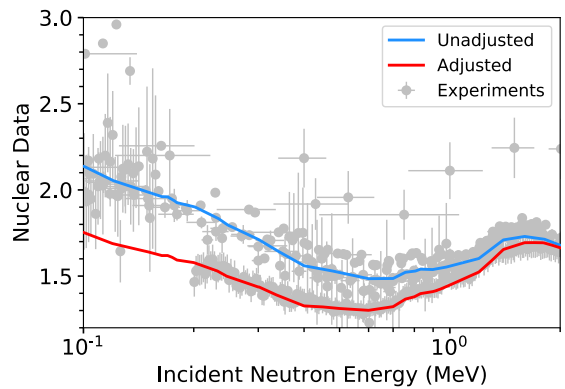
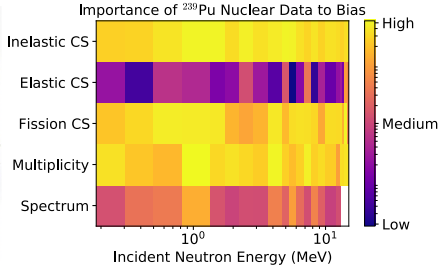
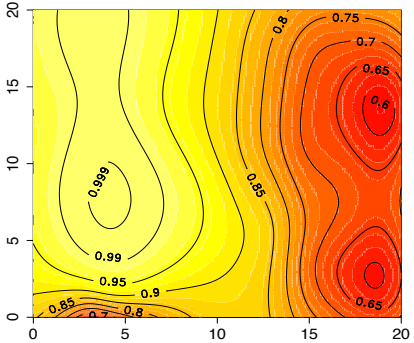



Los Alamos
NATIONAL LABORATORY

Delivering science and technology
to protect our nation
and promote world stability

LDRD
LABORATORY DIRECTED
RESEARCH & DEVELOPMENT

NNSA

Los Alamos
NATIONAL LABORATORY

# Getting sensitivities for various integral responses supporting nuclear data validation and adjustment

J. Hutchinson, J. Alwin, A. Clark, T. Cutler, M. Grosskopf, W. Haeck, M. Herman, N. Kleedtke, J. Lamproe, R.C. Little, I. Michaud, D. Neudecker M. Rising, T. Smith, N. Thompson, S. Vander Wiel

CSEWG 2021, November 15

LA-UR-21-31279

# EUCLID uses and developed tools to get sensitivities for various different measurement

| 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 which can help to disentangle compensating errors and improve overall validation of nuclear data.

# Using existing sensitivity tools to obtain a diverse collection of sensitivity profiles

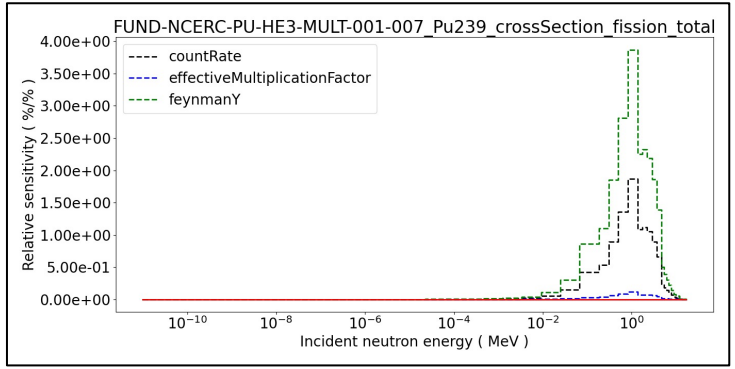
- Brute-force sensitivities with FRENDY/SANDY
  - Direct modification of ENDF/ACE files
  - Requires individual isotope-reaction-energy perturbations and independent MCNP calculations
  - O. Cabellos and A.R. Clark computed pulsed-sphere sensitivities with this methodology*

*D.Neudecker, ANE **159**, 108345, (2021).

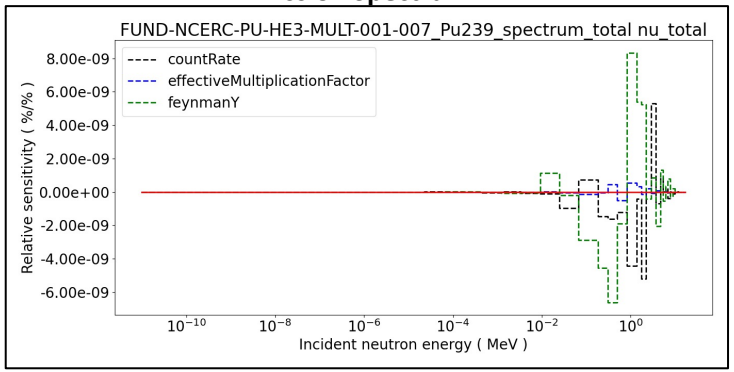
- SENSMG
  - Tool wrapped around the LANL deterministic transport code PARTISN
  - Requires using multi-group cross sections
  - Computed reaction rates, spectral indices (J. Alwin), and subcritical multiplication (A.R. Clark) sensitivities

**BeRP Subcritical Multiplication**

**Fission Cross Section**




**Fission Spectrum**




Tools for sensitivities of different responses

Use cases

# Deriving and computing more sensitivities through existing capabilities

Using $k_{eff}$ sensitivities, T. Cutler, J. Hutchinson, N. Kleedtke have derived and simulated other response sensitivities

- Beta-effective

$$\beta = 1 - \frac{k_p}{k}$$

- Reactivity coefficients

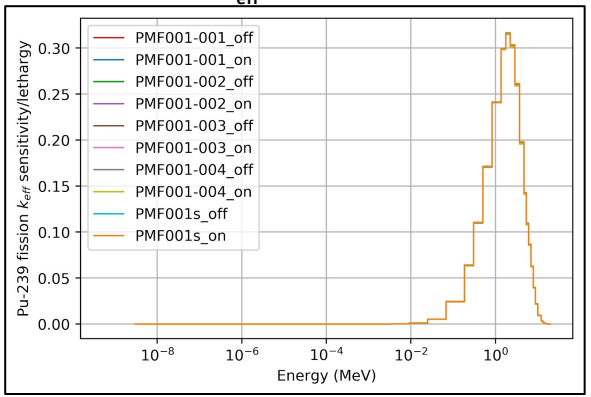
$$\Delta\rho_{a-b} = \left(1 - \frac{1}{k^{(a)}}\right) - \left(1 - \frac{1}{k^{(b)}}\right)$$

