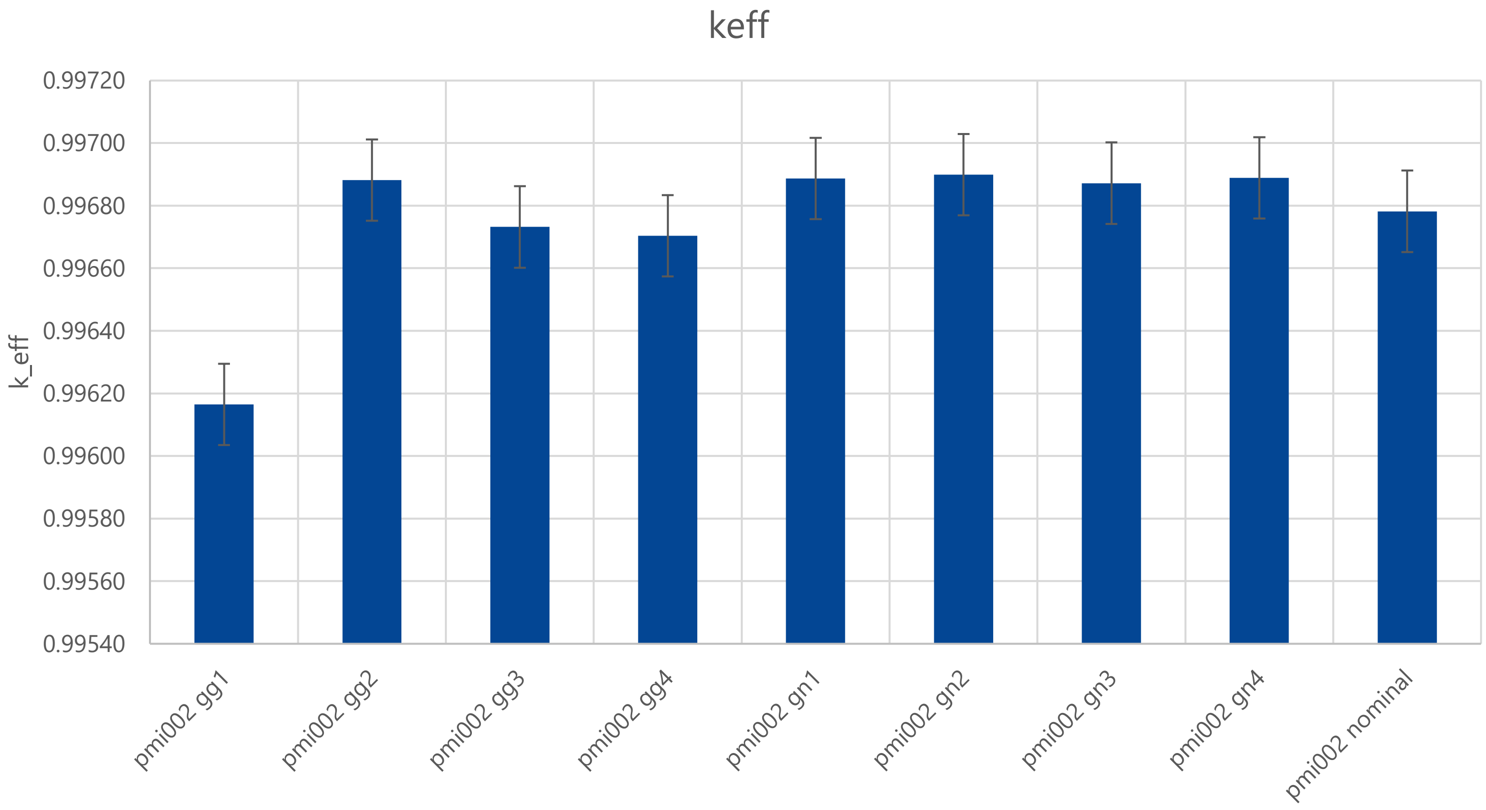
Results

- Microscopic measurement: nTOF
- Vary the first Γ_γ width (E=4 keV)
- Calculate chi-squared on measurement





Sensitivity to Gg (PMI002)



Introduction

ND Evaluation

Evaluated ND (mean values and covariance)

