LA-UR-25-26753

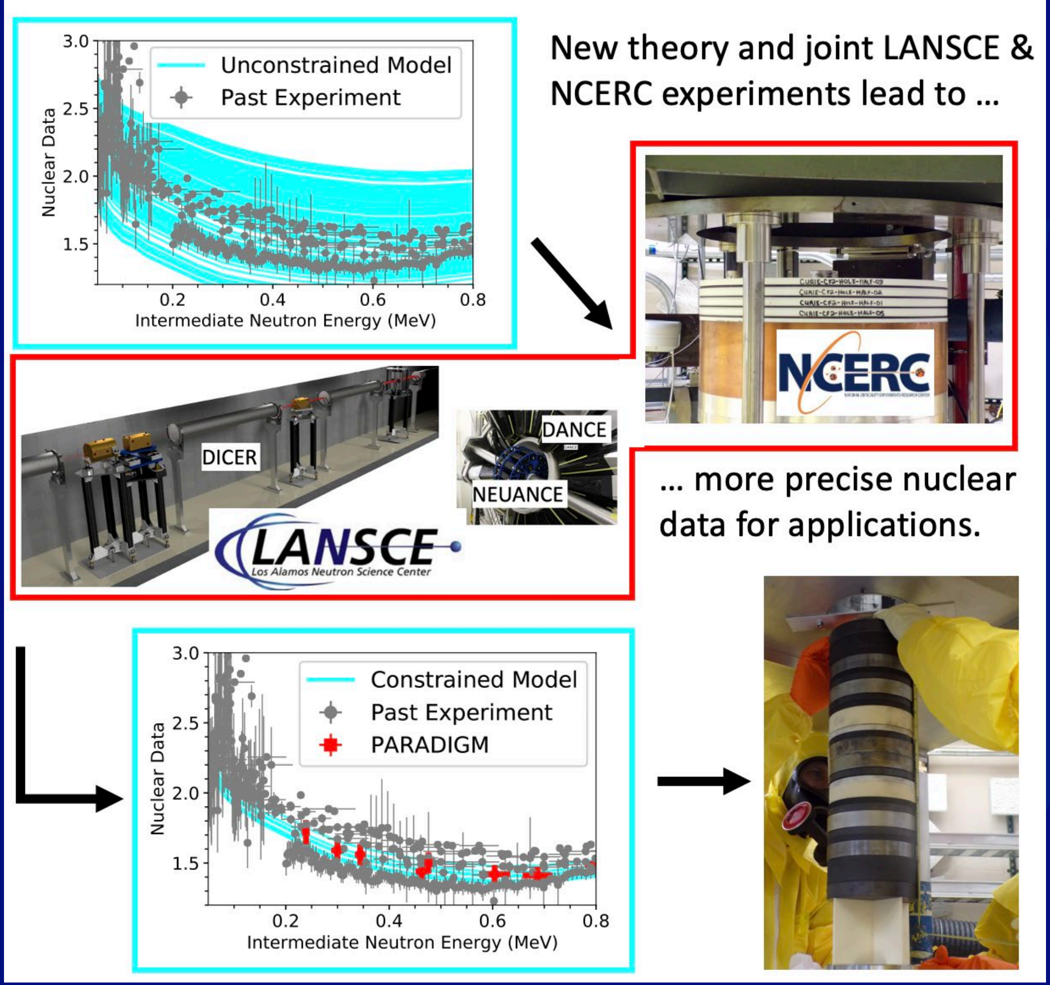
Approved for public release; distribution is unlimited.

Title: PARADIGM Differential and Integral Experiments Aiming to Reduce 239Pu Nuclear Data Uncertainties from 1-600 keV

Author(s): Cutler, Theresa Elizabeth; Neudecker, Denise; Thompson, Elizabeth Christine; Bell, Brian Wesley; Brain, Peter Jacob; Devlin, Matthew James; Fujio, Kazuki; Gibson, Nathan Andrew; Grosskopf, Michael John; Herman, Michal W.; Hutchinson, Jesson D.; Kawano, Toshihiko; Khatiwada, Ajeeta; Kleedtke, Noah Andrew; Leal Cidoncha, Esther; Little, Robert Currier; Lovell, Amy Elizabeth; McHugh, Annamaria Rose; Stamatopoulos, Athanasios; Vander Wiel,

