Selecting a Pair of Differential and Integral Experiments that Reduce Uncertainties in Intermediate-Energy Nuclear Data

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Objectives

What is the goal?

- Optimally select a pair of candidate LANSCE (differential) and NCERC (integral) experiments that would best reduce uncertainties in intermediate energy nuclear data (ND).
  - Particular interest in ^{239}Pu from 1-600keV.
  - Concept of differential and integral data introduced later.

- A key component of understanding ^{239}Pu ND from the perspective of integral data is fission data (PFNS, $\bar{\nu}$, and fission cross section).
  - Fission observables are key data (among most sensitive) to simulate integral data.
  - We also explore a differential fission experiment.

- Ultimately, this is an example of how to select the best experiments to understand application needs tied to fission.

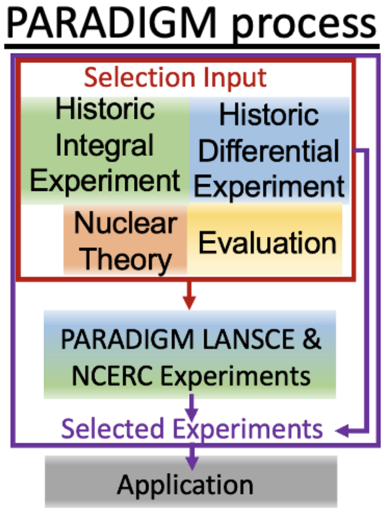
Objectives

What is the goal?

- Optimally select a pair of candidate LANSCE (differential) and NCERC (integral) experiments that would best reduce uncertainties in intermediate energy ND (particularly ^{239}Pu from 1-600keV).

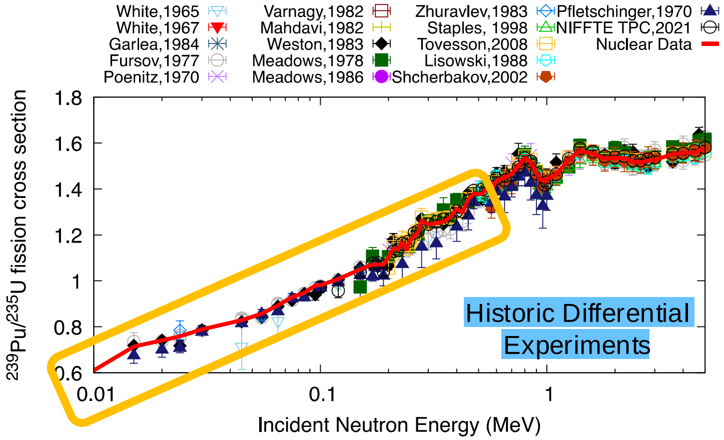
How will we accomplish this?

- Combine theory model curves with historic differential and integral benchmark experiments to initially constrain ND.
  - Use of historic data avoids repeating existing experiments.
  - Integral experiments are maximally sensitive to ^{239}Pu fission cross section.
- Compare additional improvements from candidate experiments to what has been attained through adjustments to historic data.