- Rossi-alpha

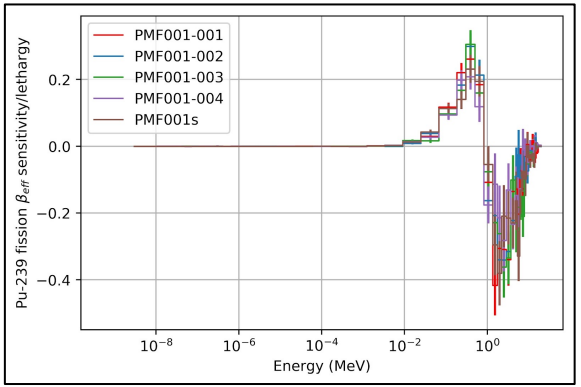
$$\alpha = \frac{k_p - 1}{l}$$

**PMF001 (Jezebel)**

**$k_{eff}$ sensitivities**




**$\beta_{eff}$ sensitivities**



# M. Rising developed new fixed-source sensitivity in MCNP for easier execution and faster run-time.

- Central difference, brute force calculations (FRENDY/SANDY codes)
  - Difficult to distinguish Monte Carlo statistics from small perturbations
  - Computationally expensive

- Differential operator (PERT card)

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

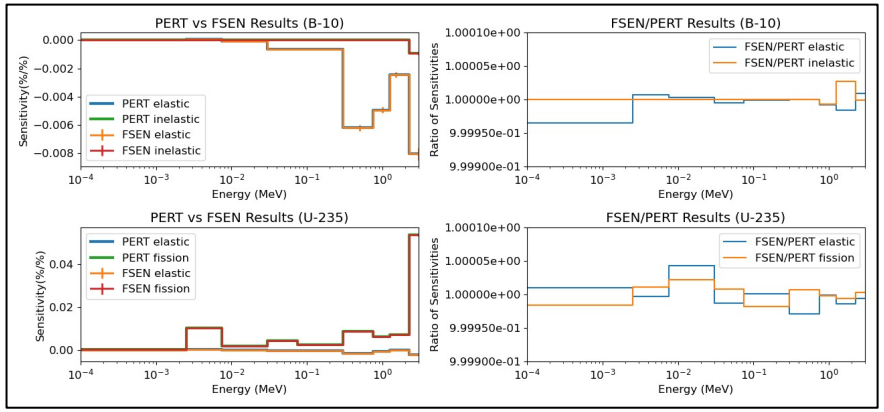
  - More complicated to use (many input cards needed = isotope x reaction x energy)
  - Limited to reactions (no multiplicity, spectrum or angular distributions)

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

```
c
fsen1 xs  iso=5010 92235  rxn=2 4 18
           erg=0.00000E+00 2.53000E-08
               5.00000E-03 1.00000E-02
               5.00000E-02 1.00000E-01
               5.00000E-01 1.00000E+00
               1.50000E+00 3.00000E+00
c
```

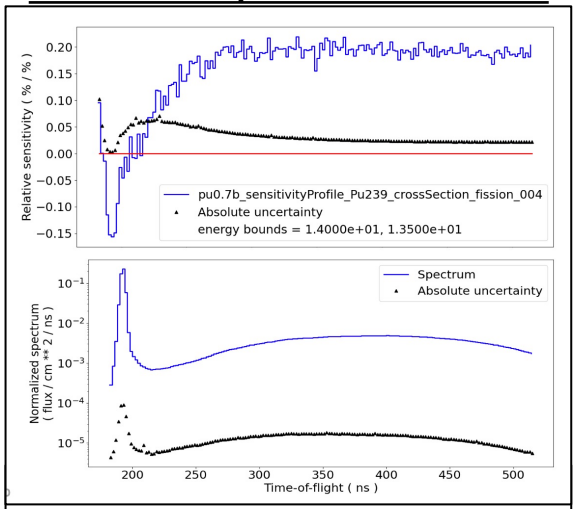
# Verification of the new sensitivity methodology has been undertaken.

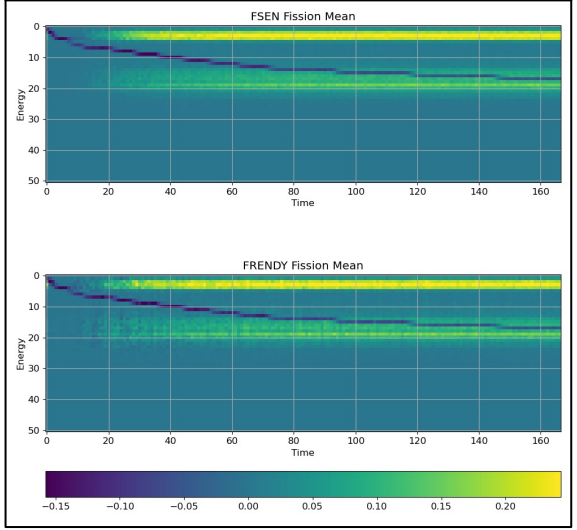
- Performing extensive verification to provide a robust and accurate capability
  - Comparison between FSEN and PERT




- Comparison between FSEN and central difference
  - Verification of FSEN using FRENDY results

**LLNL Pulsed Sphere of 0.7 MFP Pu**



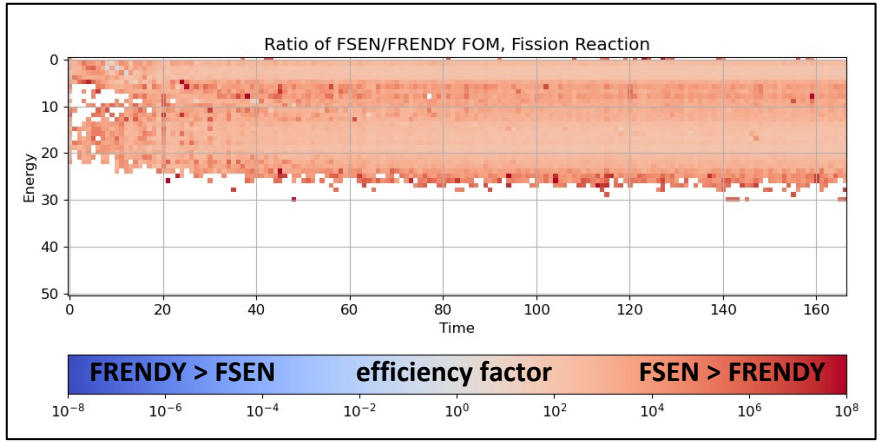

Tools for sensitivities of different responses Use cases

# Computational benefits of the new MCNP6 sensitivity methodology are promising

- FRENDY/SANDY vs. FSEN efficiency
  - Figure of merit $(FOM)$
    - Measure of Monte Carlo calculational efficiency
    - $FOM = \dfrac{1}{\mathrm{Time}(CPU) \cdot \mathrm{Var}(S)}$
    - Average efficiency gain for fission reaction

$$\boxed{7.3 \cdot 10^5 \text{ x}}$$

**LLNL Pulsed Sphere of 0.7 MFP Pu**




- PERT vs. FSEN efficiency
  - Computational cost is roughly equivalent
  - Pre- and post-processing of PERT results not automated
  - No optimization of the prototype FSEN capability (yet)

Human cost to use PERT may be higher with how easy it is to use the new FSEN capability

Tools for sensitivities of different responses

Use cases

# W. Haeck programmed FAUST tool that processes all different output formats into common json format.

- FAUST
  - Input / output processing of MCNP, SENSMG results
  - Handling of all sensitivity data for use in nuclear data adjustment and experiment design optimization
  - Common and easy to use JSON format support (new MCNP6 FSEN output also available in JSON)
  - Crater tool used to **rapidly** study impact of nuclear data changes on validation benchmarks

