Using Whisper-1.1 to Guide Improvements to Nuclear Data Evaluations

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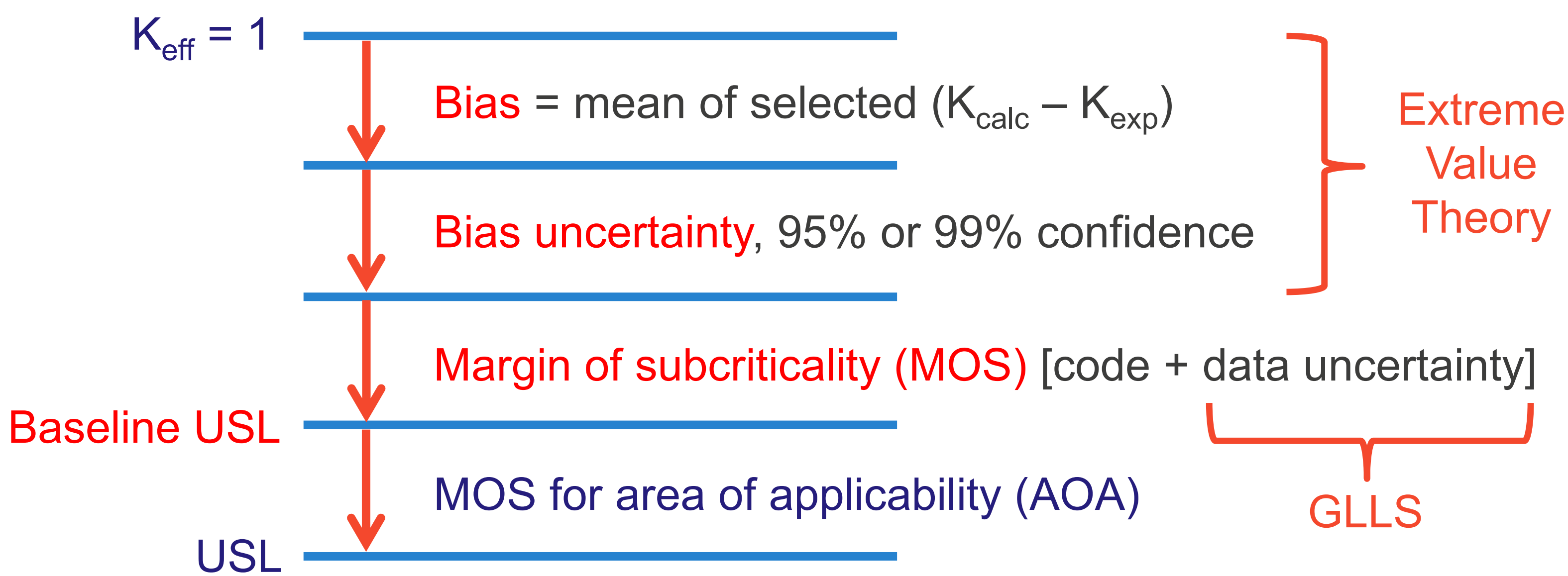
Outline

- **Introduction**
- **Motivation**
- **Background**
    - Uranium-233 nuclear data and benchmarks
    - Whisper-1.1 catalogue data
    - Generalized Linear-Least-Squares (GLLS) method
- **Numerical results**
- **Conclusions & future work**

Introduction

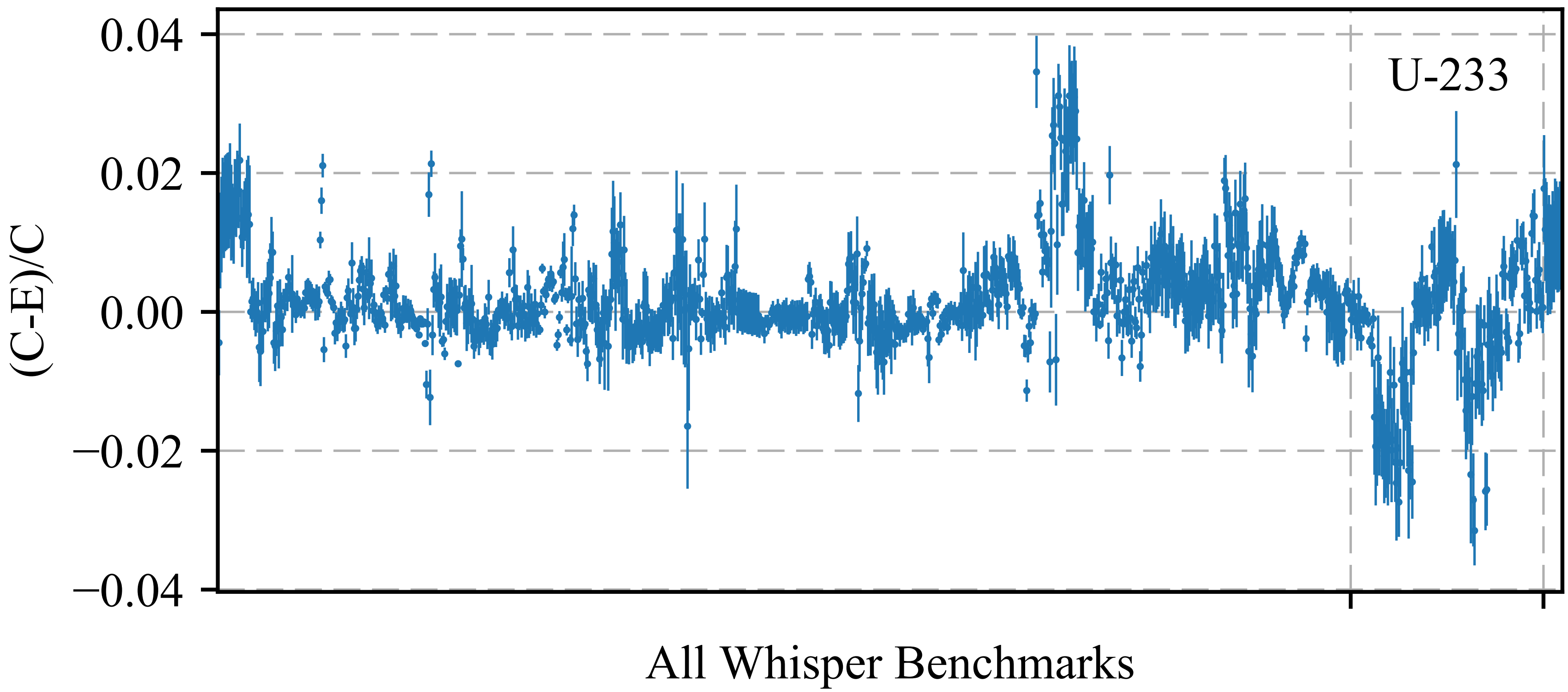
- **What is Whisper-1.1?**
  - Statistical analysis code included with MCNP6.2 to determine baseline USL