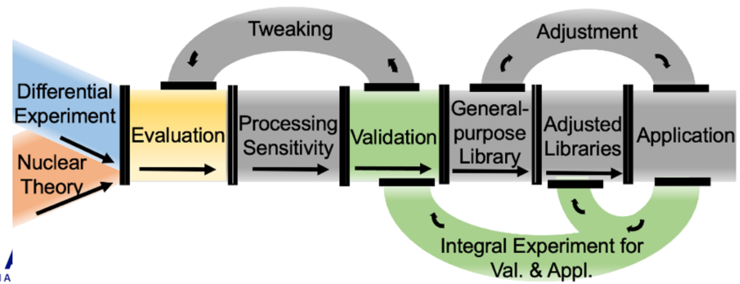
Intermediate-energy ND

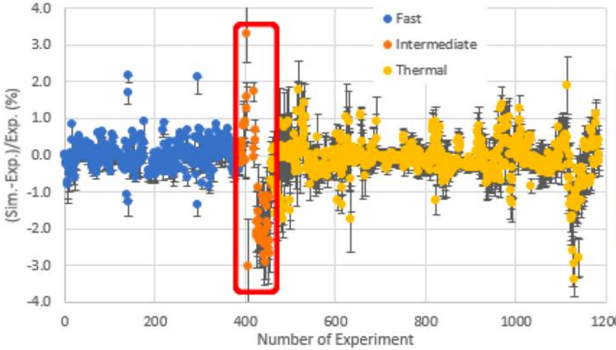
- Intermediate ND are poorly understood due to:
  - **Nuclear theory:** LANL developing current model to smoothly connect between theories for the various energy ranges.
  - **Differential experiments:** scarce and uncertain due to low neutron flux.
  - **Integral experiments:** sensitivities to this range are sparse (only 5% of ICSBEP benchmarks).



Database from Neutron Data Standards (IAEA)

The linear ND pipeline





Historic Integral Experiments

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

How do we better understand the intermediate energy range?

- We are interested in performing 1-2 **integral** benchmark experiments with supporting **differential** experiment that focus on ^{239}Pu from 1-600keV.
  - **Integral:** Candidate experiment designs with ZPPR Pu plates and Cu reflector are investigated by a genetic algorithm and several materials interstitials (including boron) are observed.
    - Optimized to be maximally sensitive to ^{239}Pu fission cross sections from 1-600 keV.
  - **Differential:** Candidate experiments focused on reaction channels for ^{239,240}Pu and ^{63,65}Cu and ^{10}B(n,tot).

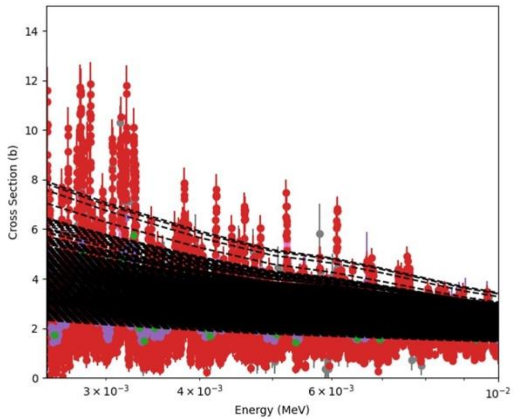
- Consider optimistic and conservative (e.g. experiment uncertainties, contaminated beam, increased background) point of view for each candidate experiment.

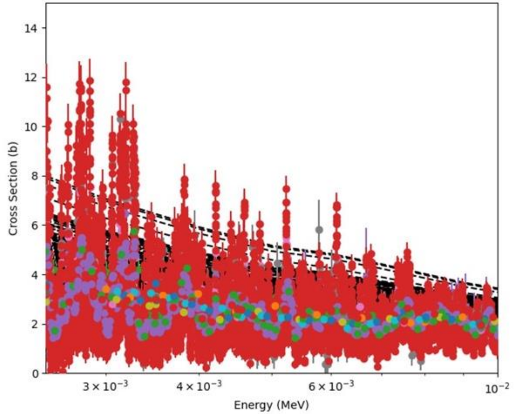
Nuclear Theory: Sampled curves via Hauser-Feshbach statistical theory

- CoH_3 is used to calculate average cross sections in the unresolved resonance region for $^{239,240}Pu$ and $^{63,65}Cu$.
  - Reactions include total elastic, inelastic, capture, (n,2n), fission cross sections; elastic and inelastic angular distributions.

- Hauser-Feshbach statistical theory cannot provide unresolved resonance region structures.
  - Covariance is too strongly correlated, imposing strict smoothness on cross sections.

^{239}Pu Fission Cross Section





Summary of historic differential and integral experiments

- **Differential:** EXFOR database used for historic experiments.

