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Title: Investigating Fission Reaction Rate Ratio Sensitivities

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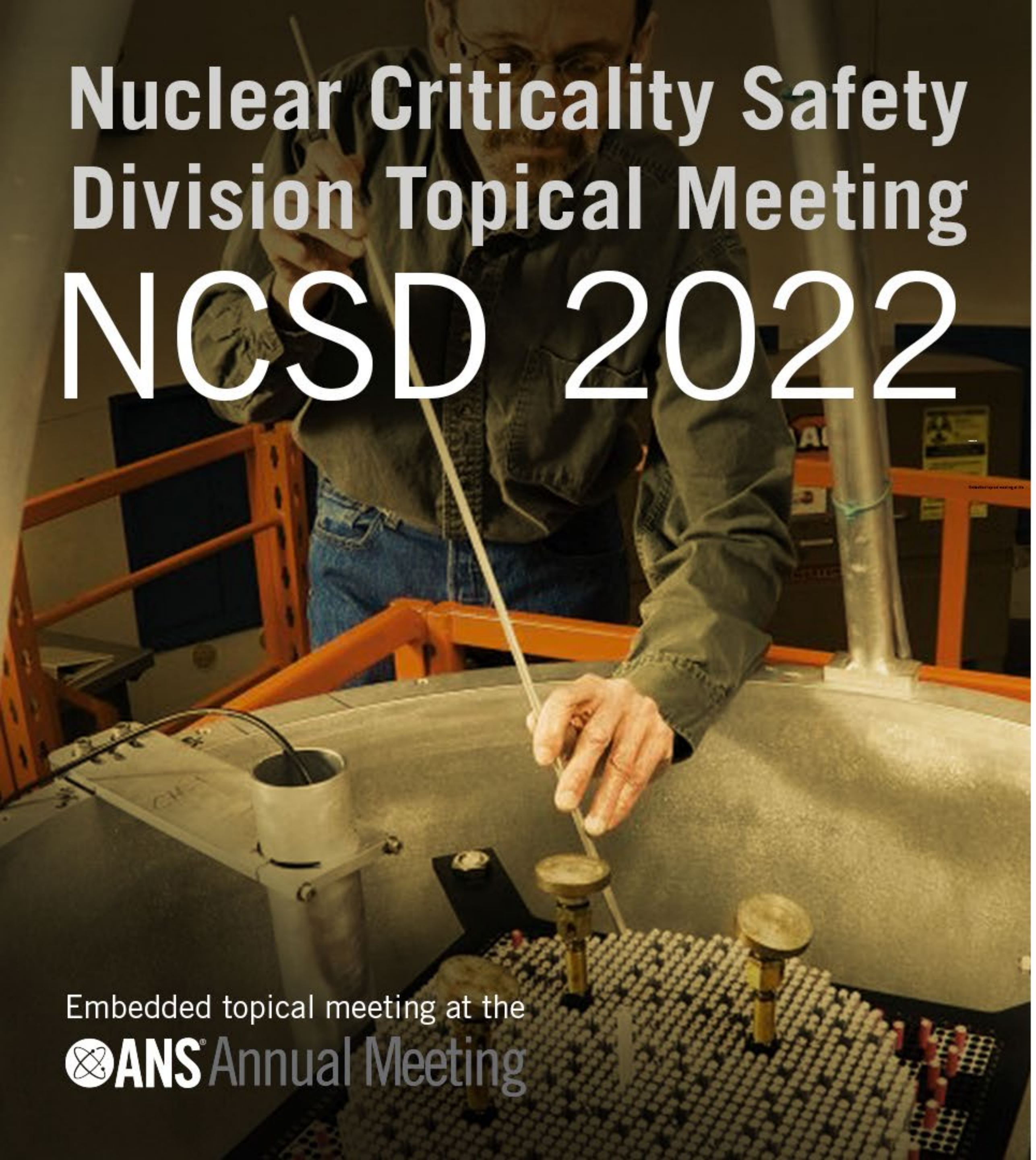

Investigating Fission Reaction Rate Ratio Sensitivities

J. Alwin, J. Hutchinson, N. Kleedtke, A. Clark, T. Cutler, W. Haeck, R. Little, D. Neudecker, M. Rising, T. Smith, N. Thompson

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Fission Reaction Rate Ratios

- Why Investigate Reaction Rate Ratios?
  - Part of broader effort: EUCLID LANL Laboratory Directed R&D (LDRD)
  - Subset of data in EUCLID sensitivity library
- Integral Experiment Measurements
- Calculational methods
  - Results
  - Sensitivities
- Development of Capabilities
  - Experiment optimization
  - Tools for understanding impact and adjustment
  - Future MCNP6 capability - FSEN
- Conclusions and Future Work

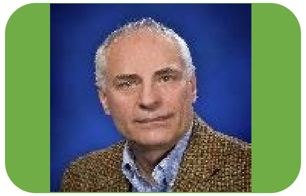
EUCLID Team

Experiments **U**nderpinned by **C**omputational **L**earning for **I**mprovements in nuclear **D**ata

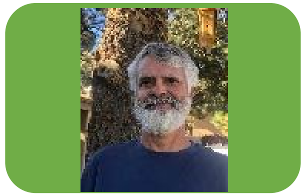
Goal: design validation experiments optimized to resolve compensating errors & adjust nuclear data to experiments

Nuclear Data

Wim Haeck



Michal Herman



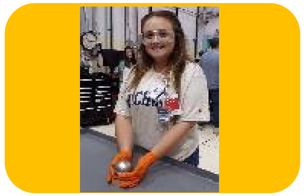
Robert Little

Denise Neudecker

Simulations

Jennifer Alwin

Alexander Clark



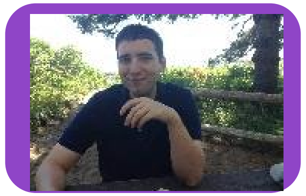
Juliann Lamproe

Michael Rising

Machine Learning

Michael Grosskopf

Noah Kleedtke



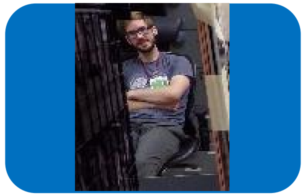
Isaac Michaud

Scott Vander Wiel

Experiments

Theresa Cutler

Jesson Hutchinson



Travis Smith

Nicholas Thompson

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Experimental Measurements

Measurement Method	Observable			
	σ	ν	β	PFNS
Critical experiments	✓	✓		✓
Neutron Multiplication Measurements	✓	✓	✓	
Reaction rate ratios	✓	✓		✓
Pulsed Spheres	✓			
Gamma/Neutron Leakage Spectra	✓			✓
Delayed Neutron Measurements			✓	
Rossi-α	✓	✓	✓	
Reactivity Coefficient	✓		✓	

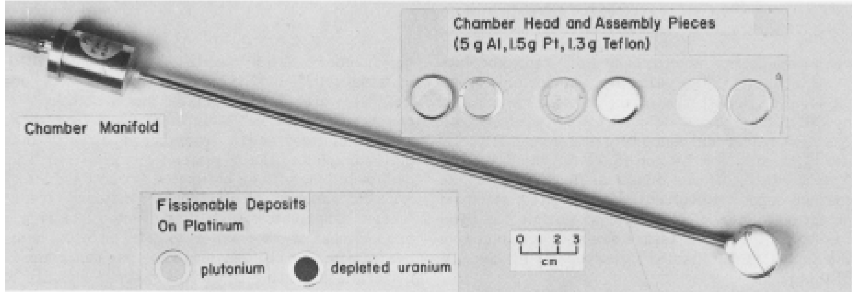
Different measurement types give complimentary data useful to constrain nuclear data and understand compensating errors.

EUCLID sensitivities for many different responses on the same grid → sensitivity library

LA-UR-22-21534

Measured Fission Reaction Rate Ratios

- Measured in central region using foils or fission chamber
  - Energy spectrum dependent, referred to as spectral index

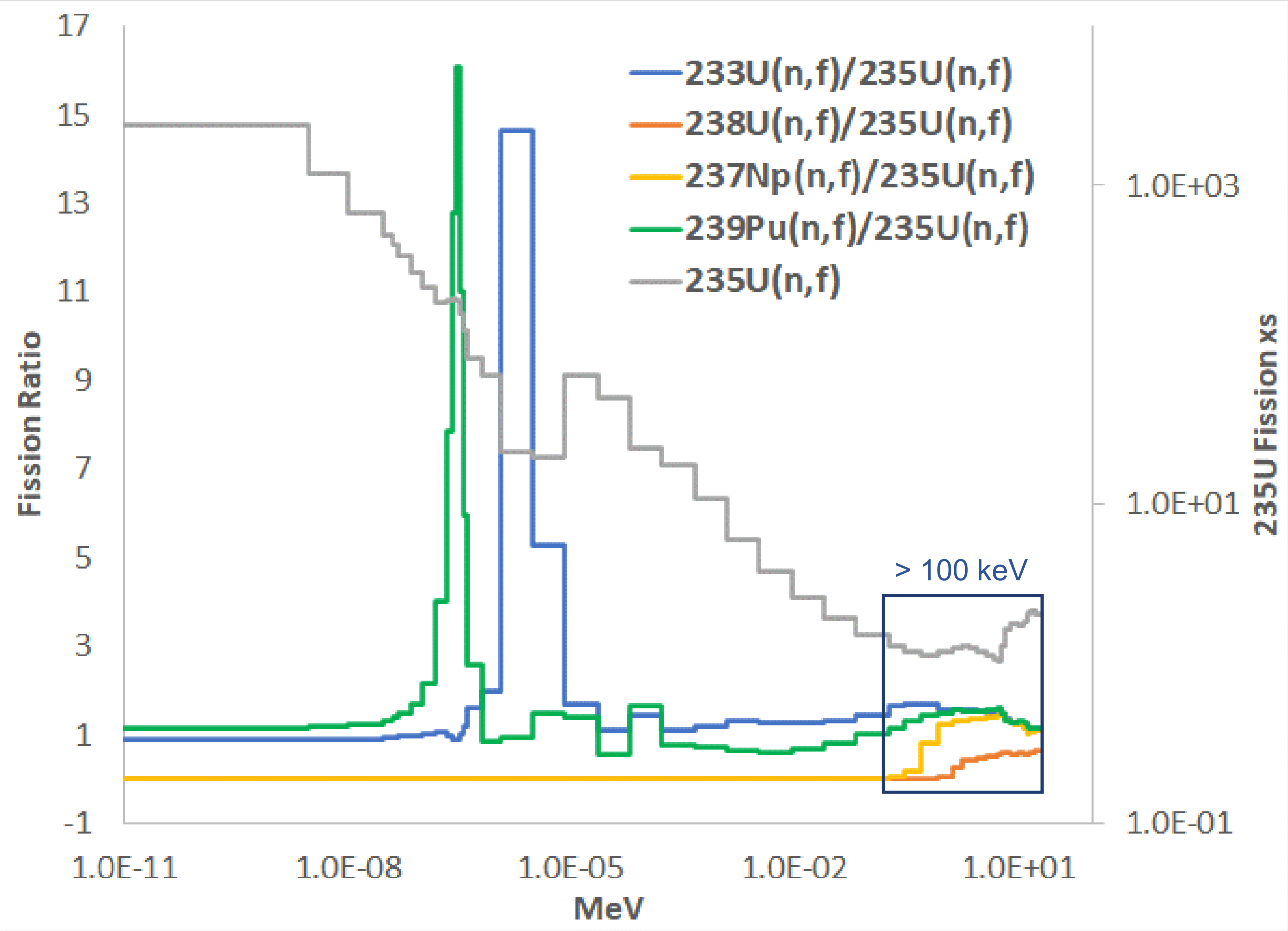


Fission Chamber with Flattop

Foils

Fission Reaction Rate Ratios

- Spectral index
- Compared with ^{235}U fission reaction rate
- ^{239}Pu reaction rate ratio peaks at much lower energy than ^{237}Np and ^{238}U
- HMF1
  - 1.46 MeV ANECF
  - 95 % fissions in fast range
- HMF28
  - 1.50MeV ANECF
  - 92% fissions in fast range
- PMF1
  - 1.92 MeV ANECF
  - 98% fissions in fast range
- PMF6
  - 1.89 MeV ANECF
  - 94% fissions in fast range



Measured Fission Reaction Rate Ratios

- Measured in central region using foils or fission chamber
- Compared with calculated ratios in SENSMG
- Sensitivities for each isotope & reaction

Assembly	Quantity	$^{238}U_f/^{235}U_f$	$^{237}Np_f/^{235}U_f$	$^{233}U_f/^{235}U_f$	$^{239}Pu_f/^{235}U_f$
HMF-001	Calc. Exp. C/E	0.1587 0.1643 ±0.0018 0.9656	0.8346 0.8516 ±0.012 0.9800	1.5748 1.59 ±0.03 0.9905	1.3816 1.4152 ±0.014 0.9763
HMF-028	Calc. Exp. C/E	0.1453 0.1492± 0.0016 0.9741	0.7789 0.7804 ±0.01 0.9981	1.5729 1.608 ±0.003 0.9782	1.3597 1.3847 ±0.012 0.9820
PMF-001	Calc. Exp. C/E	0.2110 0.2133 ±0.0023 0.9893	0.9744 0.9835 ±0.014 0.9907	1.5636 1.578 ±0.027 0.9909	1.4241 1.4609 ±0.013 0.9748
PMF-006	Calc. Exp. C/E	0.1725 0.1799 ±0.002 0.9935	0.8469 0.8561 ±0.012 1.0032	1.5618 - -	1.3796 - -

Calculated Fission Reaction Rate Ratios

- Reaction rate ratio sensitivities for each isotope & reaction over 51 energy groups
- Calculated in SENSMG
  - 1st order sensitivities using Generalized Perturbation Theory using PARTISN multigroup discrete-ordinates code
  - 1-D spherical or slab & 2-D cylindrical geometries

$$R = \frac{R_1}{R_2} = \frac{\int_V dV \sum_{g=1}^{G} \Sigma_1^g(r)\phi^g(r)}{\int_V dV \sum_{g=1}^{G} \Sigma_2^g(r)\phi^g(r)}$$

