Improving Nuclear Data with Advanced Computational Capabilities

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WANDA

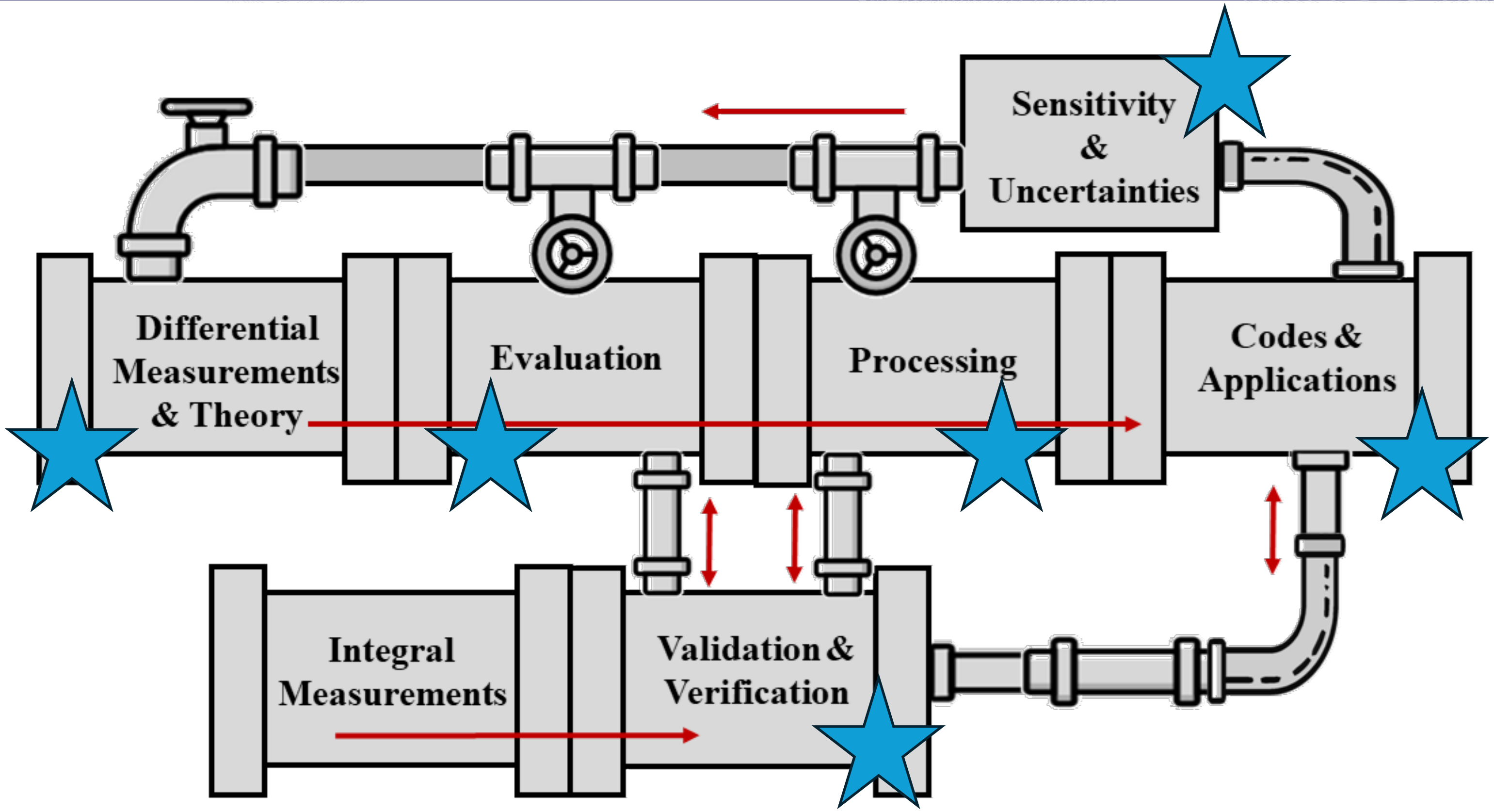
February 10, 2025

Outline

- Nuclear Data Pipeline
- Current activities
- Future needs

Nuclear Data Pipeline (NA-114 perspective)