Nuclide	Reactions
^{239}Pu	PFNS, $\bar{\nu}$, (n,f), (n,tot), (n,g), (n,el), (n,inl) cs
^{240}Pu	PFNS, $\bar{\nu}$, (n,f), (n,tot), (n,g), (n,el), (n,inl) cs
^{63}Cu	(n,tot), (n,g), (n,p) (n,el), (n,inl) cs
^{65}Cu	(n,tot), (n,g), (n,el), (n,inl) cs

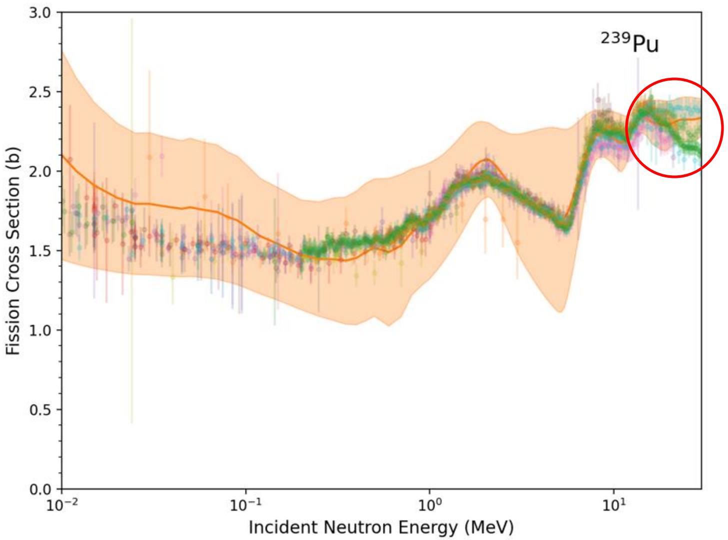
Detailed UQ is undertaken for each experiment by experts to correctly judge impact of candidate experiment vis-a-vis existing data.

- **Integral:** Whisper benchmark suite of ~1100 ICSBEP models and 30 experiments performed at NCERC used for historic experiments.

Series	Name
HEU-MET-FAST	028-001, 047-001, 048-011 059-002, 072-001, 072-003, 073-001, 084-002, 084-004, 084-006, 084-007, 084-017, 085-001, 085-002, 100-002, 102-001, 104-001
HEU-MET-INTER	006-001—004, 011-001—005
PU-MET-MIXED	002-001, 002-003, 003-001, 003-003
PU-MET-INTER	003-001, 004-001
PU-MET-FAST	001-001, 006-001, 024-001, 027-001, 032-001, 038-001, 047-001
PU-SOL-THERM	011-001, 011-005, 011-008
PU-COMP-MIXED	002-005, 002-006
Other	euclid-3x2-crit, euclid-8x1-crit

Challenges of the data

- Discrepancies from missing model structure and between experiments:
  - **Theory** curves do not capture true resonance structure.
  - **Differential** data often do not agree with one another within their reported uncertainties.
- High dimensional data over different energy grids:
  - **Theory/ENDF/B-VIII.0:** 12,200+ values spanning 15 nuclides.
  - **Differential:** 8,400+ observables spanning 122 experiments.
  - **Integral:** 46 experiments with sensitivities to 12,200+ ND inputs.



Notation for model

Initial ND quantities

- $\boldsymbol{\sigma}$ = initial uncertain ND.
- $\boldsymbol{\sigma_{init}}$ = mean from theory curves and ENDF/B-VIII.0.
- $\boldsymbol{V_{init}}$ = covariance from theory curves and ENDF/B-VIII.0.

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Differential ND quantities

- $\boldsymbol{y_{diff}}$ = differential observations.
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- $\boldsymbol{L}$ = linear interpolation matrix from the evaluation grid to observed data.

