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Title: The EUCLID Sensitivity Library

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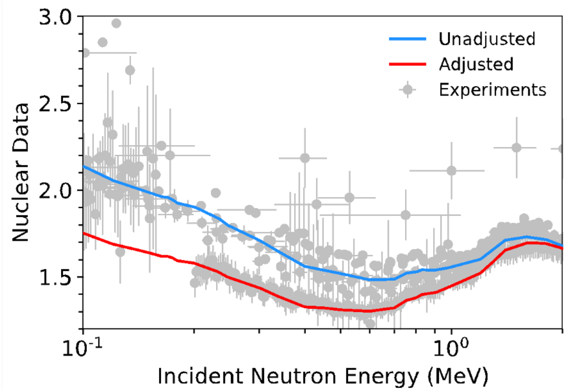

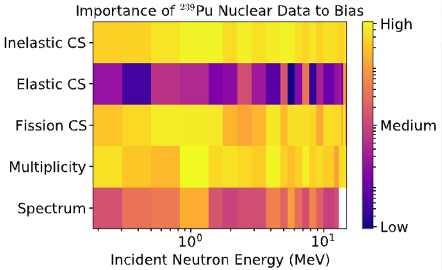

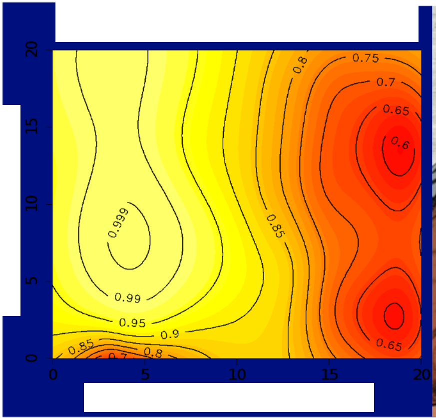

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The EUCLID Sensitivity Library

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

March 15, 2022 WPEC SG-46

LDRD

Team

Experiments
Underpinned by
Computational
Learning for
Improvements in nuclear
Data

- PI/Co-PIs in blue.
- Speakers in **bold underline**.

Nuclear Data

Wim Haeck

Michal Herman

Robert Little

Denise Neudecker

Simulations

Jennifer Alwin

Alexander Clark

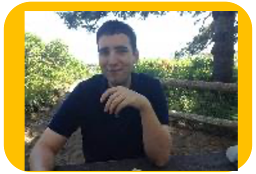
Juliann Lamproe

Michael Rising

Machine Learning

Michael Grosskopf

Noah Kleedtke



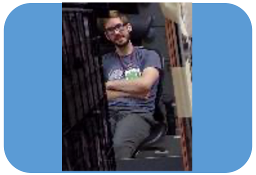
Isaac Michaud

Scott Vander Wiel

Experiments

Theresa Cutler

Jesson Hutchinson



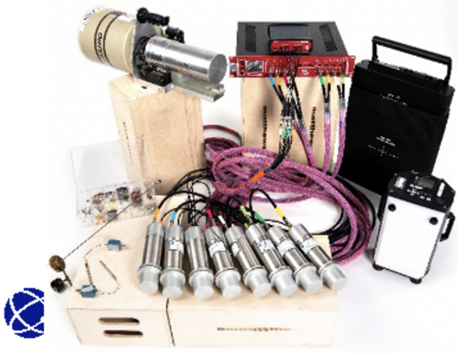
Travis Smith

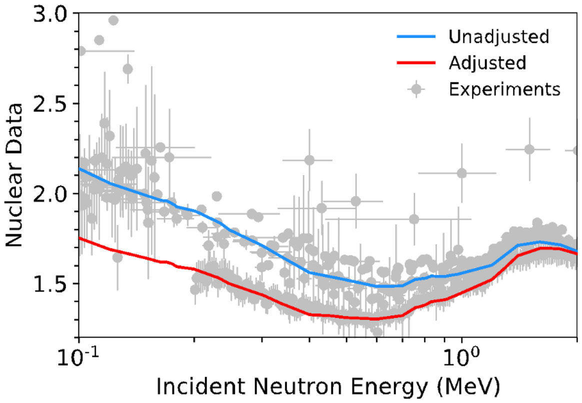
Nicholas Thompson

EUCLID aims to design validation experiments optimized to resolve compensating errors & adjust nuclear data to experiments

Neutron Transport Simulation (MCNP)