1. **Benchmark selection: use benchmark and application correlations (c_k) computed using <u>nuclear data sensitivity profiles</u> and <u>covariance data</u>**
2. **Compute bias and bias uncertainty based on selected benchmarks using Extreme Value Theory**
3. **Additional margin for nuclear data uncertainty estimated by <u>GLLS</u>**

Motivation

- At 2017 DOE NCSP TPR in Washington, D.C. at least two presenters (Leal @ IRSN and Kahler @ LANL) mentioned poor agreement between simulated ^{233}U ICSBEP benchmarks
- Whisper-1.1 contains 1101 benchmarks, 158 of which contain significant amounts of ^{233}U



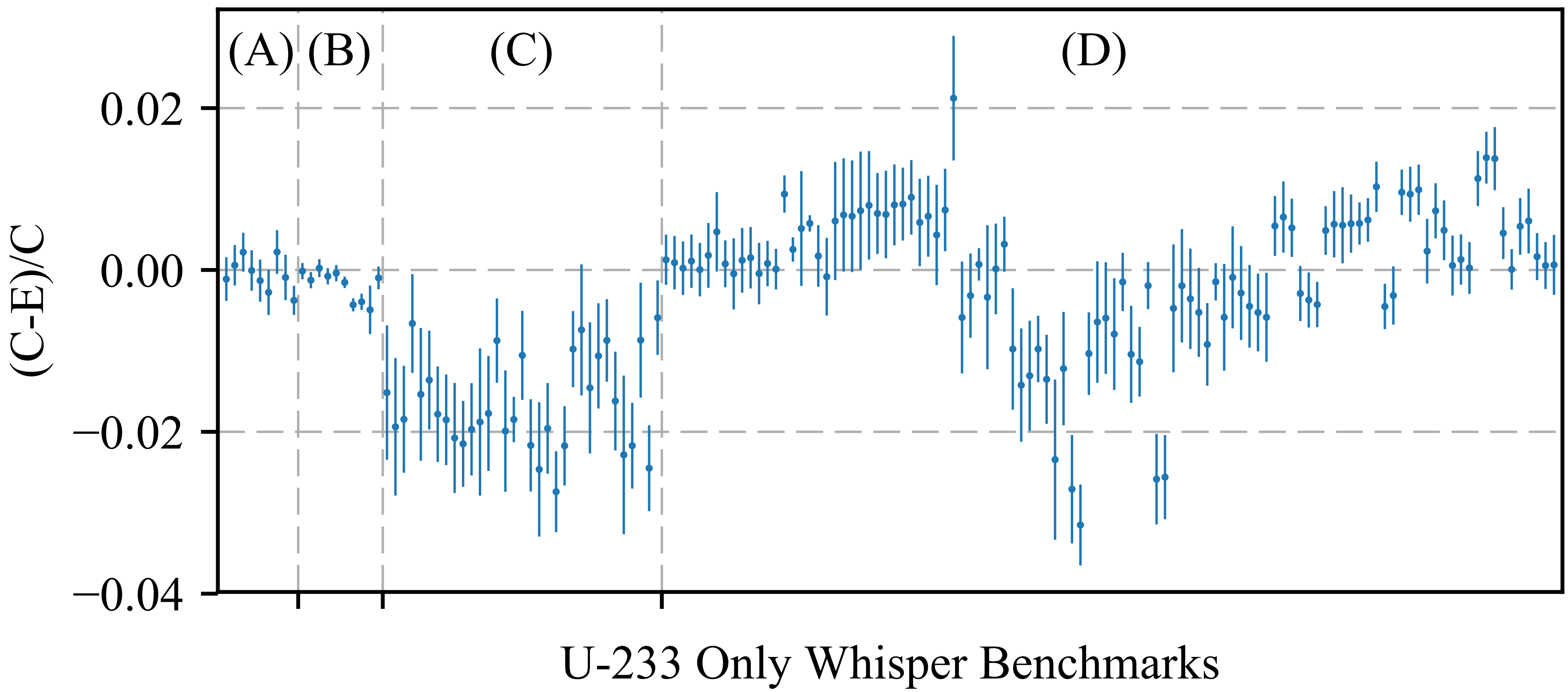
Motivation

(A) **U233-COMP-THERM**
(B) **U233-MET-FAST**
(C) **U233-SOL-INTER**
(D) **U233-SOL-THERM**

χ^2	4.61
RMS	0.0106

Note these discrepancies are defined as

$$d_i = \frac{k_i - m_i}{k_i}$$



Background

- **^{233}U nuclear data and benchmarks**
  - ENDF/B-VII.1 data
  - 158 ^{233}U benchmarks

- **Whisper-1.1 catalogue data**
  - 1101 benchmarks with simulated and benchmark K_{eff}
  - 44-group nuclear data sensitivity profiles
  - BNL-LANL-ORNL (BLO) low-fidelity covariance data

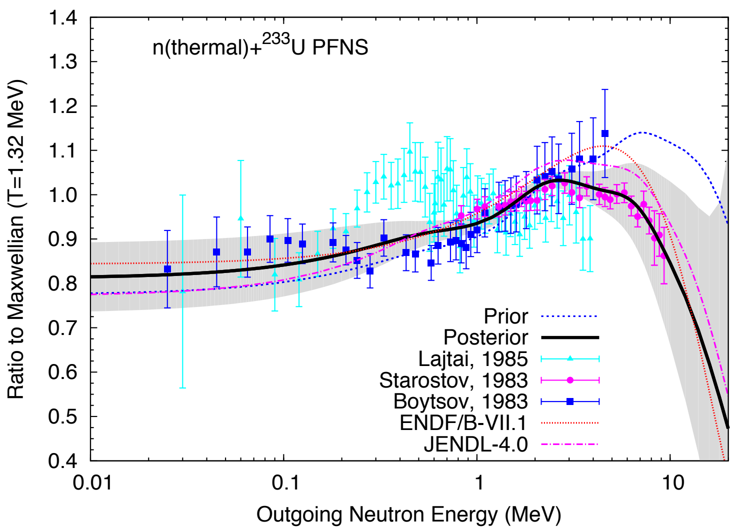
- **Generalized linear-least-squares**
  - Can be used for data adjustment/assimilation
  - Whisper-1.1 uses GLLS to estimate MOS_{data}