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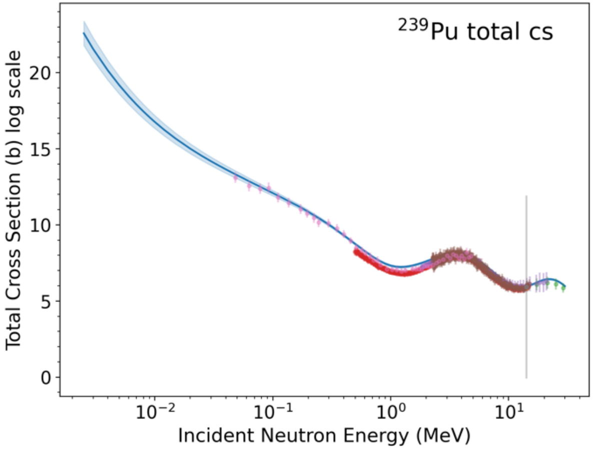
Integral ND quantities

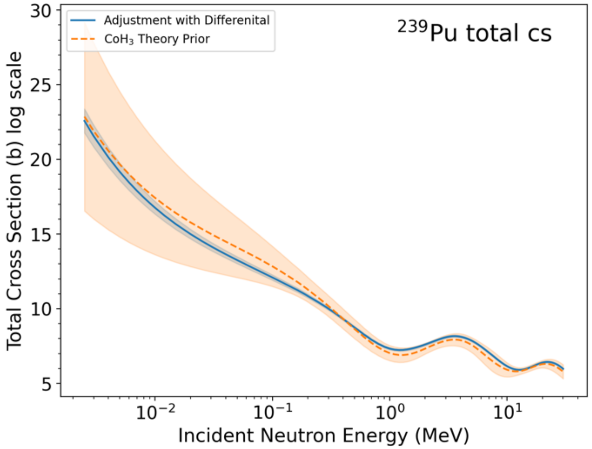
- $\boldsymbol{y_e}$ = set of experimentally measured values of integral benchmarks.
- $\boldsymbol{y_c}$ = set of calculated values of integral benchmarks.
- $\boldsymbol{S}$ = response sensitivity matrix with respect to ND inputs.

Three sources of input represent multivariate Gaussian distributions and are assumed to be independent.

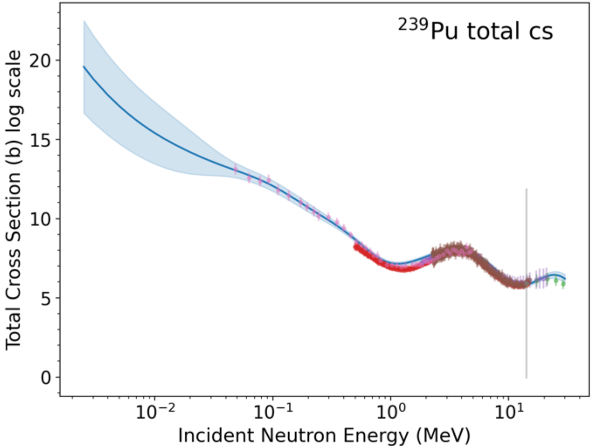
Impact of GPs on adjustment

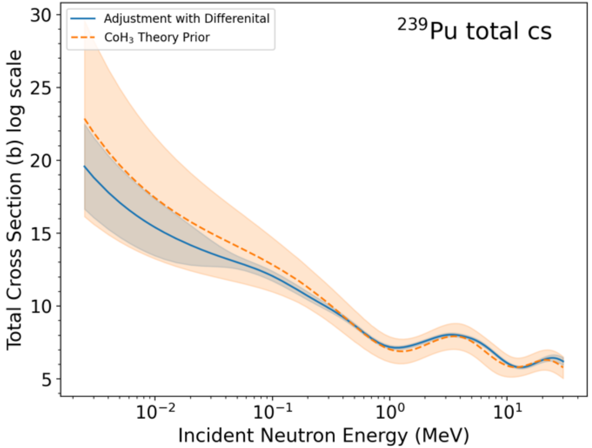
No GPs on **initial** or **differential** covariances





