Designing experiments predicted to significantly reduce uncertainties on a chosen application

Denise Neudecker

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

The scientific goals described in this talk are:

1) **We, as a field, want to accelerate the timeline to progress on solving application questions.**
2) **We do that by designing and selecting experiments predicted to reliably reduce uncertainties on an application quantity of interest.***

*Experiments are expensive and time intensive. You better be sure up-front they have the desired impact on your application.

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We show an example from the LANL LDRD-DR *PARADIGM* project. Its framework can be used for projects across the complex and is not tied to LANL. **This example shows that the field can do it IF WE HAVE THE RIGHT RESOURCES (data, codes, people, funding, etc.).**

*Experiments are expensive and time intensive. You better be sure up-front they have the desired impact on your application.

PARADIGM's goals are an example of the broader question we are trying to answer for the field:

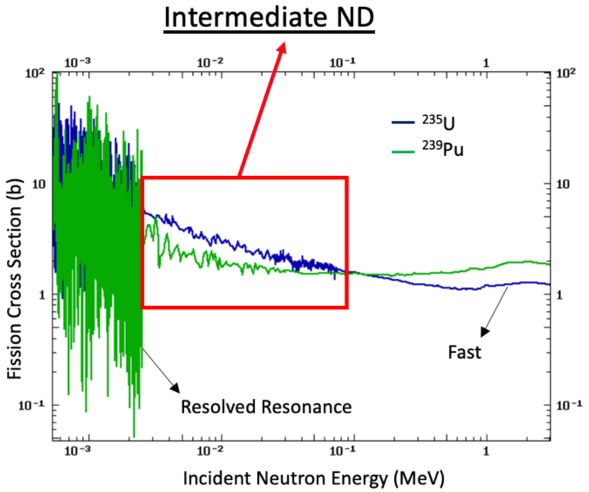
1) **We, as a field, want to accelerate the timeline to progress on solving application questions.**
2) **We do that by designing and selecting experiments predicted to reliably reduce uncertainties on an application quantity of interest.**

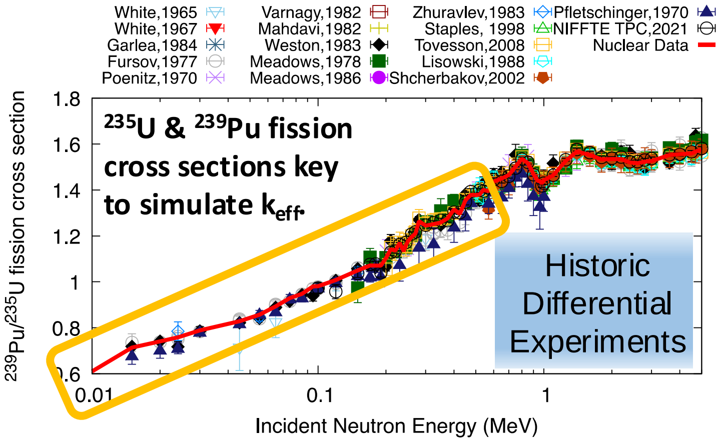
PARADIGM goals:

1) We want to accelerate progress on understanding ^{239}Pu 1-600 keV nuclear data from 25 to 3 years.
2) We want to reliably reduce ^{239}Pu nuclear data uncertainties by 50% by selecting an optimal differential and integral experiment combination to do so.

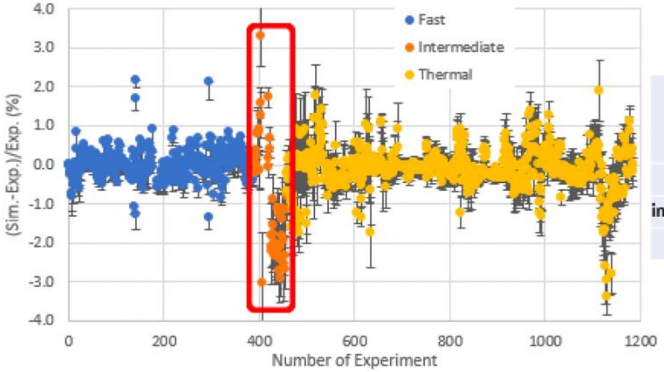
Our target nuclear data are biased & uncertain because supporting data poor.