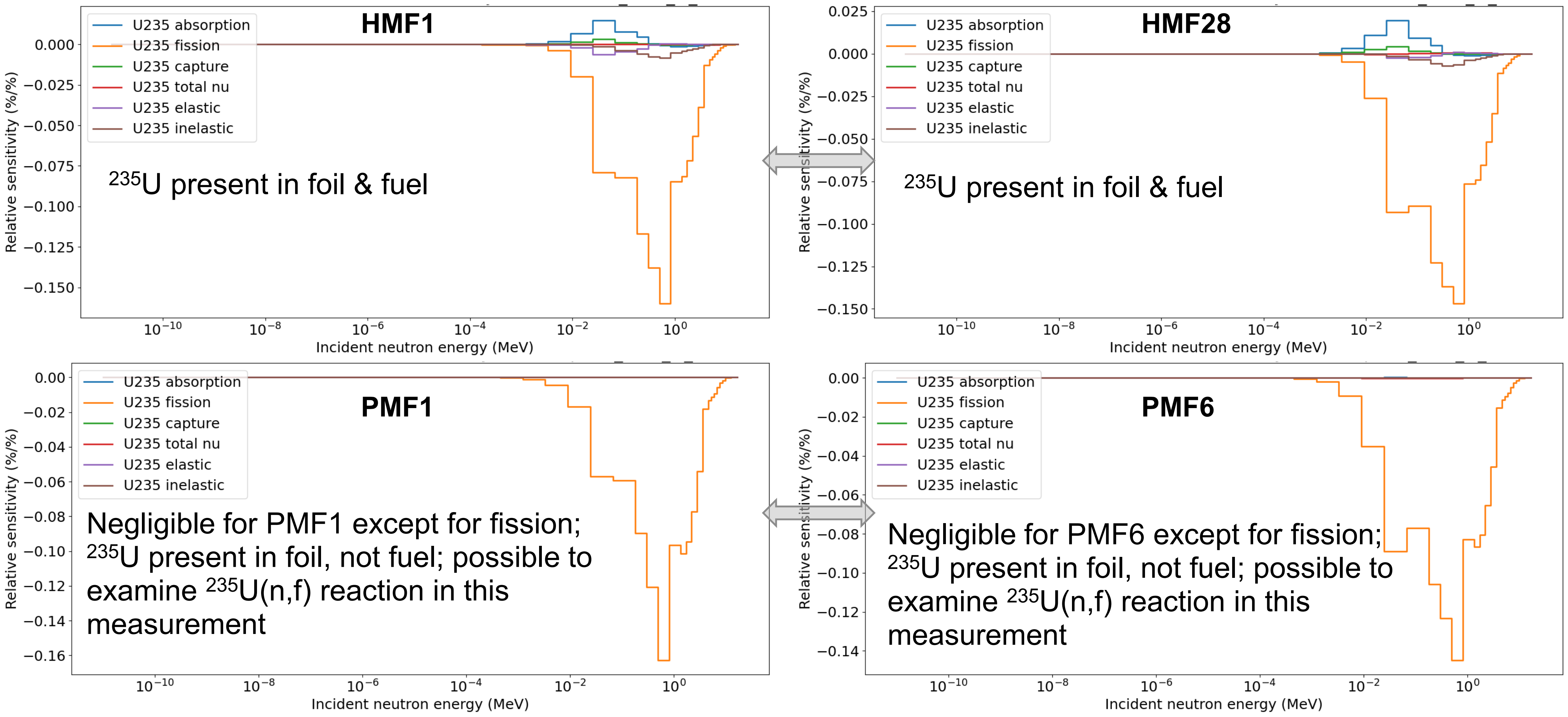
R	= reaction rate ratio,
V	= problem volume,
r	= point within V,
G	= number of g energy groups,
Σ_1^g, Σ_2^g	= reaction cross sections, and
$\phi^g(r)$	= scalar flux in g at r

Total 1st order sensitivity of R to reaction x is the sum of the relative sensitivity, $S_{R,x}^g \equiv \frac{\sigma_{x,0}^g}{R_0} \frac{\partial R}{\partial \sigma_x^g}\Big|_{\sigma_x^g=\sigma_{x,0}^g}$ over energy groups

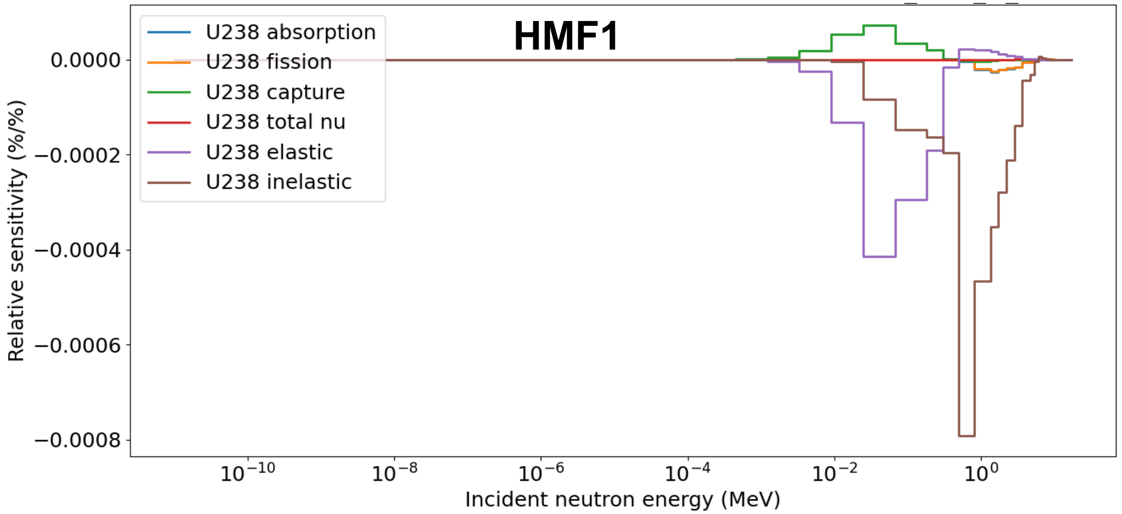
$$S_{R,x} = \sum_{g=1}^{G} S_{R,x}^g$$

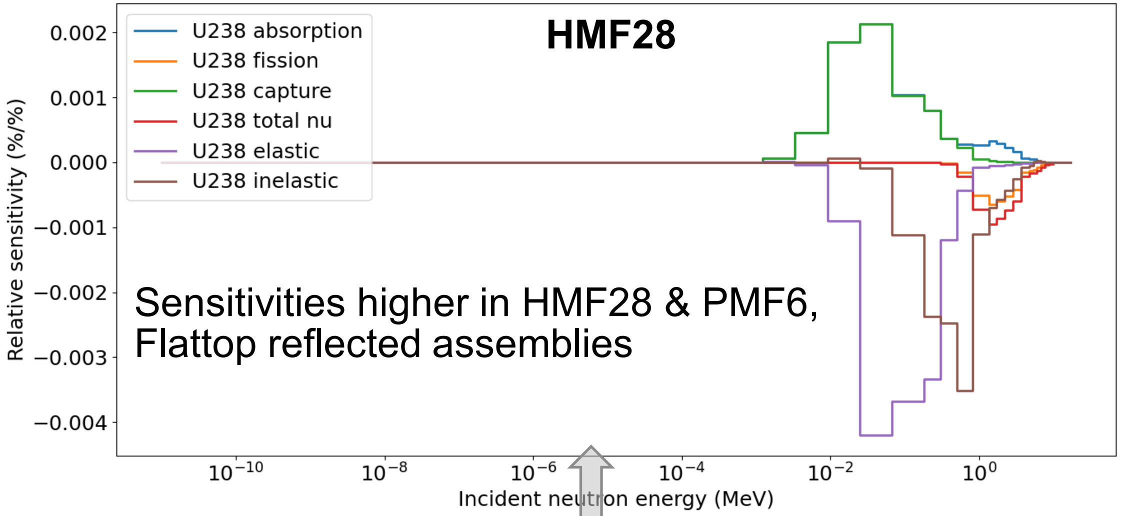
- MCNP6.2 to calculate flux in central region of assembly and reaction rates

^{239}Pu(n,f)/^{235}U(n,f) Sensitivity to ^{235}U

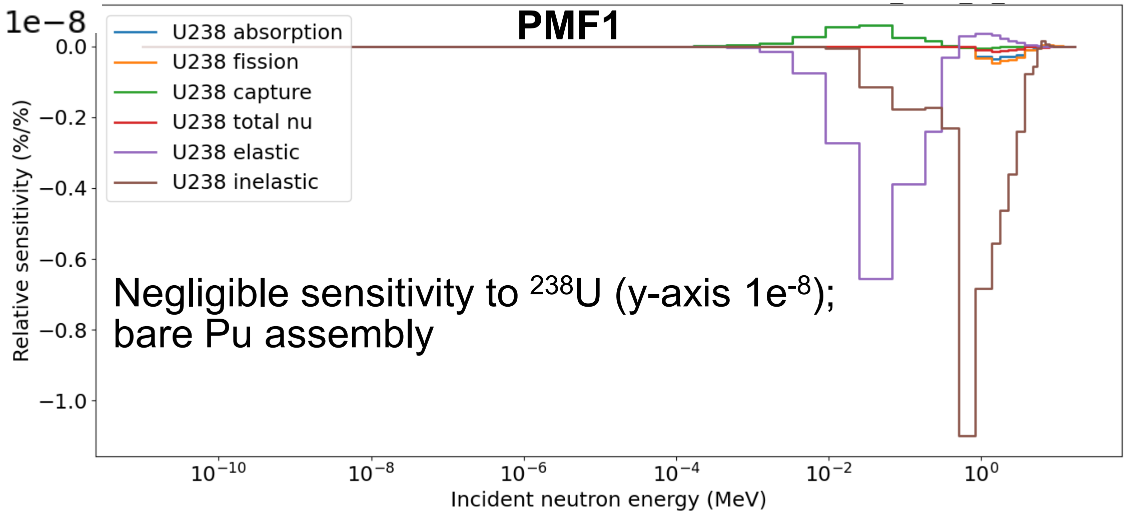


^{239}Pu(n,f)/^{235}U(n,f) Sensitivity to ^{238}U

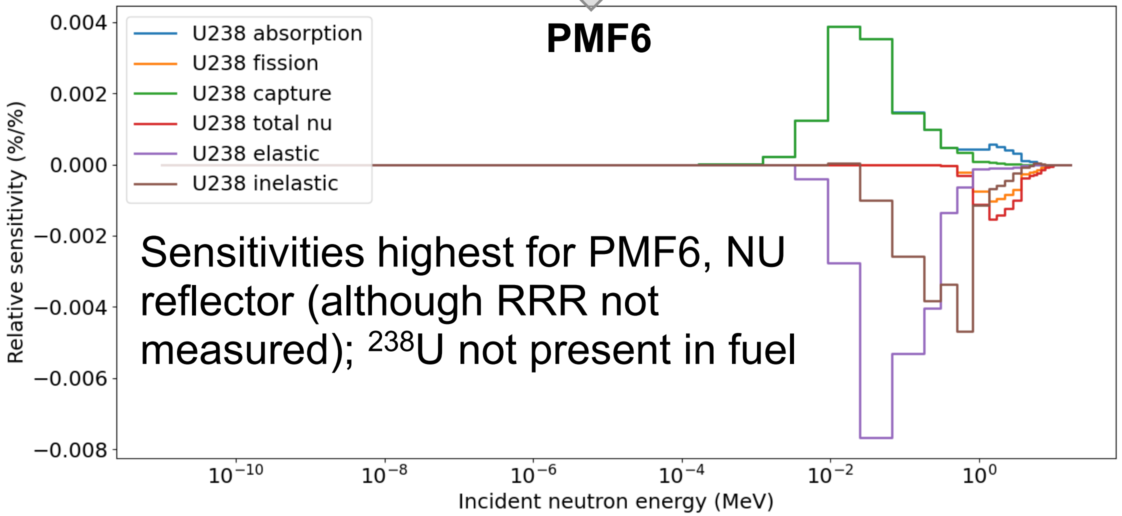




Sensitivities higher in HMF28 & PMF6, Flattop reflected assemblies

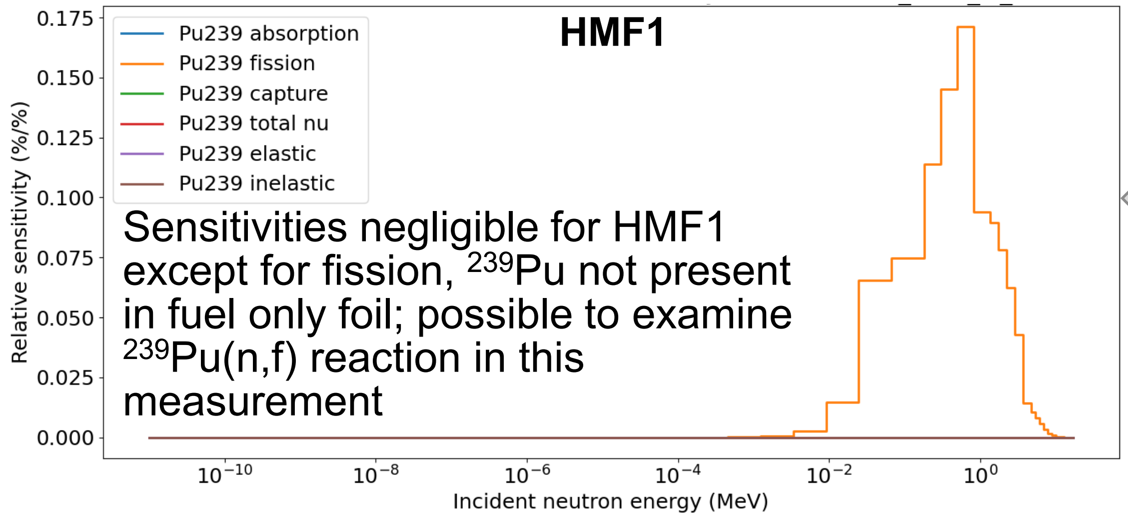


Negligible sensitivity to ^{238}U (y-axis 1e^{-8}); bare Pu assembly

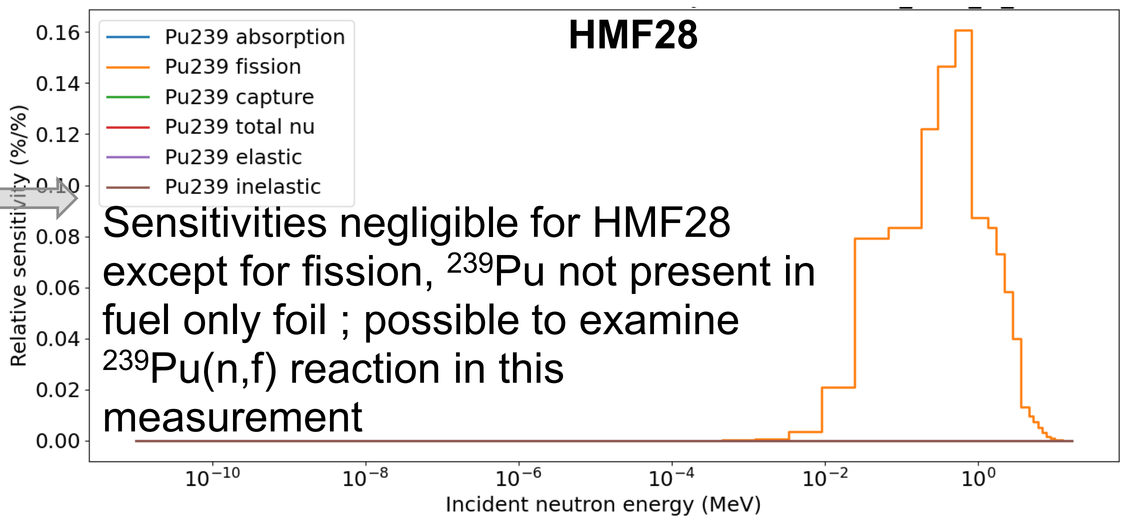


Sensitivities highest for PMF6, NU reflector (although RRR not measured); ^{238}U not present in fuel

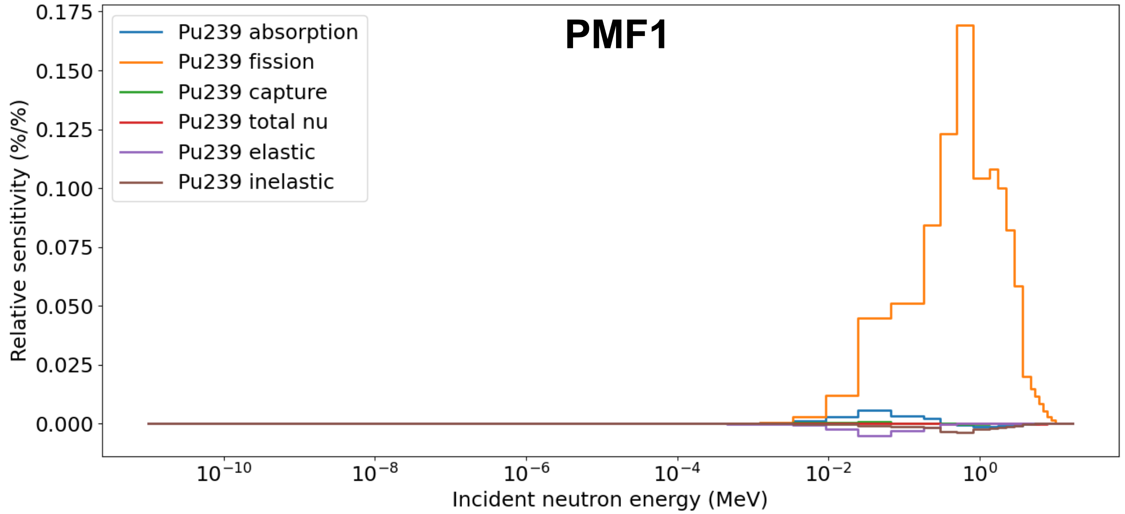
^{239}Pu(n,f)/^{235}U(n,f) Sensitivity to ^{239}Pu