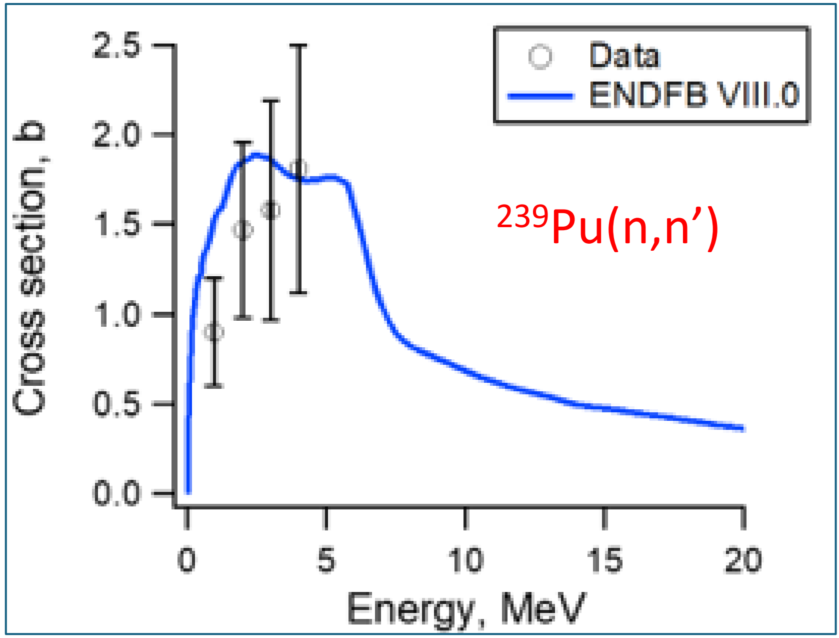
- Advanced Simulation and Computing (NA-114) supports a spectrum of efforts in support of the U.S. deterrent across the nuclear data pipeline
- Modern methods and diagnostic platforms increase "good" data
- Machine Learning/Artificial Intelligence (ML/AI) provides new opportunities for improved accuracy and reduced timelines



Both LLNL and LANL maintain a complete and integrated nuclear data pipeline to achieve Defense Program goals – NA-114 directly funds multiple technical activities

Evaluations remain a key activity

- Evaluation of reactions: Use nuclear theory reaction codes, constrained by measured differential data and validated against integral data, to determine accurate mean values and uncertainties
- Identify priorities based on sensitivity and **uncertainty studies**, specific requests, and available capabilities (both experiment and theory)
- Strong need to revisit evaluation/processing/benchmark workflow/pipeline to become more agile and robust
- Should we be tuning evaluations to specific benchmarks?