- Nuclear theory: no reliable URR model.
- Differential exp.: scarce/uncertain due to low neutron flux.
- Integral experiments sensitive to this range are sparse and poorly calculated.





Historic Differential Experiments



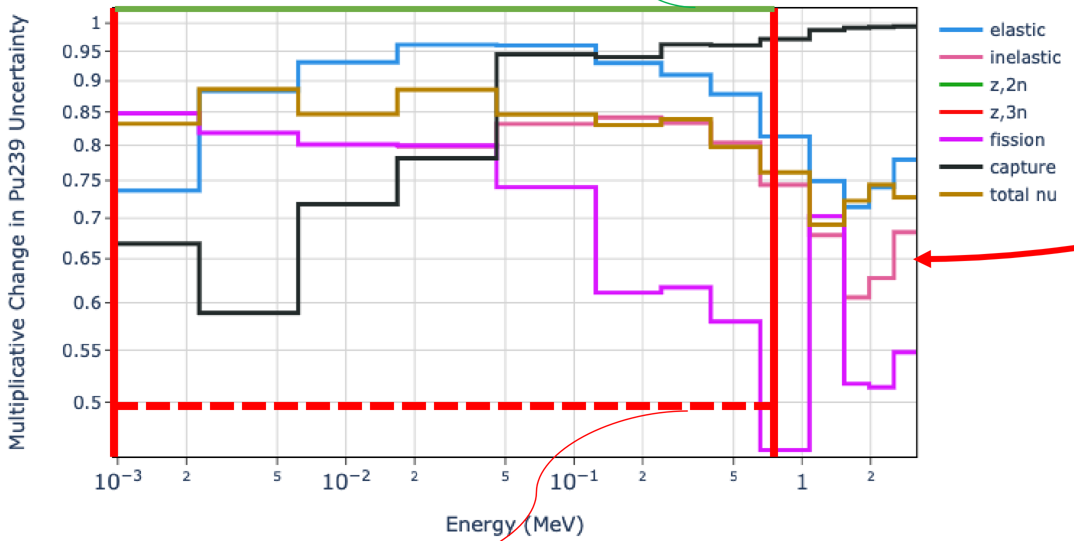
Historic Integral Experiment

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

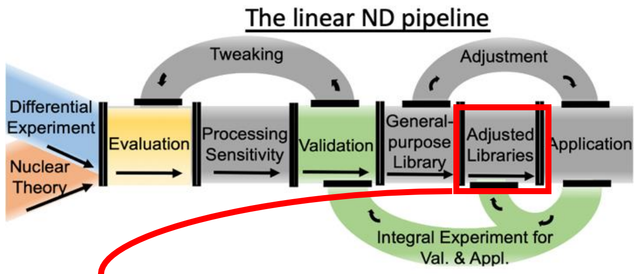
Intermediate ^{239}Pu ND are crucial input for the weapons program, criticality safety, etc.!

ND unc. on application simulations can be reduced via adjustment to related integral exp. *IF YOU TRUST THEM*.

ENDF/B-VIII.0 unchanged unc.



We want to reduce ^{239}Pu ND below that line.

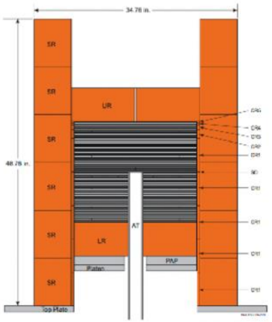


For PARADIGM, we are close to reducing the uncertainties by 50% with current integral data, but we don't fully trust them.

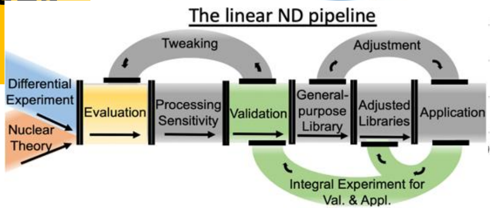
Having an integral experiment that we trust is the challenge.

Historic example: Understanding large bias in precise intermediate Zeus crit took 25 years thanks to slow pipeline!

