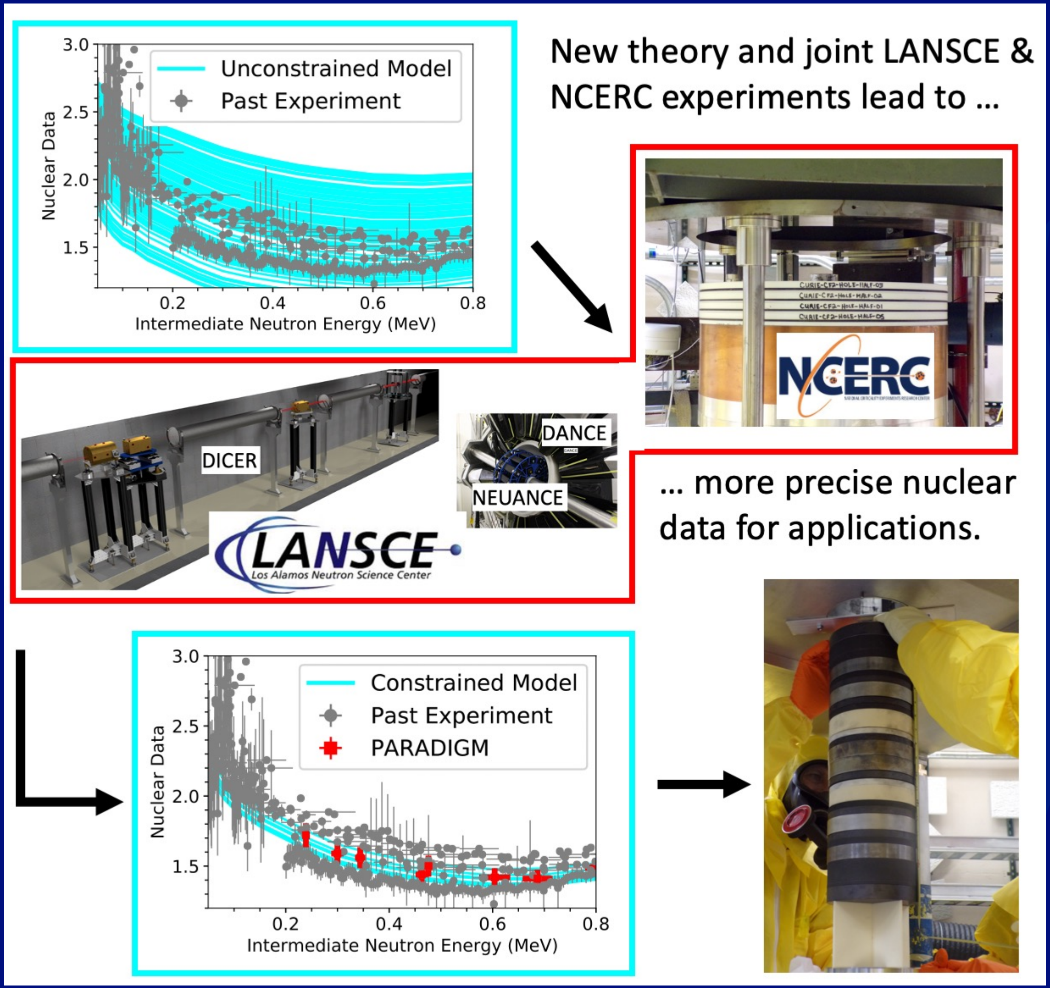
Los Alamos
NATIONAL LABORATORY



PARADIGM

PARallel Approach of Differential and InteGral Measurements

LDRD

Machine learning selection of differential and integral experiments to optimally reduce nuclear data uncertainties

PARADIGM team: D. Neudecker (PI), C. Thompson, K. Amundson, B. Bell, P. Brain, T. Cutler (co-PI), 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

NCSP TPR, Dec. 3-5, 2024

This project is funded by the LANL LDRD program.
Thank you very much, NCSP, for covering the NCERC facility cost for PARADIGM!