With GPs on **initial** and **differential** covariances





Generalized least squares (GLS) model to initially constrain ND

Step 1: Adjust to historic differential data

We update the **initial** ND quantities as

$$\boldsymbol{\sigma}_{diff} = \boldsymbol{\sigma}_{init} + \boldsymbol{V}_{init}\boldsymbol{L}^T(\boldsymbol{L}\boldsymbol{V}_{init}\boldsymbol{L}^T + \boldsymbol{\Delta})^{-1}(\boldsymbol{y}_{diff} - \boldsymbol{L}\boldsymbol{\sigma}_{init})$$

$$\boldsymbol{V}_{diff} = \boldsymbol{V}_{init} - \boldsymbol{V}_{init}\boldsymbol{L}^T(\boldsymbol{L}\boldsymbol{V}_{init}\boldsymbol{L}^T + \boldsymbol{\Delta})^{-1}\boldsymbol{L}\boldsymbol{V}_{init}$$

Step 2: Calibrate to historic integral benchmark experiments

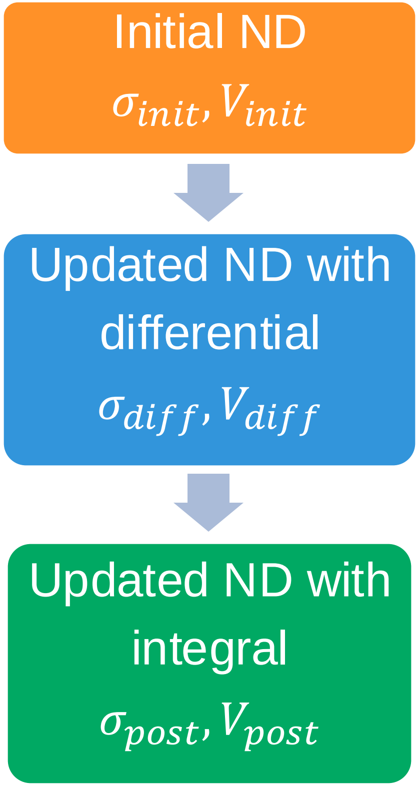
We update the **differential** adjusted ND quantities using

$$(\boldsymbol{y}_e - \boldsymbol{y}_c) \sim N(0, \boldsymbol{S}\boldsymbol{V}_{diff}\boldsymbol{S}^T + \boldsymbol{\Sigma}_e)$$

to obtain

$$\boldsymbol{\sigma}_{post} = \boldsymbol{\sigma}_{diff} + \boldsymbol{V}_{diff}\boldsymbol{S}\left(\boldsymbol{S}^T\boldsymbol{V}_{diff}\boldsymbol{S} + \boldsymbol{\Sigma}_e\right)^{-1}(\boldsymbol{y}_e - \boldsymbol{y}_c)$$

$$\boldsymbol{V}_{post} = \boldsymbol{V}_{diff} - \boldsymbol{V}_{diff}\boldsymbol{S}\left(\boldsymbol{S}^T\boldsymbol{V}_{diff}\boldsymbol{S} + \boldsymbol{\Sigma}_e\right)^{-1}\boldsymbol{S}^T\boldsymbol{V}_{diff}$$



Experiment selection

Step 3: Use D-optimality criterion to guide experiment selection

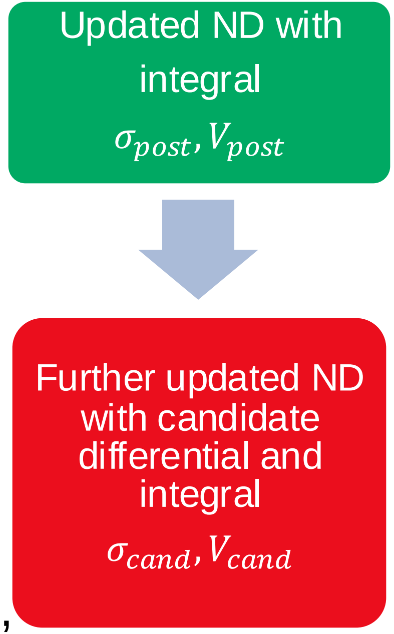
- A D-optimal set of experiments will best reduce the uncertainty volume in the intermediate range after adjustment to all reliable historic experiments.