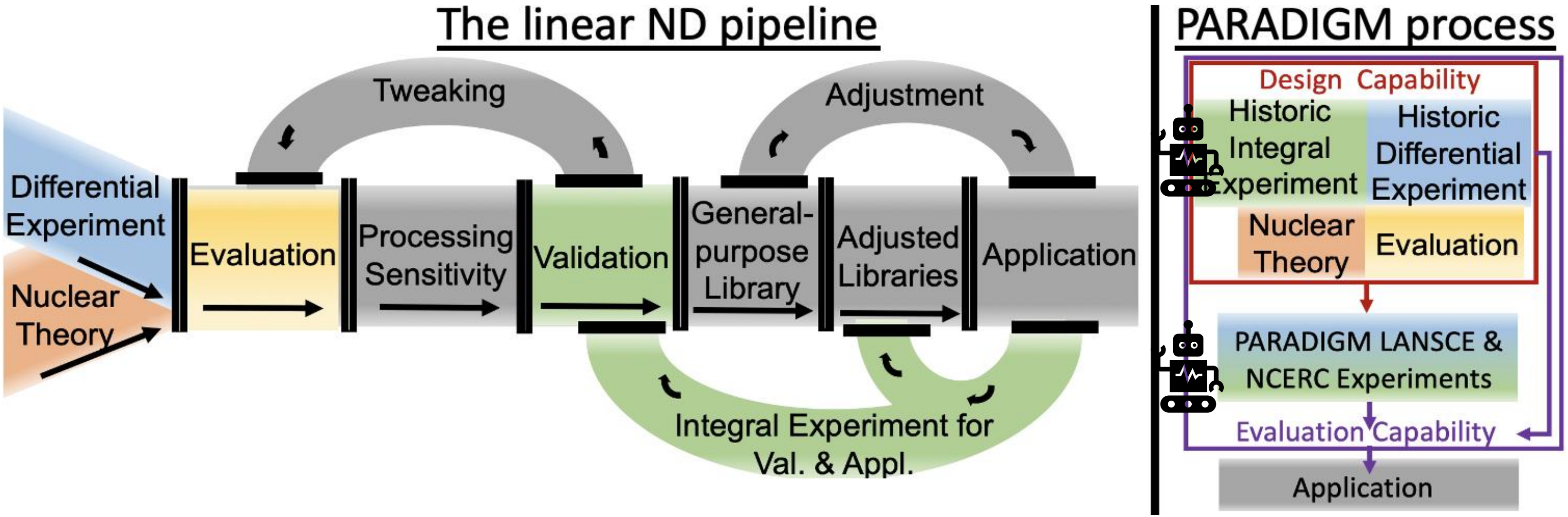
- **Challenge: to go to intermediate energies, we need reflector materials that are not well-understood.**
- Example Zeus experiment:
  - 1998 at TA-18, filled integral experiment gap in HEU intermediate ND with reliable exp. unc. of <0.1 %.
  - Halving the 10-sigma bias in Zeus (trusted unc!) took ~25 years, because of multiple iterations of the linear pipeline to understand that large C/E linked to poor ^{235}U ***& Cu*** (reflector) ND.



If differential AND integral experiments AND theory were developed simultaneously, the Zeus issue could have been resolved in 3 years.



The key step to accelerate understanding nuclear data is executing a decision-making tool for exp. selection. It turns around the pipeline.

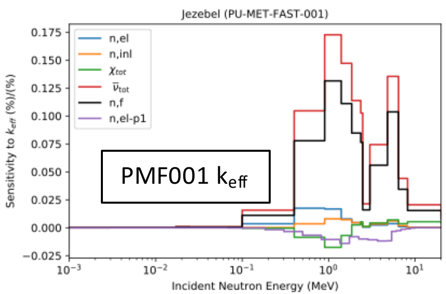


We investigate at the get-go what differential and integral experiments along with theory improvements will reliably reduce unc. in ND. Acceleration of process requires:

- **Having a team that delivers input data from all parts of the pipeline.**
- **Machine learning to select optimal experiments to reduce unc.**

AI/ML is required as the selection process includes high-dimensional input data to avoid repeating past experiments.

