Los Alamos
NATIONAL LABORATORY

Optimal experiment design and nuclear data validation with diverse benchmarks

Alexander R. Clark, Ph.D., E.I.

XCP-5: Materials and Physical Data

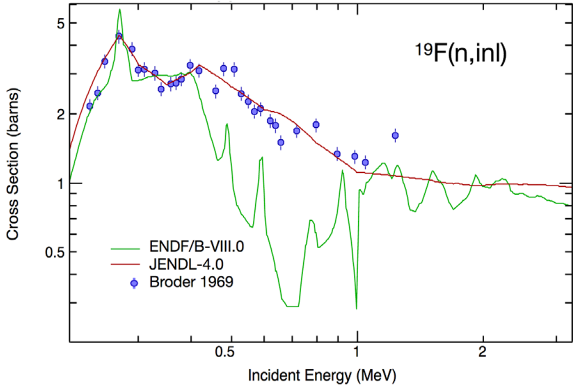
February 23rd-25th, 2021

NCSP TPR 2021 meeting

LA-UR-21-21446

Identification of discrepant nuclear data with machine learning

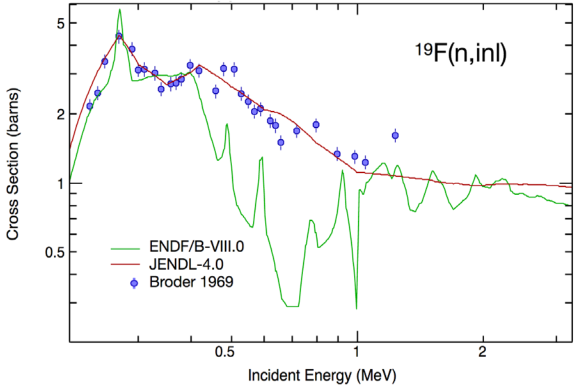
- Deficiencies in nuclear data can have significant impact on many applications, including determining USLs for criticality safety
- Previous Machine Learning project had already identified discrepant nuclear data that most contributed to bias between measured and simulated critical benchmark responses (funded by NCSP-ASC [ATDM-PEM-V&V])
- LDRD-DR project, EUCLID, objective is “to design small-scale experiments that address needs and deficiencies in nuclear data”

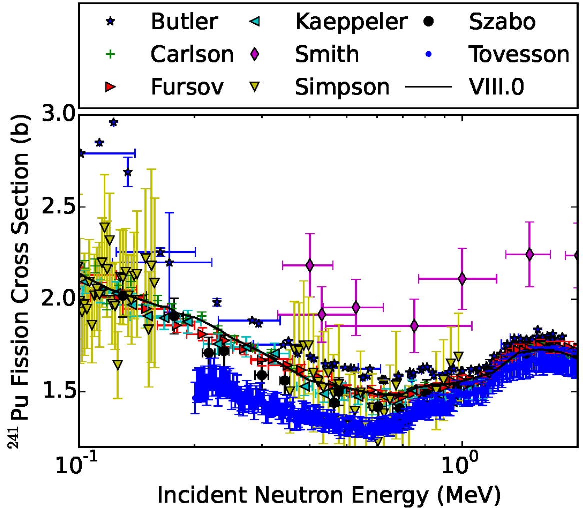


1. P. Grechanuk, M. E. Rising, and T. S. Palmer, “Using Machine Learning Methods to Predict Bias in Nuclear Criticality Safety,” *J. Comput. Theor. Transp.*, 47:4-6, 552-565
2. D. Neudecker, O. Cabellos, A. R. Clark et al., “Enhancing Nuclear Data Validation Analysis by Using Machine Learning,” Submitted Sept. 2019 to *Nucl Data Sheets*

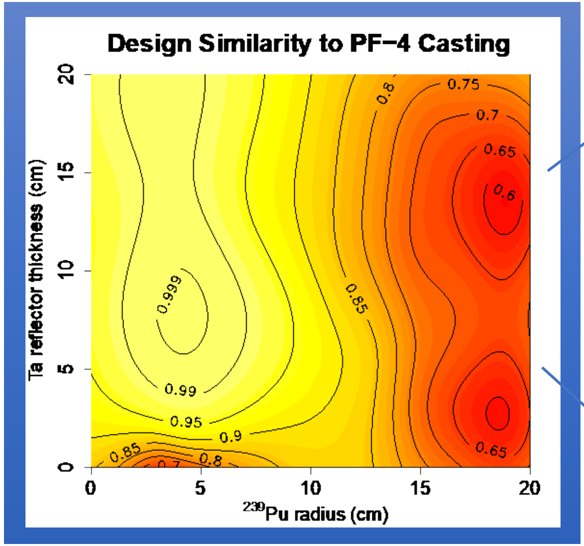
Identification of discrepant nuclear data with machine learning