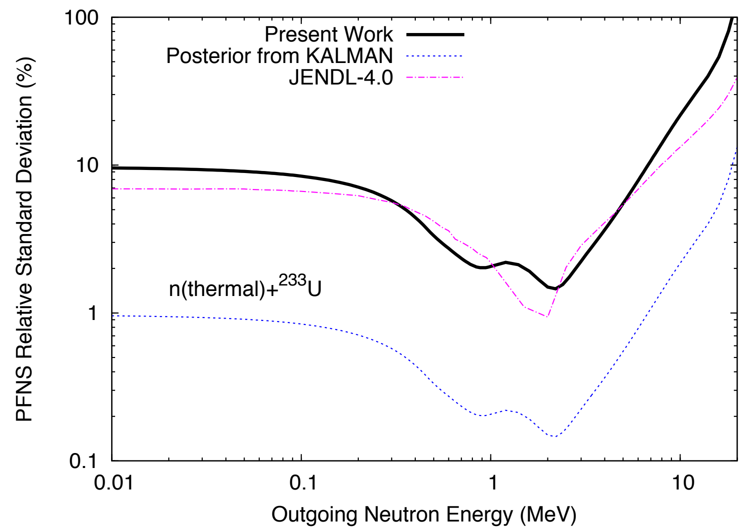
Background – ^{233}U Nuclear Data and Benchmarks

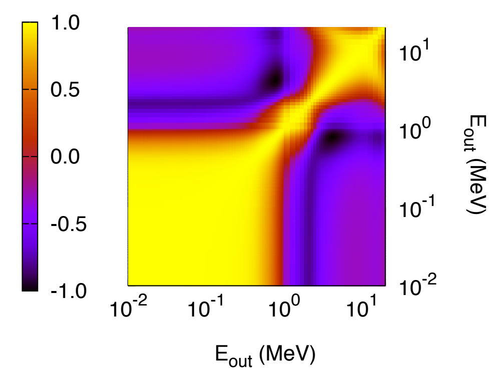
- **Example of dated/inconsistent ^{233}U nuclear data in ENDF/B-VII.1**
  - Info on PFNS, taken from JENDL-3.3 based on Madland-Nix model
  - Actual PFNS, data is energy-dependent Watt spectrum, no uncertainties reported

```
 0.000000+0 0.000000+0          0          0          0          09222 0  0    0
 9.223300+4 2.310377+2          0          0          1          09222 5 18    1
-3.000000+7 0.000000+0          0         11          1          29222 5 18    2
          2          2                                            9222 5 18    3
 1.000000-5 1.000000+0 3.000000+7 1.000000+0                      9222 5 18    4
 0.000000+0 0.000000+0          0          0          1          119222 5 18    5
         11          2                                            9222 5 18    6
 1.000000-5 9.770000+5 1.500000+6 9.770000+5 2.000000+6 9.800000+59222 5 18    7
 5.000000+6 1.010000+6 7.000000+6 9.700000+5 1.000000+7 9.800000+59222 5 18    8
 1.220000+7 1.010000+6 1.500000+7 1.000000+6 1.800000+7 1.040000+69222 5 18    9
 2.000000+7 1.060000+6 3.000000+7 1.060000+6                      9222 5 18   10
 0.000000+0 0.000000+0          0          0          1          119222 5 18   11
         11          2                                            9222 5 18   12
 1.000000-5 2.546000-6 1.500000+6 2.546000-6 2.000000+6 2.532000-69222 5 18   13
 5.000000+6 2.412000-6 7.000000+6 2.571000-6 1.000000+7 2.474000-69222 5 18   14
 1.220000+7 2.612000-6 1.500000+7 2.652000-6 1.800000+7 2.689000-69222 5 18   15
 2.000000+7 2.620000-6 3.000000+7 2.620000-6                      9222 5 18   16
 0.000000+0 0.000000+0          0          0          0          09222 5  099999
```

```
>> MF=5 ENERGY DISTRIBUTIONS OF SECONDARY PARTICLES                   9222 1451  395
                                                                     9222 1451  396
MT=18: Prompt Fission Neutron Spectrum Matrix                        9222 1451  397
   The MT=18 spectra are taken from the JENDL-3.3 evaluation         9222 1451  398
(Ma02). That evaluation utilizes a modified form (Oh92) of the       9222 1451  399
Madland and Nix Los Alamos model (MN82). The compound nucleus        9222 1451  400
formation cross sections for fission fragments (FF) were            9222 1451  401
calculated using Becchetti-Greenlees potential (Be69).  Up to       9222 1451  402
4th-chance-fission were considered at high incident neuttron        9222 1451  403
energies.  The Ignatyuk formula (Ig79) were used to generate the    9222 1451  404
level density parameters.                                           9222 1451  405
Parameters adopted:                                                 9222 1451  406
     Total average FF kinetic energy = 172.311-0.0212*E(MeV)        9222 1451  407
     Average energy release          = 188.438 MeV                  9222 1451  408
     Average mass number of light FF =  95                          9222 1451  409
     Average mass number of heavy FF = 139                          9222 1451  410
     Level density of the light FF   =  9.999- 10.094               9222 1451  411
     Level density of the heavy FF   = 11.89 - 12.20                9222 1451  412
Note that the parameters vary with the incident energy within the   9222 1451  413
indicated range.                                                    9222 1451  414
```





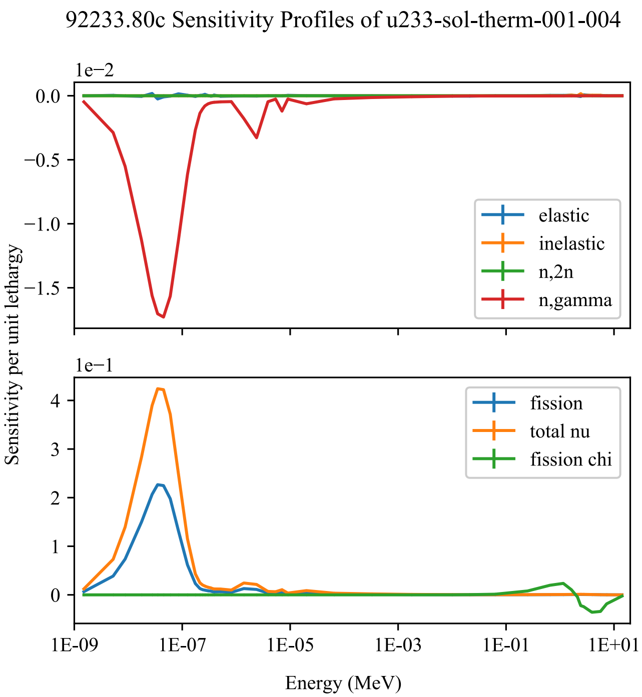


Plots taken from
M.E. Rising *et al*. NSE **175**, 81-93.