Experimental input

Experiment correlations

Capture yield measurements

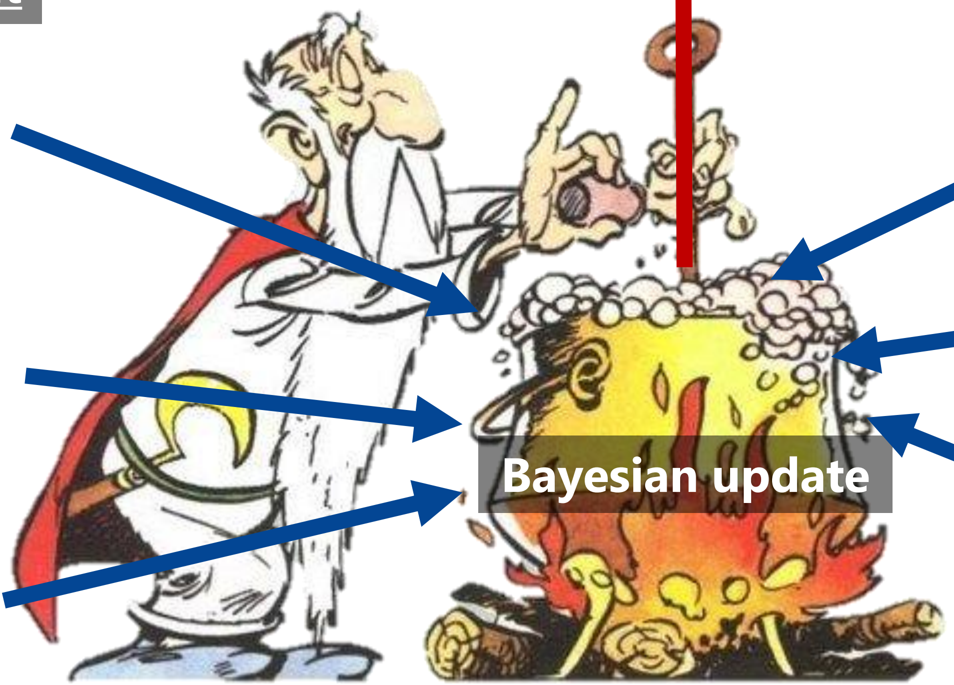
Transmission measurements

Prior knowledge

Model defects

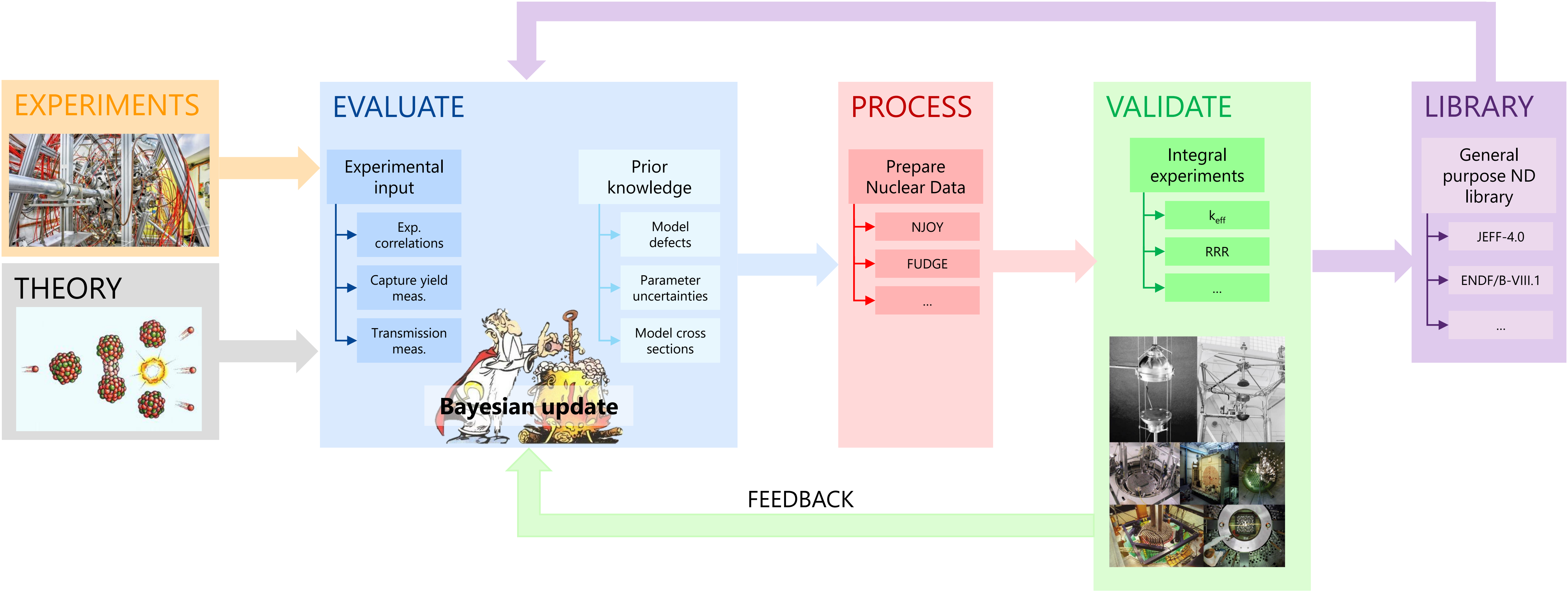
Parameter uncertainties

Model cross sections



from D. Neudecker et al..