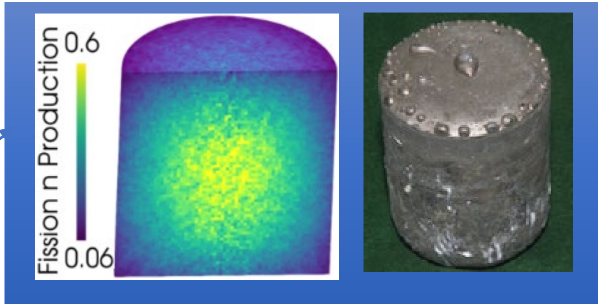
- Deficiencies in nuclear data can have significant impact on many applications, including determining USLs for criticality safety
- Previous Machine Learning project had already identified discrepant nuclear data that most contributed to bias between measured and simulated critical benchmark responses (funded by NCSP-ASC [ATDM-PEM-V&V])
- LDRD-DR project, EUCLID, objective is “to design small-scale experiments that address needs and deficiencies in nuclear data”

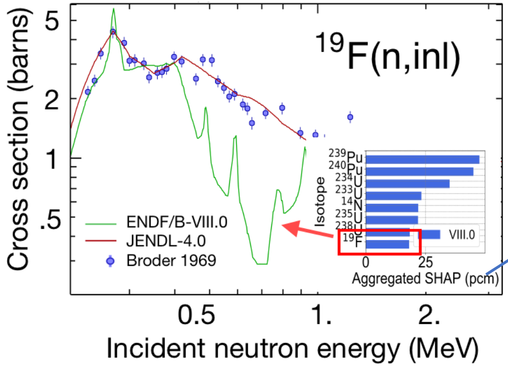


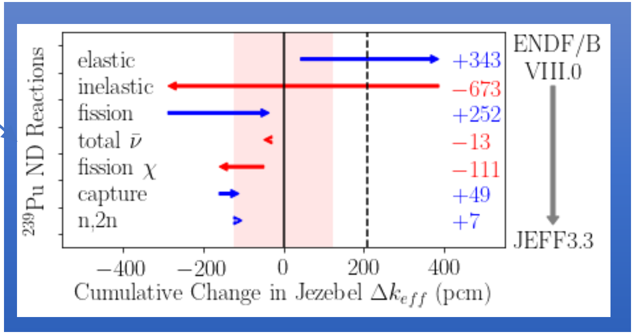


Optimal experiment design



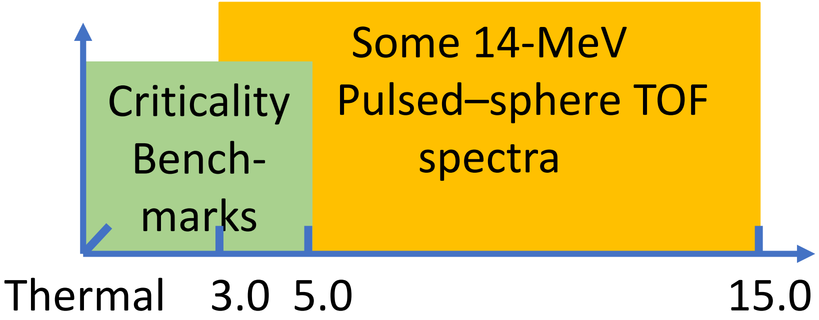




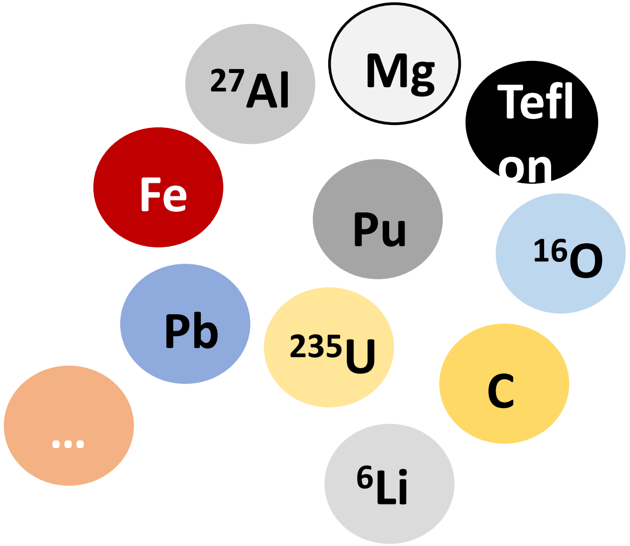


Justification for inclusion of diverse benchmarks