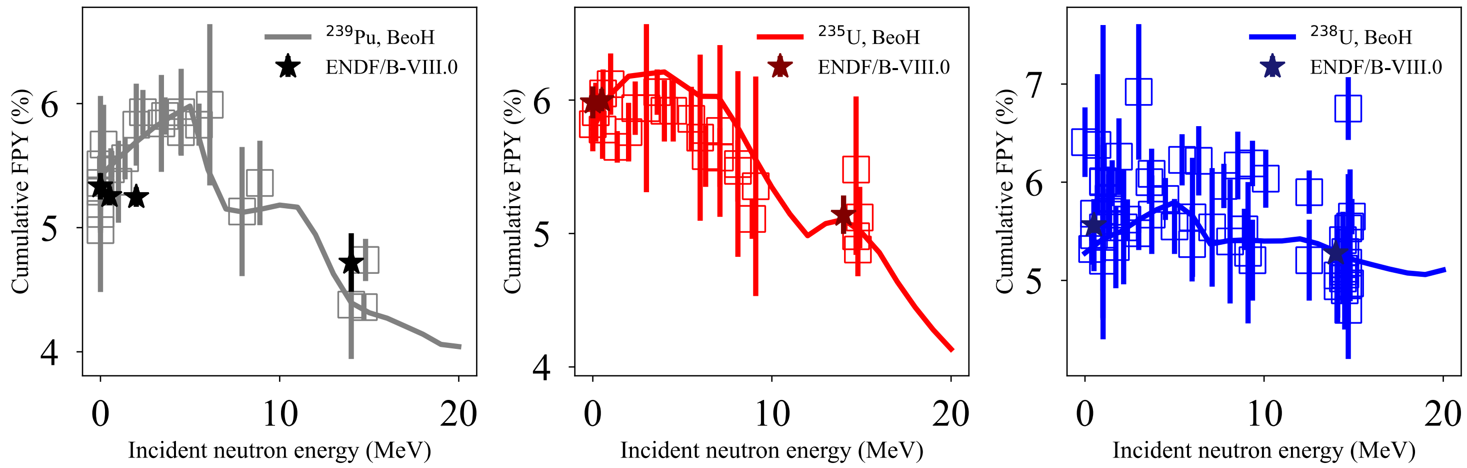


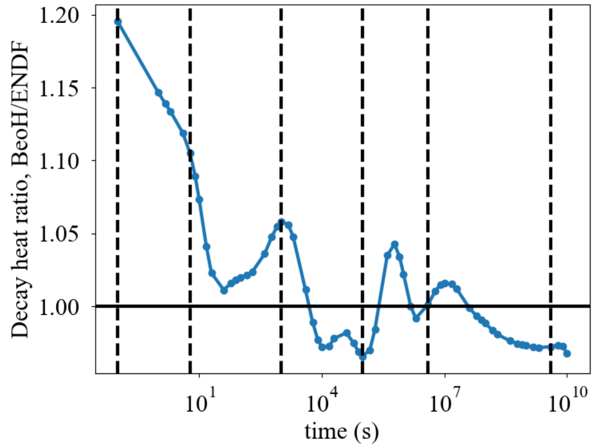
Neutron inelastic scatter measurements (points with error bars) and evaluated cross section from ENDF/B-VIII.0

Evaluation and validation for fission product yields underway

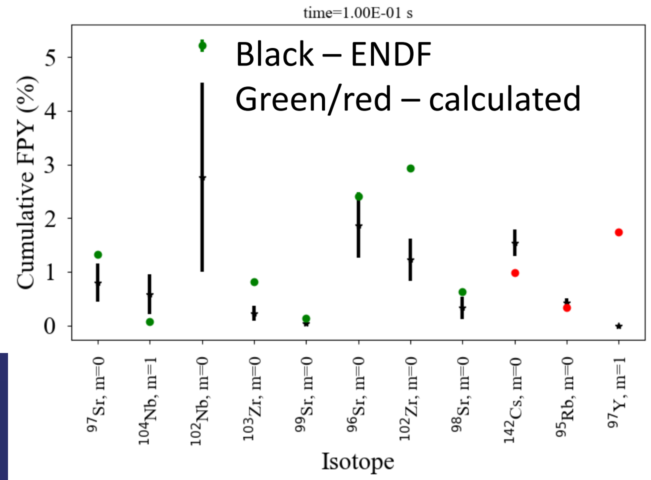
- Advanced theory models calculate prompt and delayed fission observables – fission product yield (FPY) evaluations are being made consistent with decay data and other prompt/delayed observables

^{97}Zr fission products from ENDF/B-VIII.0 compared to theory predictions





Decay heat provides an important validation; example for ^{239}Pu



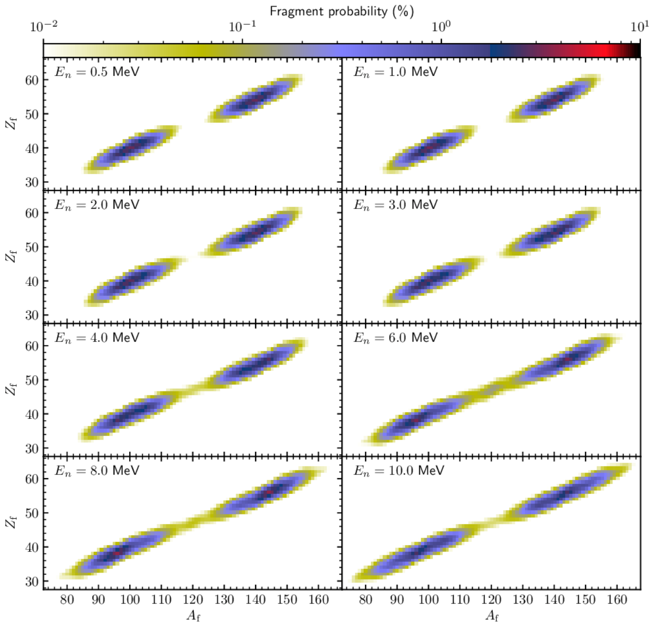
- Differences in decay heat between ENDF/B data and new calculations identify nuclei that should be studied further