Some long-term outcomes of this project are of interest for the NCSP program:

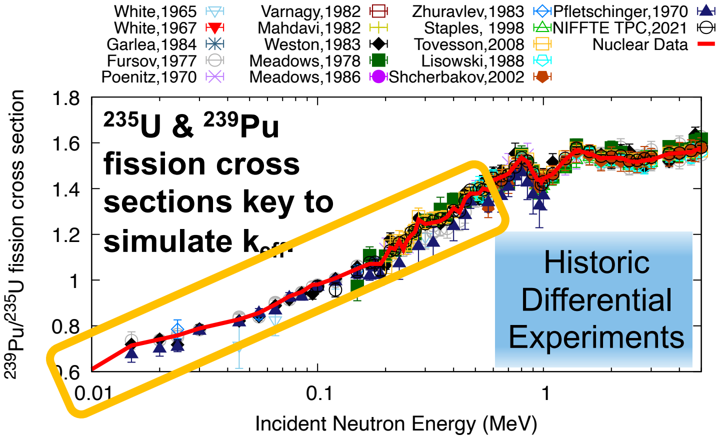
- We developed AI/ ML ***methodology to quantitatively decide which combination of differential and integral experiments can best reduce ND uncertainties*** of interest for applications. Such a methodology can be used to more tightly couple IE/ ND efforts to answer NCSP application needs. It also accelerates progress in resolving issues in ND.
- We are ***studying*** ^{239}***Pu and*** ^{63}***Cu ND via differential and integral experiment from 1-600 keV*** which is also of interest for NCSP.
- ***URR theory*** developed for this project can be also used for future NCSP evaluations.

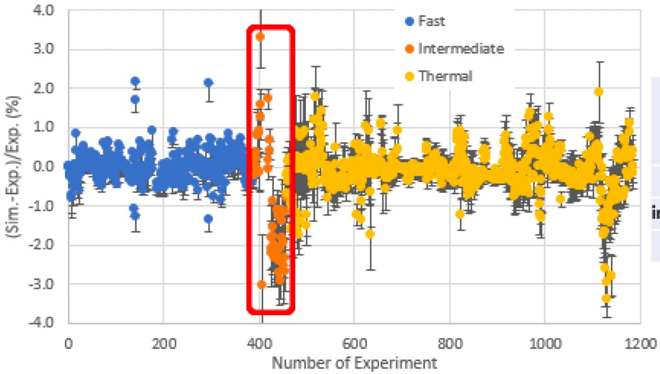
How do we accelerate scientific progress in the ND field?

By selecting via 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: sparse and poorly calculated (only 5% of ICSBEP benchmarks).





Historic Integral Experiment

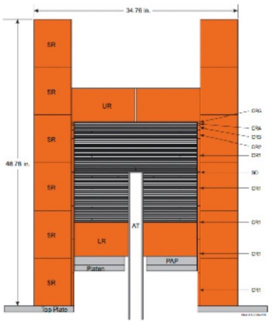
Energy Range	# Cases	Average (Sim.-Exp.)/ Exp. (%)
Fast	382	0.029
intermediate	55	-0.74
Thermal	728	-0.24

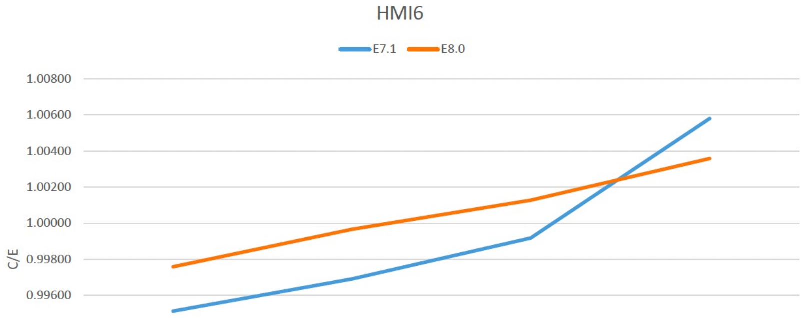
Intermediate actinide ND are crucial input for various programs including NCSP.