- Sometimes difficult to “disentangle” which nuclear data contributes to bias in critical benchmark
  - Single integral response from critical benchmark requires ~10^6 differential nuclear data points to simulate
  - Difficult to consider structural/moderator/reflector material separately from fissile core
  - Sensitive to a specific region of incident neutron energies
- One approach is to apply machine learning to a diverse set of measurements
  - Integral and differential observables (e.g. k_{eff} and TOF spectrum)
  - Composed of fissile and non-fissile materials
  - Sensitive to nuclear data in different energy regions
- Can improve nuclear data and benefit criticality safety

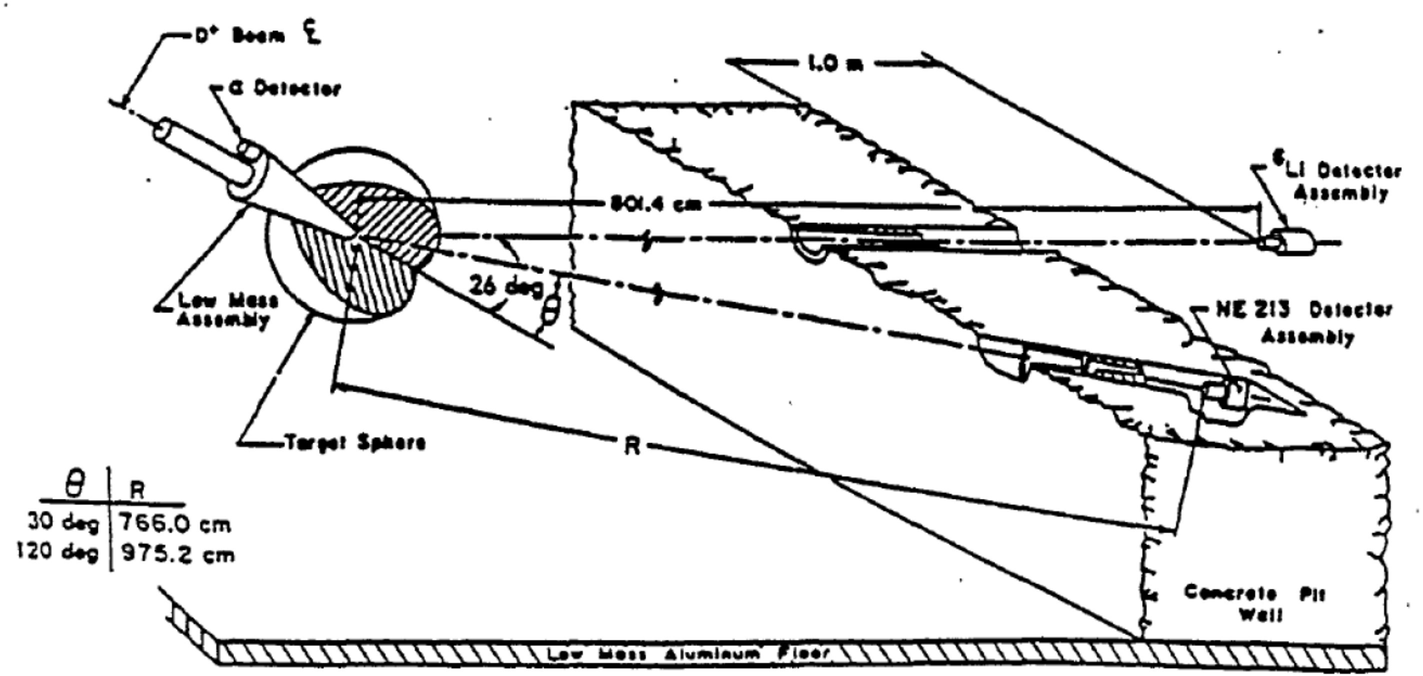


Nuclear data energy range to which simulations are sensitive (MeV)