- Further update $\boldsymbol{V}_{post} \rightarrow \boldsymbol{V}_{cand}$ by running Steps 1-2 with uncertainties for a pair of candidate experiments.

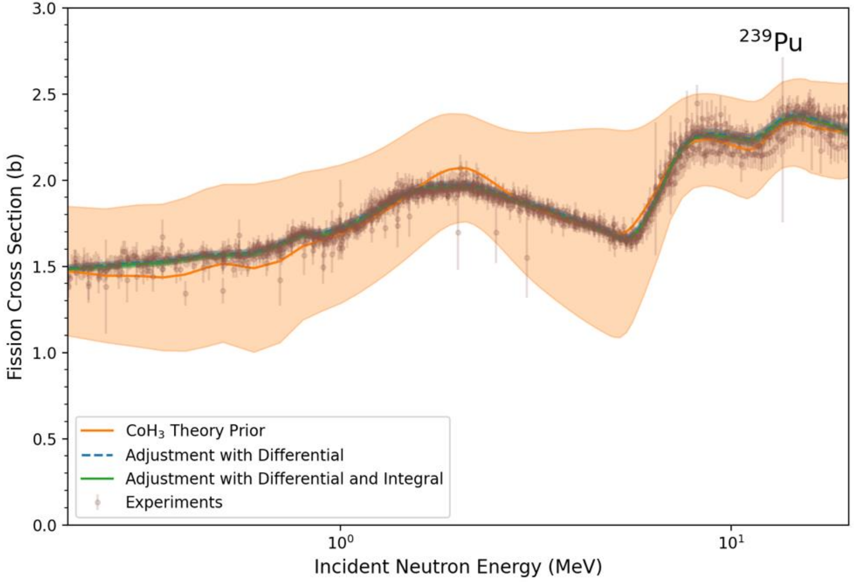
- Subset $\boldsymbol{V}_{post}$ and $\boldsymbol{V}_{cand}$ to only include isotopes appearing in the candidate **integral** experiments (PARADIGM isotopes) from1-600keV.

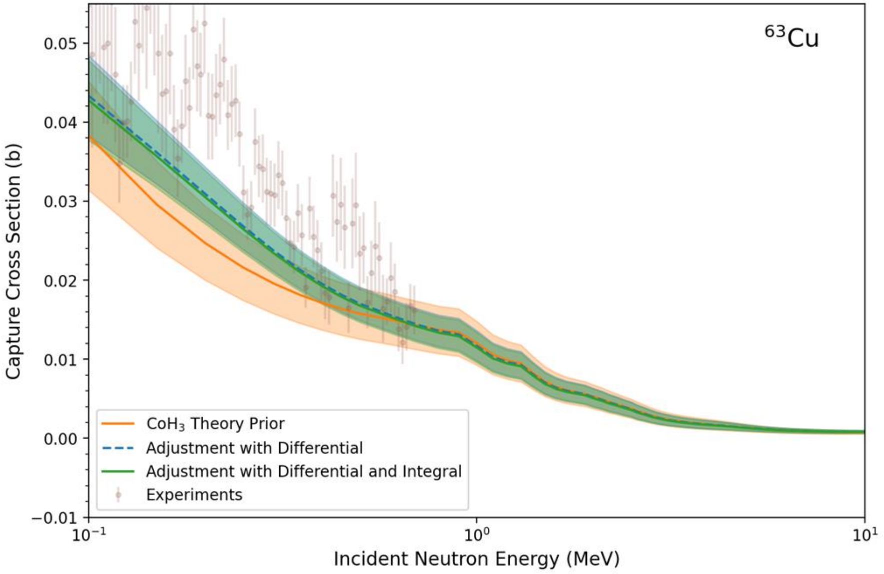
- For each pair of candidate **integral** and **differential** experiments, compute

$$\boldsymbol{D}_{cand} = \log\det \boldsymbol{V}_{post} - \log\det \boldsymbol{V}_{cand}$$