Los Alamos NATIONAL LABORATORY

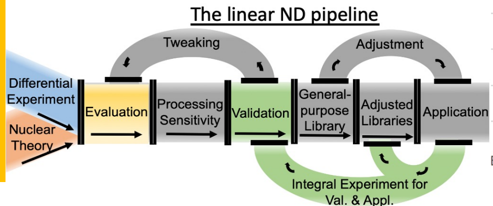
Adjusting ^{239}Pu ND to k_{eff} reduces unc. by 50%, but needs to understand *all* ND of integral exp. Zeus shows challenge.

- If we adjust to Pu existing intermediate k_{eff} values, our ^{239}Pu ND unc. reduce by 50%
- But we don’t trust the data because we don’t fully understand ND queried by the integral exp.
- Challenge: to go to intermediate energies, we need reflector materials that are not well-understood.
- Example: Reducing the 10-sigma bias in Zeus (trusted unc!) took ~25 years, because it took us time to understand that large C/E linked to poor ^{235}U ***<u>& Cu</u>*** (reflector) ND.

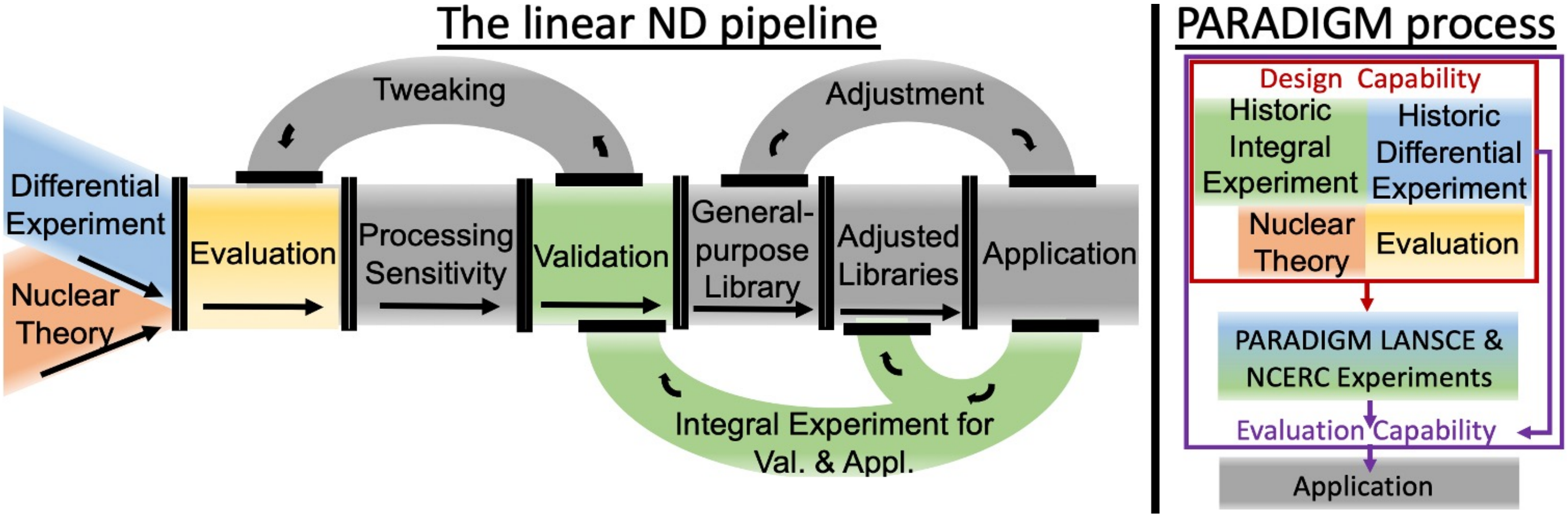




If differential AND integral experiments AND theory were developed simultaneously, the Zeus issue could have been resolved in < 5 years.