LLNL 14-MeV pulsed spheres

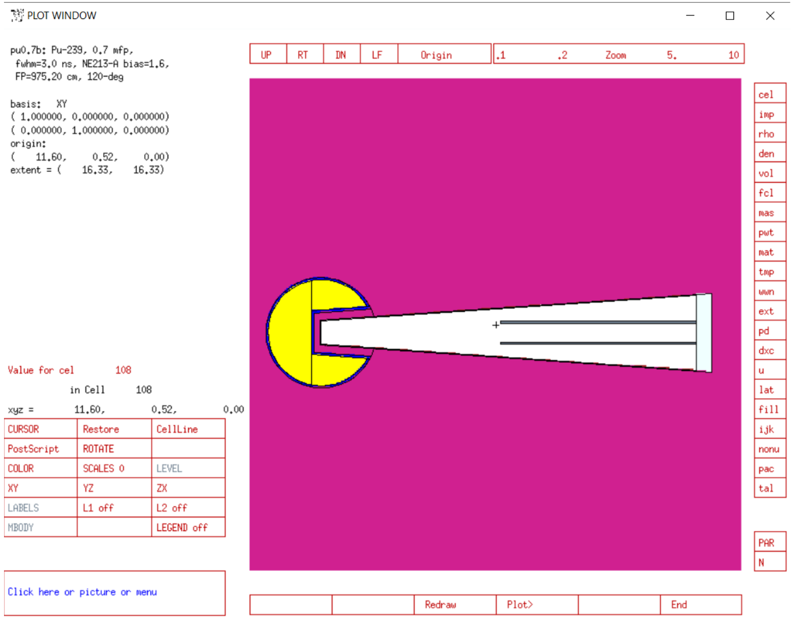
LLNL pulsed-sphere experimental setup



θ	R
30 deg	766.0 cm
120 deg	975.2 cm

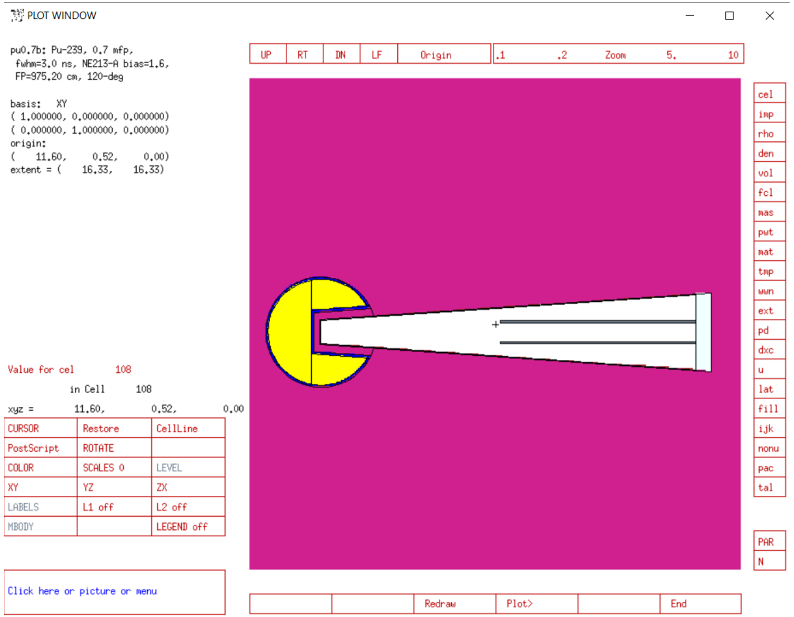
1. Tanja Goričanec et al. "Analysis of the U-238 Livermore Pulsed Sphere Experiments Benchmark Evaluations," International Nuclear Data Committee Report INDC(NDS)-0742 (2017)