Intended for: MCNP Users Symposium

Issued: 2025-07-14



PARADIGM

PARallel Approach of Differential and InteGral Measurements

PARADIGM Differential and Integral Experiments Aiming to Reduce ^{239}Pu Nuclear Data Uncertainties from 1-600 keV

PARADIGM team: T. Cutler (co-PI), D. Neudecker (PI), C. Thompson, B. Bell, P. Brain, M. Devlin (co-PI), K. Fujio, N. Gibson, M. Grosskopf, M.W. Herman, J. Hutchinson, T. Kawano, A. Khatiwada, N. Kleedtke, E. Leal Cidoncha, B. Little, A.E. Lovell, A. McHugh, A. Stamatopoulos, S.A. Vander Wiel

MCNP User Symposium, July 7-10, 2025

This project is paid by the LANL LDRD program.

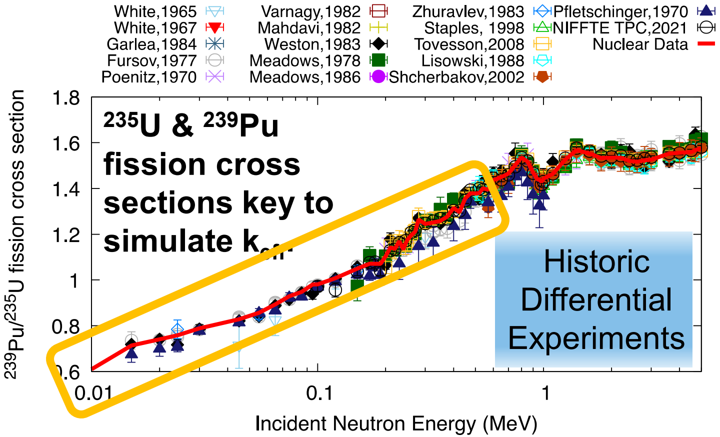
Thank you very much, NCSP, for covering the NCERC facility cost for PARADIGM!

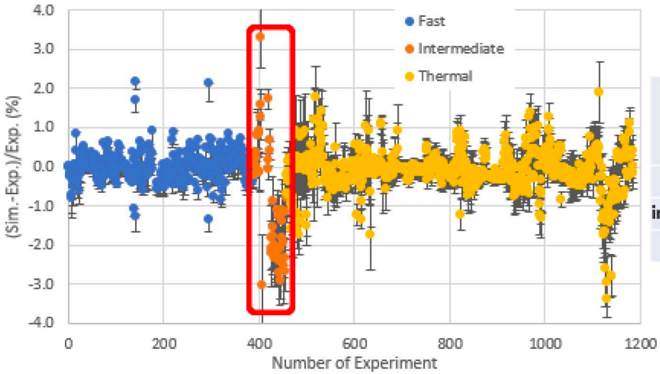
How do we accelerate scientific progress in the Nuclear Data (ND) field?

By selecting via Machine Learning (ML) an optimum combination of differential and integral experiments to reduce ND uncertainties.

Goal: PARADIGM will credibly reduce ^{239}Pu ND uncertainty from 1-600 keV by 50%. This is a challenge because:

- Differential experiments: scarce and uncertain due to low neutron flux.
- Nuclear theory: no reliable URR model implemented to smoothly connect RRR to fast.
- Integral experiments sensitive to this range are sparse and poorly calculated (only 5% of ICSBEP benchmarks).