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

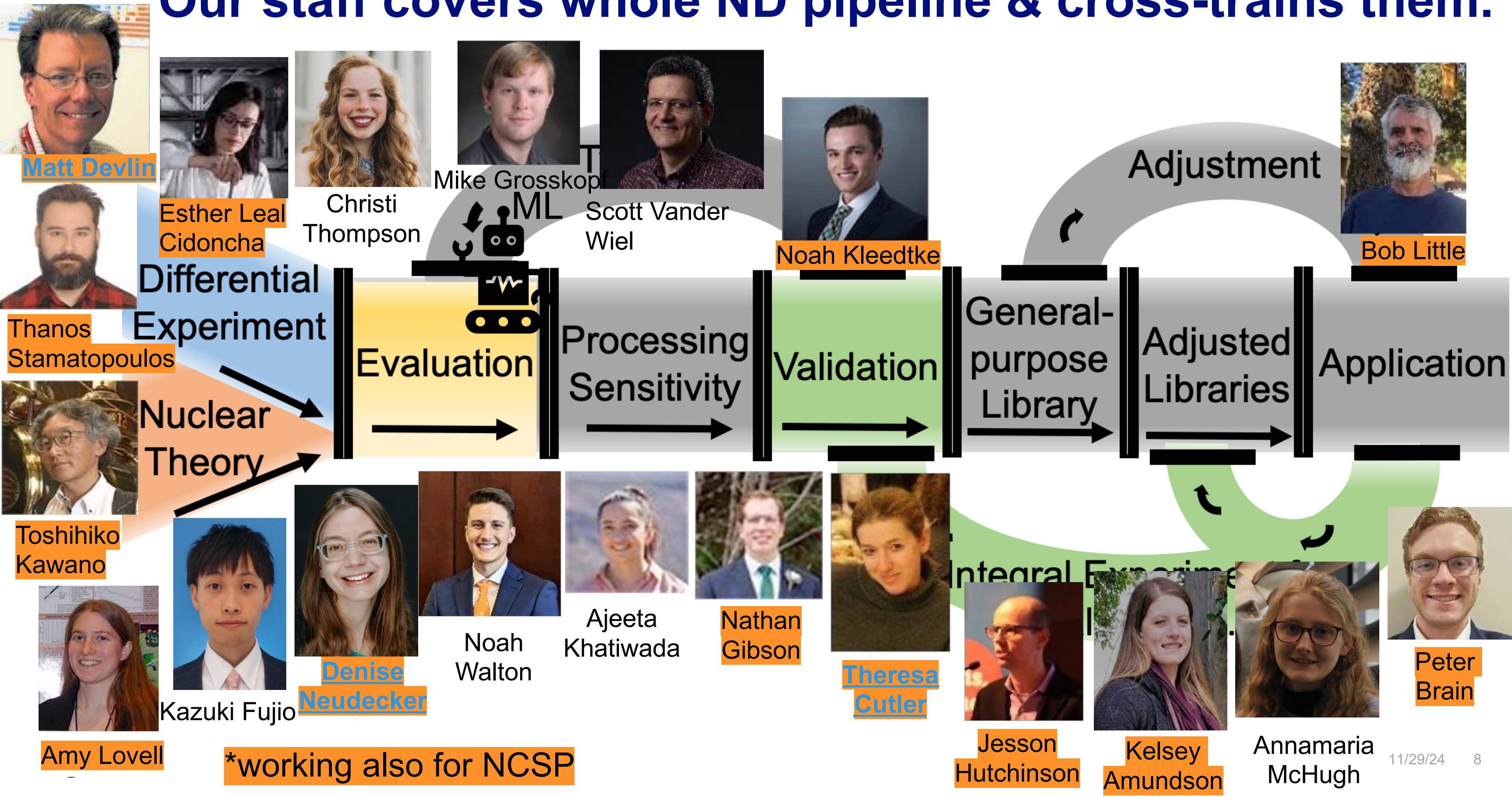


We investigate at the get-go what differential and integral experiments along with theory developments are key to reduce unc. in ND.