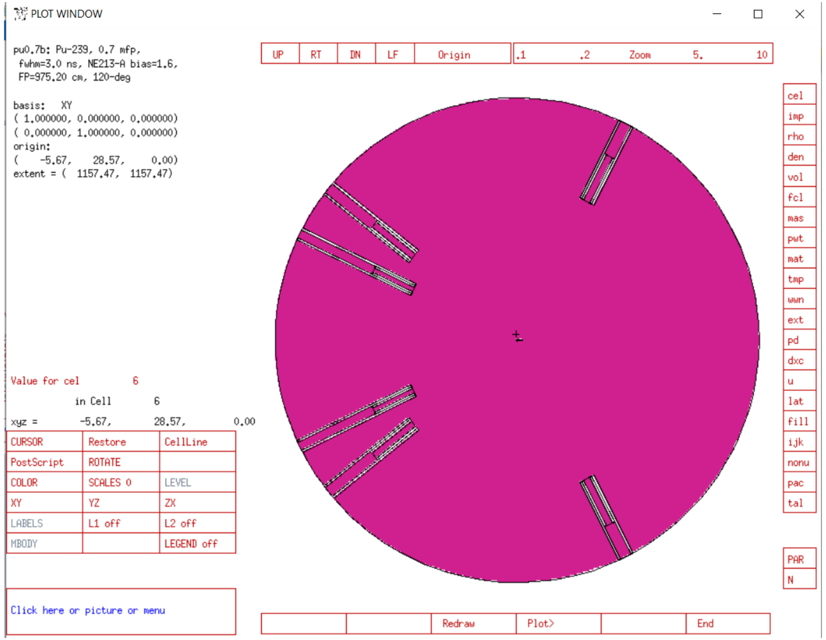
Pulsed-sphere MCNP model



1. S.C. Frankle, “Possible Impact of Additional Collimators on the LLNL Pulsed Sphere Experiments (U)," LANL Report LA-UR-05-5877 (2005).
2. S.C. Frankle, “LLNL Pulsed Sphere Measurements and Detector Response Functions (U)," LANL Report LA-UR-05-5878 (2005).
3. S.C. Frankle, “README file for Running a LLNL Pulsed-Sphere Benchmark," LANL Report LA-UR-05-5879 (2005).

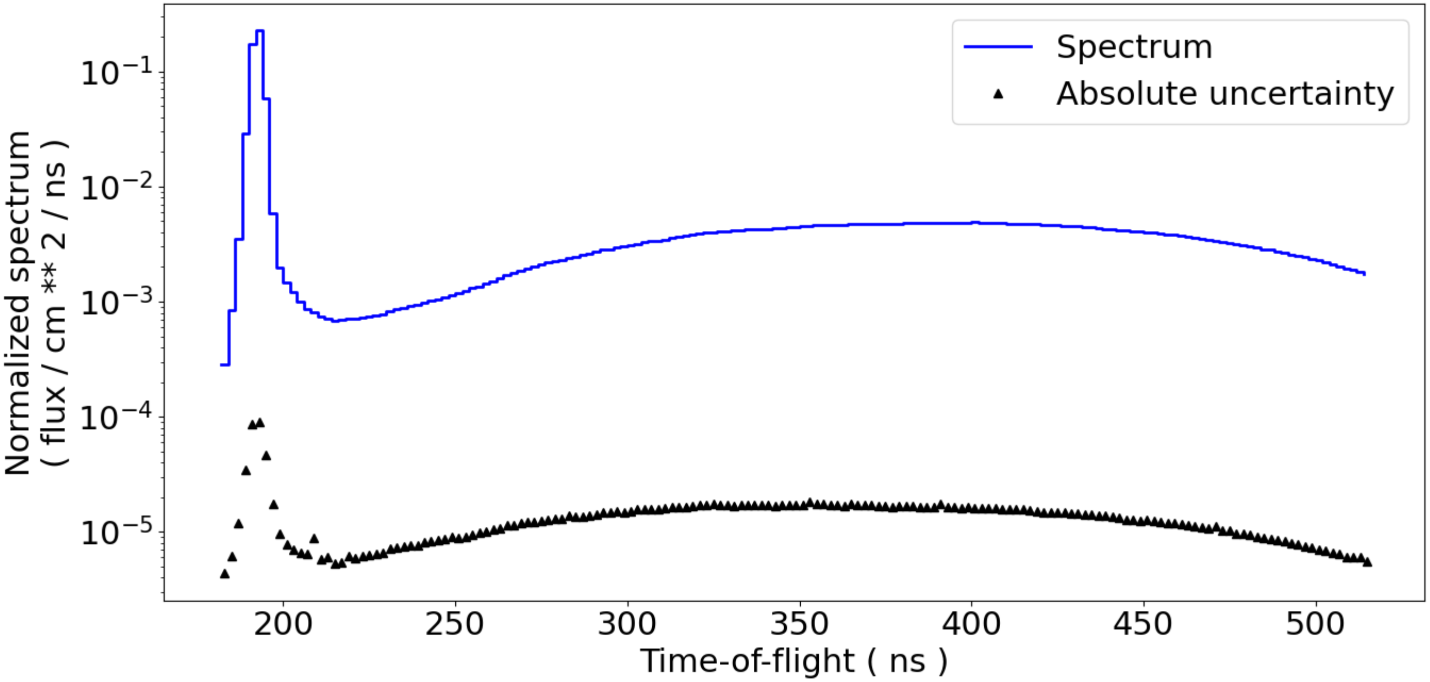
Pulsed-sphere MCNP model





1. S.C. Frankle, “Possible Impact of Additional Collimators on the LLNL Pulsed Sphere Experiments (U)," LANL Report LA-UR-05-5877 (2005).
2. S.C. Frankle, “LLNL Pulsed Sphere Measurements and Detector Response Functions (U)," LANL Report LA-UR-05-5878 (2005).
3. S.C. Frankle, “README file for Running a LLNL Pulsed-Sphere Benchmark," LANL Report LA-UR-05-5879 (2005).