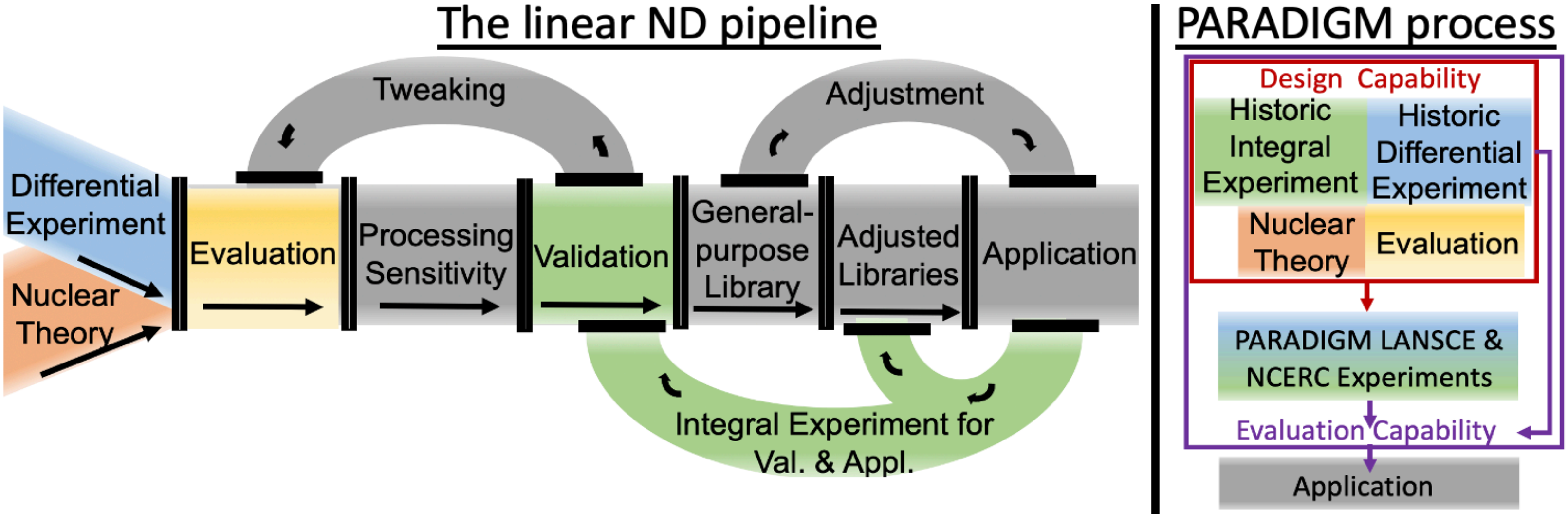


Historic Integral Experiment

Energy Range	# Cases	Average (Sim.-Exp.)/ Exp. (%)
Fast	382	0.029
intermediate	55	-0.74
Thermal	728	-0.24

Intermediate actinide ND are crucial input for various programs including NCSP.

We cut down the time for understanding biases in ND from 25 to 3 years by developing a decision-making tool for experiment selection.



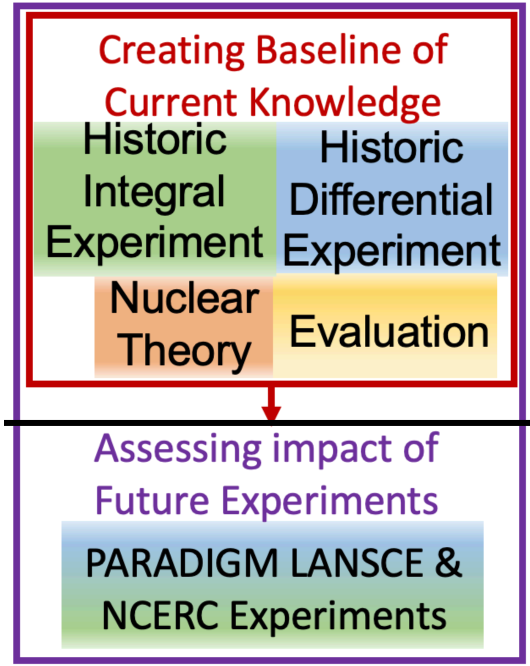
We investigate at the get-go what differential and integral experiments along with theory developments are key to reduce unc. in ND.

This acceleration of process requires:

- **Turning around the ND pipeline (and having a team to do it).**
- **Machine learning to select optimal LANSCE & NCERC exps. to reduce unc.**

Experiment selection is a multi-step process using ML (GLS augmented with Gaussian process, D-optimality).

PARADIGM Experiment Selection Tool



Step 0: Define initial ND from nuclear theory and ENDF/B-VIII.0.

Step 1: Adjust to historic differential data using GLS & Gaussian process.

Step 2: Calibrate to historic integral benchmarks using GL.

Step 3: Use D-optimality criterion to guide selection of pairs of candidate experiments.

We have high-dimensional input data for our ML-enhanced adjustment.