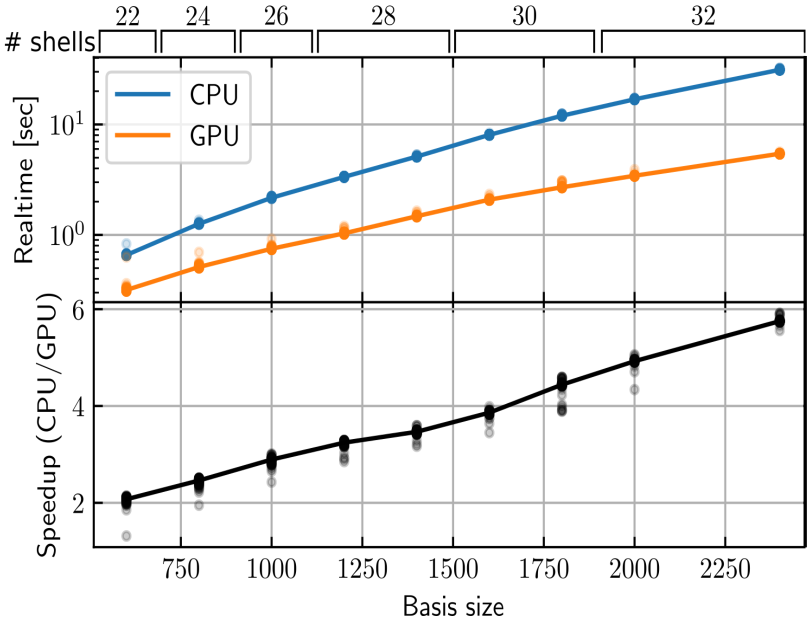
Leading-edge methods and computation platforms advance predictive theory capabilities

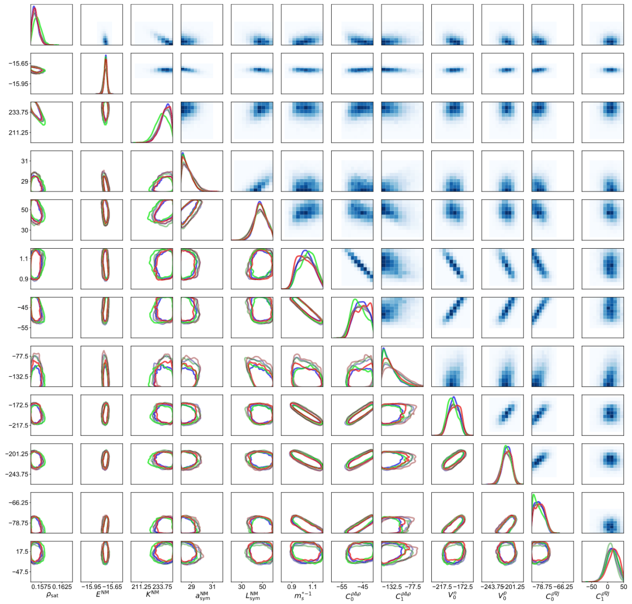
Nuclear density functional theory is a fully consistent framework to predict fission properties – from FPY to deexcitation

Calculations of nuclear properties in large phase spaces require next-generation HPC machines – and porting codes!

Bayesian techniques and AI/ML emulators enable the quantification of uncertainties in theoretical predictions







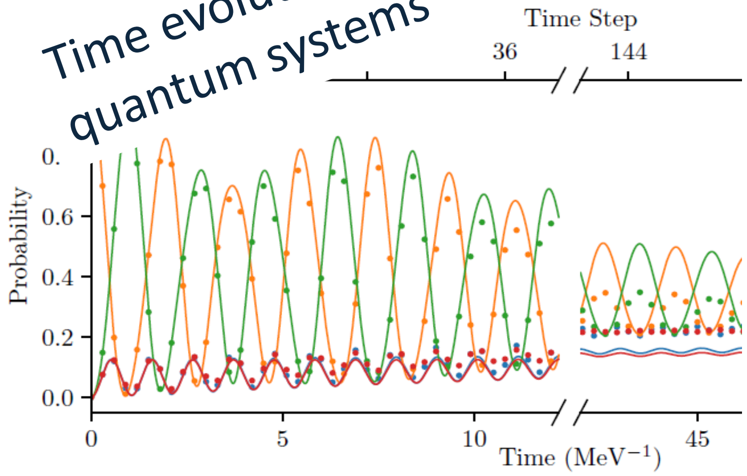
HPC capabilities and AI/ML techniques are the two pillars supporting a rigorous theory UQ pipeline

Quantum computing will allow for the next leap in modeling and prediction capabilities for nuclear data

- Quantum computing and simulations are poised to:
  - Address grand computational problems in nuclear physics
  - Enhance classical-computational nuclear physics