Simulated pulsed-sphere time-of-flight spectrum for plutonium pulsed sphere



1. D. Neudecker, O. Cabellos, A. R. Clark et al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," *manuscript submitted to ann. nucl. energy*, Jan. 6, 2021
2. W. Haeck, A. R. Clark, and M. Herman, “Calculating the impact of nuclear data changes with Crater,” *Trans. Am Nucl. Soc. Winter Meeting*, Online, Nov. 15-19, 2020

Estimating sensitivities with central-difference calculations

- Sensitivity of pulsed-sphere time-of-flight spectrum to group-wise nuclear data is defined as

$$S_{R_t,\alpha_g} = \frac{\alpha_{g,0}}{R_t|_{\alpha=\alpha_{g,0}}} \frac{\partial R_t}{\partial \alpha_g}\bigg|_{\alpha=\alpha_{g,0}}$$

  - R_t = Time-of-flight spectrum at time bin t
  - α_g = Nuclear data parameter at group g

- Sensitivity can be numerically estimated to second-order in perturbation size with central-differences

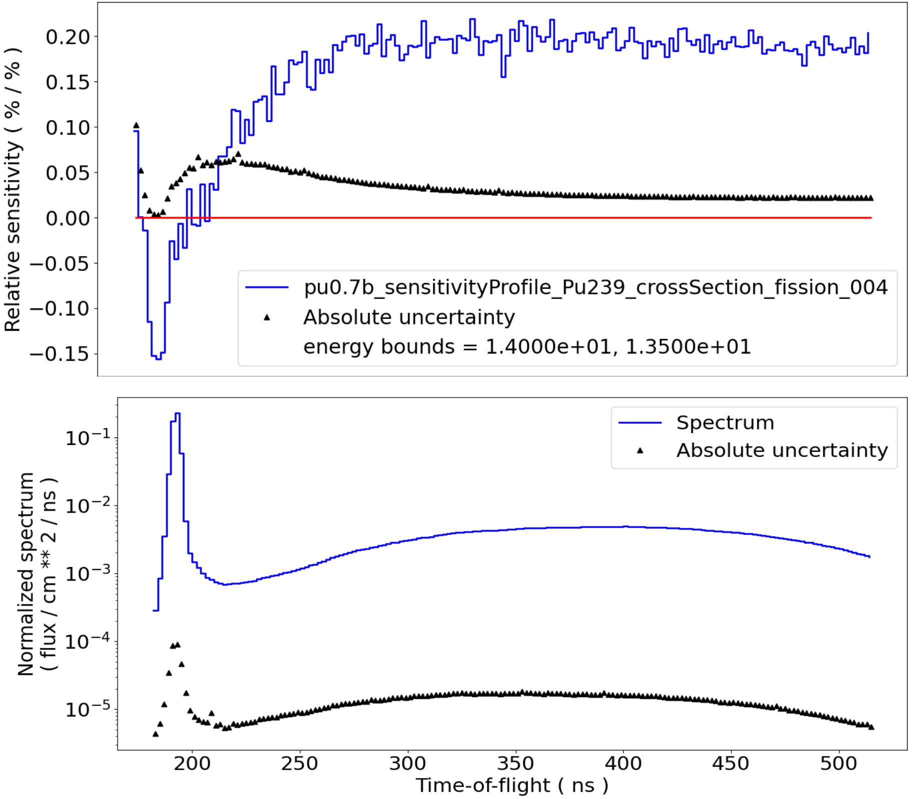
$$S_{R_t,\alpha_g} = \frac{\alpha_{g,0}}{R_t|_{\alpha=\alpha_{g,0}}} \frac{R_t|_{\alpha=\alpha_{g,0}+\Delta\alpha_g} - R_t|_{\alpha=\alpha_{g,0}-\Delta\alpha_g}}{2\Delta\alpha_g} + \mathcal{O}(\Delta\alpha^2)$$

Sensitivity analysis procedure

1. Obtain ENDF files from nndc.bnl.gov
2. Perturb nuclear data with one of two codes
   - FRENDY[1,3]
     - Process ENDF file into ACE format with NJOY
     - FRENDY directly perturbs ACE file
     - Operates on MF1,3
   - SANDY[2,3]
     - Process ENDF file into PENDF format with NJOY
     - SANDY perturbs either ENDF or PENDF file
     - Process ENDF and PENDF files in ACE format with NJOY
     - Operates on MF3,4
3. Generate MCNP input decks with Faust
4. Perform MCNP runs on HPC machine, Snow
5. Post-process MCTAL files with Faust to compute sensitivities[4]