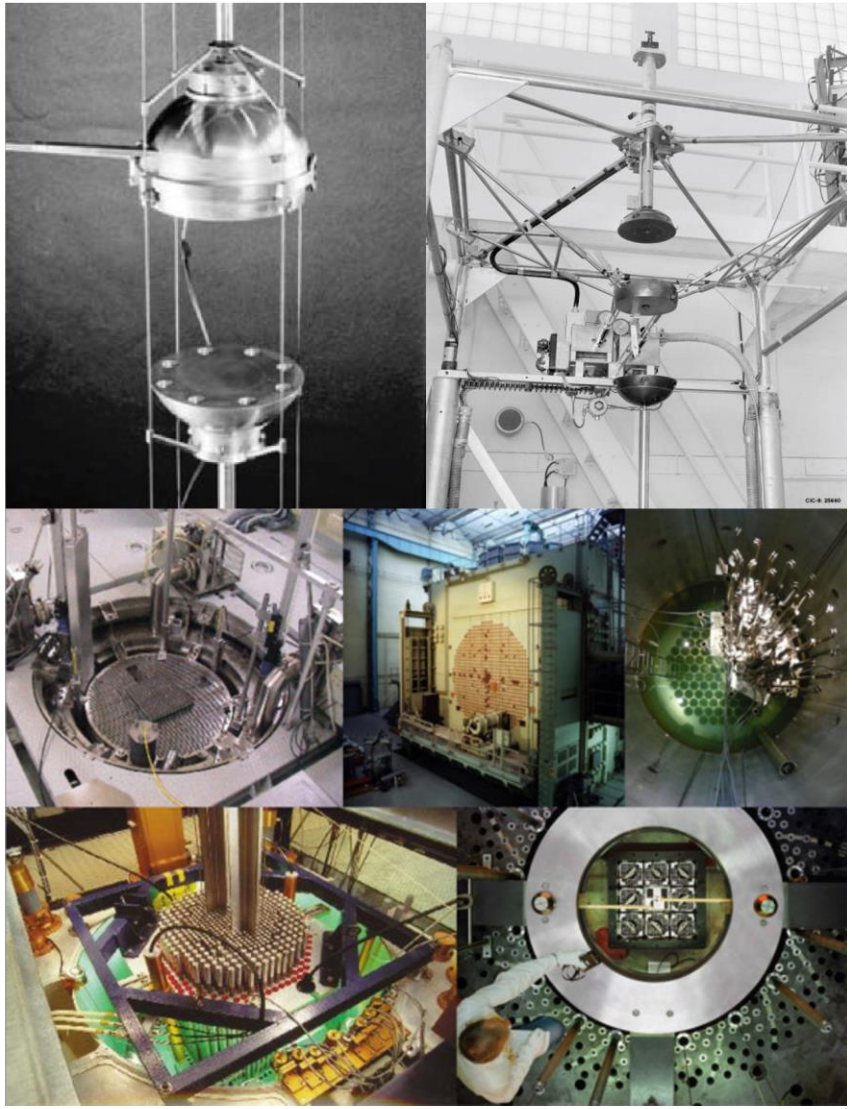
Intoduction



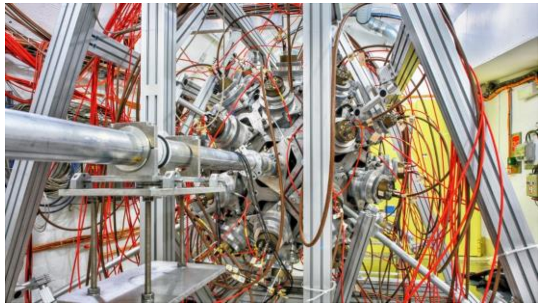
Introduction

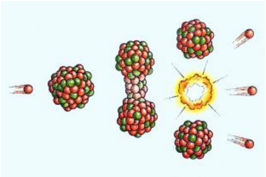
Validation on integral experiments

- Well-known benchmarks
- Calculate C/E:
  - Critical assemblies
  - Pulsed spheres
  - Shielding benchmarks
- Inverse modelling to provide feedback

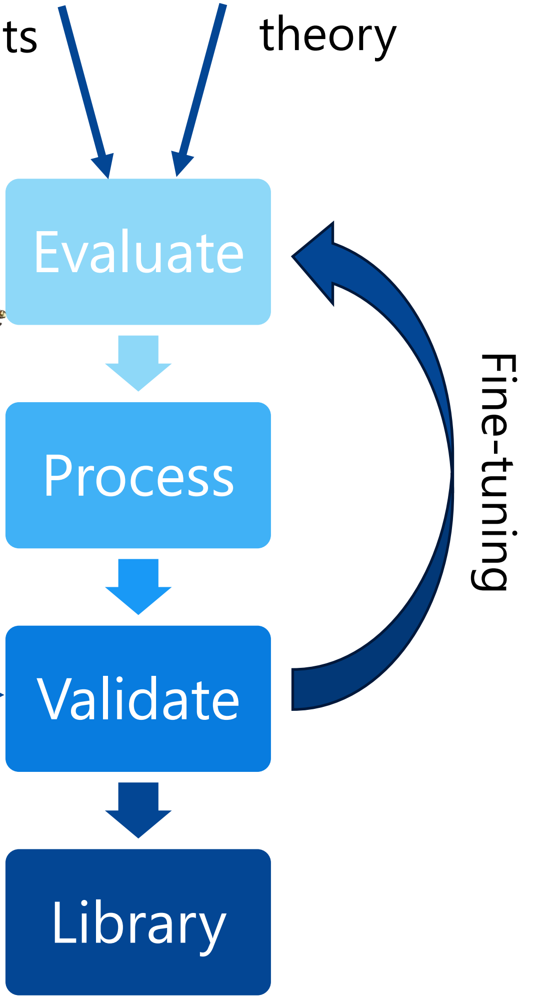


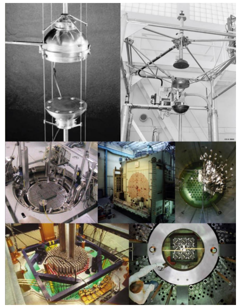
Introduction





- Nuclear data evaluation process
  - Multi-step process
  - Evaluation ➔ Bayesian approach
  - Integral experiments used for validation





Experimental observables

		$\Gamma_r \gg \Gamma_n$	$\Gamma_r \ll \Gamma_n$
• Transmission	$A_{t,thin} \propto g\Gamma_n$	$g\Gamma_n$	$g\Gamma_n$
$\ell = 0$ assignment scattering radius	$A_{t,thick} \propto \sqrt{g\Gamma_n \Gamma}$	$\sqrt{g\Gamma_n \Gamma_r}$	$\sqrt{g\Gamma_n}$
	$\Rightarrow g\Gamma_n, \Gamma$	$g\Gamma_n, \Gamma_r$	g, Γ_n
• Reaction	$A_{r,thin} \propto g\frac{\Gamma_n \Gamma_r}{\Gamma}$	$g\Gamma_n$	$g\Gamma_r$
Higher sensitivity for weak resonances	$\Rightarrow$	$g\Gamma_n, \Gamma_r$	g, Γ_n, Γ_r

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