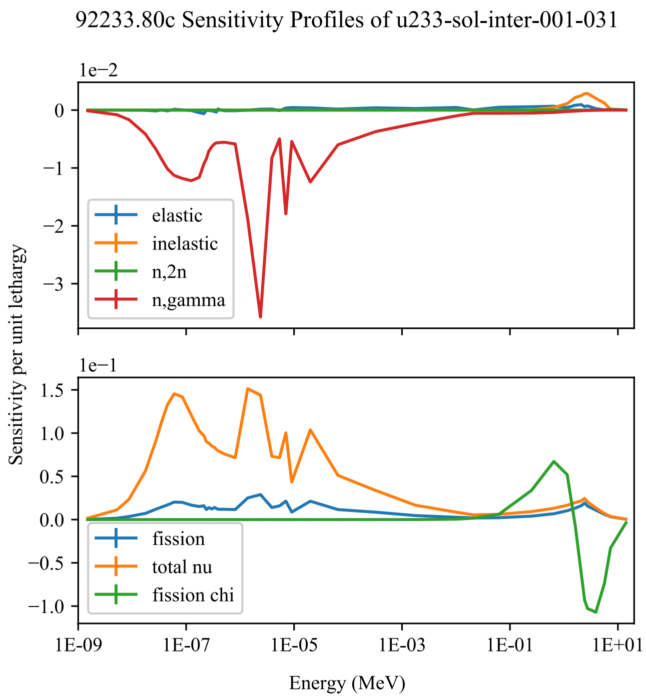
Background – ^{233}U Nuclear Data and Benchmarks

- **158 ^{233}U benchmarks and sensitivity profiles from 4 different series**
  - U233-SOL-THERM, U233-SOL-INTER, U233-MET-FAST, U233-COMP-THERM (not shown below)