This acceleration of process requires:

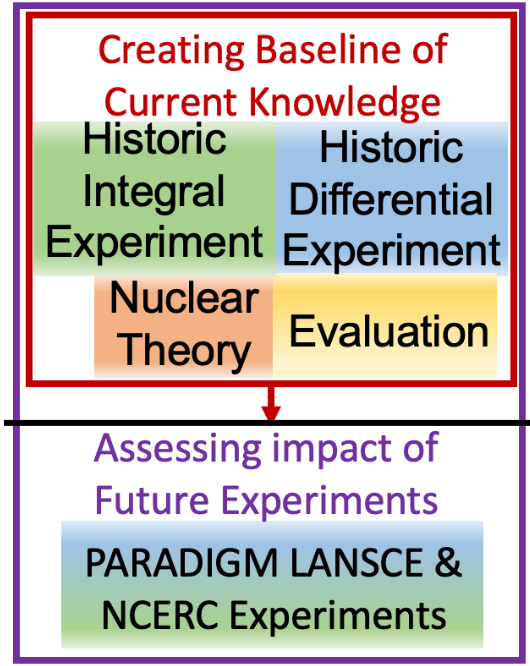
- **Turning around the ND pipeline (and having a team to do it).**
- **Machine learning to select optimal LANSCE & NCERC exps. to reduce unc.**

Our staff covers whole ND pipeline & cross-trains them.



Experiment selection is a multi-step process using ML (Generalized least squares with Gaussian process, D-optimality).

PARADIGM Experiment Selection Tool



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

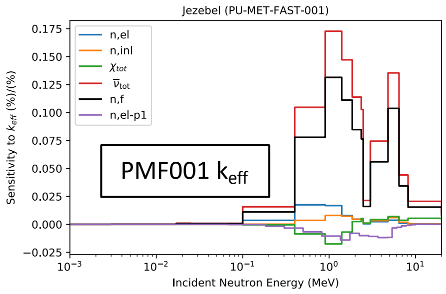
Step 1: Adjust to historic differential data using GLS & Gaussian process.

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***)*



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

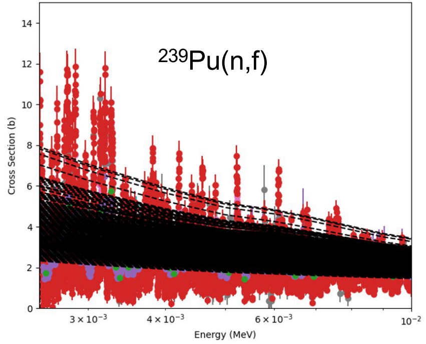
Nuclear Theory

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)***

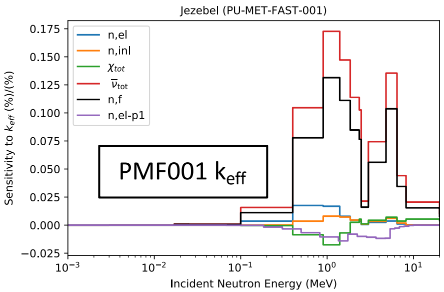


*Sensitivity database planned to be released to WPEC SG-52

**Curated data sets are planned to be released to WPEC SG-54

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

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



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

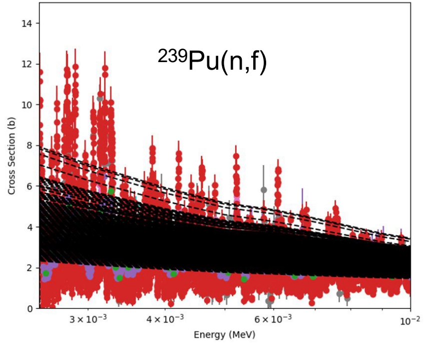
Nuclear Theory

Assessing impact of Future Experiments

PARADIGM LANSCE & NCERC Experiments

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

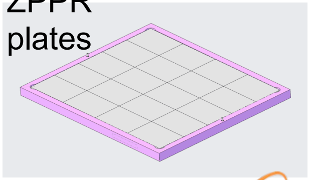
^{63,65}Cu, ^{239,240}Pu model data ***(~2,200)***



20 potential differential exp.