**Output from Crater Tool within FAUST**

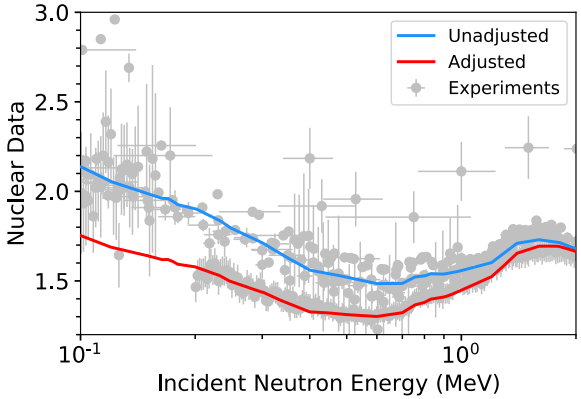
```
====   Pu239   ====
Modified reaction(s):  ['total nu']

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
```

# EUCLID

## Uses sensitivities for many use-cases.

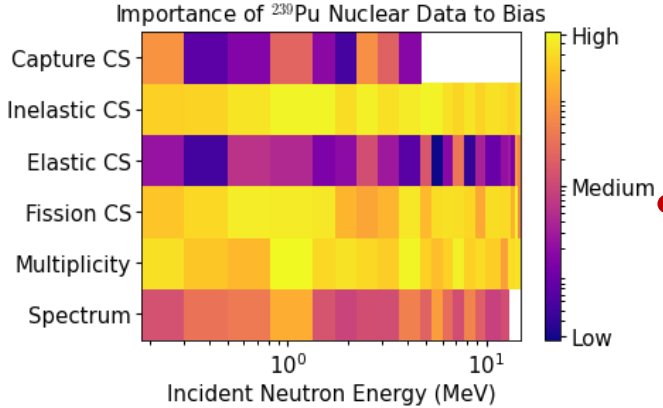
**Neutron Transport Simulation (MCNP)**

**Validation Experiments**

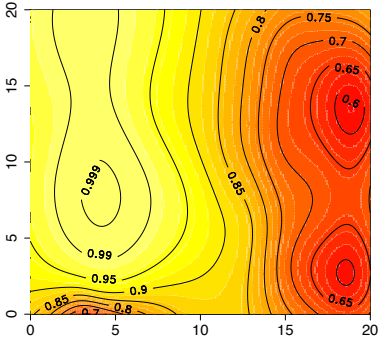



**Experiment Refines Nuclear Data to Improve Simulations**

**ML-Augmented Search for Compensating Errors**




**ML-Optimized Experiment to Resolve Compensating Errors**




Tools for sensitivities of different responses

Use cases

# One use-case is adjustment: we can filter to and select from our diverse set of benchmarks for adjustment

Adjustment tool developed by Mike Grosskopf.

◉ Original ○ Inflate Uncertainty for Labeled Questionable Benchmarks
◉ No Correction ○ Pulsed Sphere GP Correction for Long TOF

Set Gaussian Process TOF Correlation Length (ns):

10.0 25.0 50.0 100.0 150.0 200.0 400.0

Set TOF Gaussian Process Standard Deviation (cm^-2 ns^-1):