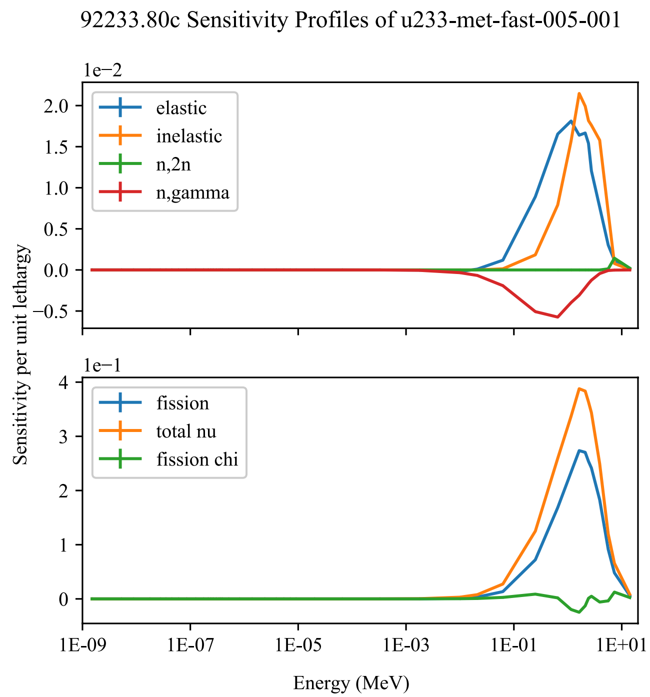
Thermal



Intermediate

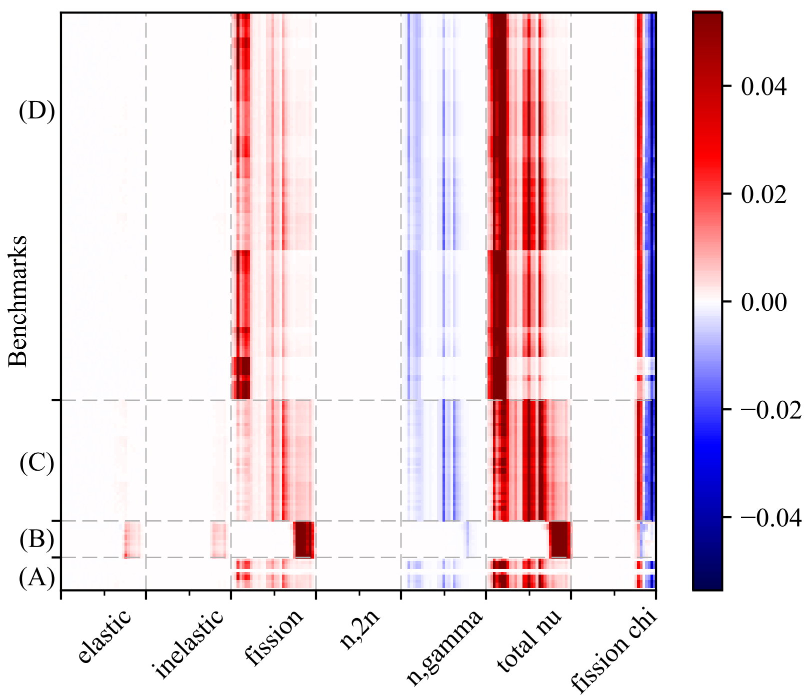


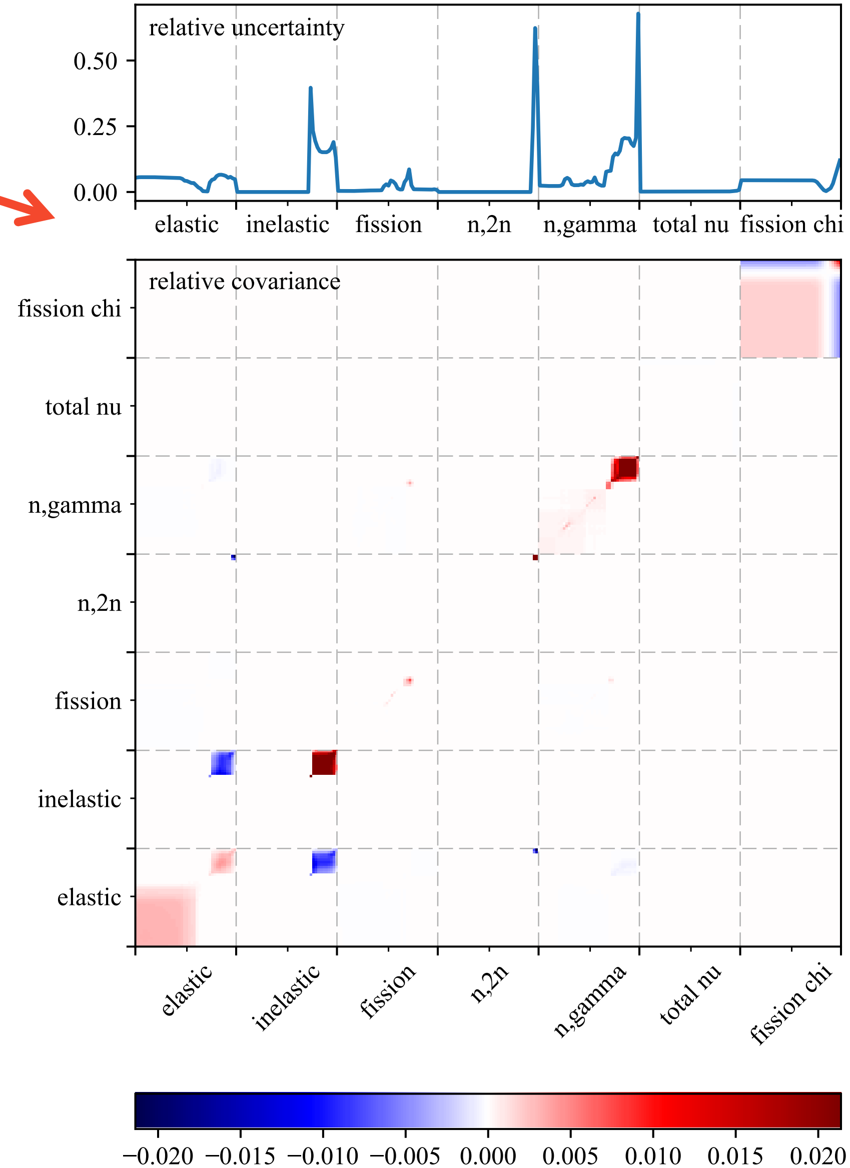
Fast



Background – Whisper-1.1 Catalogue Data

- **BLO covariance data**
- **All ^{233}U sensitivity profiles**
  - (A) **U233-COMP-THERM**
  - (B) **U233-MET-FAST**
  - (C) **U233-SOL-INTER**
  - (D) **U233-SOL-THERM**





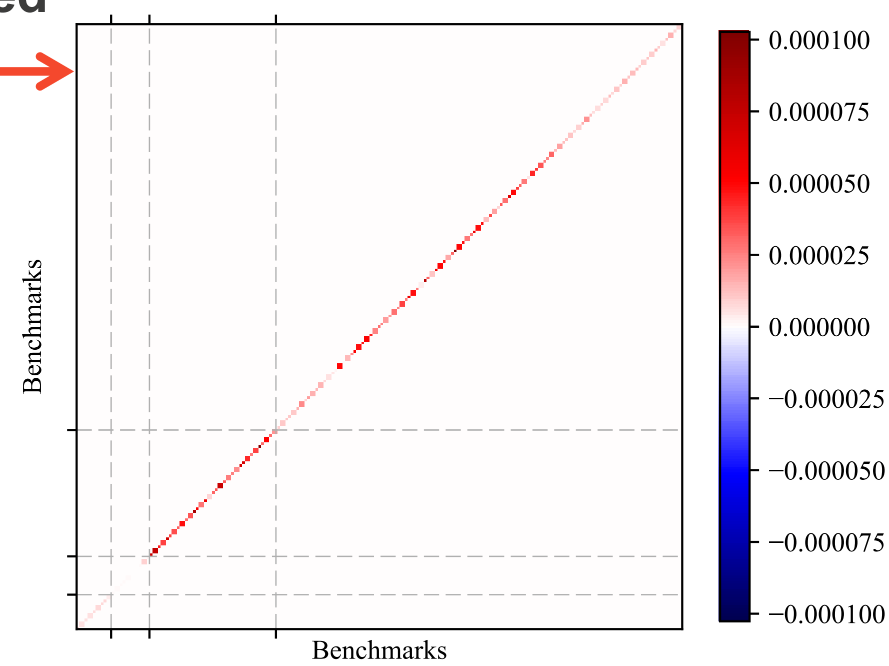
Background – GLLS

- Goal is to minimize discrepancies between simulated and measured K_{eff} while constrained by the nuclear data covariance matrices

$$\chi^2 = \mathbf{\Delta k}^T \mathbf{C}_{\mathbf{mm}}^{-1} \mathbf{\Delta k} + \mathbf{\Delta}\sigma^T \mathbf{C}_{\sigma\sigma}^{-1} \mathbf{\Delta}\sigma$$

$\mathbf{\Delta k} =$ Discrepancy between posterior (adjusted) and measured K_{eff}

$\mathbf{C}_{\mathbf{mm}} =$ Covariance matrix of measured benchmarks



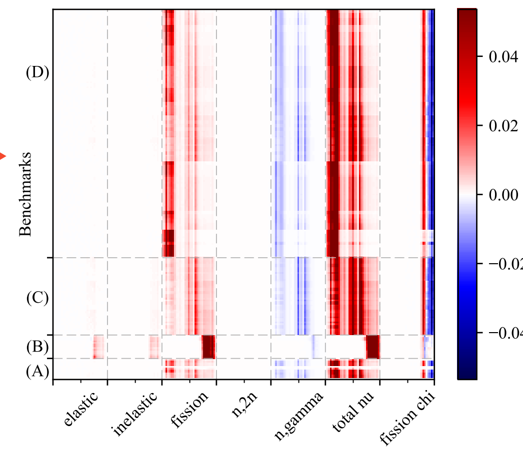
$\mathbf{\Delta}\sigma =$ Difference between prior and posterior nuclear data

$\mathbf{C}_{\sigma\sigma} =$ Covariance matrix of nuclear data (previous slide)

Background – GLLS

- With the sensitivity profiles defining how each benchmark K_{eff} changes with respect to the nuclear data,

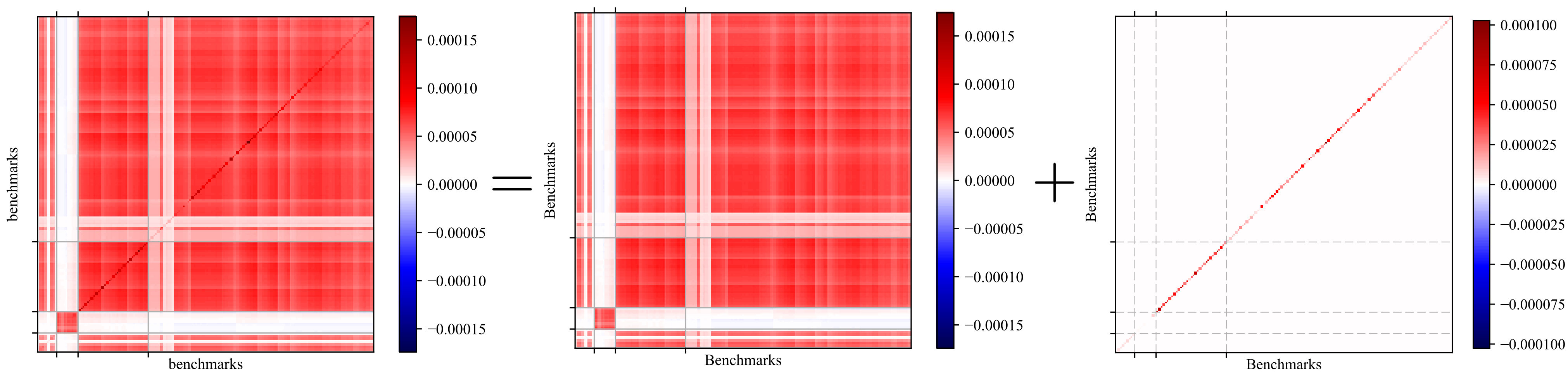
$$S_{i,j} = \frac{\sigma_j}{k_i}\frac{\partial k_i}{\partial \sigma_j}$$