6 potential integral exp.

ZPPR plates

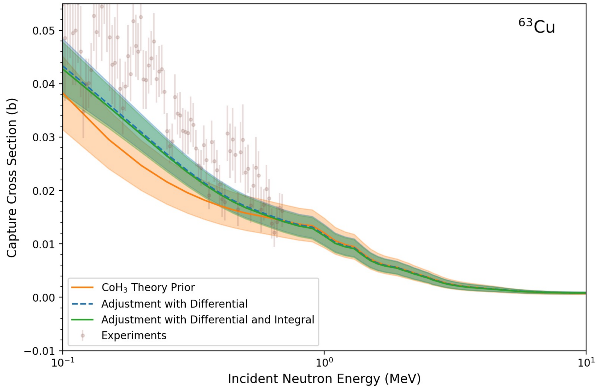


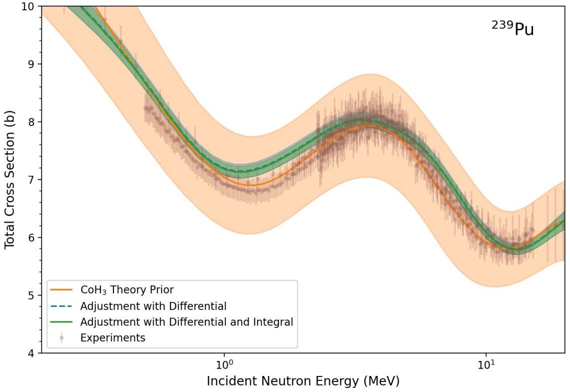
Comet

NCERC

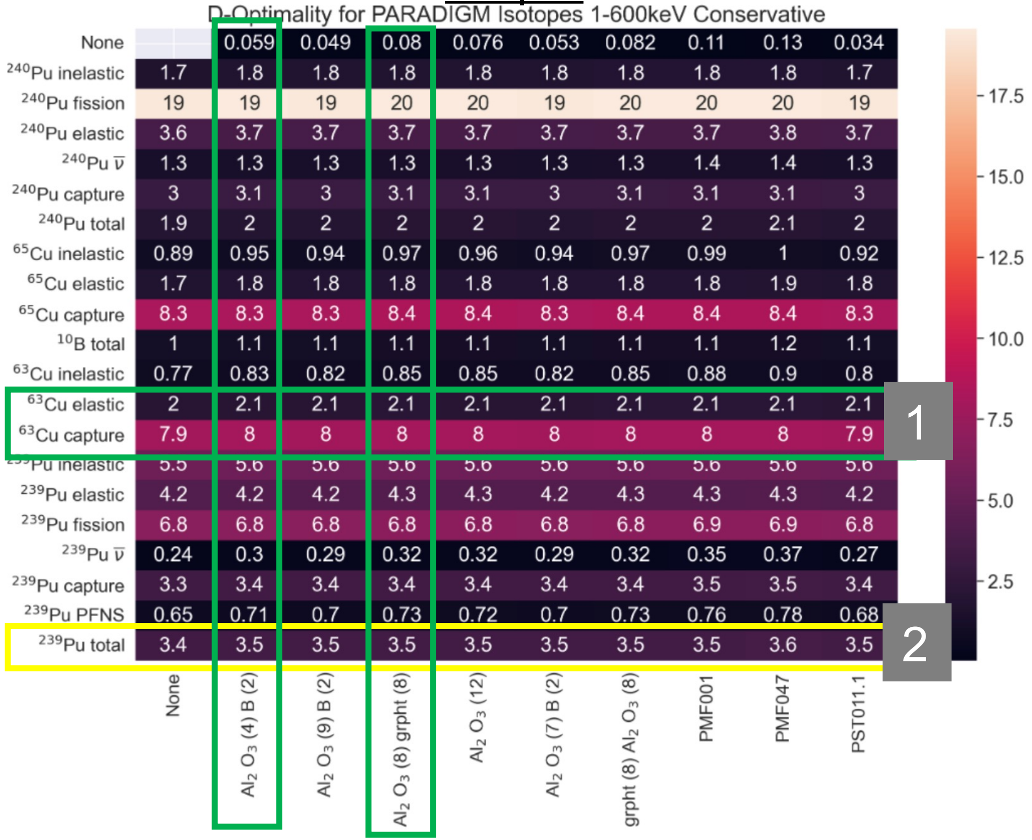
LANSCE and NCERC experiments are chosen based on AI/ ML tool with GLS, Gaussian processes and D-optimality*.