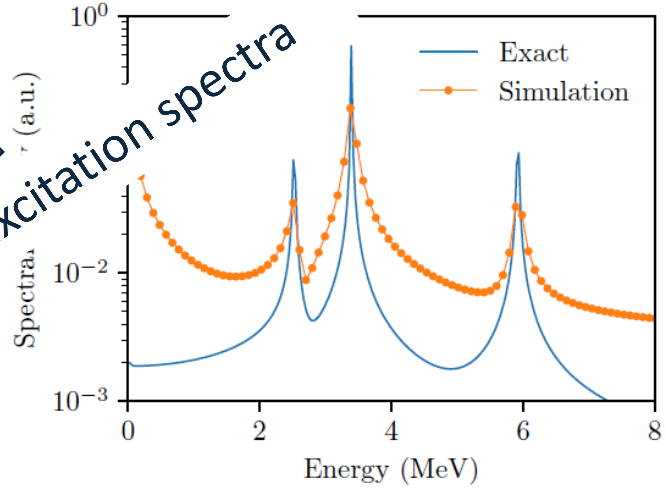
Quantum Information Science and Technology for Nuclear Physics:
Input into U.S. Long-Range Planning
https://arxiv.org/abs/2303.00113

Time evolution of quantum systems



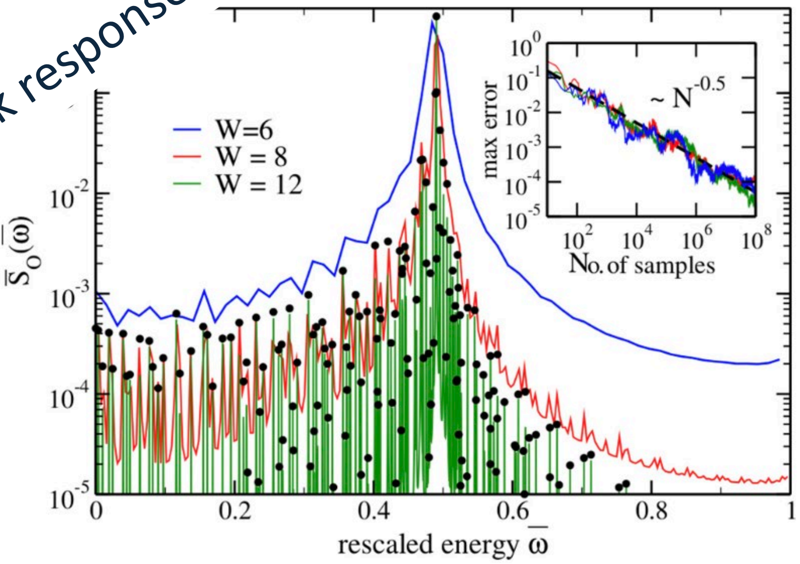
FFT

Excitation spectra



Holland, Wendt et al. (2020), Phys. Rev. A 101, 062307

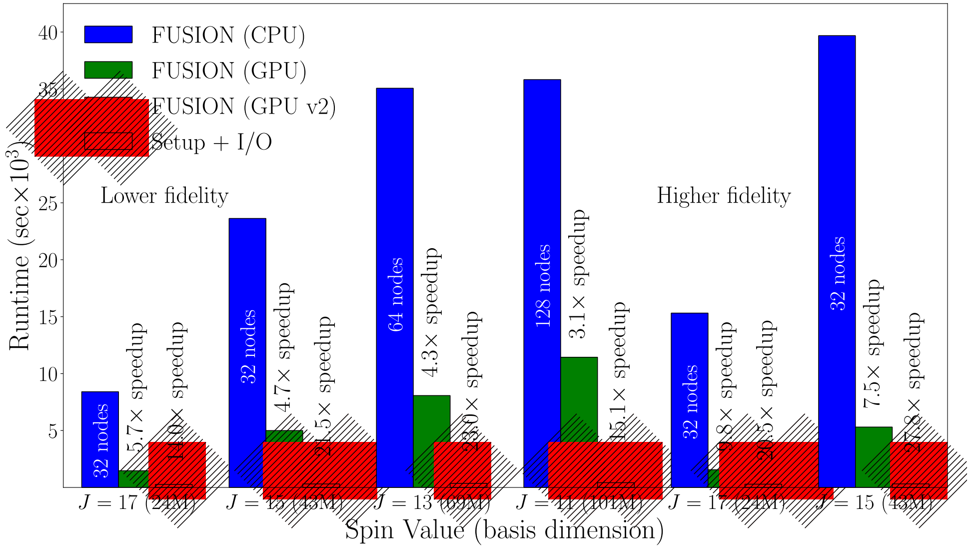
Electroweak responses

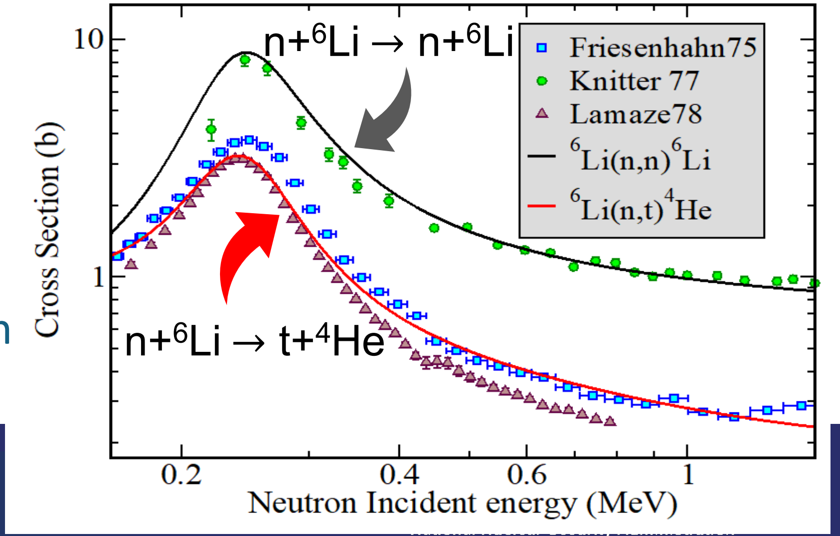


Roggero A. & Carlson, J (2019), Phys. Rev. C 100, 034610

Software quality is increasingly important

- Software capabilities continue to grow: need for improved software engineering
  - Need to extend software lifetime
  - Version control
  - Changing computational architectures
- Support for challenging design iteration timescales:
  - Take advantage of advanced architectures
  - Need high-quality and robust workflows
  - Increased sharing provides critical leveraging and peer review





GPU-enabled ab initio evaluation of n+^{6}Li; Kravvaris *et al.*

Data science efforts continue to grow

- Nuclear data community continues to expand and improve uncertainty efforts
- Activities across the pipeline support uncertainty analysis and reduction -- templates for differential measurements an excellent example
- Community has developed unique infrastructure to enable machine learning investigations
- Common formats (e.g. GNDS, ENDF) a significant success
- How can we expand these benefits to other scientific communities?

(n,tot); (n,xn); (n,γ) and (n,z); PFNS and nu-bar:
EPJ Nuclear Sciences and Technologies 2023


EPJ Nuclear Sci. Technol. **9**, 35 (2023)
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https://doi.org/10.1051/epjn/2023014

Templates of Expected Measurement Uncertainties: a CSEWG Effort, Cyrille De Saint Jean and Denise Neudecker (Guest editors)

Available online at: https://www.epj-n.org

REGULAR ARTICLE · OPEN ACCESS