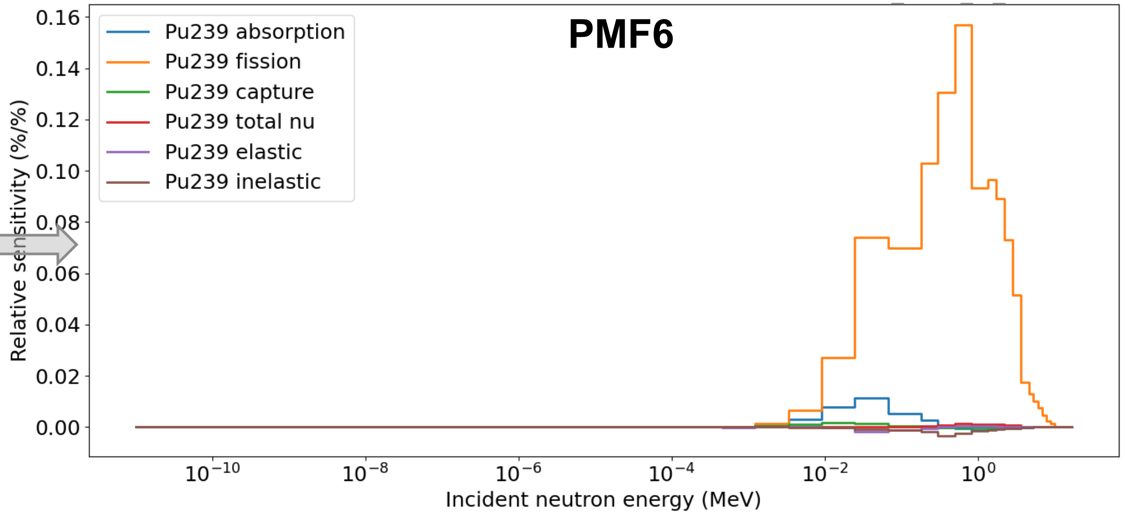


Sensitivities negligible for HMF1 except for fission, ^{239}Pu not present in fuel only foil; possible to examine ^{239}Pu(n,f) reaction in this measurement

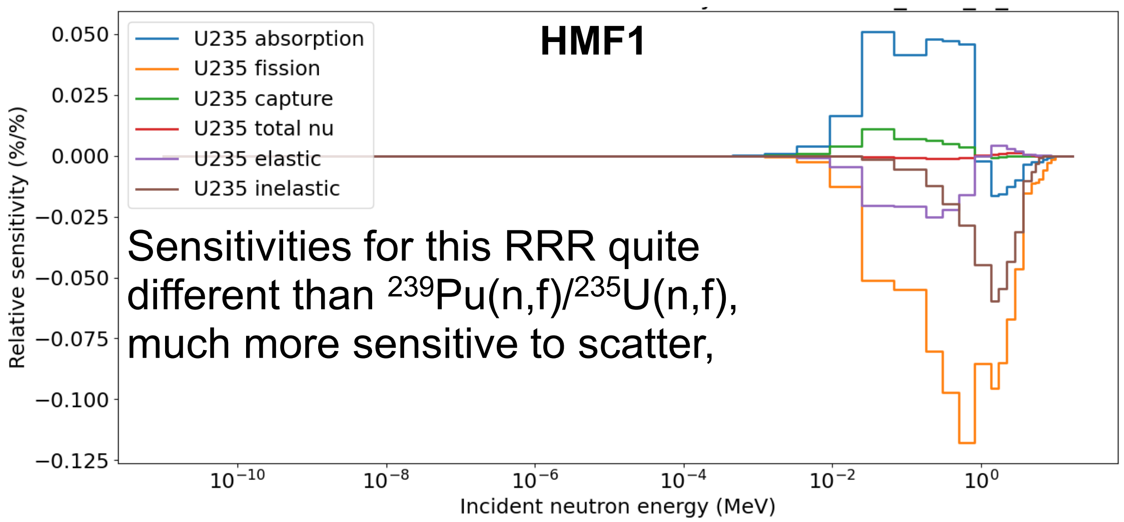


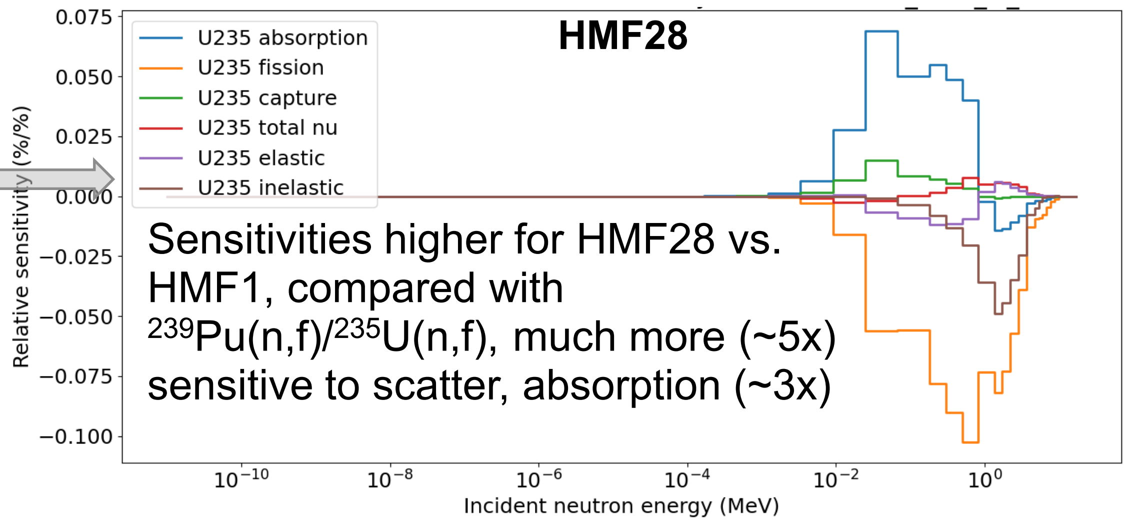
Sensitivities negligible for HMF28 except for fission, ^{239}Pu not present in fuel only foil ; possible to examine ^{239}Pu(n,f) reaction in this measurement

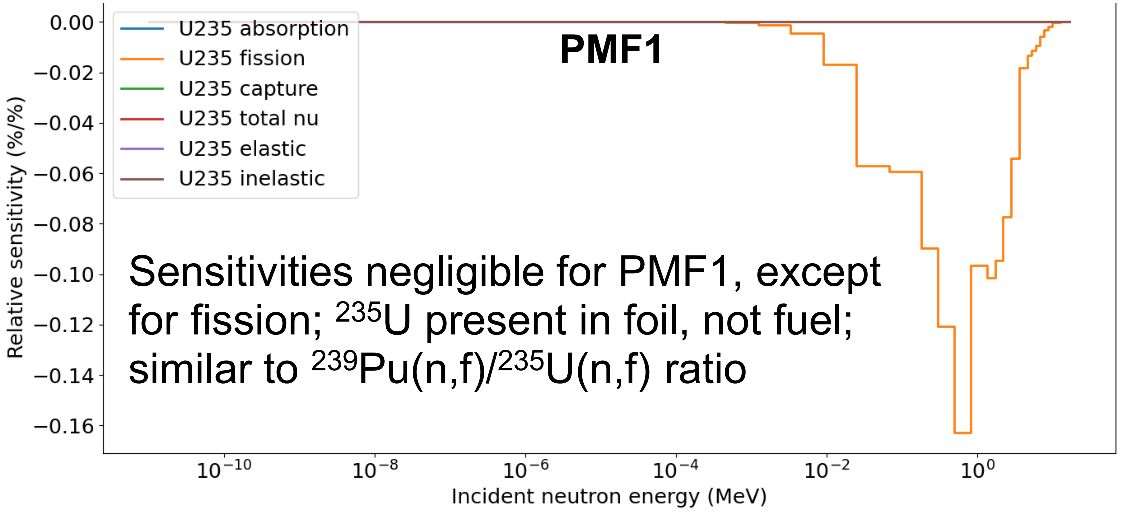


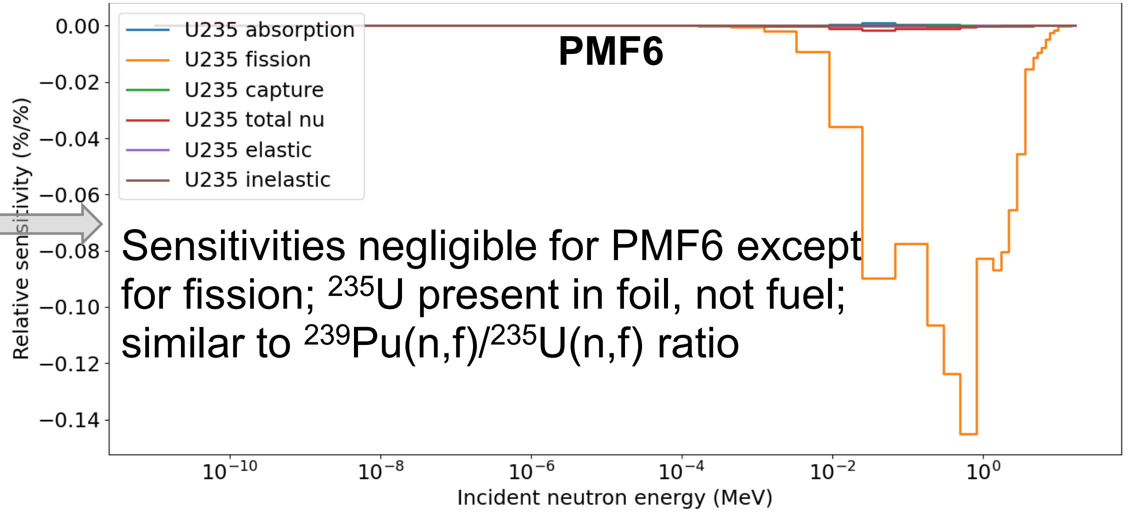


^{238}U(n,f)/^{235}U(n,f) Sensitivity to ^{235}U









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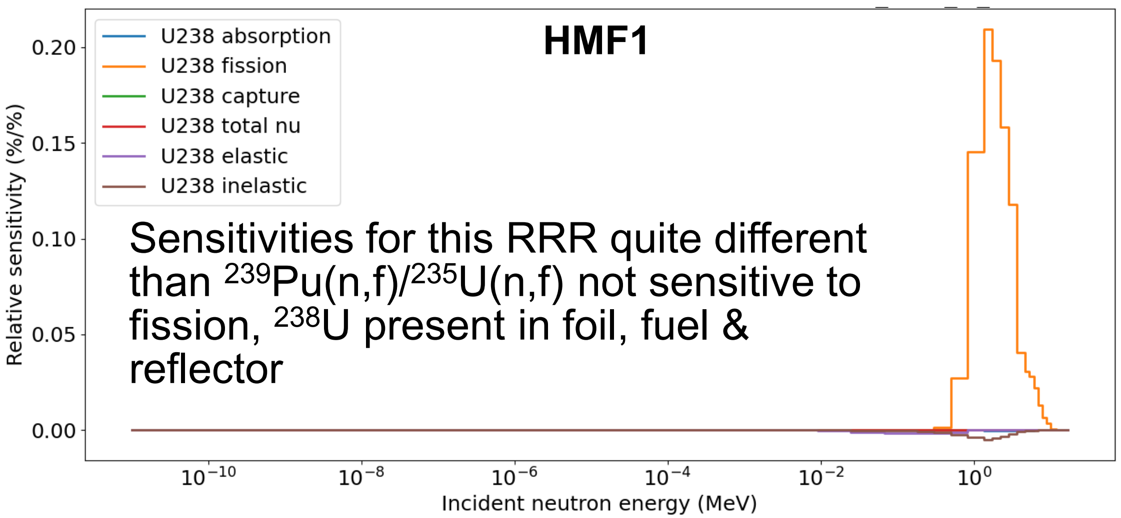
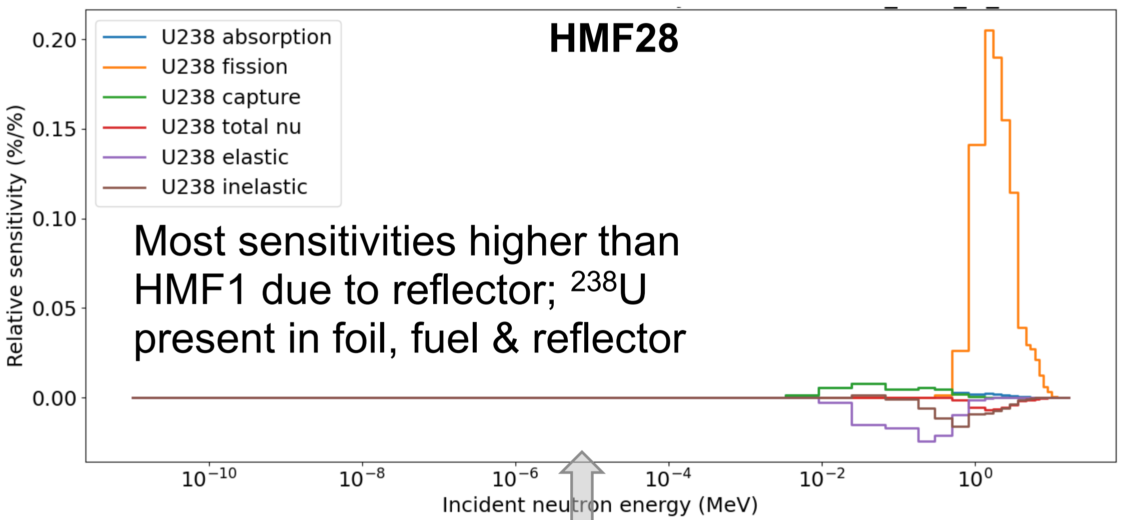
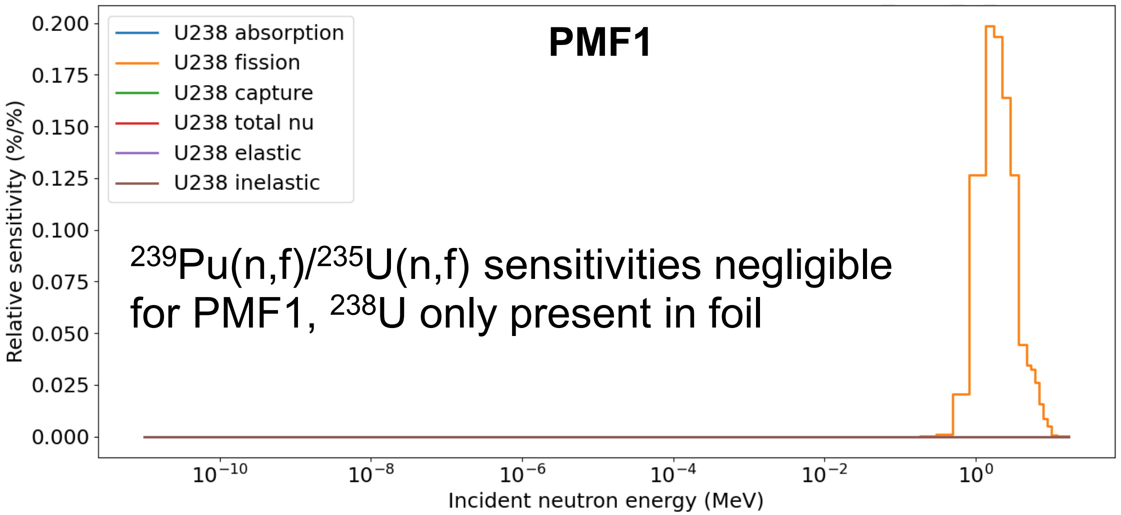
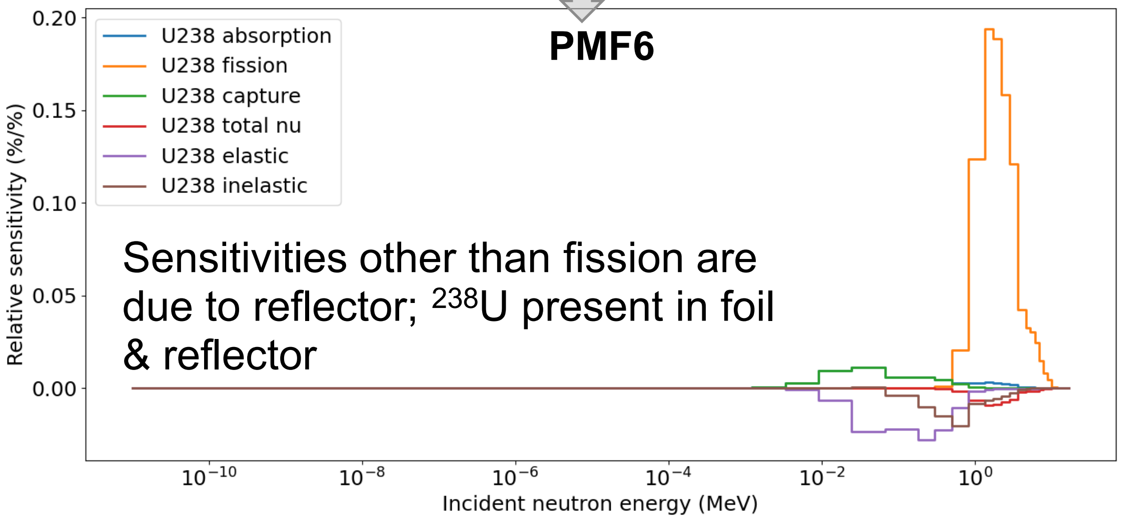
^{238}U(n,f)/^{235}U(n,f) Sensitivity to ^{238}U