1. K. Tada et al., “Development and Verification of a New Nuclear Data Processing System FRENDY,” *J.Nucl. Sci. Technol.*, **54**(7), pp. 806-817 (2017).
2. L. Fiorito, et al., “Nuclear data uncertainty propagation to integral responses using SANDY,” *Ann. Nucl. Energy*, Volume 101, 2017, Pages 359-366, ISSN 0306-4549.
3. O. Cabellos and L. Fiorito, “Examples of Monte Carlo Techniques applied for Nuclear Data Uncertainty Propagation,” *EPJ Web Conf.*, 211 (2019) 07008
4. W. Haeck, A. R. Clark, and M. Herman, “Calculating the impact of nuclear data changes with Crater,” *Trans. Am Nucl. Soc. Winter Meeting*, Online, Nov. 15-19, 2020

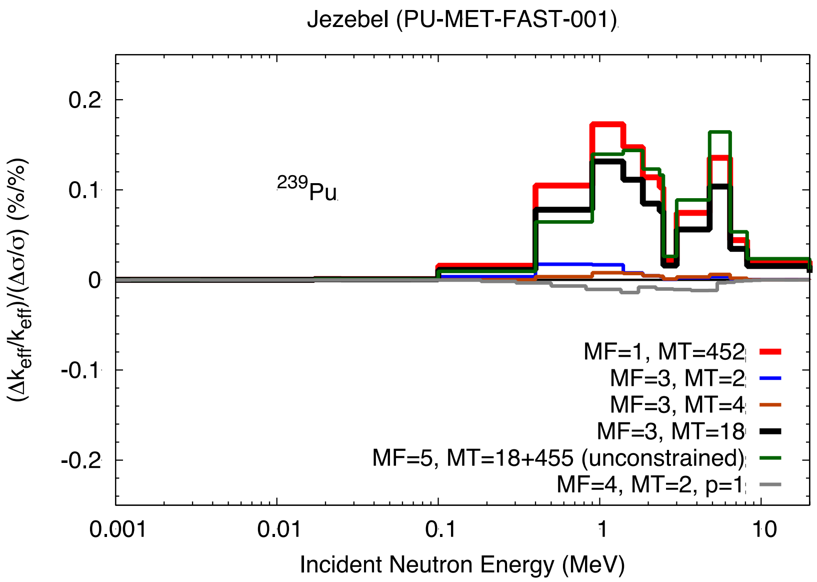
Sensitivity to fission cross section



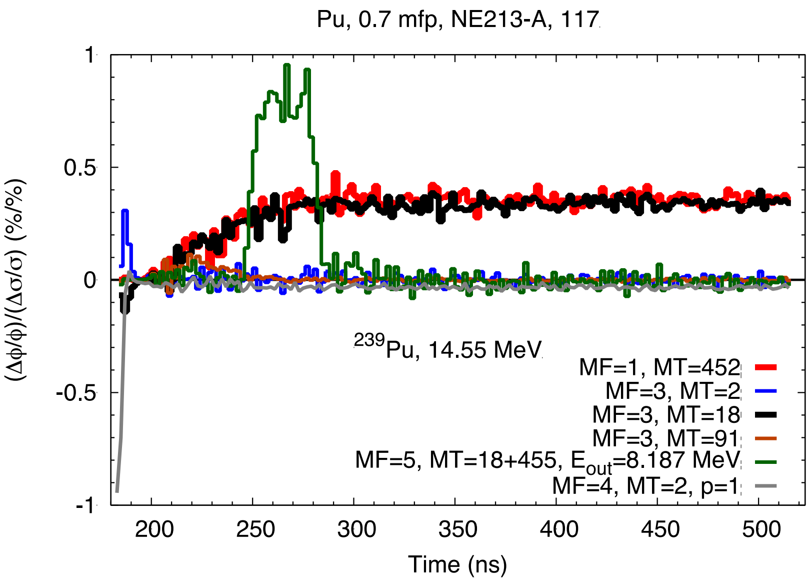
1. D. Neudecker, O. Cabellos, A. R. Clark et al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," *manuscript submitted to ann. nucl. energy*, Jan. 6, 2021
2. W. Haeck, A. R. Clark, and M. Herman, “Calculating the impact of nuclear data changes with Crater,” *Trans. Am Nucl. Soc. Winter Meeting*, Online, Nov. 15-19, 2020

Pulsed Sphere TOF spectra enable studying fission-source term observables and angular distributions differently than criticality.