Templates of expected measurement uncertainties

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Received: 28 April 2023 / Received in final form: 19 July 2023 / Accepted: 7 August 2023

Abstract. The covariance committee of CSEWG (Cross Section Evaluation Working Group) established templates of expected measurement uncertainties for neutron-induced total, (n,γ), neutron-induced charged-particle, and (n,xn) reaction cross sections as well as prompt fission neutron spectra, average prompt and total fission neutron multiplicities, and fission yields. Templates provide a list of what uncertainty sources are expected for each measurement type and observable, and suggest typical ranges of these uncertainties and correlations based on a survey of experimental data, associated literature, and feedback from experimenters. Information needed to faithfully include the experimental data in the nuclear-data evaluation process is also provided. These templates could assist (a) experimenters and EXFOR compilers in delivering more complete uncertainties and measurement information relevant for evaluations of new experimental data, and (b) evaluators in achieving a more comprehensive uncertainty quantification for evaluation purposes. This effort might ultimately lead to more realistic evaluated covariances for nuclear-data applications. In this topical issue, we cover the templates coming out of this CSEWG effort–typically, one observable per paper. This paper here prefaces this topical issue by introducing the concept and mathematical framework of templates, discussing potential use cases, and giving an example of how they can be applied (estimating missing experimental uncertainties of ^{235}U(n,f) average prompt fission neutron multiplicities), and their impact on nuclear-data evaluations.

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Thank You