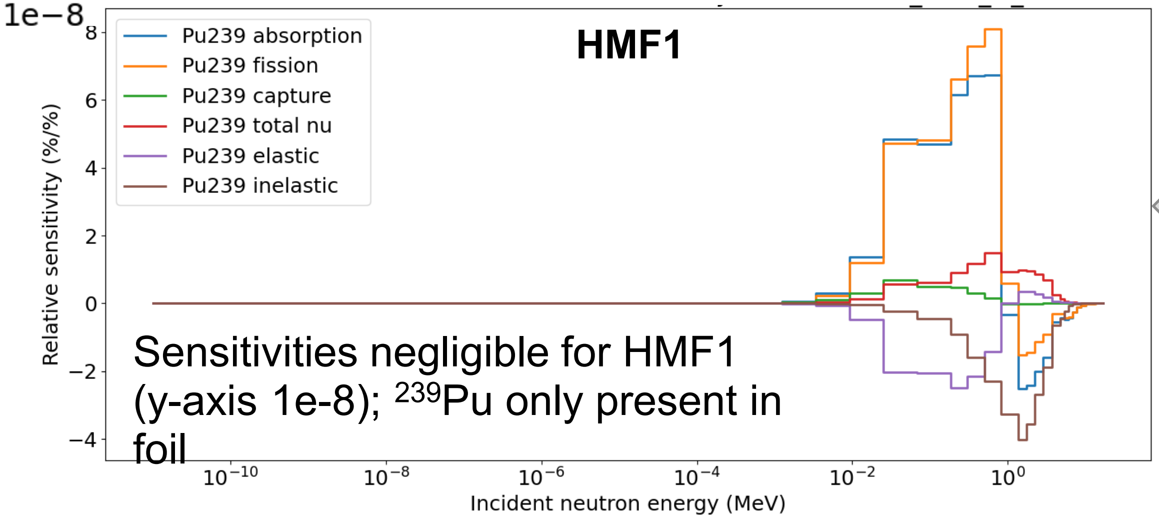




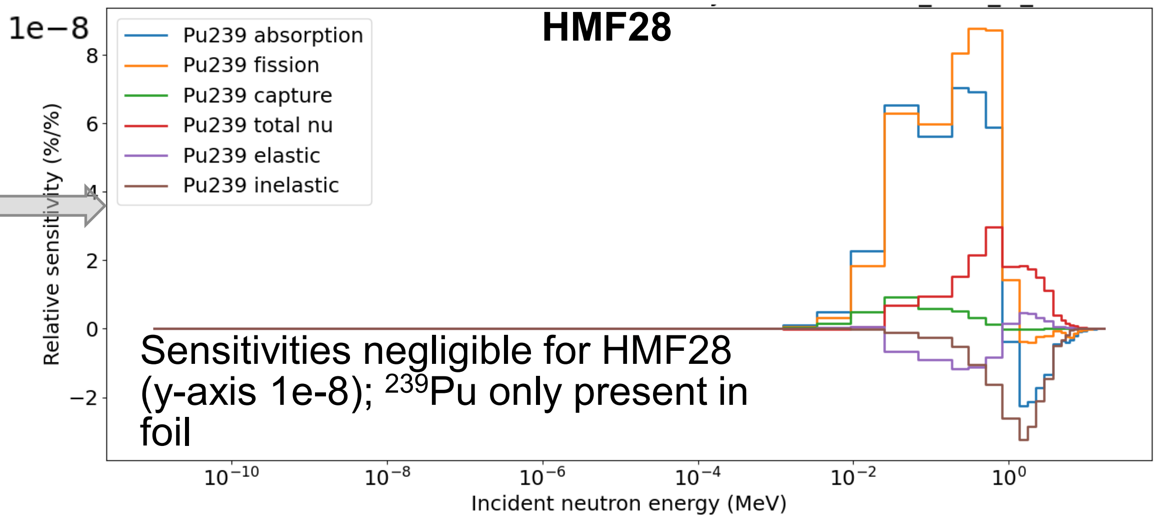




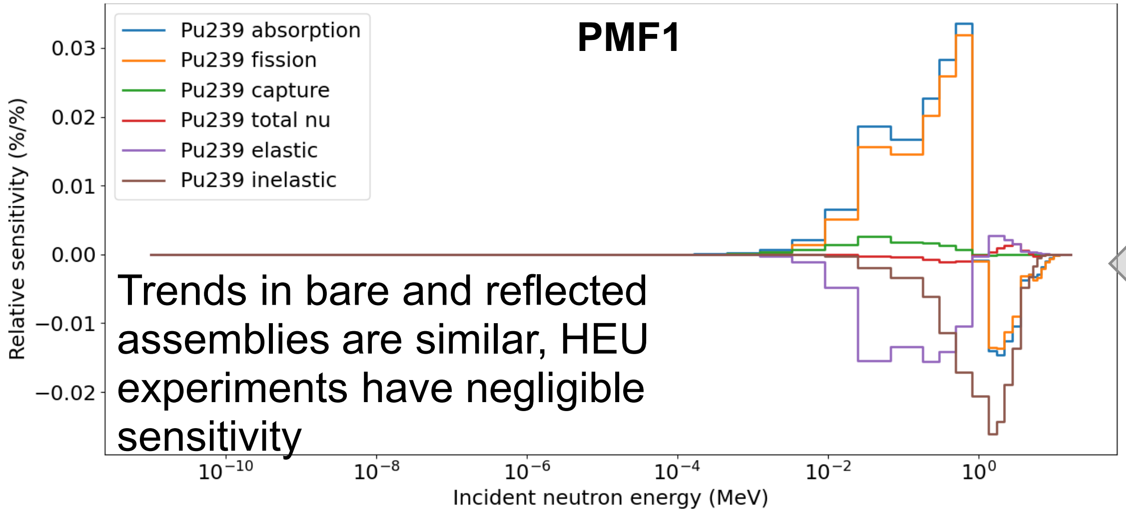
^{238}U(n,f)/^{235}U(n,f) Sensitivity to ^{239}Pu



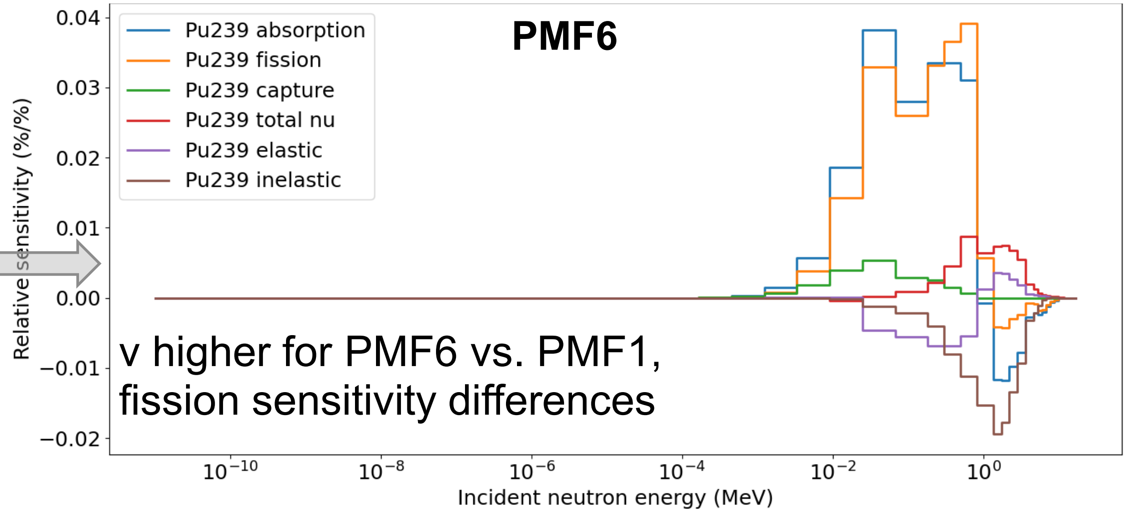
Sensitivities negligible for HMF1 (y-axis 1e-8); ^{239}Pu only present in foil



Sensitivities negligible for HMF28 (y-axis 1e-8); ^{239}Pu only present in foil



Trends in bare and reflected assemblies are similar, HEU experiments have negligible sensitivity



ν higher for PMF6 vs. PMF1, fission sensitivity differences

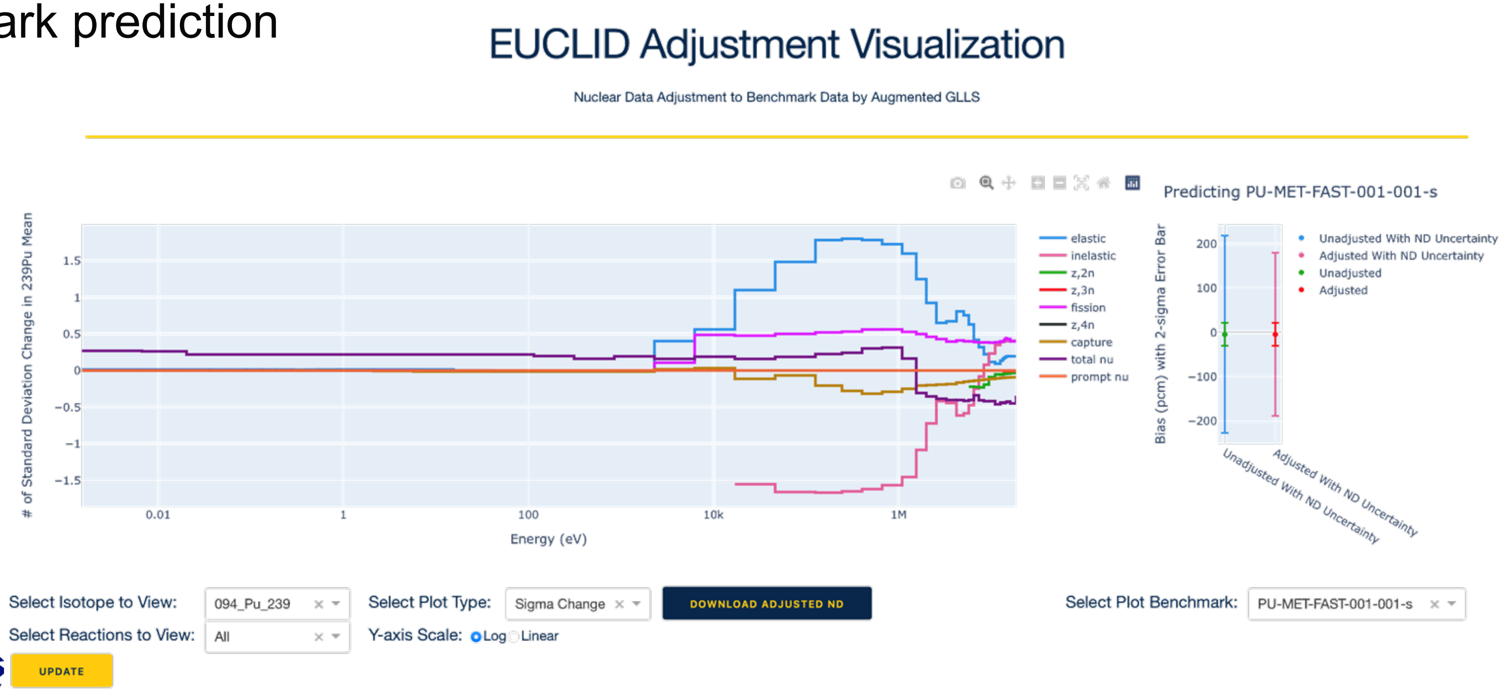
EUCLID Sensitivity library

- Reaction rate ratio sensitivities added to library, also includes:
  - k_{eff}
  - Pulsed Spheres
  - β_{eff}
  - Reactivity Coefficients
  - Subcritical Measurements
- EUCLID Sensitivities can be used to help:
  - Identify unconstrained physics spaces where compensating errors can hide,
  - Design experiments optimized to answer nuclear questions for applications,
  - Validate nuclear data and provide essential feedback to CSEWG how to improve the library
- This exchange format has been formalized
  - Description document : LA-UR-19-32580 report
  - Standardized schema for validation is available (https://json-schema.org)
  - See https://git.oecd-nea.org/science/wpec/sg45/documents

Capabilities using Sensitivity library

- Tool for exploring adjustment with many different responses
- Leverages GLLS-based adjustment with several expanded capabilities
  - 2111 total benchmark observations
  - 2579 nuclear data observables (isotope, reaction, energy group combinations)
- Explore first-order impact of adjustment on benchmark prediction

- Capability to explore several additional sources of uncertainty to assess impact on adjustment
  - Uncertainty on sensitivities
  - Enlarged uncertainties for observations based on ML-augmented benchmark review
  - Shape and time-of-flight uncertainty for pulsed sphere observations



- Currently uses ENDF/B-VIII.0 nuclear data and covariances (51 group structure).
- Observations simulated using MCNP6.2 and SENSMG.