46 k_{eff} benchmarks. with sensitivities (dim: ***46x>12,200***)

PMF001 k_{eff}

VIII.0 ND: ^{1}H, ^{9}Be, ^{10,11}B, ^{12}C, ^{16}O, ^{27}Al, ^{52}Cr, ^{56}Fe, ^{208}Pb, ^{235,238}U VIII.0 ND. ***(~10,000)***

PARADIGM Experiment Selection Tool

Creating Baseline of Current Knowledge

Historic Integral Experiment

Historic Differential Experiment

Evaluation

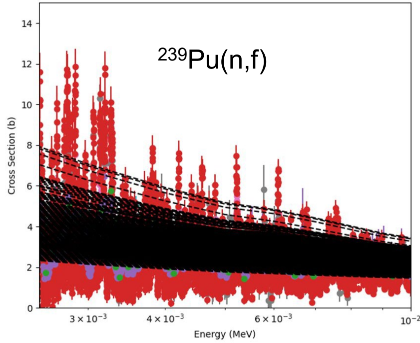
Nuclear Theory

Assessing impact of Future Experiments

PARADIGM LANSCE & NCERC Experiments

122 differential data sets ***(~8,400 data points)***

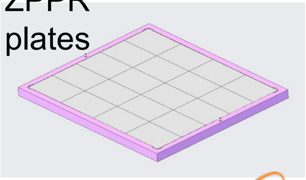
^{63,65}Cu, ^{239,240}Pu model data (***~2,200***)



20 potential differential exp.

6 potential integral exp.