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

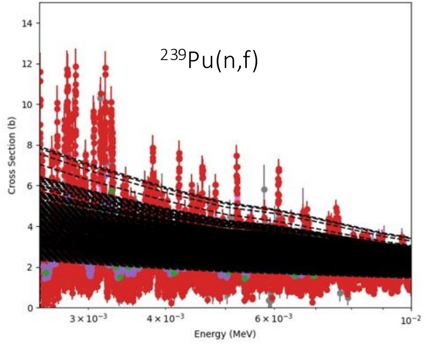
- Historic Integral Experiment
- Historic Differential Experiment
- Evaluation
- Nuclear Theory

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***)

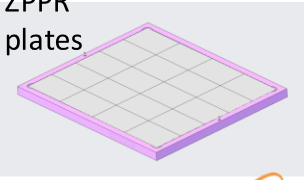


20 potential differential exp.

LANSCE Los Alamos Neutron Science Center

6 potential integral exp.

ZPPR plates



Comet

NCERC

Experiments were selected within a year with AI/ ML metrics.

NCERC: Cu reflector, Pu fuel
- Alumina for 30-600 keV.
- Alumina/Graphite for 1-30 keV.

LANSCE: DICER measurement of ^{63}Cu(n,tot) cross section and analysis of ^{63}Cu(n,g) cross section.

D-Optimality for PARADIGM Isotopes 1-600keV Optimistic

Candidate Differential Experiments (rows) / Candidate Integral Experiments (columns)

	None	Al_2 O3 (4) B (2) opt.	Al_2 O3 (9) B (2) opt.	Al_2 O3 (8) grpht (8) opt.	Al_2 O3 (12) opt.	Al_2 O3 (7) B (2) opt.	grpht (8) Al_2 O3 (8) opt.
None		0.19	0.15	0.2	0.2	0.17	0.21
^{240}Pu inelastic	2.9	3.1	3.1	3.1	3.1	3.1	3.1
^{240}Pu fission	24	24	24	24	24	24	24
^{240}Pu elastic	5.3	5.5	5.4	5.5	5.5	5.5	5.5
^{240}Pu $\bar{\nu}$	5.1	5.3	5.3	5.3	5.3	5.3	5.3
^{240}Pu capture	4.8	5	5	5	5	5	5
^{240}Pu total	3.8	4	4	4	4	4	4
^{65}Cu inelastic	2.2	2.3	2.3	2.4	2.3	2.3	2.4
^{65}Cu elastic	2.7	2.9	2.9	2.9	2.9	2.9	2.9
^{65}Cu capture	4.5	4.7	4.7	4.7	4.7	4.7	4.7
^{10}B total	2.7	2.9	2.8	2.9	2.9	2.8	2.9
^{63}Cu inelastic	1.7	1.9	1.9	1.9	1.9	1.9	1.9
^{63}Cu elastic	5.9	6.1	6.1	6.1	6.1	6.1	6.1
^{63}Cu capture	9.3	9.4	9.4	9.5	9.5	9.4	9.5
^{239}Pu inelastic	7.5	7.7	7.7	7.7	7.7	7.7	7.7
^{239}Pu elastic	5.8	6	6	6	6	6	6
^{239}Pu fission	10	11	11	11	11	11	11
^{239}Pu $\bar{\nu}$	3.4	3.6	3.6	3.6	3.6	3.6	3.6
^{239}Pu capture	5.1	5.3	5.2	5.3	5.3	5.3	5.3
^{239}Pu PFNS	0.69	0.89	0.85	0.9	0.89	0.86	0.9
^{239}Pu total	4.4	4.6	4.6	4.6	4.6	4.6	4.6

Color scale: 5, 10, 15, 20

1

2

Yes, the field can answer : What experiment can reliably reduce uncertainties of my application quantity of interest!

	What made it possible for this example:	What is needed for the future:
Team	Having team across the pipeline.	Have expertise across the pipeline and complex as needed.
Input data	Historic experiments, mean values and covariance. Please consider that we had a well-defined (smaller) scope than other applications might have!	• Curated and comprehensive differential and integral experiments are needed→ Evaluators need to share their input data and open database is needed. • Complete libraries of model curves or mid-fi covariances! • Sensitivity libraries tying nuclear data to applications!
Algorithms	AI/ ML to digest 12,000 x 12,000 problem.	• Algorithms to deal with higher-dimensional data. • AI/ML codes to deal with metadata features.
Codes	We had adjustment tools, NJOY, MCNP, CoH available.	• Community tools for adjustments, sensitivities, processing, modeling are needed. • Comprehensive framework needs to be able to use them!

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*Dedicated funding for this kind of work is needed as this work is non-trivial!

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