Comparison with differential experiments overlayed

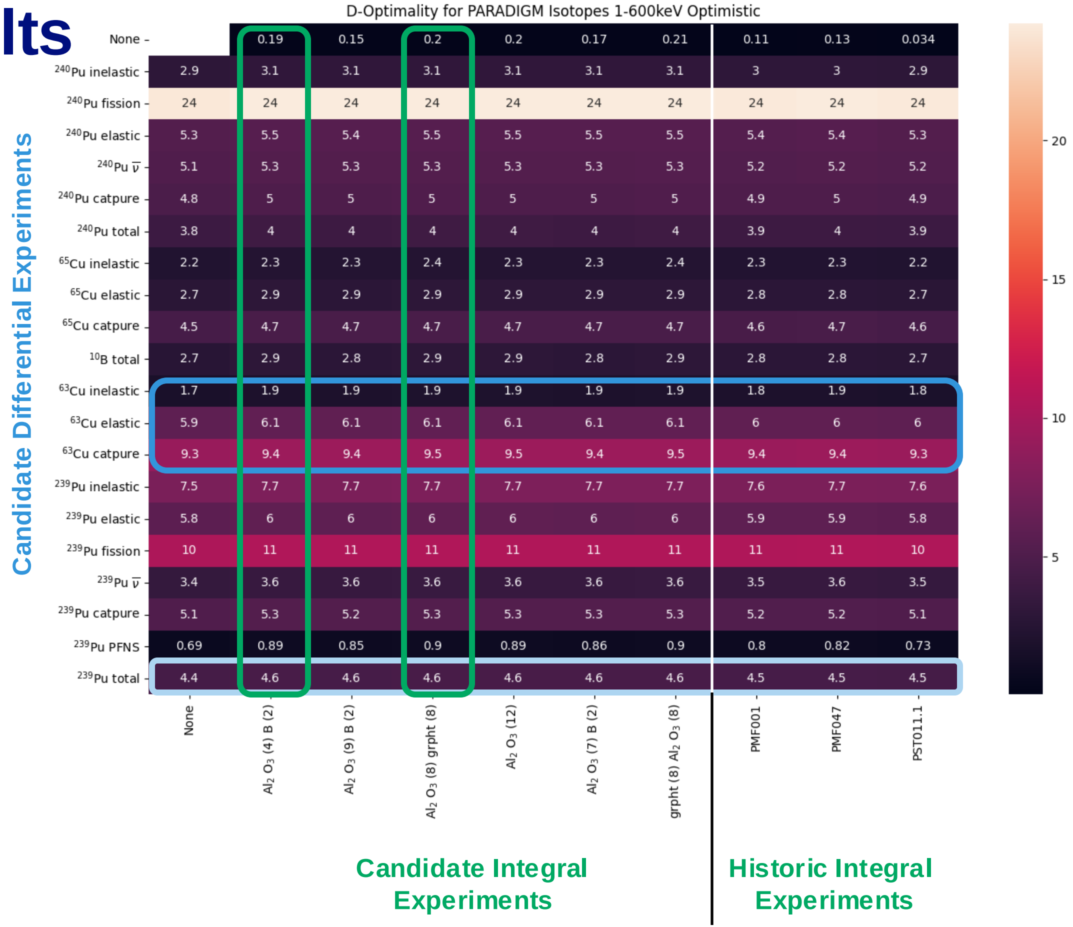




Adjustments are mostly driven by differential data with minor influence from integral data.

D-optimality (D-opt) results

- The higher the D-opt, the more impact from candidate experiments.
- **Differential** candidates are the big drivers of D-opt relative to **integral** candidates with minor and nearly equal improvements.
    - Several direct measurements vs single indirect measurement.
- Final decision for combination of experiments based on D-opt and feasibility constraints.