Step 0-2





Step 3



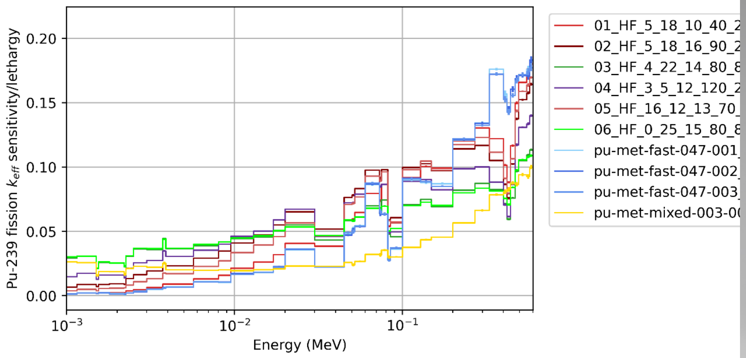
	None	Al_2O_3 (4) B (2)	Al_2O_3 (9) B (2)	Al_2O_3 (8) grpht (8)	Al_2O_3 (12)	Al_2O_3 (7) B (2)	grpht (8) Al_2O_3 (8)	PMF001	PMF047	PST011.1
None		0.059	0.049	0.08	0.076	0.053	0.082	0.11	0.13	0.034
^{240}Pu inelastic	1.7	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.7
^{240}Pu fission	19	19	19	20	20	19	20	20	20	19
^{240}Pu elastic	3.6	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.8	3.7
^{240}Pu $\bar{\nu}$	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.4	1.4	1.3
^{240}Pu capture	3	3.1	3	3.1	3.1	3	3.1	3.1	3.1	3
^{240}Pu total	1.9	2	2	2	2	2	2	2	2.1	2
^{65}Cu inelastic	0.89	0.95	0.94	0.97	0.96	0.94	0.97	0.99	1	0.92
^{65}Cu elastic	1.7	1.8	1.8	1.8	1.8	1.8	1.8	1.8	1.9	1.8
^{65}Cu capture	8.3	8.3	8.3	8.4	8.4	8.3	8.4	8.4	8.4	8.3
^{10}B total	1	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.2	1.1
^{63}Cu inelastic	0.77	0.83	0.82	0.85	0.85	0.82	0.85	0.88	0.9	0.8
^{63}Cu elastic	2	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1
^{63}Cu capture	7.9	8	8	8	8	8	8	8	8	7.9
^{239}Pu inelastic	5.5	5.6	5.6	5.6	5.6	5.6	5.6	5.6	5.6	5.6
^{239}Pu elastic	4.2	4.2	4.2	4.3	4.3	4.2	4.3	4.3	4.3	4.2
^{239}Pu fission	6.8	6.8	6.8	6.8	6.8	6.8	6.8	6.9	6.9	6.8
^{239}Pu $\bar{\nu}$	0.24	0.3	0.29	0.32	0.32	0.29	0.32	0.35	0.37	0.27
^{239}Pu capture	3.3	3.4	3.4	3.4	3.4	3.4	3.4	3.5	3.5	3.4
^{239}Pu PFNS	0.65	0.71	0.7	0.73	0.72	0.7	0.73	0.76	0.78	0.68
^{239}Pu total	3.4	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.6	3.5