ZPPR plates

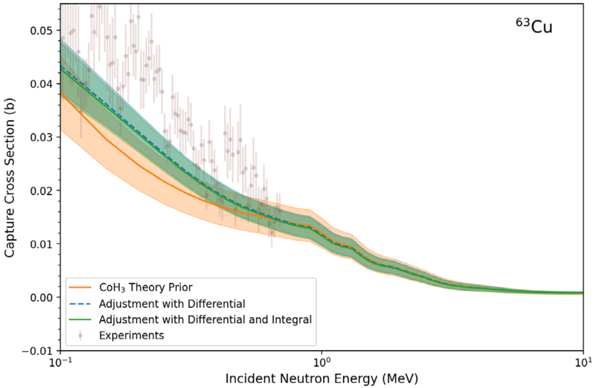


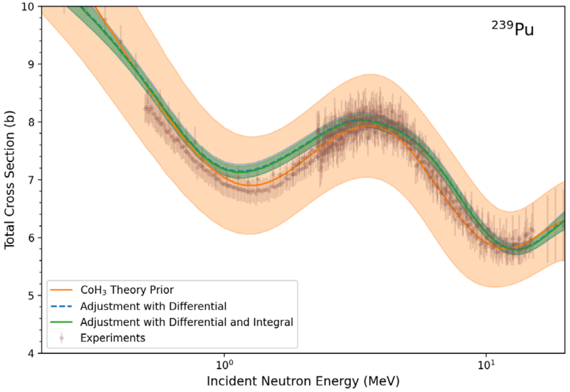
Comet

NCERC

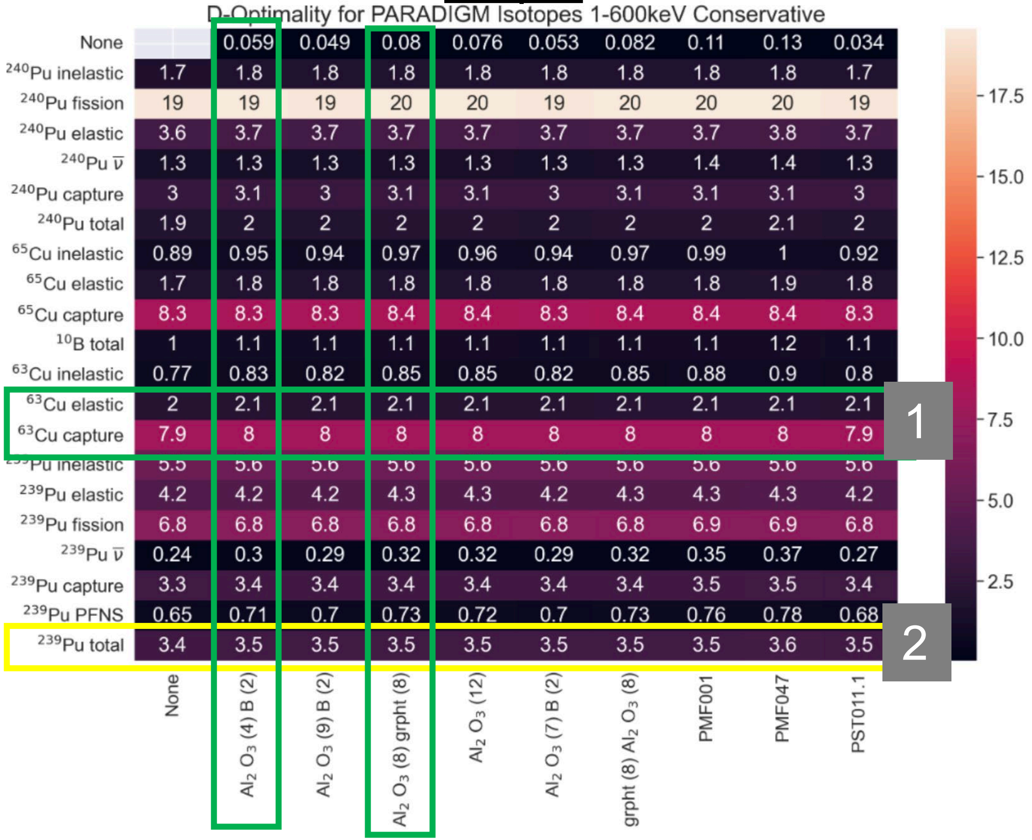
LANSCE and NCERC experiments are chosen based on AI/ ML tool with GLS, Gaussian processes and D-optimality*.

Step 0-2





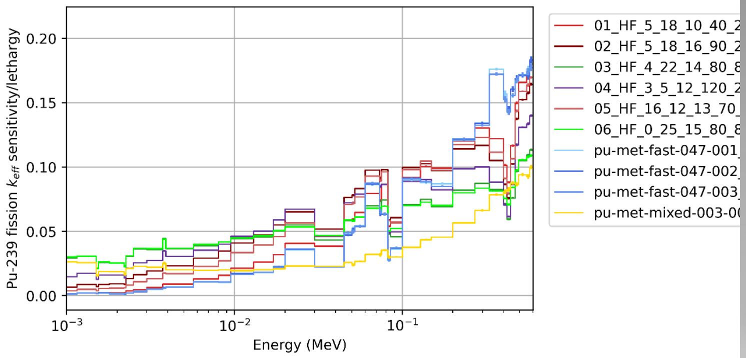
Step 3

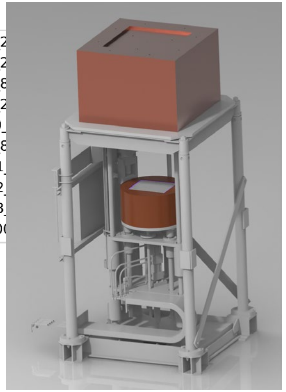


*The higher D-opt, the more impact of experiment.

Los
NATIONAL LABORATORY

The NCERC integral experiment has Pu fuel and thick Cu reflector. We study both also by differential experiments.





NCERC: Cu reflector, Pu fuel

- Alumina for 30-600 keV.
- Alumina/ Graphite for 1-30 keV.