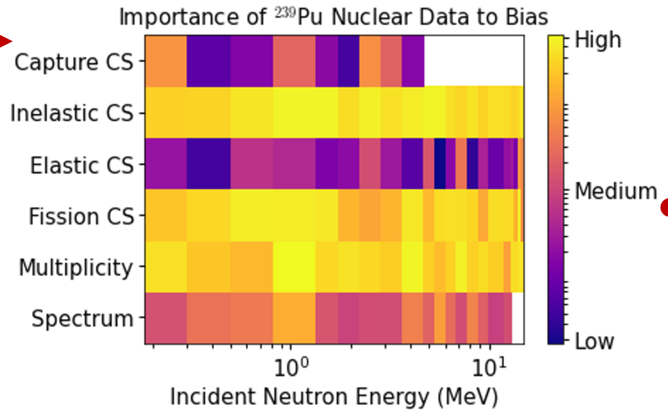
Validation Experiments



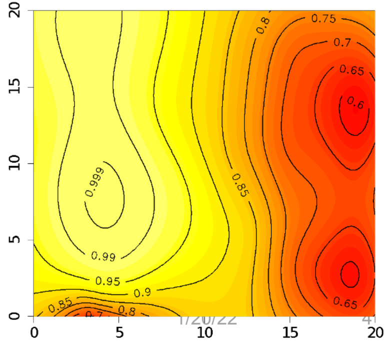


Experiment Refines Nuclear Data to Improve Simulations

ML-Augmented Search for Compensating Errors



ML-Optimally Designed Experiment to Resolve Compensating Errors



EUCLID provides sensitivities for many measurement responses. We are happy to share them through the NEA.

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 we will use to constrain nuclear data and tease out compensating errors.

We needed for EUCLID applications sensitivities for many different responses on the same grid and for the same observables -> made a sensitivity library.

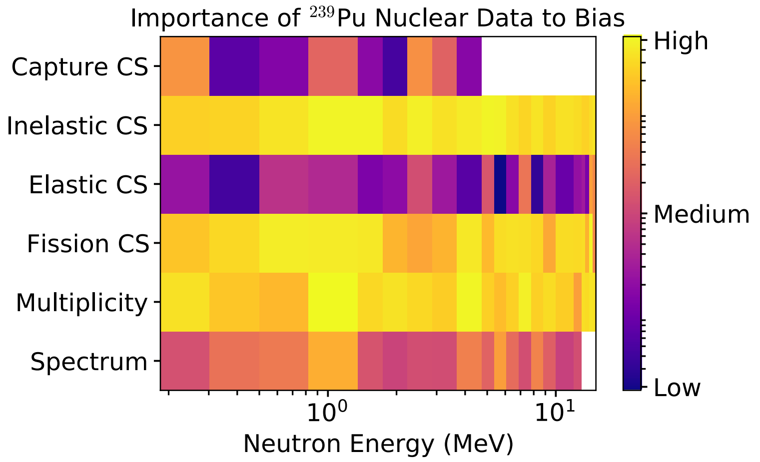
EUCLID Sensitivity Database

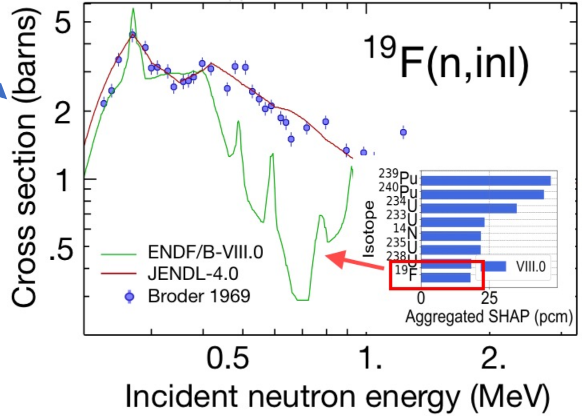
- Denise Neudecker: EUCLID use-cases for sensitivities (5 min)
- Sensitivities: (5 min each)
  - Wim Haeck: k_{eff}
  - Jennifer Alwin: reaction rates
  - Jesson Hutchinson: $beta_{eff}$
  - Theresa Cutler: reactivity coefficients
  - Noah Kleedtke: rossi alpha
  - Alex Clark: subcrits sensitivities
  - Alex Clark: LLNL pulsed-sphere neutron-leakage spectra
- Wim Haeck: Format and Library (10 min)
- Mike Rising: New capabilities for sensitivities (10 min)

EUCLID Use Cases for Sensitivities

Sensitivity database was used for large-scale validation and identifying unconstrained physics spaces with ML.