- Linear error propagation, "sandwich" rule,

$$\mathbf{C_{kk}} = \mathbf{S}\mathbf{C}_{\sigma\sigma}\mathbf{S}^T$$

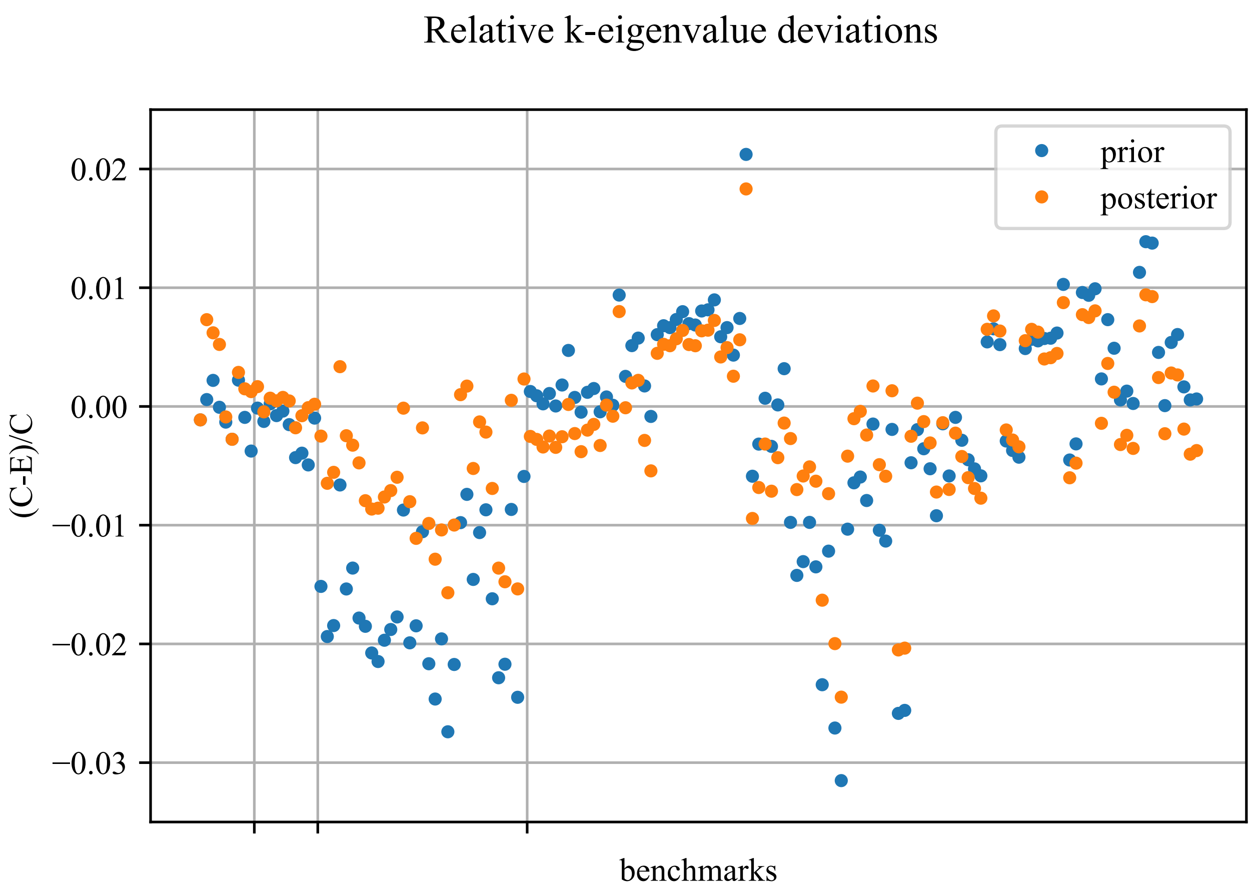
- Covariance of the prior discrepancies: $\mathbf{C_{dd}} = \mathbf{C_{kk}} + \mathbf{C_{mm}}$



Numerical Results

- **The final results of the GLLS minimization process, improved agreement between simulation and measurement**