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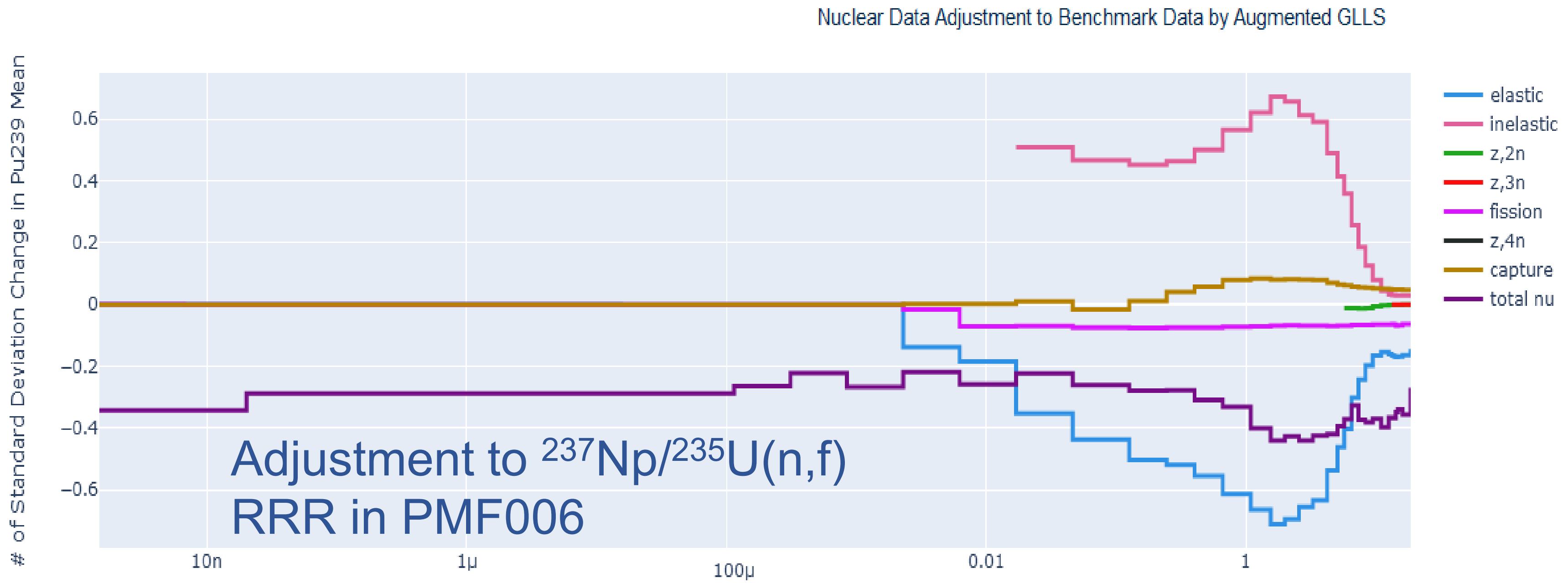
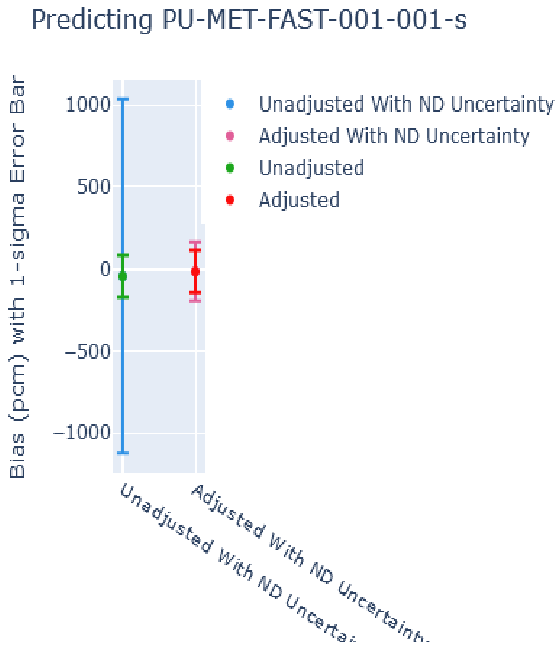
Capabilities using Sensitivity library

- **Exploring** adjustment: k_{eff} & reaction rate ratios (also pulsed spheres, β_{eff}, reactivity coefficients, subcrit.)
- R&D tool to increase understanding
- CSEWG – ENDF/B-VIII.1 will be general-purpose library
  - Evaluated from differential experimental data and theory, small hand-tweaks w/in constraints of few observables

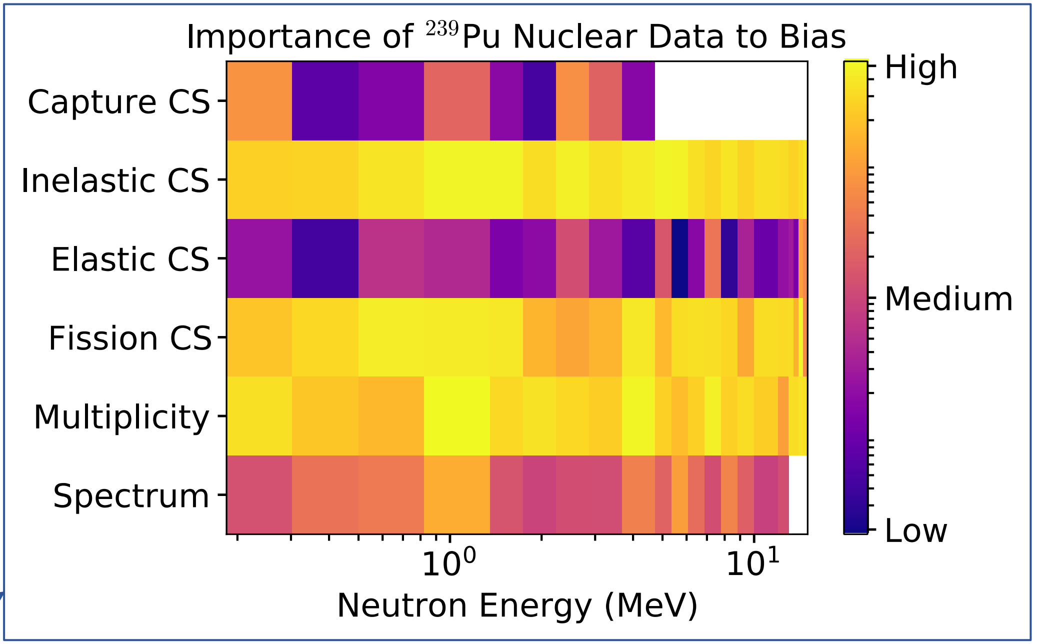
EUCLID Adjustment Visualization

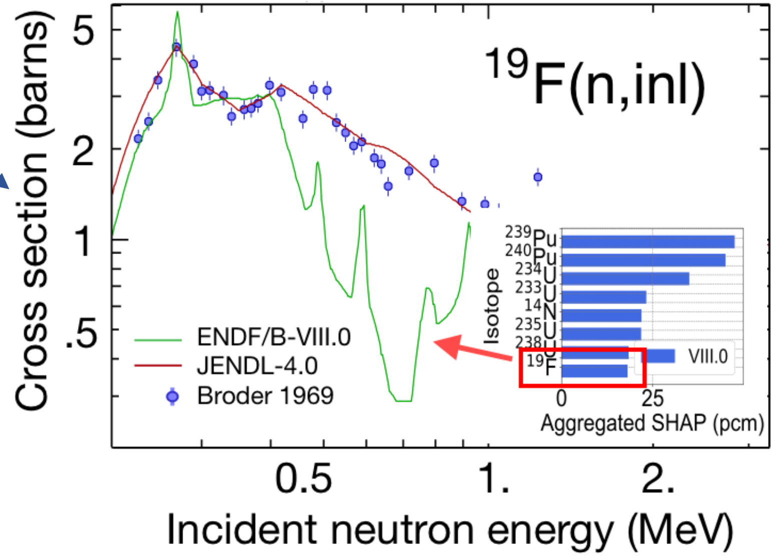




Capabilities using Sensitivity library

	RAFIEKI
Applies	Random forest & SHAP
Input	integral responses and sensitivities
Output	which nuclear data likely related to bias
Publication	DN, NDS 167, 36 (2020), DN, PRC 104, 034611 (2021)
Tool	Will eventually be open-source





Capabilities using Sensitivity library

	FAUST & CRATER
Applies	1st-order forward-propagation
Input	integral responses and sensitivities
Output	impact of changes in nuclear data on simulated responses
Publication	W. Haeck, Trans. Am. Nucl. Soc. 123, 723 (2020)
Tool	Will eventually be open-source

```
====   Pu239   ====
Modified reaction(s):  ['total nu']

Benchmark Name              | Diff.   Old     New
                            |         Bias    Bias
                            | (pcm)   (pcm)   (pcm)
MIX-COMP-FAST-002-001       |  -27  |  -494  |  -521
MIX-COMP-FAST-003-001       |  -28  |   -73  |  -101
MIX-MET-INTER-004-001       |  -18  |   426  |   408
MIX-MET-MIXED-001-001       |   -3  |    81  |    78
. . .
PU-MET-FAST-001-001-s       |  -15  |    44  |    29
PU-MET-FAST-002-001         |  -14  |   133  |   119
PU-MET-FAST-005-001         |  -20  |   -73  |   -93
PU-MET-FAST-006-001         |  -22  |   -30  |   -52
PU-MET-FAST-008-001         |  -20  |  -239  |  -259
PU-MET-FAST-011-001         |  -13  |    77  |    64
PU-MET-FAST-012-001         |  -24  |   106  |    82
PU-MET-FAST-013-001         |  -23  |  -559  |  -582
PU-MET-FAST-015-001         |  -20  |   -39  |   -59
PU-MET-FAST-045-006-s       |  -19  |   723  |   704
PU-MET-FAST-045-007-s       |  -19  |   691  |   672
. . .
PU-MET-INTER-002-001        |  -20  |  1696  |  1676
PU-MET-INTER-003-001        |  -19  |   154  |   135
PU-MET-INTER-004-001        |  -19  |   -71  |   -90

====   Pu239   ====
Manually set changes
Modified reaction:  ['total nu'] 0.999 68-500 keV
90 experiments with absolute change > 0.0 pcm
                Old      New
St. Deviation:  495  =>  490 pcm
Average Bias :  191  =>  176 pcm
```

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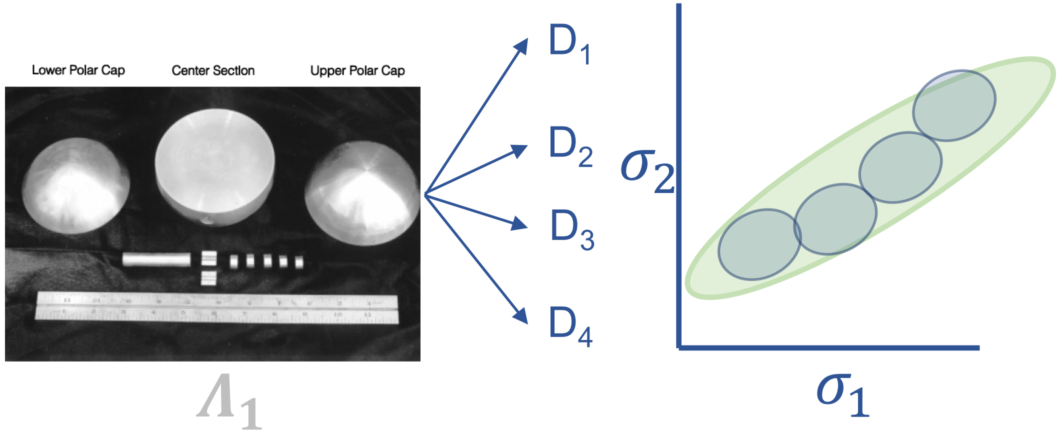
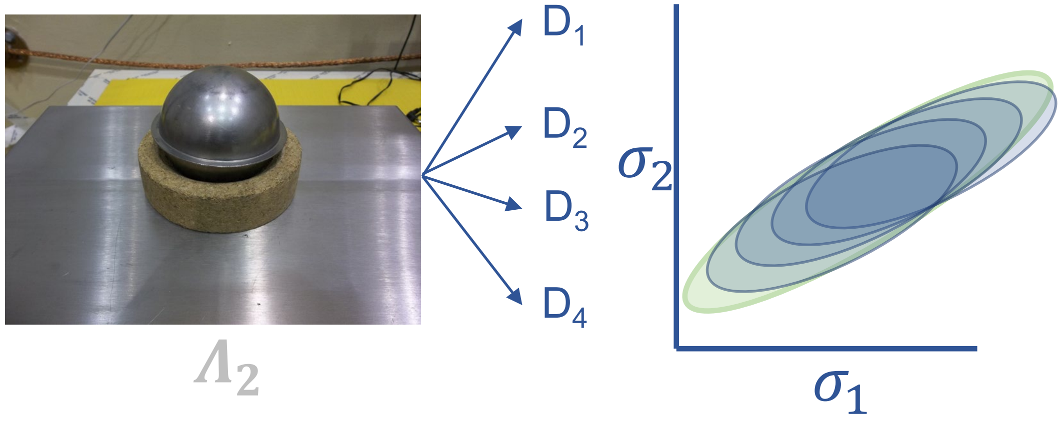
Capabilities using Sensitivity library

- Testing impact of new proposed experiment designs
  - Question: what new experimental data would lead to the most constrained nuclear data or application?
  - Combining statistical design of experiments with ML-driven design optimization
- Incorporating all information from ENDF/B-VIII.0 and previous integral data into an optimization
- Quantifying impact of proposed experiments on nuclear data adjustment/validation
- Explored to determine impact of reaction rate ratios





Conclusions and Future Work

- One EUCLID project goal is to create a **NEW** capability in the MCNP6 code
- Being tested on reaction rate sensitivities and compared with SENSMG results

What?	Why?	Who?
Current focus on a new fixed-source sensitivity capability with a **new MCNP6 FSEN** option	More approachable and efficient for general purpose applications	The EUCLID team is the first beneficiary of this new capability
Similar to the existing k-eigenvalue sensitivity method used by Whisper-1.1	Use of same tool for predictive simulation as sensitivity calculations	Already interest at LANL outside of EUCLID: XCP, P, W, NEN divisions, etc.
Extensible to general tallies in k-eigenvalue simulations	More computationally efficient and easier to use	**A production capability will be released in a future public version of the MCNP6 code**

Conclusions and Future Work

- Comparison of various fixed-source sensitivity methodologies
- Central difference, brute force calculations (FRENDY/SANDY codes)
  - Difficult to distinguish Monte Carlo statistics from small perturbations
  - Computationally expensive
- Differential operator (PERT card)
  - More complicated to use (many input cards needed = isotope x reaction x energy)
  - Limited to reactions (no multiplicity, spectrum or angular distributions)

```
689 c
690 pert101:n method=2  cell=1 2  mat=9999  rxn=2
691              rho=-3.0358e+01  erg=1e-11 2.96937e-09
692 c
```

- **Adjoint-weighting (new FSEN card)**
  - **Easy to use with accurate results (like KSEN)**
  - **Reactions, multiplicity, and energy / angular distributions all available**

```
29 c
30 fsen1 xs  iso=5010 92235  rxn=2 4 18
31             erg=0.00000E+00 2.53000E-08
32                 5.00000E-03 1.00000E-02
33                 5.00000E-02 1.00000E-01
34                 5.00000E-01 1.00000E+00
35                 1.50000E+00 3.00000E+00
36 c
```

Conclusions and Future Work

- Reaction rate ratio sensitivities added to EUCLID sensitivity library
  - Investigated to determine value toward designing optimized experiments aimed at reducing compensating errors in nuclear data
- The use of adjustment using multiple responses (and underlying/required capabilities) may benefit many applications
  - Tool for adjustment using multiple integral responses: ND adjustment and validation community.
  - Sensitivities of additional responses: ND adjustment and validation community.
  - Sensitivity capabilities: users in many application areas including safeguards/nonproliferation, criticality safety, etc.
  - Experiment optimization capability: applications which can benefit from integral experiments (criticality safety, advanced reactors, etc.)
- Working to build and test future tools and understanding of compensating errors