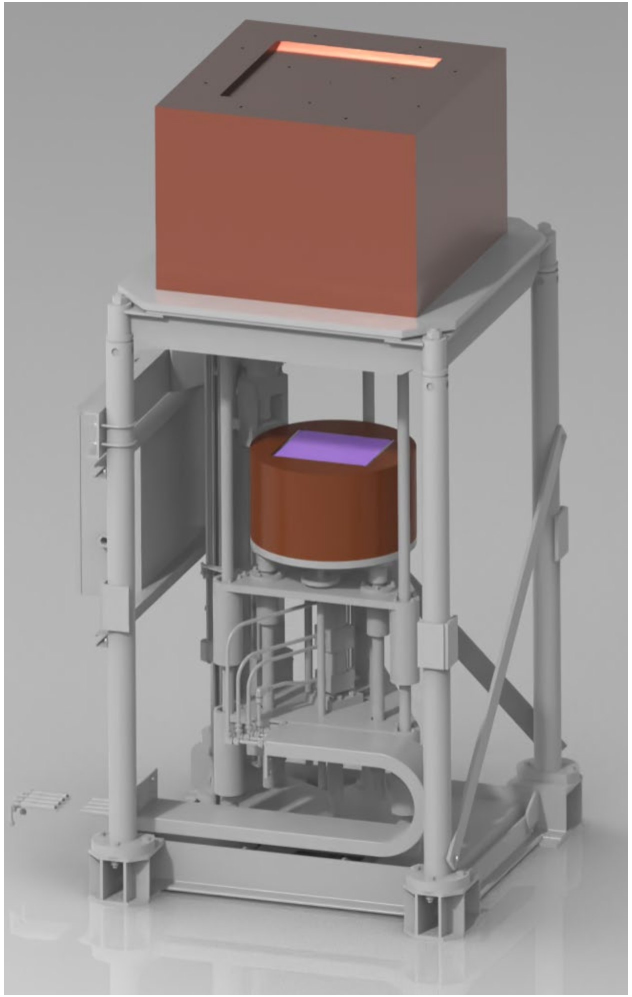
LANSCE: Cross section data.

1. ^{63}Cu(n,tot) cross section via DICER.
2. ~~^{239}Pu(n,tot) cross section if we can get sample and beam*.~~
3. Analysis of raw ^{63}Cu(n,g) data from DANCE.

*This is at a higher Einc range than Thanos' NCSP measurement.

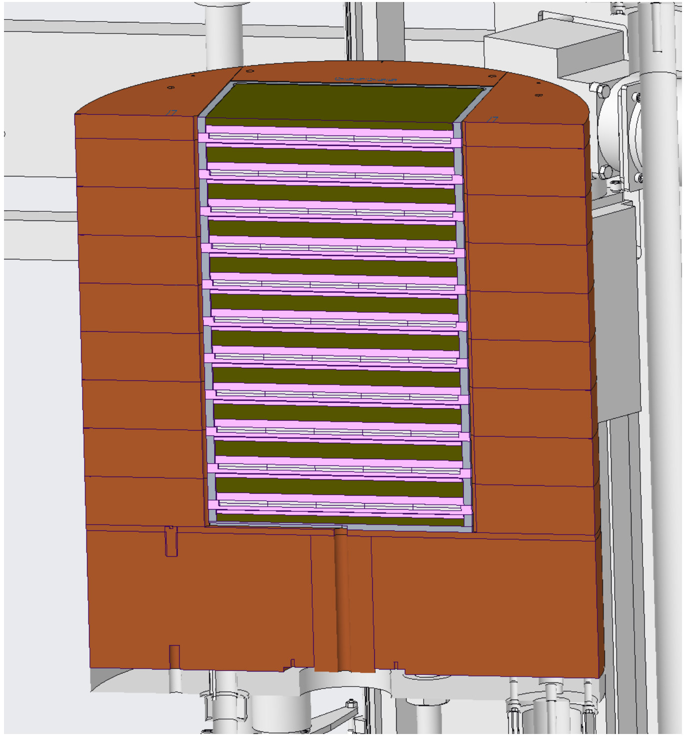
Final design

- The iterative process of adding features and checking to ensure the design meets the design requirements continues until it is “final”
- Some design changes occur given this
  - Mostly due to physical constraints and procurement issues
  - During procurement, issues with boron procurement led to a significant change
    - Uncertainty in boron physical parameters led to this
    - Removed boron completely!