1.0e-5 1.0e-4 1.0e-3 1.0e-2 1.0e-1 1.0e00

## Select Benchmarks to Adjust To:

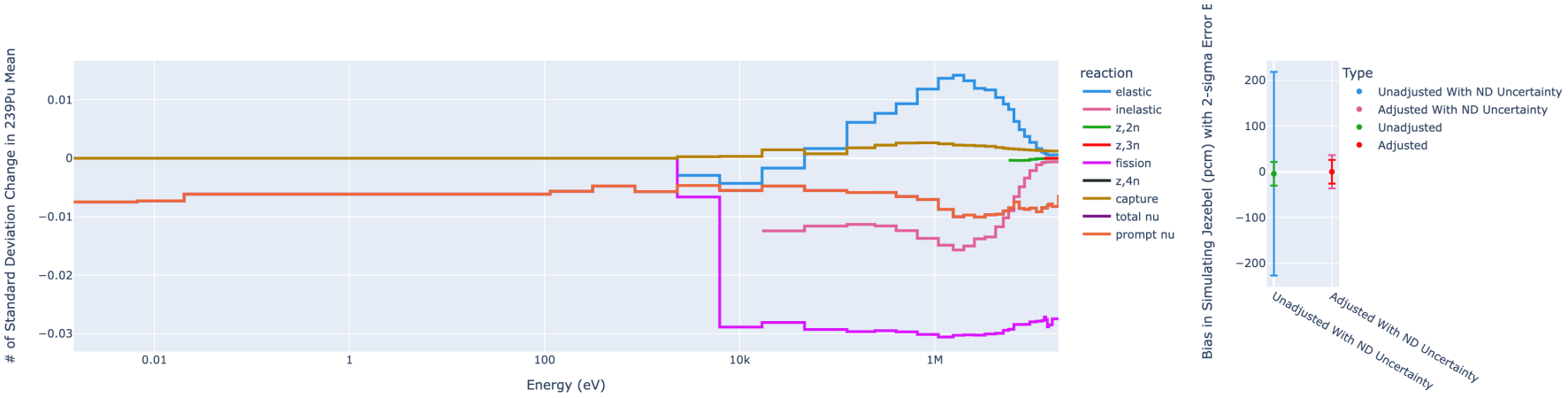
SELECT ALL | DESELECT ALL

| | Benchmark Types | Experiment Names | Experimental Value | Calculated Value | Expt. Uncertainty | Calc. Uncertainty | Total Uncertainty | Bias (sigmas) | Time-of-Flight | D-Optimality |
|---|---|---|---|---|---|---|---|---|---|---|
| | filter data... | PU-MET | | | | | | | | |
| ☑ | criticality | PU-MET-FAST-001-001-s | 1 | 1.00044 | 0.00129 | 0.00008 | 0.001292478239662 | -0.3404312633650697 | | 0.00012225205129393036 |
| ☐ | criticality | PU-MET-FAST-002-001 | 1 | 1.00133 | 0.002 | 0.00008 | 0.0020015993605114 | -0.664468637550046 | | 0.0000826247873474197 |
| ☐ | criticality | PU-MET-FAST-005-001 | 1 | 0.99927 | 0.0013 | 0.00009 | 0.0013031116606031 | 0.5601975809672006 | | 0.00010273708220366292 |
| ☐ | criticality | PU-MET-FAST-006-001 | 1 | 0.9997 | 0.003 | 0.0001 | 0.0030016662039607 | 0.09994449069790533 | | 0.0001225526093910824 |
| ☐ | criticality | PU-MET-FAST-008-001 | 1 | 0.99761 | 0.0006 | 0.00009 | 0.0006067124524847 | 3.939263138925394 | | 0.00010079873258719962 |
| ☐ | criticality | PU-MET-FAST-011-001 | 1 | 1.00077 | 0.001 | 0.00011 | 0.0010060318086422 | -0.7653833540702604 | | 0.0000932055058487017 8 |
| ☐ | criticality | PU-MET-FAST-012-001 | 1.0009 | 1.00196 | 0.0021 | 0.0001 | 0.0021023796041628 | -0.504190583803808 | | 0.00010864902908367885 |
| ☐ | criticality | PU-MET-FAST-013-001 | 1.0034 | 0.99781 | 0.0023 | 0.00009 | 0.0023017601960239 | 2.428576186892256 | | 0.00009735494910760852 |
| ☐ | criticality | PU-MET-FAST-015-001 | 1.0041 | 1.00371 | 0.0026 | 0.0001 | 0.0026019223662515 | 0.1498891761946572 | | 0.00009873491029936234 |
| ☐ | criticality | PU-MET-FAST-016-001 | 0.9974 | 1.0206 | 0.0042 | 0.00012 | 0.0042017139360027 | -5.5215562871163275 | | 0.00006938027010215084 |
| ☐ | criticality | PU-MET-FAST-016-002 | 1 | 1.01019 | 0.0038 | 0.00012 | 0.0038018942647054 | -2.680242871191348 | | 0.0000687562355783532 |
| ☐ | criticality | PU-MET-FAST-016-003 | 1 | 1.0085 | 0.0033 | 0.00011 | 0.0033018328243567 | -2.5743277907039457 | | 0.0000686450512013453 |
| ☐ | criticality | PU-MET-FAST-016-004 | 1 | 1.00787 | 0.003 | 0.00012 | 0.0030023990407672 | -2.6212371817135374 | | 0.0000688734872085301 1 |
| ☐ | criticality | PU-MET-FAST-016-005 | 1 | 1.00776 | 0.0034 | 0.00012 | 0.0034021169879943 | -2.280932733172958 | | 0.0000685881961923345 7 |

# Adjusting to Jezebel we can explore the impact on nuclear data and the propagated prediction and uncertainties for Jezebel

## EUCLID Adjustment Visualization

Nuclear Data Adjustment to Benchmark Data by Augmented GLLS




Select Isotope to View: 094_Pu_239

UPDATE

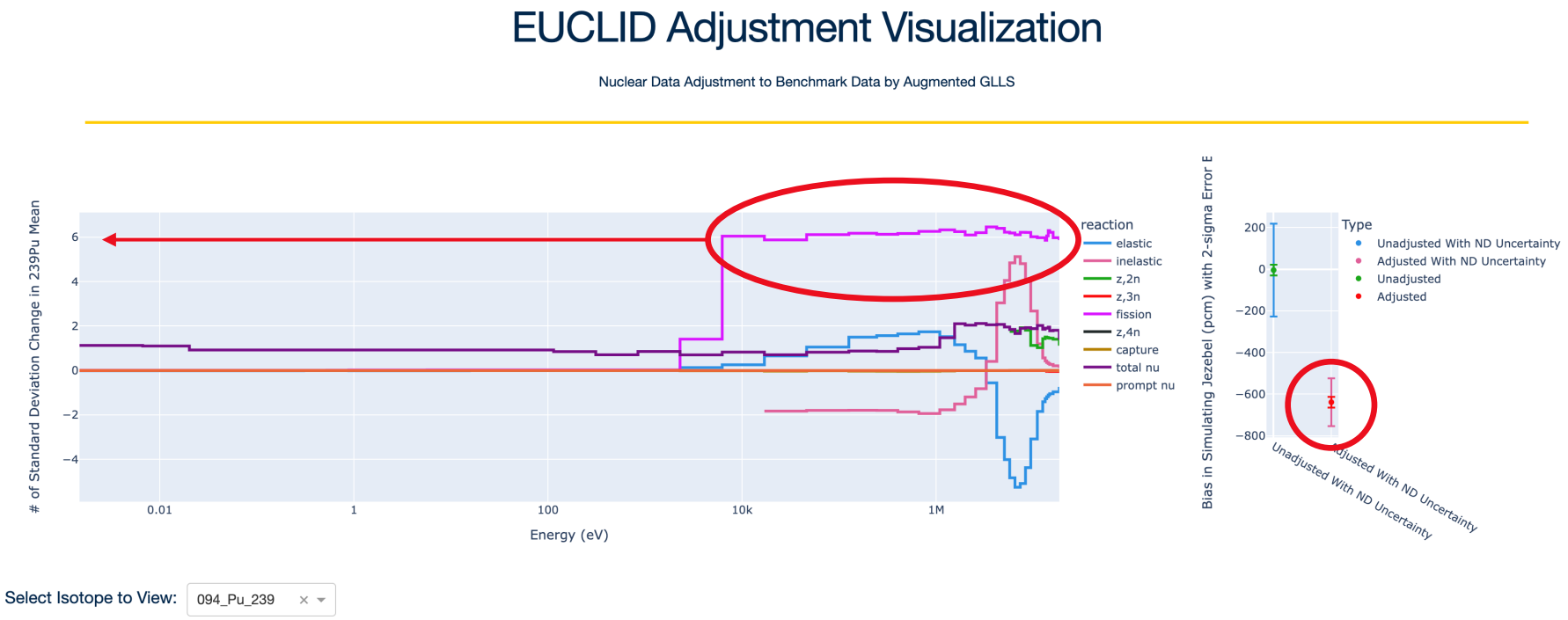
# One warning (among many): adjusting to data with unaccounted for biases leads to unreasonable results.

Select Benchmarks to Adjust To:

SELECT ALL | DESELECT ALL

| | Benchmark Types | Experiment Names | Experimental Value | Calculated Value | Expt. Uncertainty | Calc. Uncertainty | Total Uncertainty | Bias (sigmas) | Time-of-Flight |
|---|---|---|---|---|---|---|---|---|---|
| | pulse | pu | | | | | | | |
| ☑ | pulsed sphere | pu0.7b_020 | 0.0007147913970509 | 0.000681932 | 0.0000359215 | 0.000005932808399999999 | 0.00003640813614786001 | 0.9025289544472154 | 225 |
| ☑ | pulsed sphere | pu0.7b_021 | 0.0007122360609277 | 0.000682894 | 0.0000358595 | 0.0000060777566 | 0.00003637090685615144 | 0.8067453760157601 | 227 |
| ☑ | pulsed sphere | pu0.7b_022 | 0.0007600208464308 | 0.000692146 | 0.000037023 | 0.0000063677432 | 0.00003756661659587068 | 1.806786252831212 | 229 |
| ☑ | pulsed sphere | pu0.7b_023 | 0.0008498409111599 | 0.0007241289999999 | 0.0000391185 | 0.000007241289999999999 | 0.00003978307835140589 | 3.1599342325795003 | 231 |
| ☑ | pulsed sphere | pu0.7b_024 | 0.0008191129942789 | 0.000767262 | 0.00003841550000000005 | 0.0000066751794 | 0.00003899113566276551 | 1.3298149283816565 | 233 |
| ☑ | pulsed sphere | pu0.7b_025 | 0.0007823800375085 | 0.000814031 | 0.0000375555 | 0.000006837860400000006 | 0.00003817292122827238 | -0.8291469835967908 | 235 |
| ☑ | pulsed sphere | pu0.7b_026 | 0.0009983059399155 | 0.000855741 | 0.00004235550000000005 | 0.0000071882244 | 0.00004296113301898305 | 3.318463222385344 | 237 |
| ☑ | pulsed sphere | pu0.7b_027 | 0.0010256480364333 | 0.000907246 | 0.0000429255 | 0.0000075301418 | 0.00004358097733849147 | 2.716828388534677 | 239 |
| ☑ | pulsed sphere | pu0.7b_028 | 0.0010420660710246 | 0.000941066 | 0.000043263 | 0.000007810847800000001 | 0.00004396244434008151 | 2.2974170918088843 | 241 |
| ☑ | pulsed sphere | pu0.7b_029 | 0.0010045026300141 | 0.000975567 | 0.00004248550000000005 | 0.000007999649400000001 | 0.0000432320725940004 | 0.6693093409108383 | 243 |
| ☑ | pulsed sphere | pu0.7b_030 | 0.0009608063823081 | 0.00102875 | 0.000041562 | 0.000008332875 | 0.00004238911003743326 | -1.6028554888720192 | 245 |
| ☑ | pulsed sphere | pu0.7b_031 | 0.0011343775884738 | 0.00109541 | 0.00004511850000000005 | 0.000008872821 | 0.00004598267059173533 | 0.8474407417476941 | 247 |
| ☑ | pulsed sphere | pu0.7b_032 | 0.0011301612838705 | 0.00115419 | 0.0000450355 | 0.000008887263000000001 | 0.00004590402709873252 | -0.5234555146505547 | 249 |
| ☑ | pulsed sphere | pu0.7b_033 | 0.0012248364872336 | 0.00122588 | 0.000046865 | 0.000009316688 | 0.00004778209811518686 4 | -0.02183899007290044 | 251 |
| ☑ | pulsed sphere | pu0.7b_034 | 0.0012535840186192 | 0.00125507 | 0.000047407 | 0.000009538532 | 0.00004835708057477233 | -0.030729344351182287 | 253 |
| ☑ | pulsed sphere | pu0.7b_035 | 0.0012555005207115 | 0.0013207 | 0.0000474425 | 0.00000964111 | 0.0000484122072238201 | -1.3467570067001615 | 255 |
| ☑ | pulsed sphere | pu0.7b_036 | 0.0013698518122229 | 0.00136453 | 0.0000495365 | 0.000009961069 | 0.00005052808850404655 | 0.10532383829389909 | 257 |
| ☑ | pulsed sphere | pu0.7b_037 | 0.001306032292547 | 0.00141788 | 0.000048379 | 0.00000992516 | 0.00004938660184731888 | -2.264737869570025 | 259 |
| ☑ | pulsed sphere | pu0.7b_038 | 0.0014092678719227 | 0.00151701 | 0.00005024 | 0.000011377575 | 0.00005151220062160638 | -2.091584649406505 | 261 |
| ☑ | pulsed sphere | pu0.7b_039 | 0.0015691041464263 | 0.00156268 | 0.00005299 | 0.000010782492 | 0.00005407589327722719 | 0.1187987111625835 | 263 |

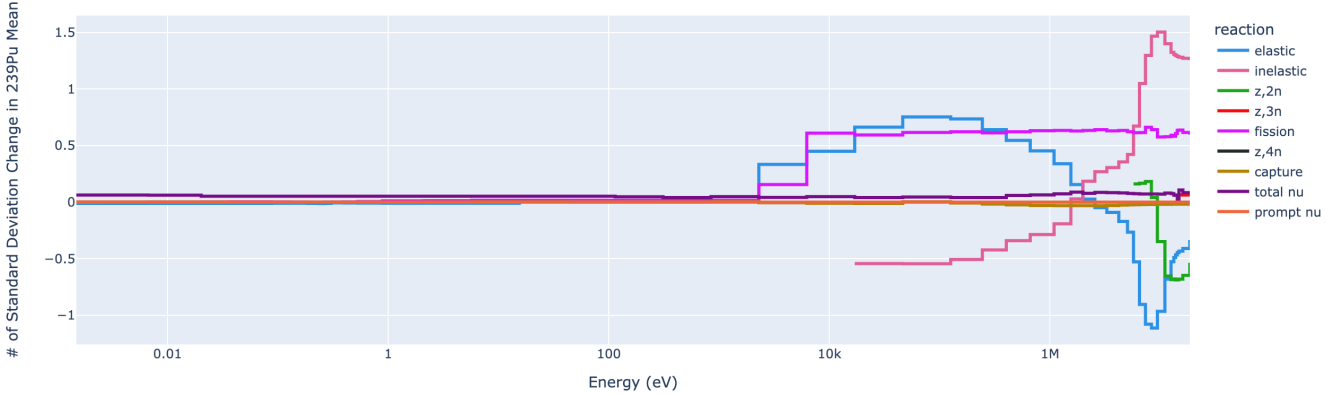
# As mentioned however, adjusting to data with unaccounted for biases leads to unreasonable results

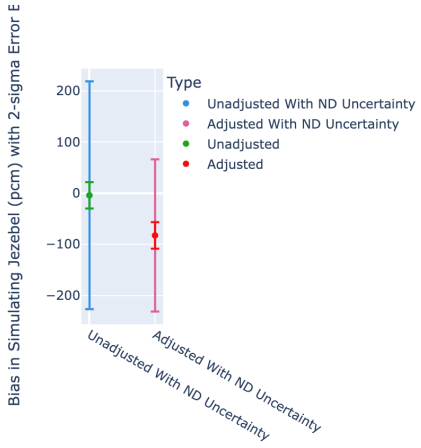


# Adding in a Gaussian process with tunable parameters to account for the bias uncertainty for long TOF mitigates this issue:

## EUCLID Adjustment Visualization

Nuclear Data Adjustment to Benchmark Data by Augmented GLLS




Select Isotope to View: 094_Pu_239

# Team

Experiments Underpinned by Computational Learning for Improvements in nuclear Data

## 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

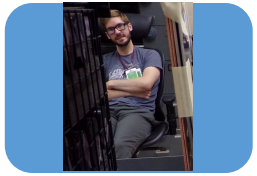
Isaac Michaud

Scott Vander Wiel

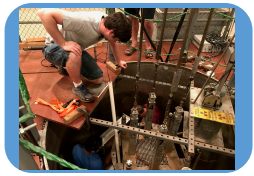
## Experiments

Theresa Cutler

Jesson Hutchinson



Travis Smith



Nicholas Thompson

# Summary

- EUCLID computed sensitivities of several integral responses to nuclear data,
- EUCLID leveraged existing tools, but new ones were also developed,
- EUCLID uses sensitivities for validation, finding where compensating errors could hide in our libraries, optimization of integral experiments and adjustment,
- We are happy to share our sensitivities after release and are establishing contact with the NEA about possible sharing these data through their tools to the community.