$$\mathbf{\Delta k = C_{mm} C_{dd}^{-1} d}$$

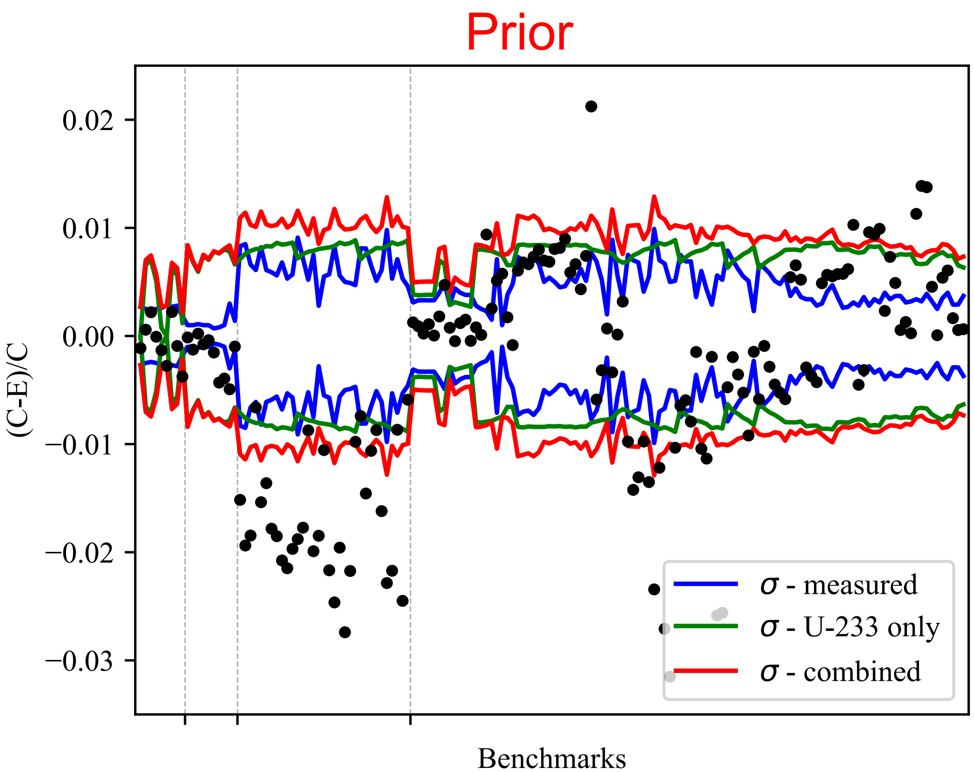


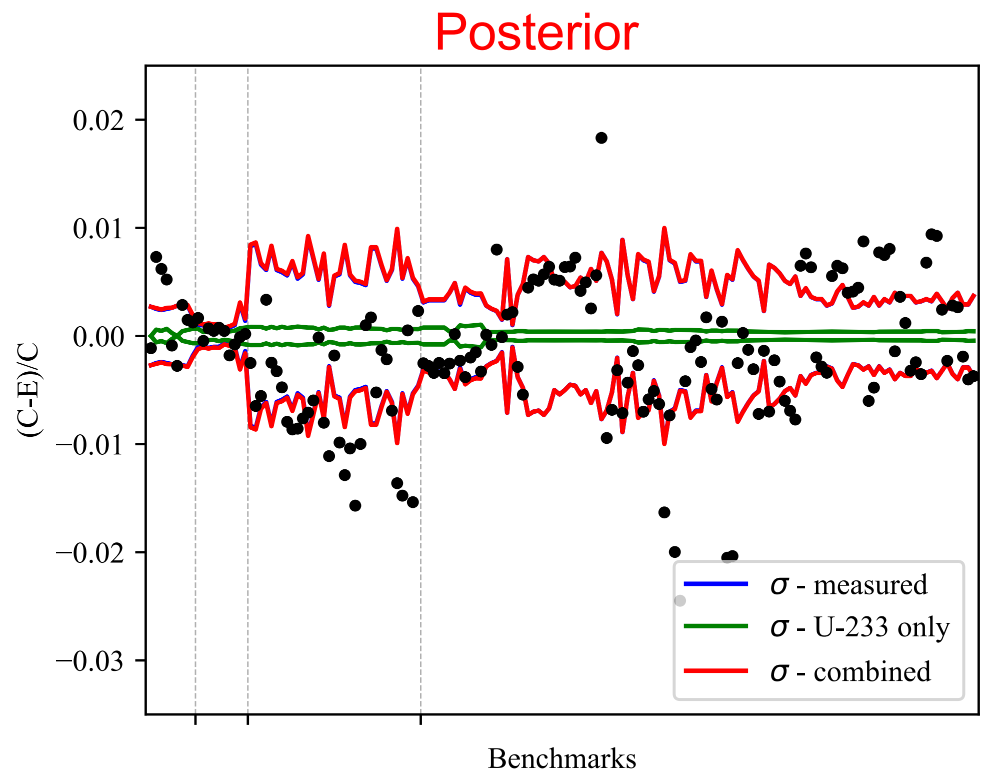
	Prior	Posterior
χ^2	4.61	2.06
RMS	0.0106	0.0066

Numerical Results

- **Reduced nuclear data induced uncertainties in benchmarks (the posterior nuclear data covariance equation is on the following slide),**