Acknowledgements

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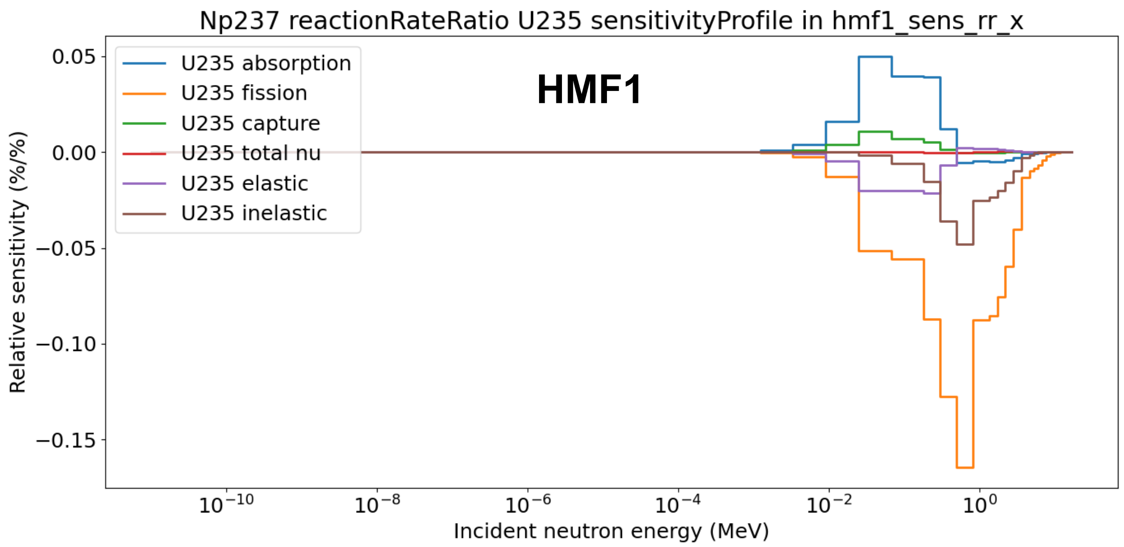
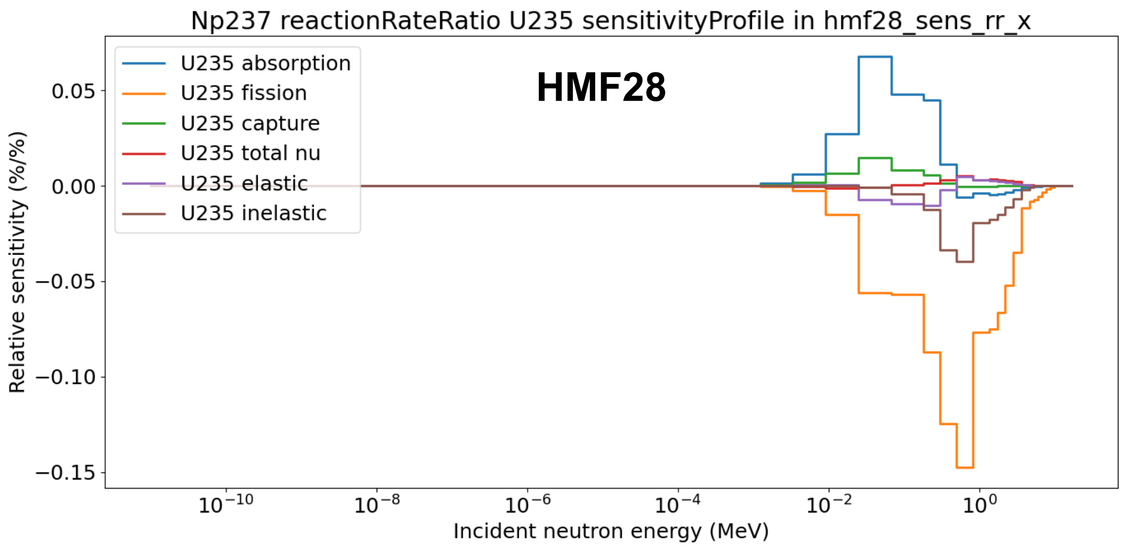
- Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of the US Department of Energy under Contract No. 89233218CNA000001.

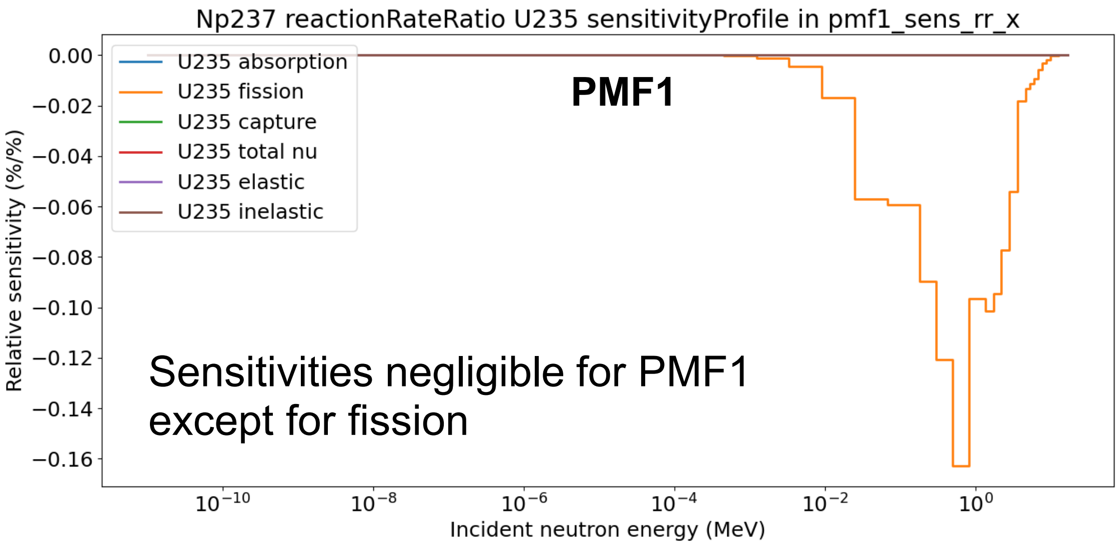
LDRD NCSP NUCLEAR CRITICALITY SAFETY PROGRAM NCERC NATIONAL CRITICALITY EXPERIMENTS RESEARCH CENTER MCNP6

Backup Slides

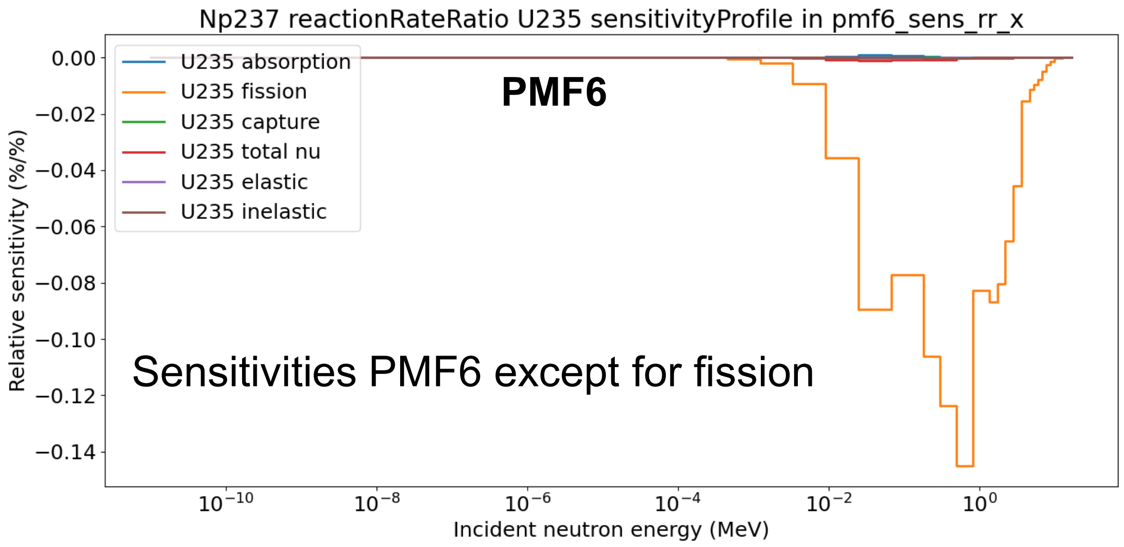
^{237}Np(n,f)/^{235}U(n,f) Sensitivity to ^{235}U





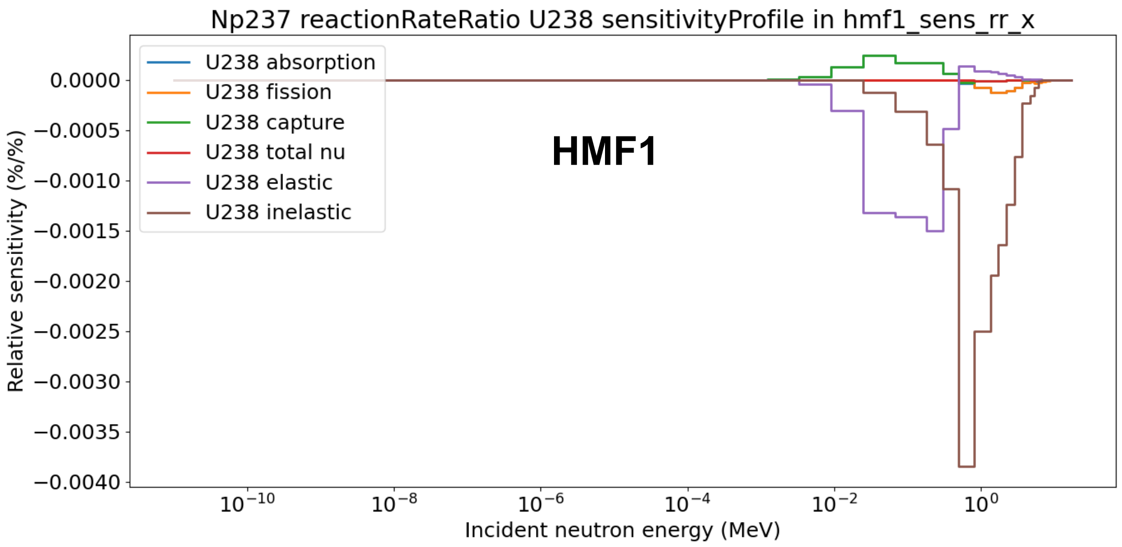


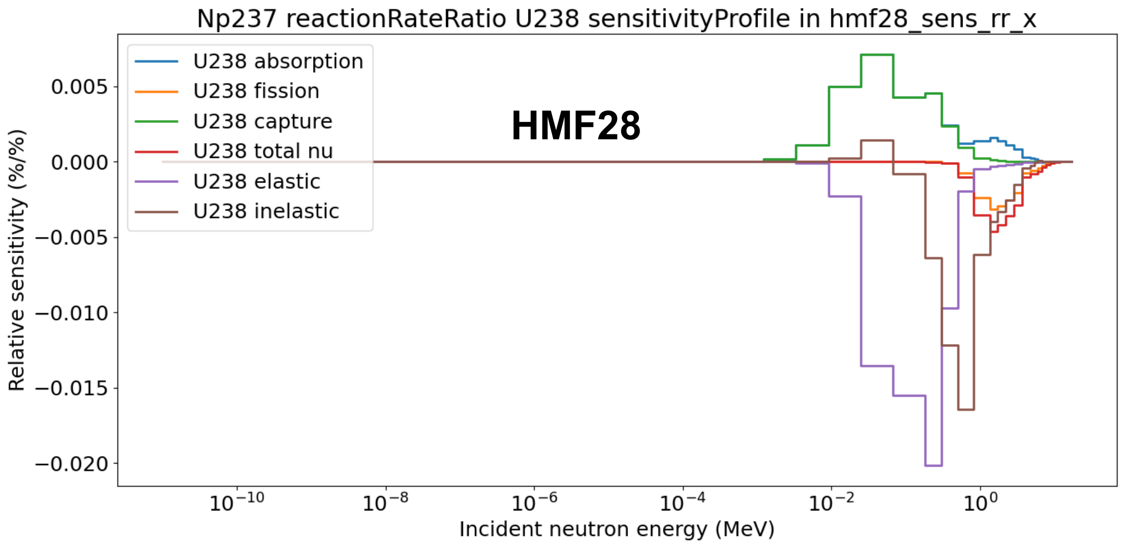
Sensitivities negligible for PMF1 except for fission

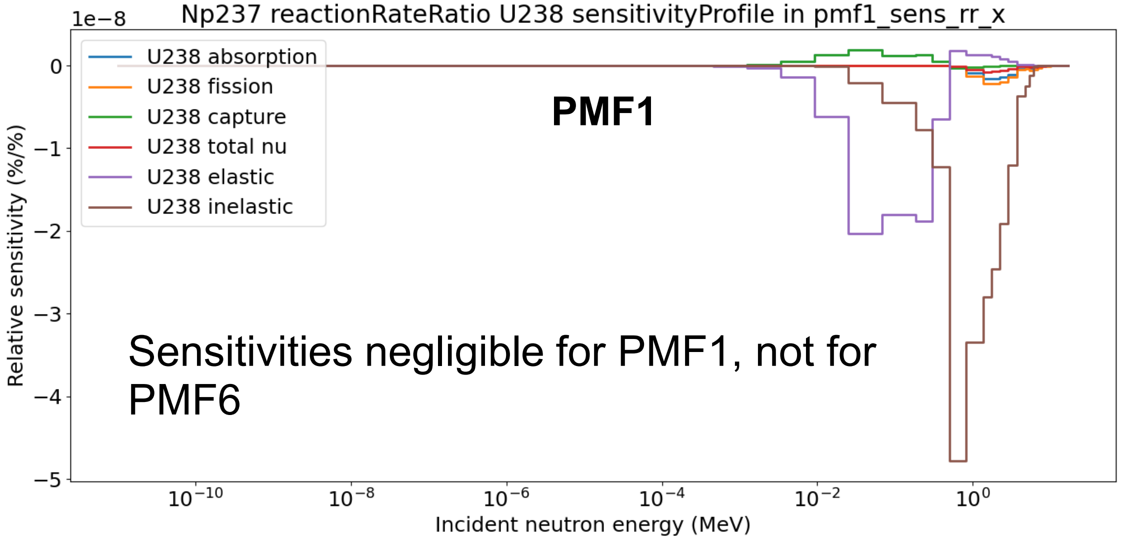


Sensitivities PMF6 except for fission

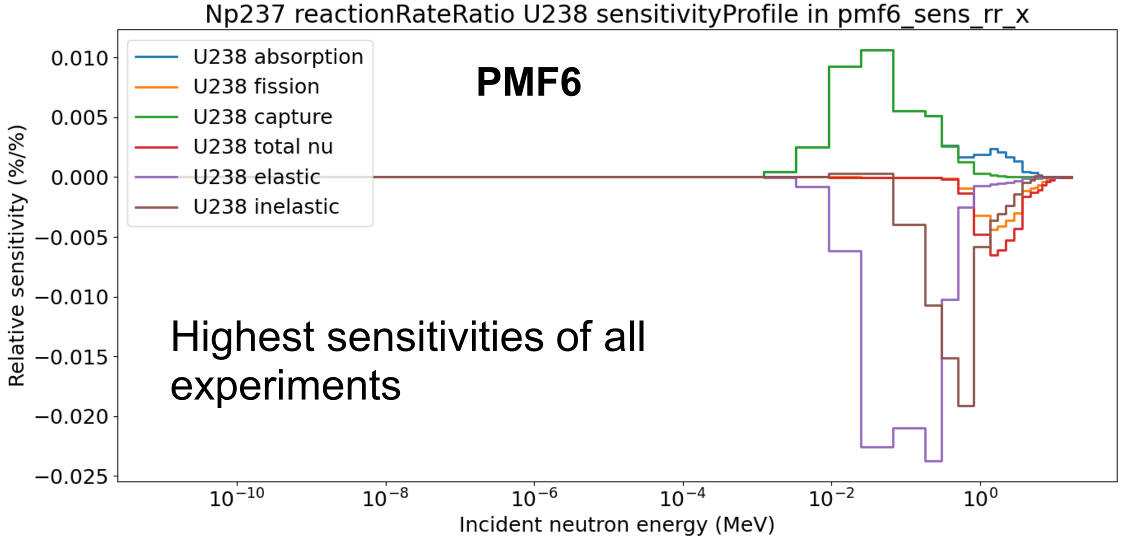
$^{237}Np(n,f)/^{235}U(n,f)$ Sensitivity to ^{238}U