# Acknowledgements

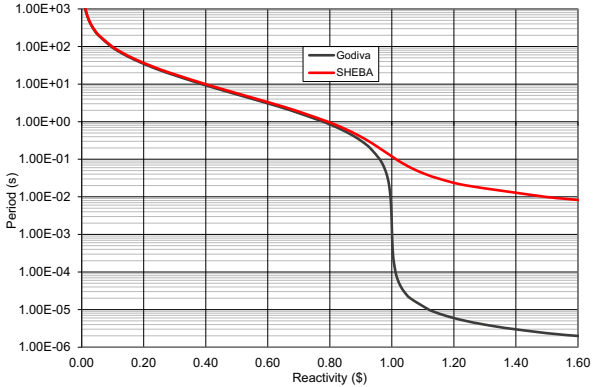

- Research reported in this publication was supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory.
- NCERC is supported by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.

# Backup

# Critical Experiments ($k_{eff}$ inference)


- At or very near delayed critical
- Convenient; uncertainties very small (~0.1%)
- Well understood
- Requires little inference
- Most common type of measurement in validation

$$\rho(\$) = \frac{\rho}{\beta_{eff}} = \frac{(k_{eff}-1)}{(k_{eff}\,\beta_{eff})} = \Lambda\omega + \sum_{i=1}^{6} \frac{\beta_i \omega}{\omega + \lambda_i}$$




- Sensitivity Simulation capabilities
  - KSEN (already developed and tested)
  - Whisper 1.1
  - Faust for analysis

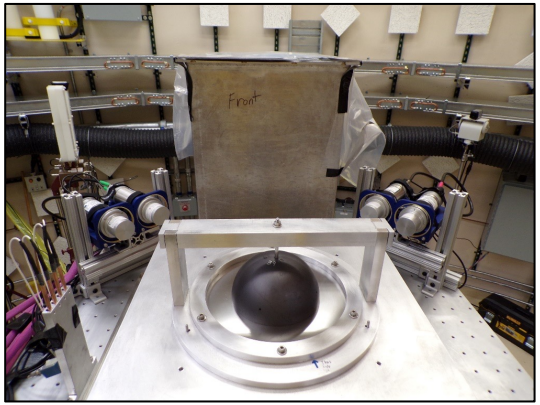
Critical experiments are the traditional metric for integral experiment response in nuclear data evaluation.

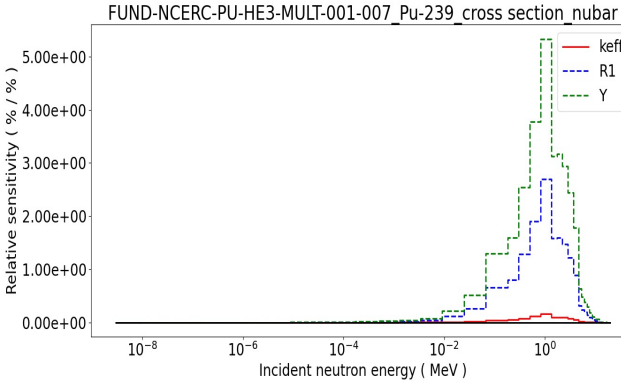
# Neutron noise experiments

- Description
  - Subcritical measurements
  - Greater Sensitivities to spontaneous fission nuclides

$$R_1 = \epsilon M_L \bar{\nu}_{S1} F_S$$

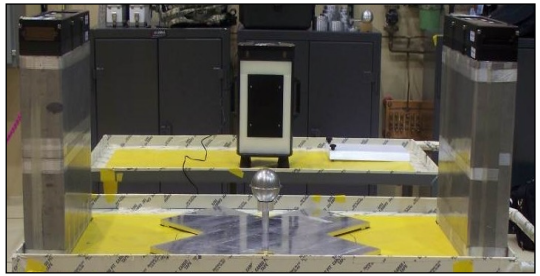
$$R_2 = \epsilon^2 M_L^2 F_S \left( \bar{\nu}_{S2} + \frac{M_L - 1}{\bar{\nu}_{I1} - 1} \bar{\nu}_{S1} \bar{\nu}_{I2} \right)$$




Sensitivity Simulation capabilities

- SENSMG
- Faust for analysis

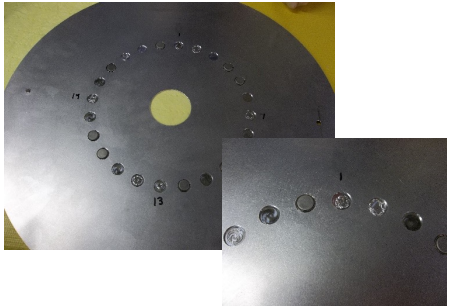


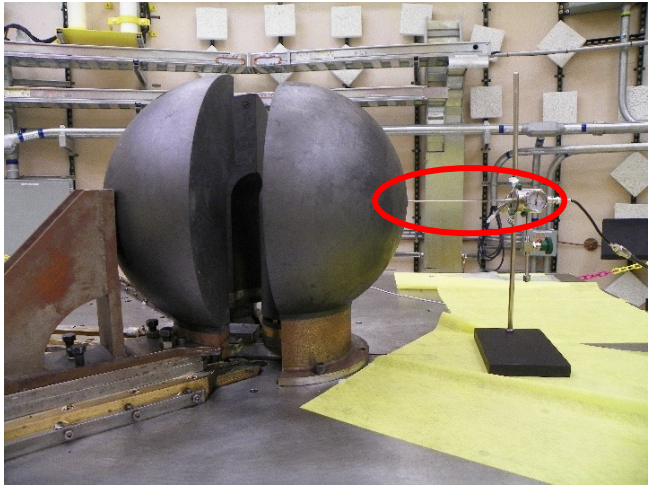
Neutron noise measurements have higher sensitivities to nuclides with significant spontaneous fission emission versus keff.

# Reaction Rate Ratios

- Description
  - comparison of reactions in two fissionable components
    - e.g. $^{239}$Pu(n,f)/ $^{235}$U(n,f)

$$\frac{\langle \sigma^x \rangle}{\langle \sigma^y \rangle} = \frac{\int \sigma^x(E)\,\psi(E)dE}{\int \sigma^y(E)\,\psi(E)dE}$$



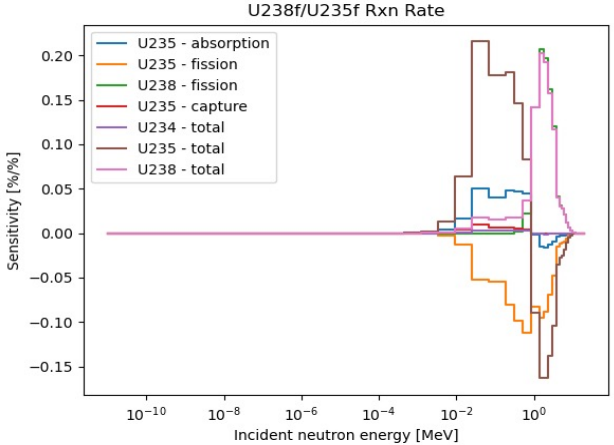


Sensitivity Simulation capabilities

SENSMG

New FSEN card in MCNP6 (developed under this project)