Conclusion and future work in developing modeling capabilities

- Combined **theory** with historic **differential** and **integral** data to constrain ND.
  - We can better understand fission data with combined knowledge from all parts of the ND pipeline.
- Steer experimental design by selecting a pair of experiments that best reduce intermediate ND using D-opt criterion.
- Additions to modeling capabilities:
  - Incorporate flux distribution for response sensitivity matrix.
  - Theory model curves to include resonance features.
  - Modify model to Bayesian framework to handle disagreements between differential experiments.
  - Include more integral responses into adjustment.

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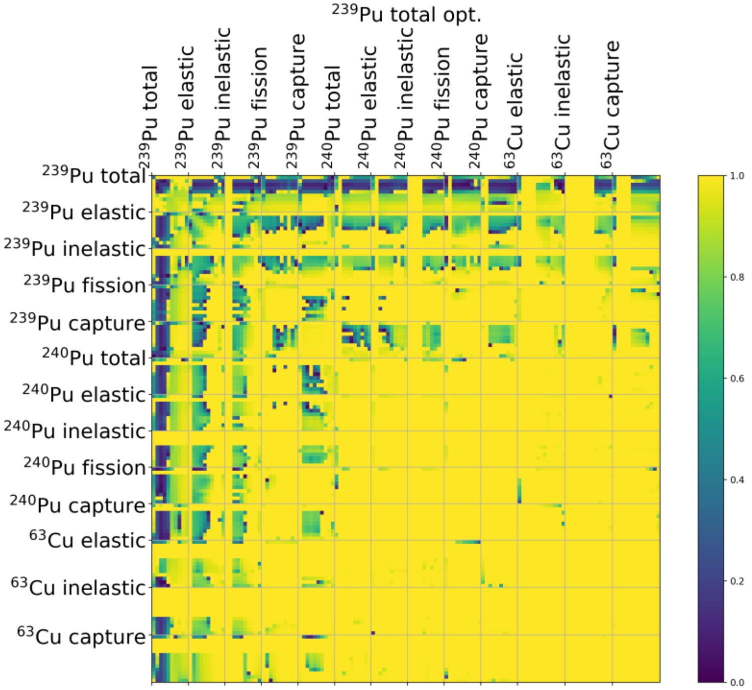
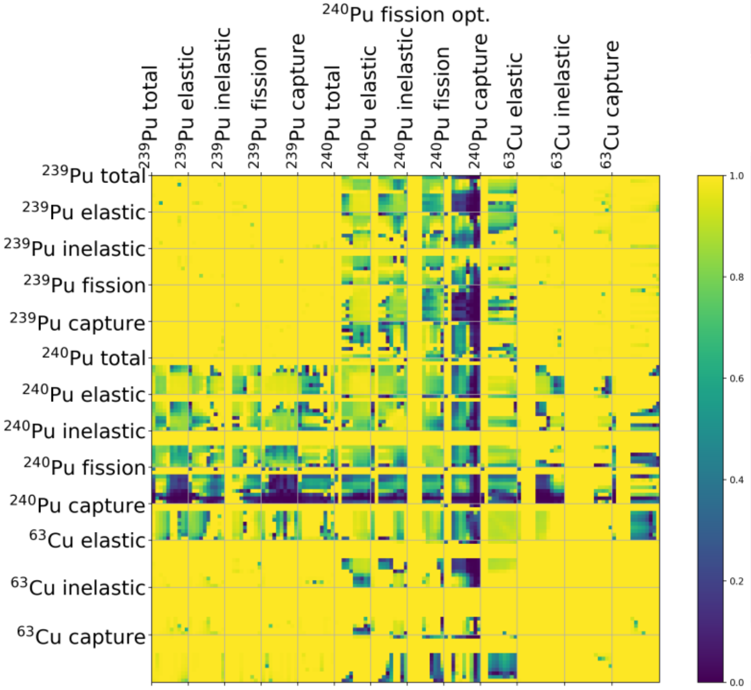
Thank you for your attention!

Backup slides

Covariance Improvements Concentrate on the Isotope Selected for the Differential Experiment - ^{239}Pu vs ^{240}Pu





Relative change in covariance: $|\frac{V_{cand}}{V_{post}}|$