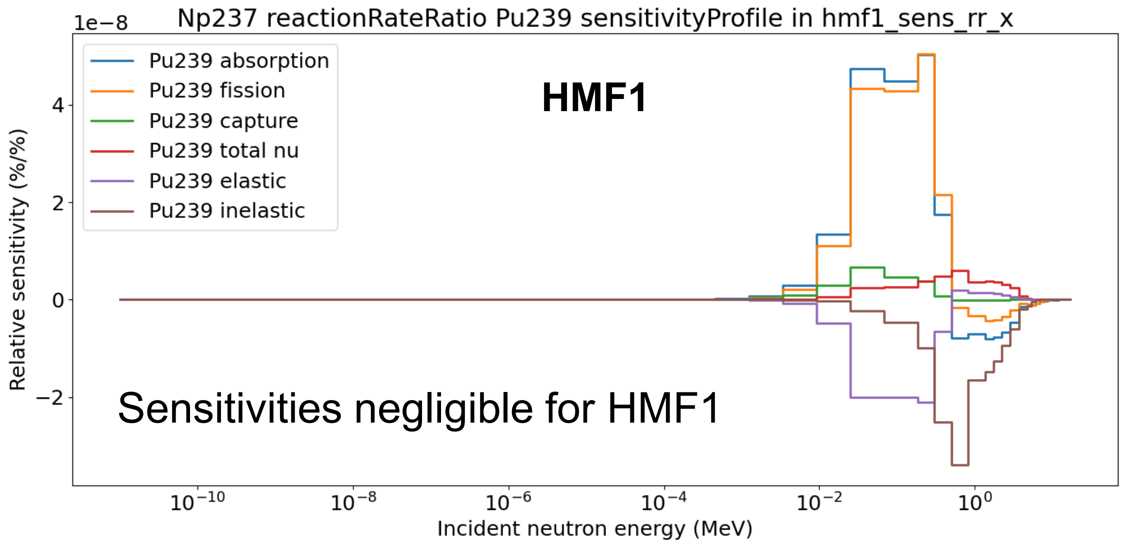


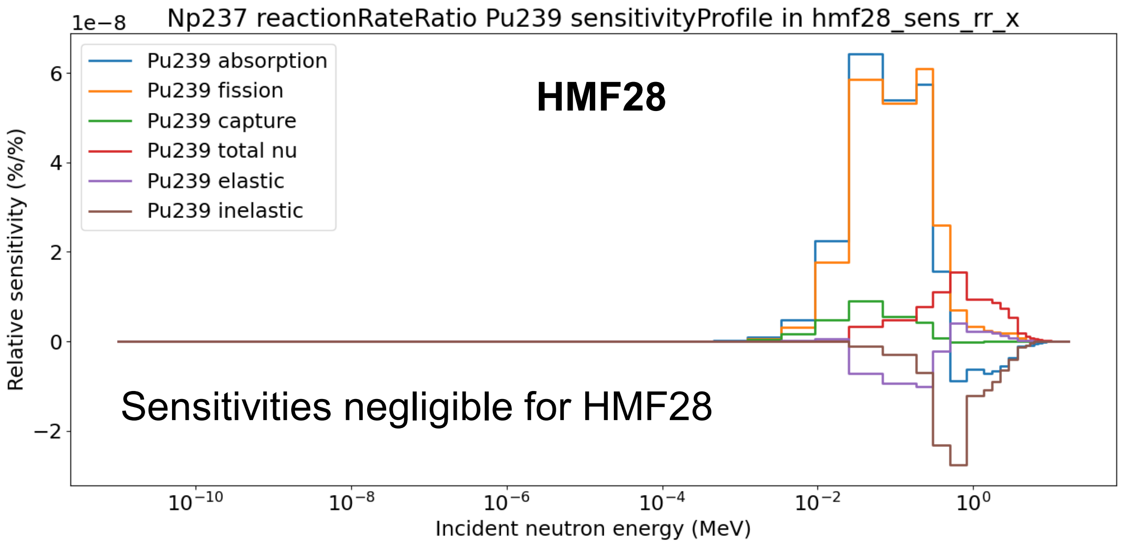
Sensitivities negligible for PMF1, not for PMF6

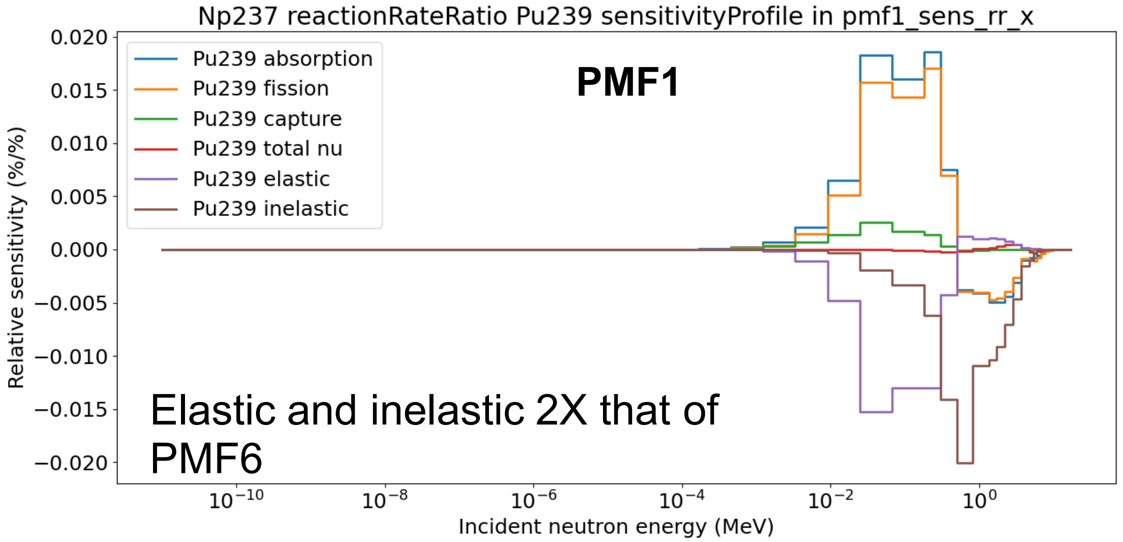


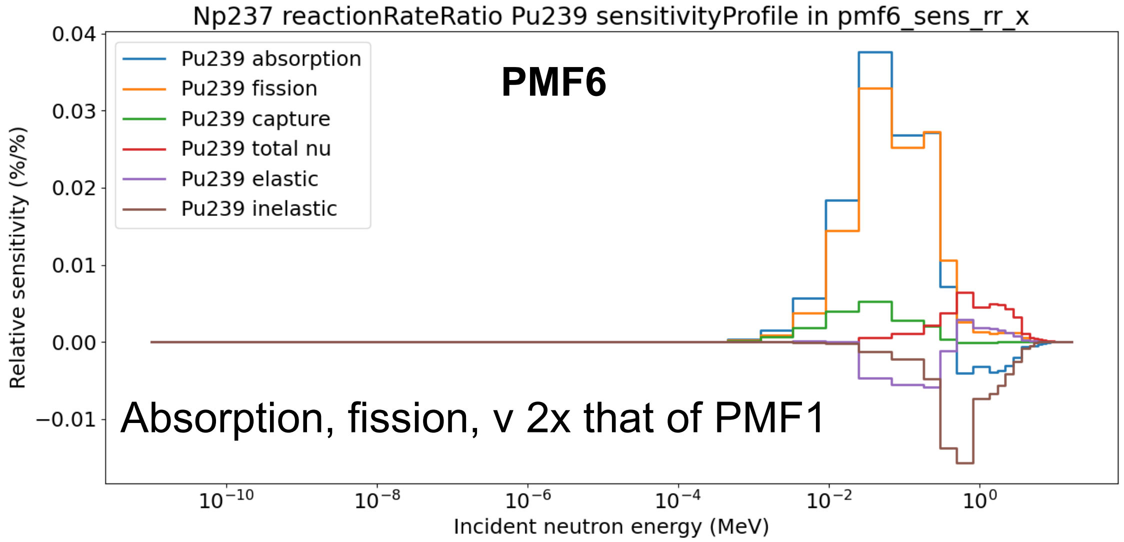
Highest sensitivities of all experiments

$^{237}Np(n,f)/^{235}U(n,f)$ Sensitivity to ^{239}Pu









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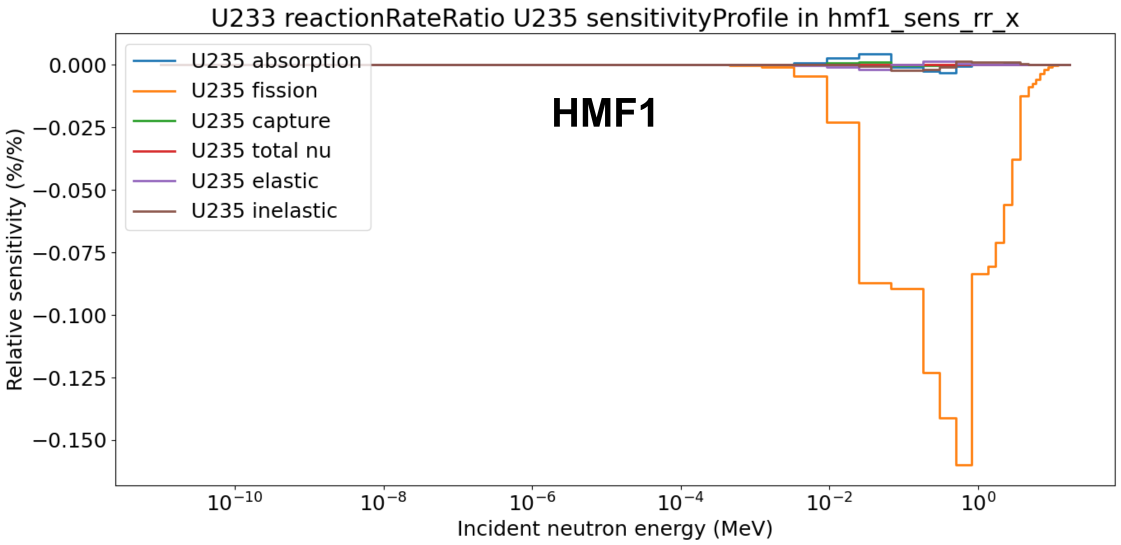
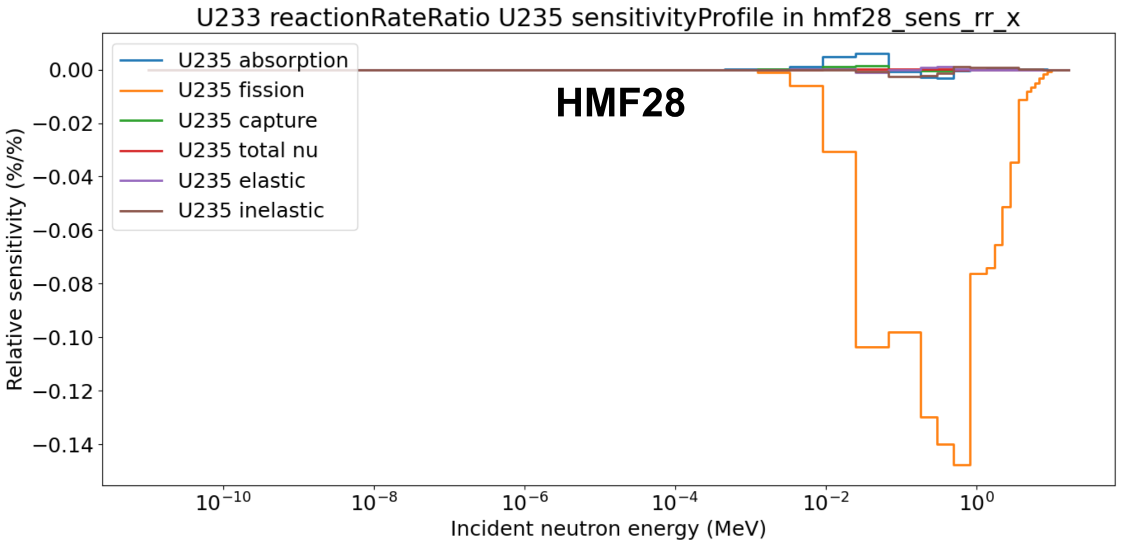
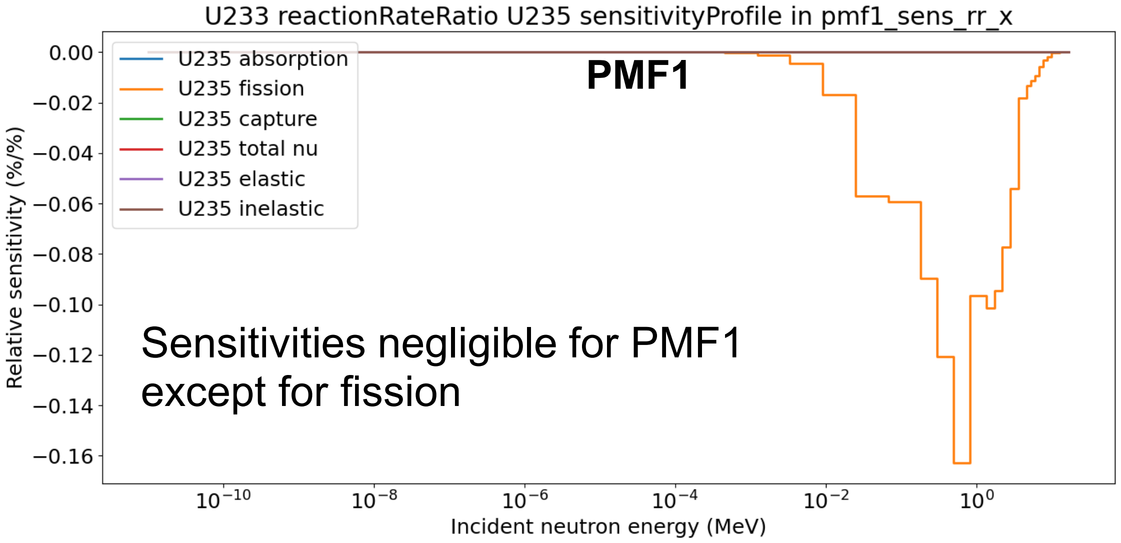
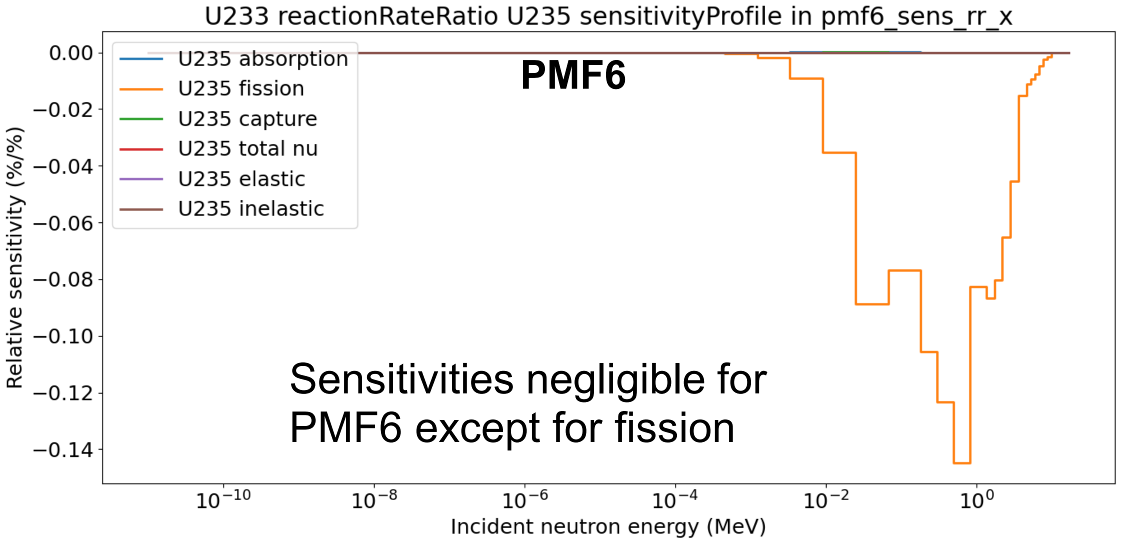
$^{233}U(n,f)/^{235}U(n,f)$ Sensitivity to ^{235}U