$$\mathbf{C}'_{\mathbf{kk}} = \mathbf{S}\mathbf{C}'_{\sigma\sigma}\mathbf{S}^T$$

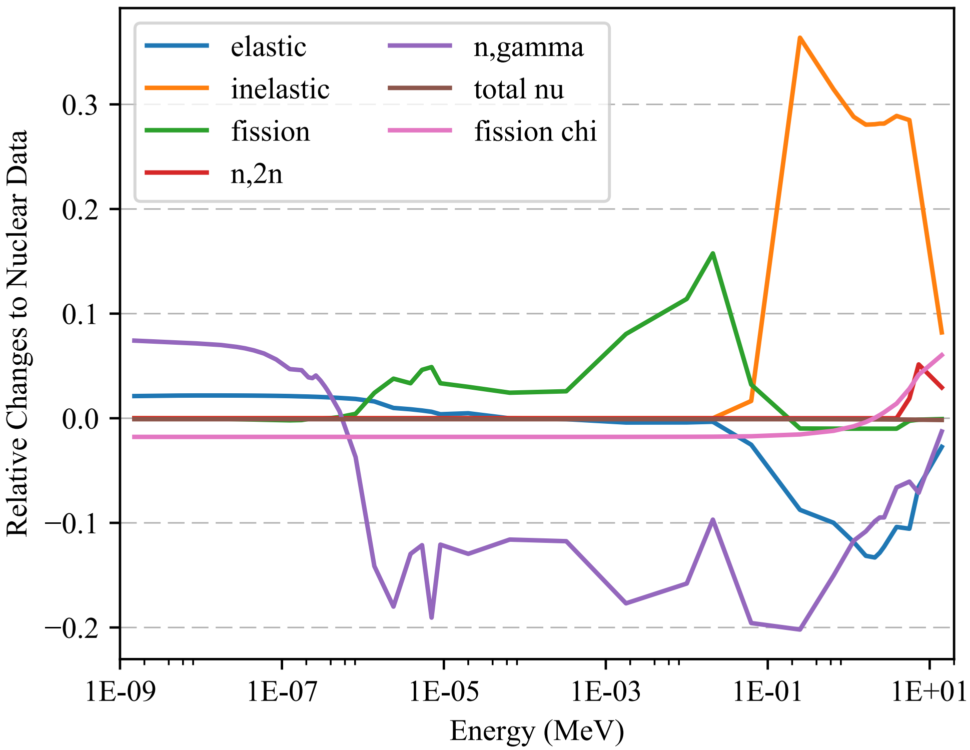


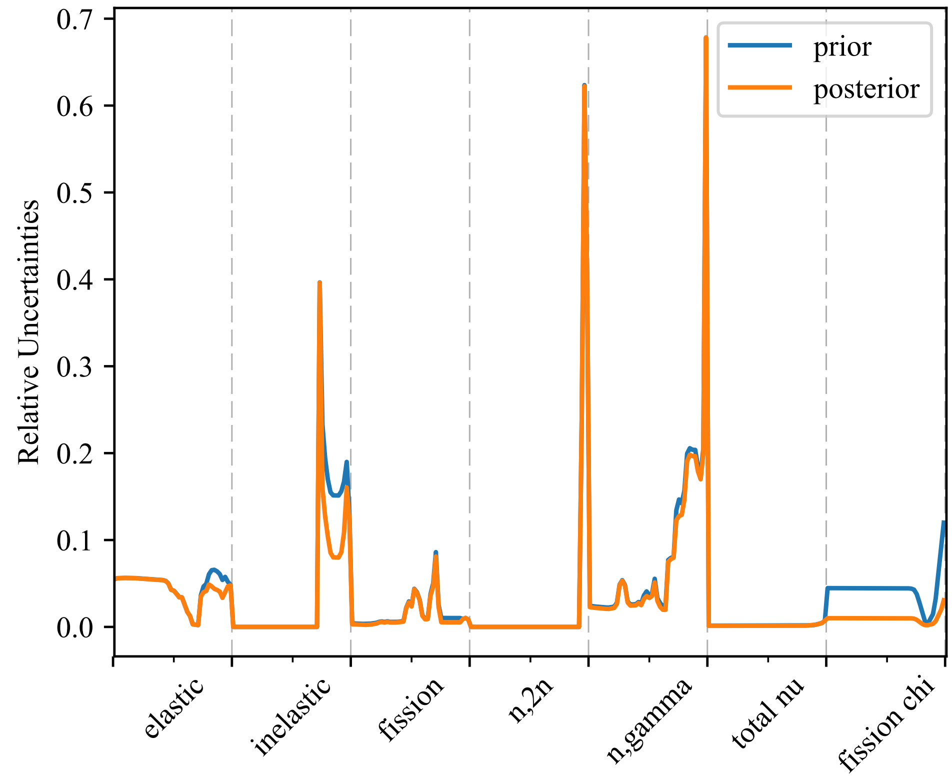


Numerical Results

- **Nuclear data and uncertainty adjustments,**

$$\boldsymbol{\Delta}\sigma = -\mathbf{C}_{\sigma\sigma}\mathbf{S}^T\mathbf{C}_{\mathbf{dd}}^{-1}\mathbf{d} \qquad \mathbf{C}'_{\sigma\sigma} = \mathbf{C}_{\sigma\sigma} - \mathbf{C}_{\sigma\sigma}\mathbf{S}^T\mathbf{C}_{\mathbf{dd}}^{-1}\mathbf{S}\mathbf{C}_{\sigma\sigma}$$





Conclusions & Future Work

- **Nuclear data is likely the largest source of bias in the ^{233}U benchmarks**
  - High energy
    - Inelastic scattering ↑ and elastic scattering ↓
    - Capture ↓
  - Intermediate energy
    - Fission ↑ and capture ↓
  - Thermal energy
    - Elastic scattering ↑ and capture ↑
  - Fission spectrum
    - Tilts ↑ above ~2 MeV, ↓ below ~2 MeV
  - Fission nubar
    - No change due to small uncertainties

^{233}U Nuclear Data Needs Work!

- **GLLS using integral experiments to constrain the nuclear data can identify places where nuclear data evaluators should focus their efforts**
- **Whisper-1.1 contains all the necessary information to do this work**

Acknowledgements

NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

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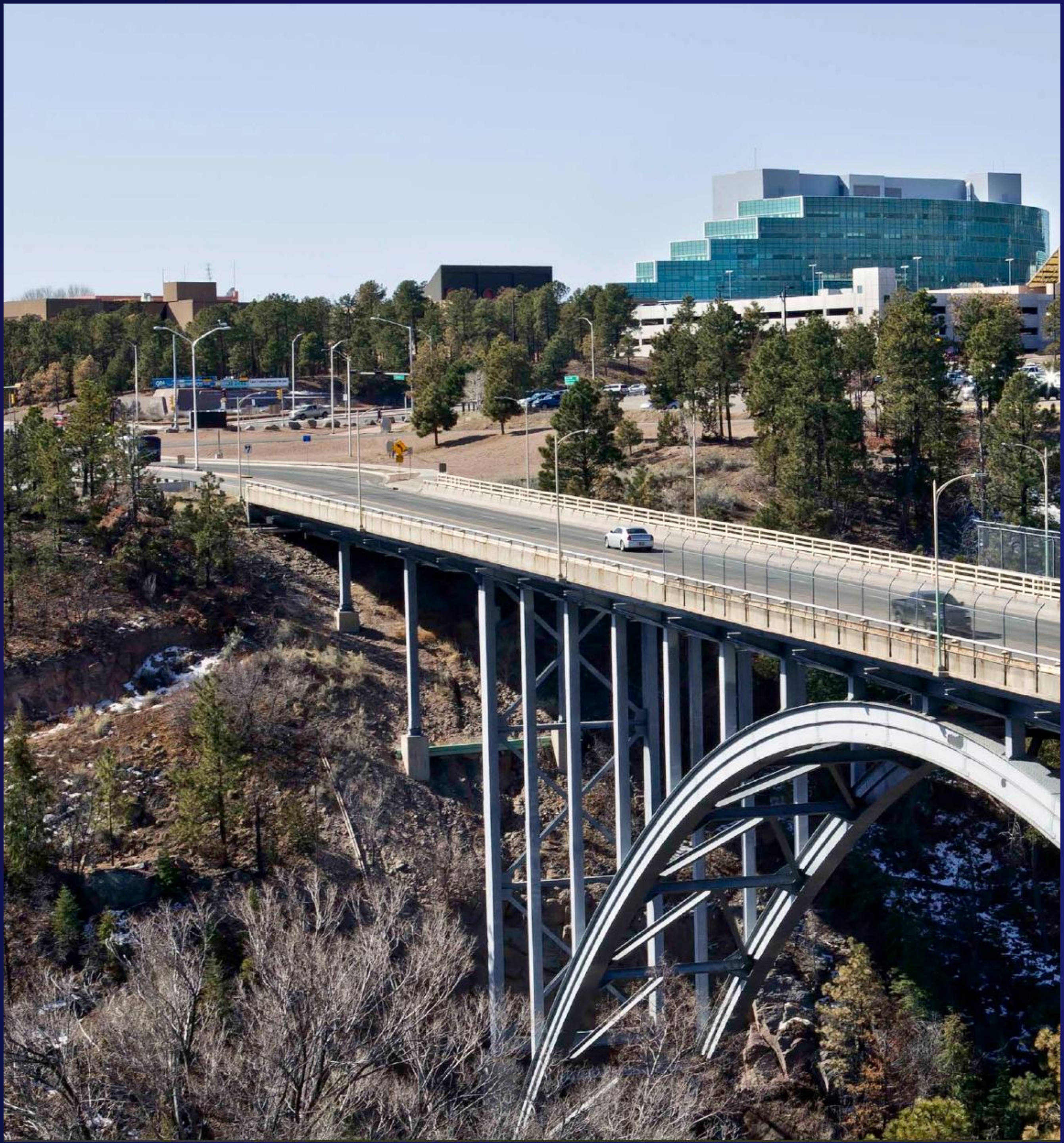

Thank you!

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