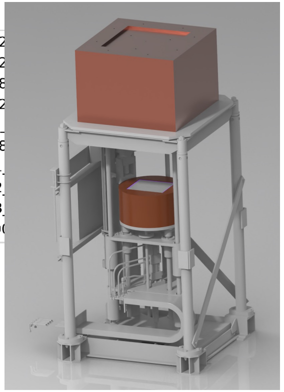
*The higher D-opt, the more impact of experiment.

Los Alamos NATIONAL LABORATORY

Experiments to be undertaken:
We study ^{239}Pu and ^{63}Cu ND via differential and integral experiment from 1-600 keV.

NCERC integral exp. highly sensitive to 1-600 keV ^{239}Pu ND. We study Pu fuel and Cu reflector by differential exp.





NCERC: Cu reflector, Pu fuel

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

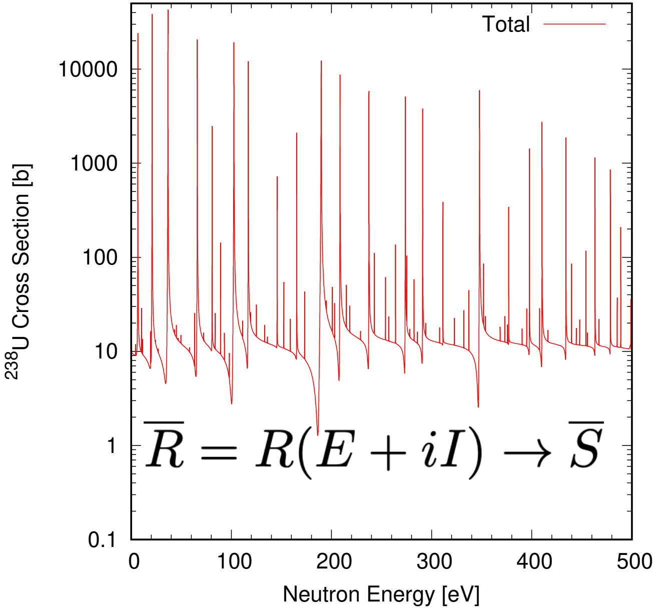
LANSCE: Cross section data.

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 E_{inc} range than Thanos' NCSP measurement.

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

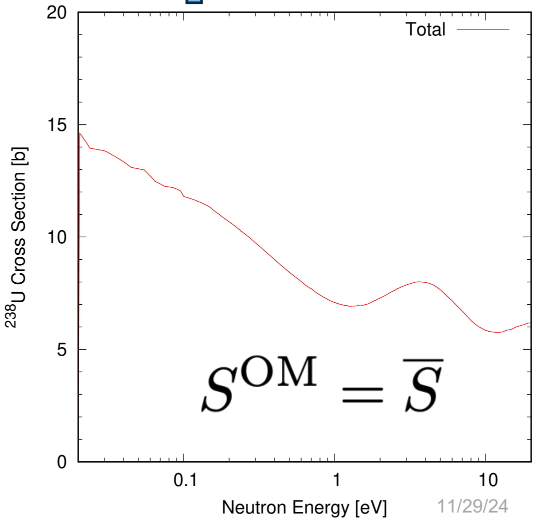
Random matrix approach is used to smoothly connect RRR and fast energy regions.



- 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

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

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



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

This project will 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/ ^{239}Pu total cross sections and ^{63}Cu capture cross sections** 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, for agreeing 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.