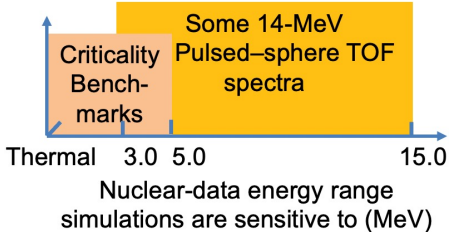
New portion of Faust for analysis

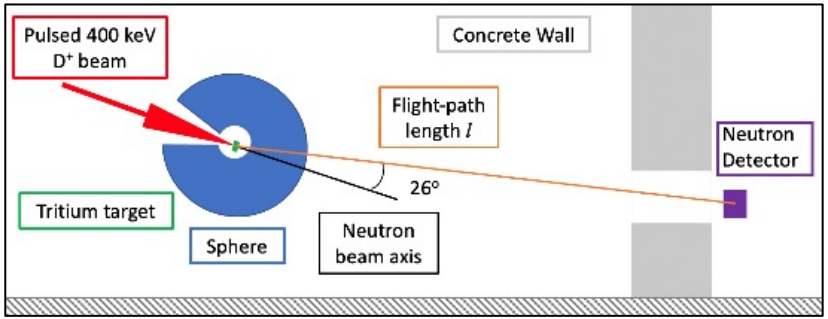



Reaction rate ratios are insensitive to the value of keff

# Pulsed Spheres

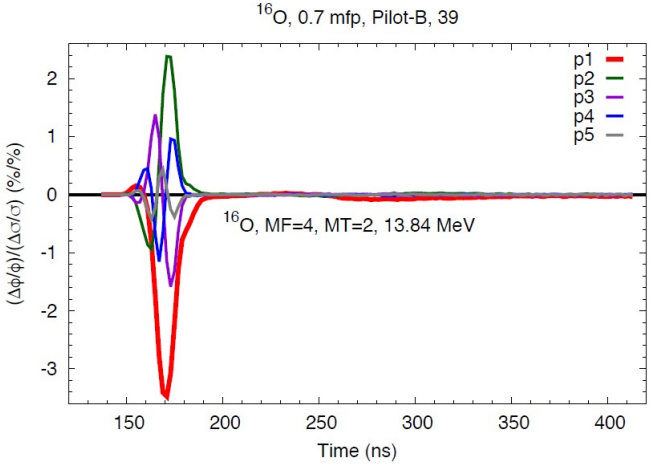
- Description
  - Decouple from fissionable isotope
  - Focus on nuclear data above 5-15 MeV
    - Dependent on thickness of material and level structure
  - High sensitivity to angular distributions and PFNS




Sensitivity Simulation capability

Faust, PERT or SANDY/ FRENDY

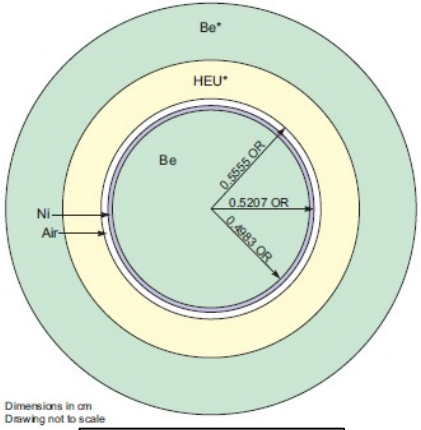



O-16 (n,el) angular sensitivity @ 13.84 MeV

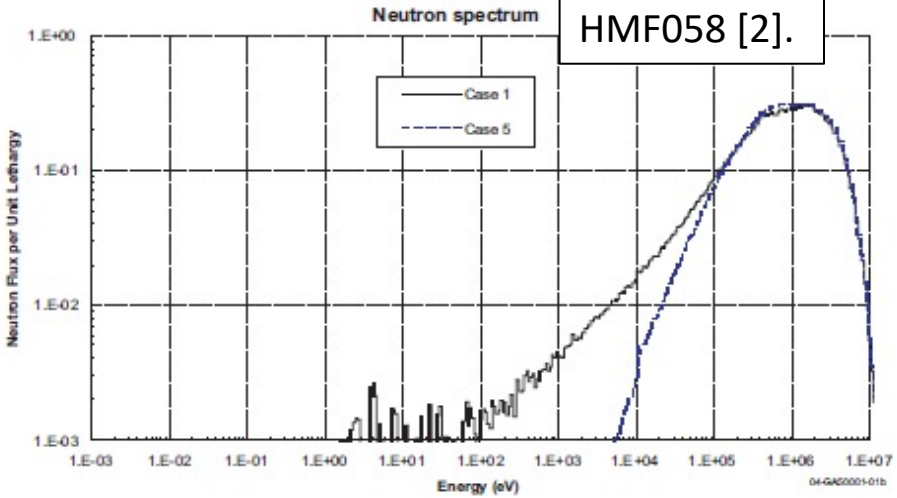
Pulsed spheres decouple sensitivity of fissionable and nonfissionable material, and significantly extend the energy range for validation.

# Gamma/ Neutron Leakage Spectra

- Description
  - Measure of the energy spectrum of the exterior of the assembly
  - Focus on gamma/ neutron energy measurements
  - Preferably subcritical system to not overwhelm detectors
  - Significant sensitivity to room return
- Sensitivity Simulation Capability
  - SENSMG
  - FSEN in MCNP6




HMF058 [2].




Leakage neutron spectra measurements focus on the energy of the neutrons, independent of keff

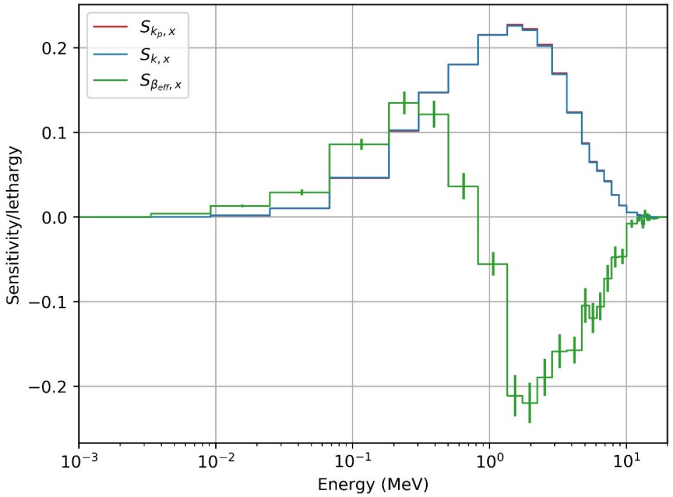
# Delayed Neutron Measurements

- Description
  - Inference of the delayed neutron fraction and groups
  - Converts measured system values (e.g. neutron e-folding time, neutron lifetime) to calculated system values (keff)
  - Determines how reliant the system is on neutrons released later in time, which makes it controllable

$$\beta_{eff} = 1 - \frac{k_p}{k_{eff}}$$

- Sensitivity Simulation Capabilities
  - Currently requires two separate simulations
    - Faust for analysis (written under this project)