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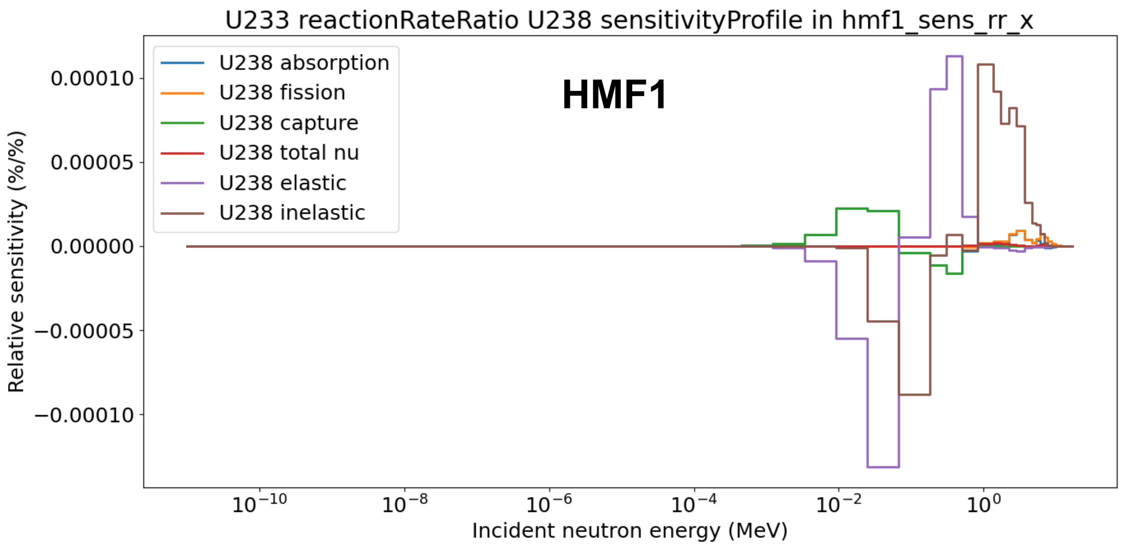
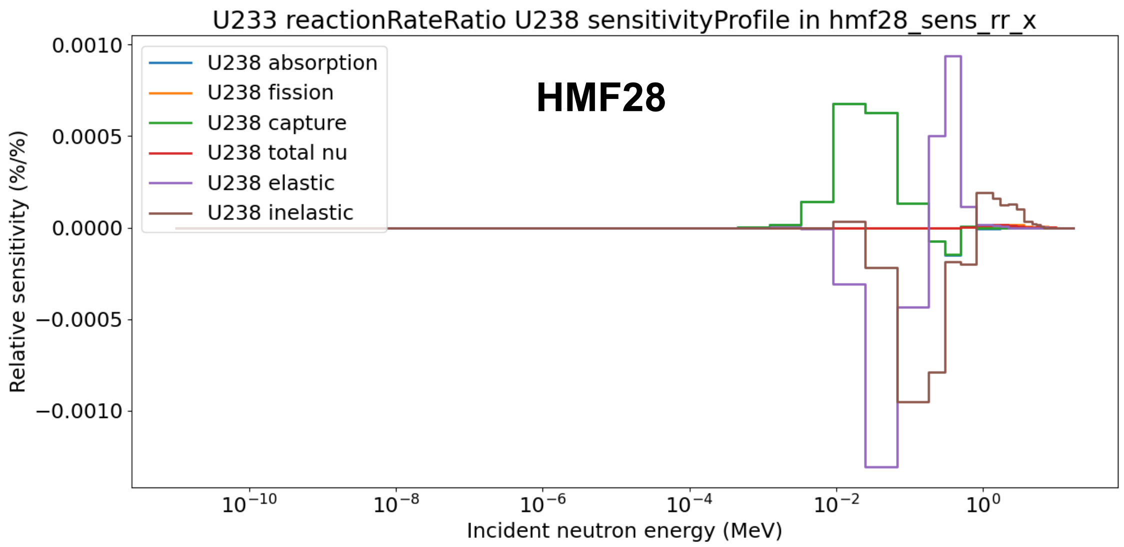
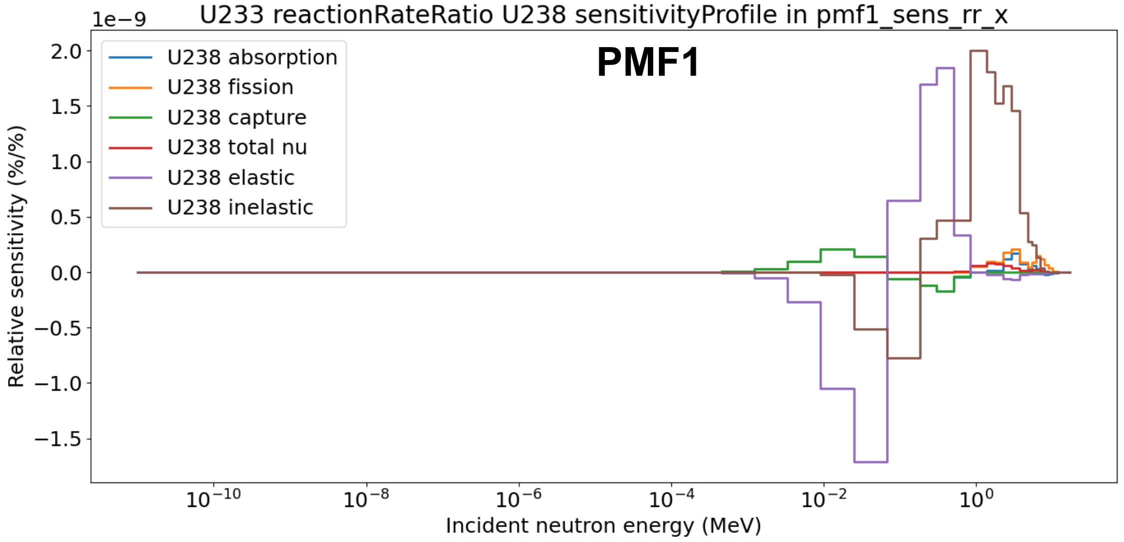
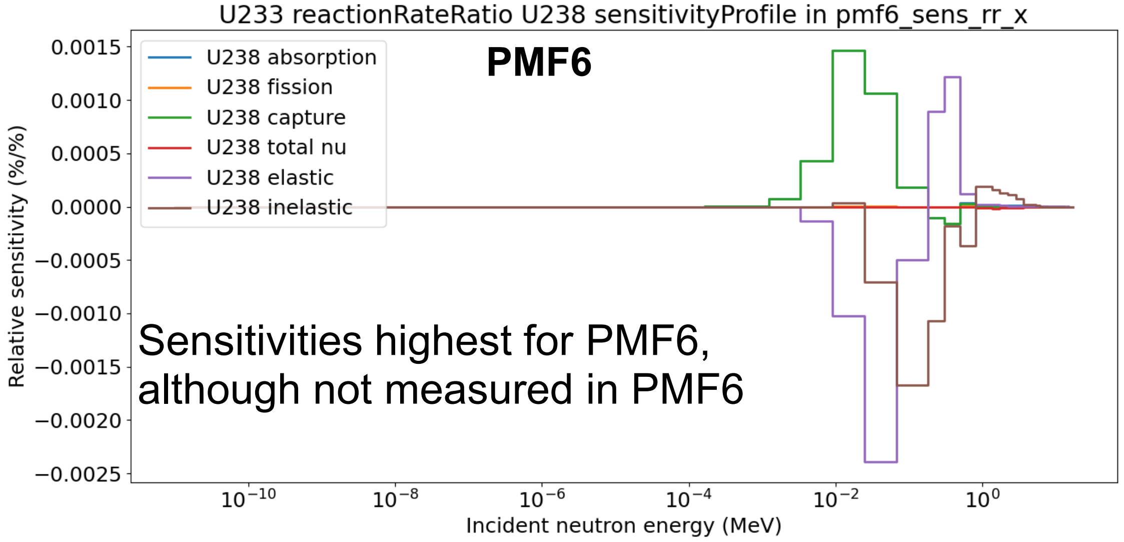
^{233}U(n,f)/^{235}U(n,f) Sensitivity to ^{238}U



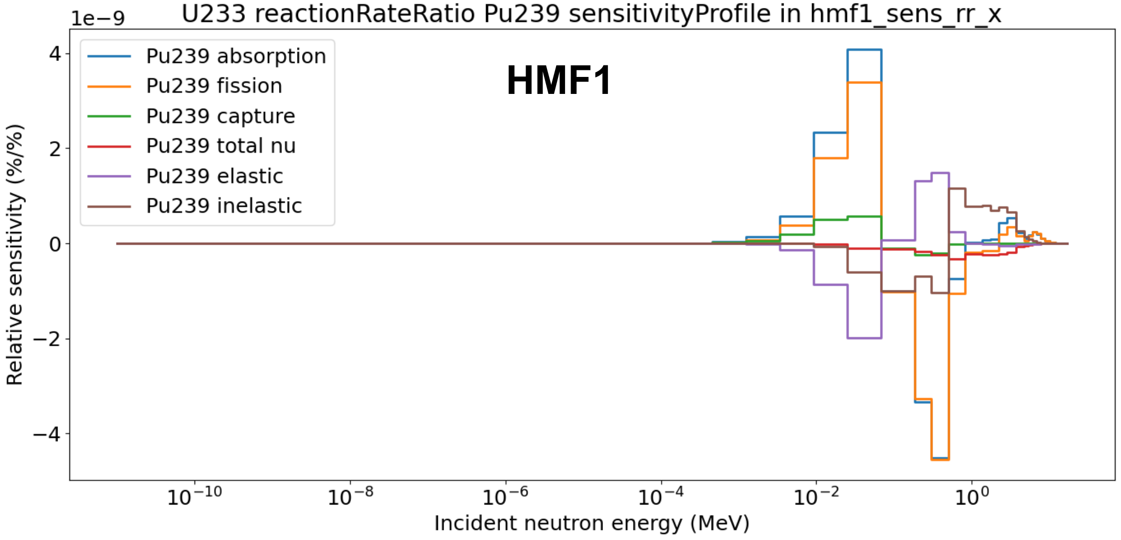


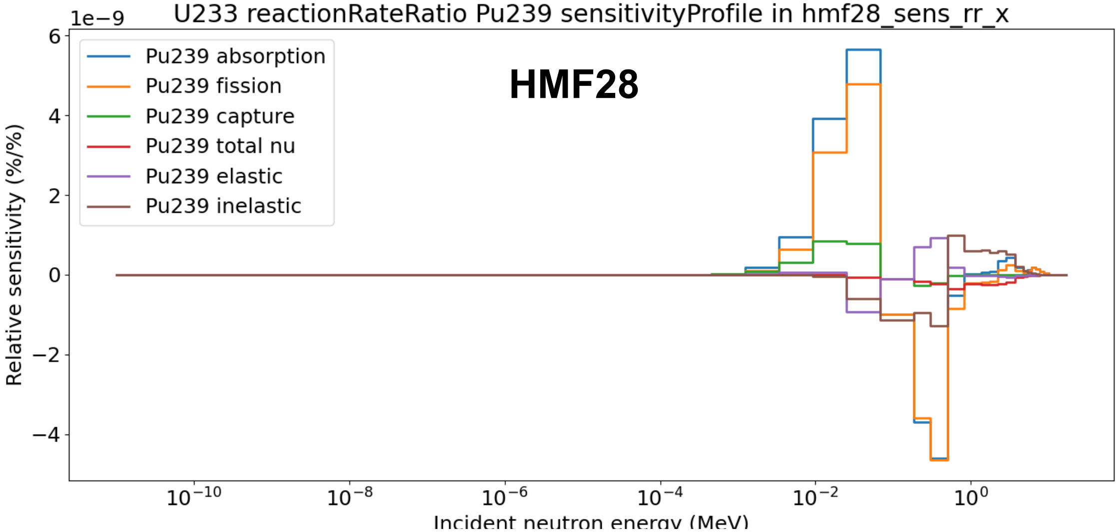


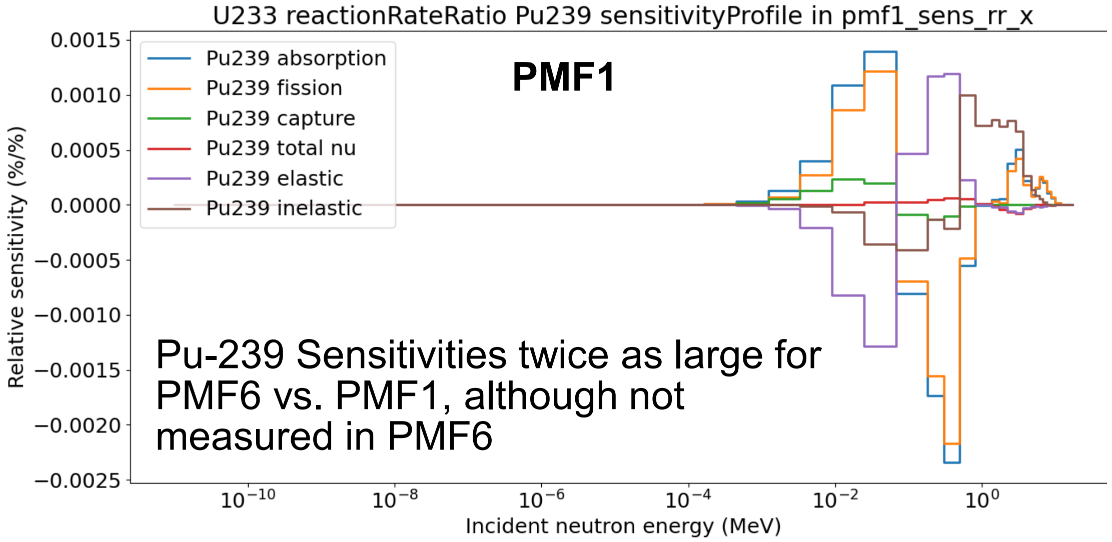


Sensitivities highest for PMF6, although not measured in PMF6

$^{233}U(n,f)/^{235}U(n,f)$ Sensitivity to ^{239}Pu







Pu-239 Sensitivities twice as large for PMF6 vs. PMF1, although not measured in PMF6