Discrete shapes and volumes

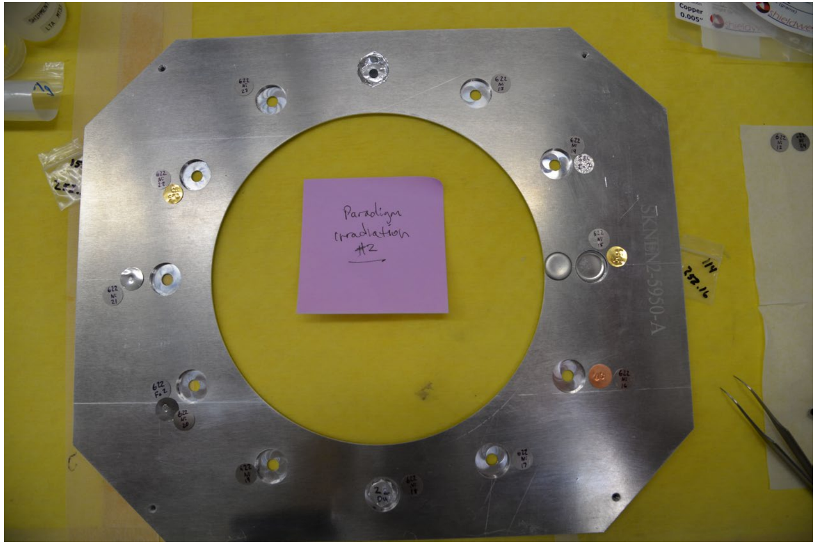
- Copper inner reflectors
  - Single pieces per layer
    - This is very wasteful from a material standpoint, and also very heavy!
    - Not guaranteed to fit, so either large gaps or not usable
    - Heavy or lots of thin layers
  - Many pieces per layer
    - Intricate design
    - Allows much greater height per layer
    - More complicated to model
- Trays holding ZPPR plates
  - Aluminum mating frames
  - Weight constraints
  - Gaps within the trays



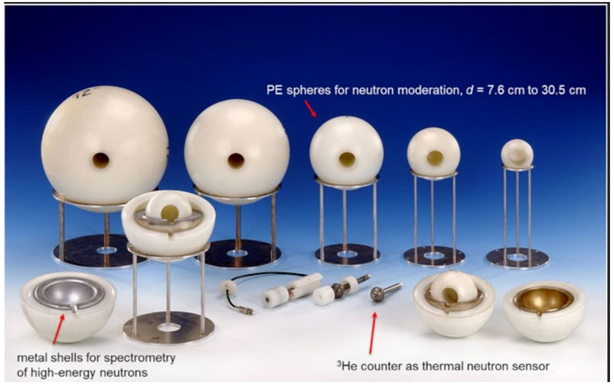
NCERC Experiment Executed in May 2025!

- The two planned configurations were measured
  - Varied in spectrum, interstitial material and fuel mass required
- Many responses measured!
  - criticality
  - Rossi-α, by two different methods
  - Reaction rate ratios
    - Activation foils and fission foils
  - Leakage Spectra via Bonner spheres
- Analysis of all methods is on-going
- Provides unique validation sets for ND and MCNP

Rossi-a and Reaction Rate Ratio Sample Plate



Bonner Sphere Measurements



Experiments to be undertaken:
We study ^{63}Cu ND via differential and integral experiment from 1-600 keV.

URR theory developed for this project can be also used for future NCSP evaluations.

Random matrix approach is used to smoothly connect RRR and fast energy regions.

- Transmission coefficients in both regions
  - it guarantees smoothly connected cross sections
  - but limited to s-wave only
- Optical model (coupled-channels)
  - for higher partial waves

$$T = 1 - |\overline{S}|^2$$

$$\overline{R} = R(E + iI) \rightarrow \overline{S}$$

GOE model provides average cross sections as well as their realistic distribution

$$S^{\mathrm{OM}} = \overline{S}$$

Based on Kawano, Talou, and Weidenmüller, *PRC* **92**, 044617 (2015); worked on by Fujio, Kawano, Lovell.

Los Alamos NATIONAL LABORATORY

This project aims to accelerate progress in the ND field by:

- We have (and plan to open source) an ML capability to quantitatively select the optimal differential and integral experiment combination to reduce ND unc. That saves us valuable time in iterating through several experiment combinations.
- We will provide the ^{63}Cu total cross section and ^{63}Cu capture cross section to EXFOR, PARADIGM NCERC experiment to CSEWG when available.
- We will publish databases of differential and integral data as allowed by LANL, helping SG-54 (curated diff. exp. database) and SG-52 (adjustment).
- We will implement URR theory in CoH which is an open-source code.

Thank you very much, NCSP, to cover the NCERC facility cost for PARADIGM.

Acknowledgements

- Research reported in this publication was supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory.
- NCERC is supported by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.