$^{235}$U fission sensitivity

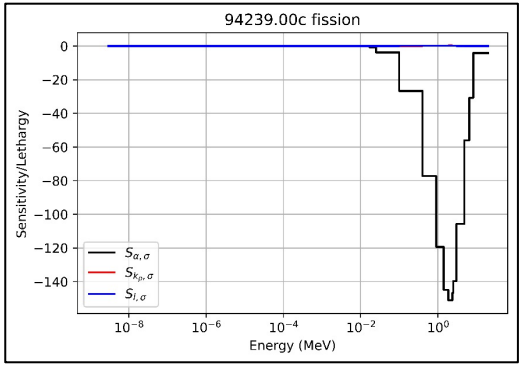



Delayed neutron sensitivities ($S_{\beta eff,x}$) exhibit very different sensitives than $k_{eff}$ ($S_{k,x}$) for the same reaction.

Prompt and delayed neutrons have different energies, resulting in unique sensitivity profiles which are different from other responses such as keff.

# Rossi-alpha Measurements

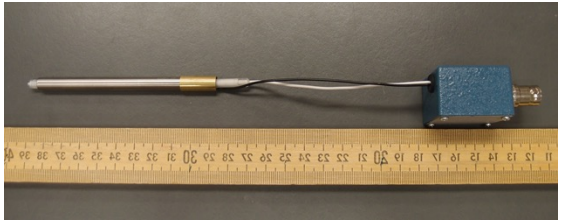
- Description
  - Measurement at delayed critical and slightly subcritical
  - rate at which the prompt neutron population changes as a function of time
  - used to infer parameter neutron lifetime, l.
  - Can be used to infer reactivity

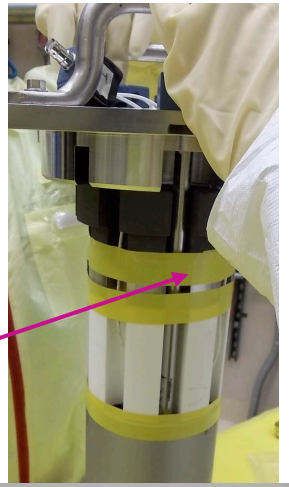



Sensitivity Simulation Capabilities

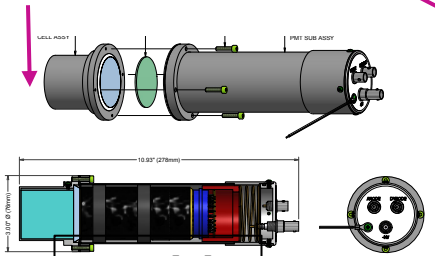
MCNP with PERT

Future: FSEN

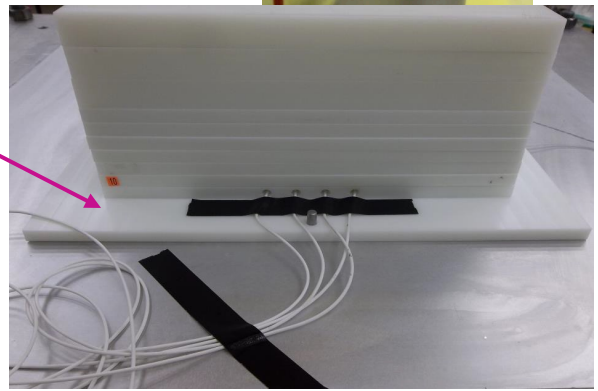




$$\alpha = \frac{k_p - 1}{l} = \frac{\beta - \rho}{\Lambda}$$



Eljen [3].



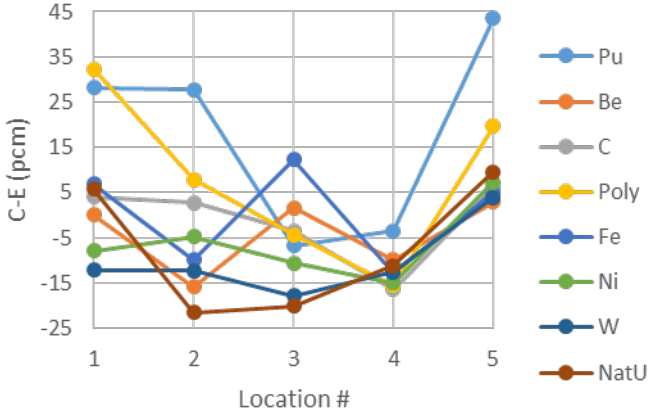
Rossi-alpha measurements probe the system lifetime, a key aspect of time dependent responses.

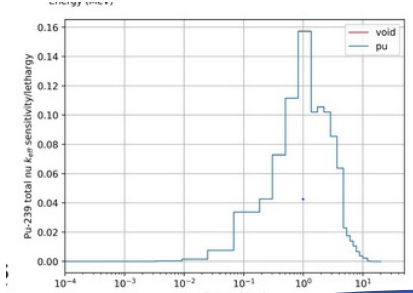
# Reactivity Coefficients

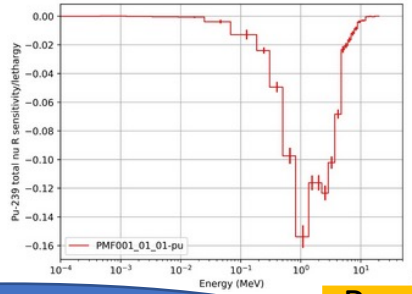
- Compare worth of a sample to worth of void in the location in the assembly
- Focused on effects from a small change (often 5-20 g)
- Removes some systematic unc

$$\Delta\rho_{a-b} = \left(\frac{1}{keff^{\,b}}\right) - \left(\frac{1}{keff^{\,a}}\right) = (\rho_a[\$] - \rho_b[\$])\beta_{eff}$$

Jezebel r.c. by radial position




Jezebel Pu sample: comparison of keff and $\Delta\rho_{a-b}$ sensitivity

## Sensitivity Simulation Capabilities

- Currently requires two separate simulations
- Faust for analysis (written under this project)

Reactivity coefficients remove some systematic uncertainties and show distinctly different sensitivities to keff

# Typical Uncertainties for the Various Measurement Methods

| Measurement Method | Typical Uncertainty (%) |
|---|---|
| Critical experiments | 0.1-0.5 |
| Neutron Multiplication Measurements | R1: 1-3,<br>R2 and Y: 2-9 |
| Reaction rate ratios | 0.9-2.0 |
| Pulsed Spheres | 5-10 |
| Gamma/Neutron Leakage Spectra | 3-20 (depending upon energy bin) |
| Delayed Neutron Measurements | 8 |
| Rossi-α | 1-3 |
| Reactivity Coefficient | 7 |

Values based on ICSBEP and IRPhEP benchmarks