Critical benchmark



14-MeV LLNL pulsed sphere



1. D. Neudecker, O. Cabellos, A. R. Clark et al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," *manuscript submitted to ann. nucl. energy*, Jan. 6, 2021

Summary

- Machine learning project had already identified problematic nuclear data
- Difficult to disentangle which nuclear data contribute to bias between measured and simulated experiments
- Inclusion of diverse benchmarks (e.g. critical and pulsed spheres) can inform nuclear data evaluation for a greater number of nuclides and energy regions to benefit criticality safety
  - 2-MeV LLNL pulsed sphere measurements
  - Experiment campaigns at NCERC
- Developed Python tool, Pulsed Sphere Sensitivity Analysis toolkit (PSSAtk)
- EUCLID using PSSAtk to design small-scale experiments that address needs/deficiencies in nuclear data
- PSSAtk can be applied to other types of problems (e.g. reaction rate foil, beta-effective)

Acknowledgements

- This work was supported in part by the DOE Nuclear Criticality Safety Program, funded and managed by the NNSA for the Department of energy
- Research reported in this publication was supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory.
- We gratefully acknowledge the support of the Advanced Simulation and Computing (ASC) program at Los Alamos National Laboratory.

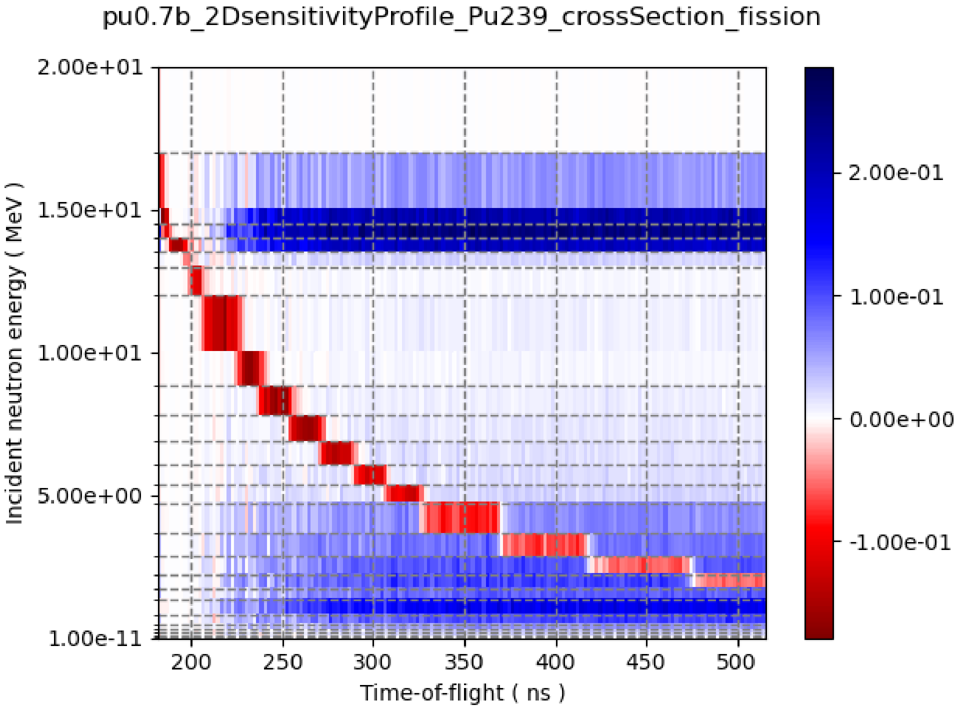
Supplemental content

Estimating sensitivities with MCNP PERT card

- Create a fictitious material
  - Nuclide weight fraction is multiplied by $1 + p$
  - Material density is multiplied by ratio of sum of modified-to-original weight fractions
- Specify METHOD=2 on the PERT card to return ΔR_t
- Calculate the relative sensitivity as

$$S_{R_t,\alpha_g} = \frac{\Delta R_t}{R_T|_{\alpha=\alpha_{g,0}} \cdot p}$$

Sensitivity to fission cross section



1. D. Neudecker, O. Cabellos, A. R. Clark et al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," *manuscript submitted to ann. nucl. energy*, Jan. 6, 2021
2. W. Haeck, A. R. Clark, and M. Herman, “Calculating the impact of nuclear data changes with Crater,” *Trans. Am Nucl. Soc. Winter Meeting*, Online, Nov. 15-19, 2020