	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



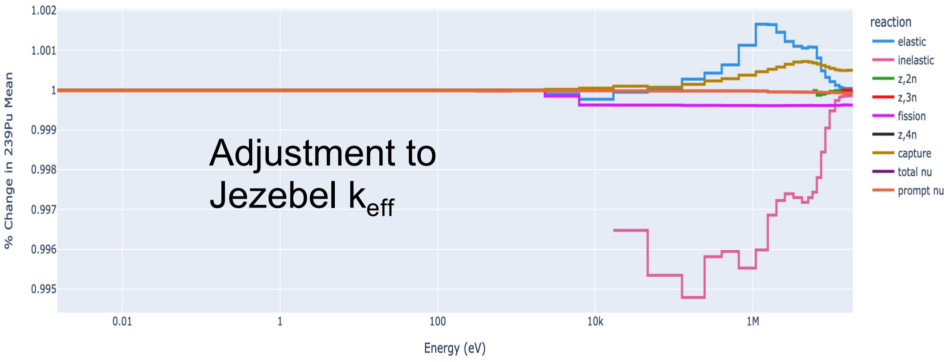


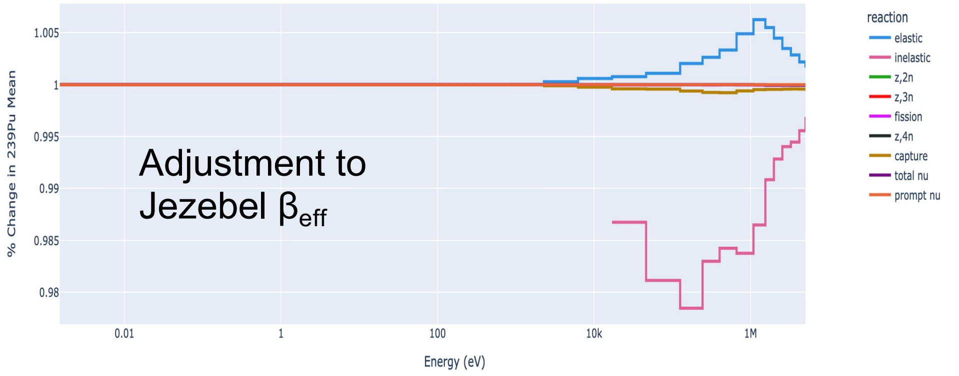
Similarly to NDAST, CRATER in FAUST uses sensitivities to quickly assess impact of ND changes on benchmarks.

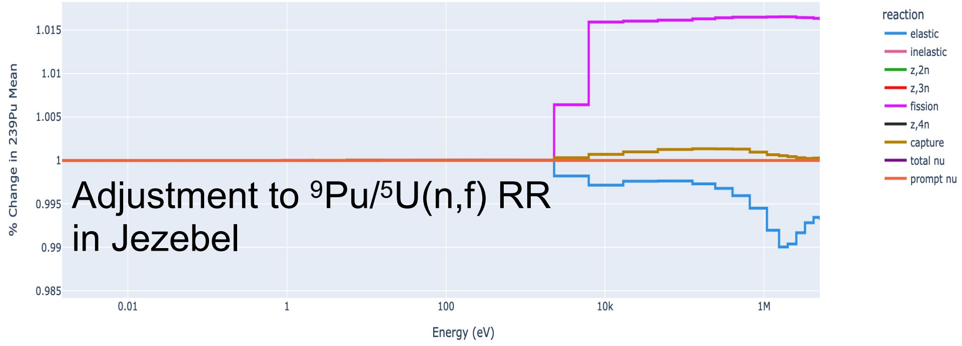
	FAUST & CRATER
Applies	1st-order forward-propagation
Input	integral responses and sensitivities
Output	impact of changes in nuclear data on simulated responses
Publication	W. Haeck, Trans. Am. Nucl. Soc. 123, 723 (2020)
Tool	Will eventually be open-source

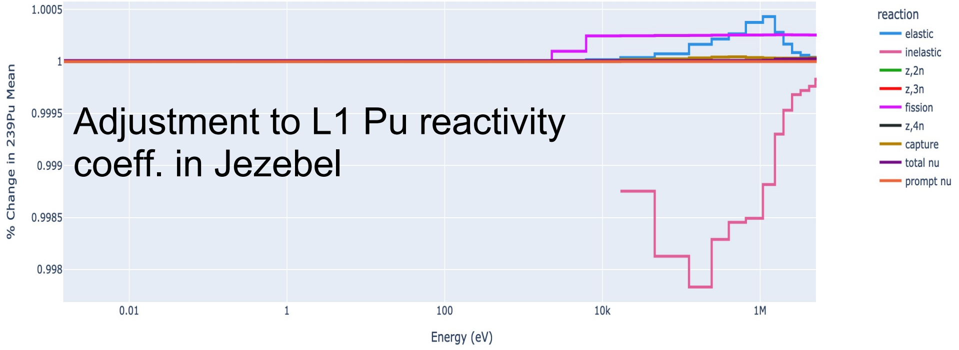
```
====    Pu239   ====
Modified reaction(s):  ['total nu']

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
```

Sensitivities for many responses enables adjustment with respect to them -> Might reduce compensating errors.



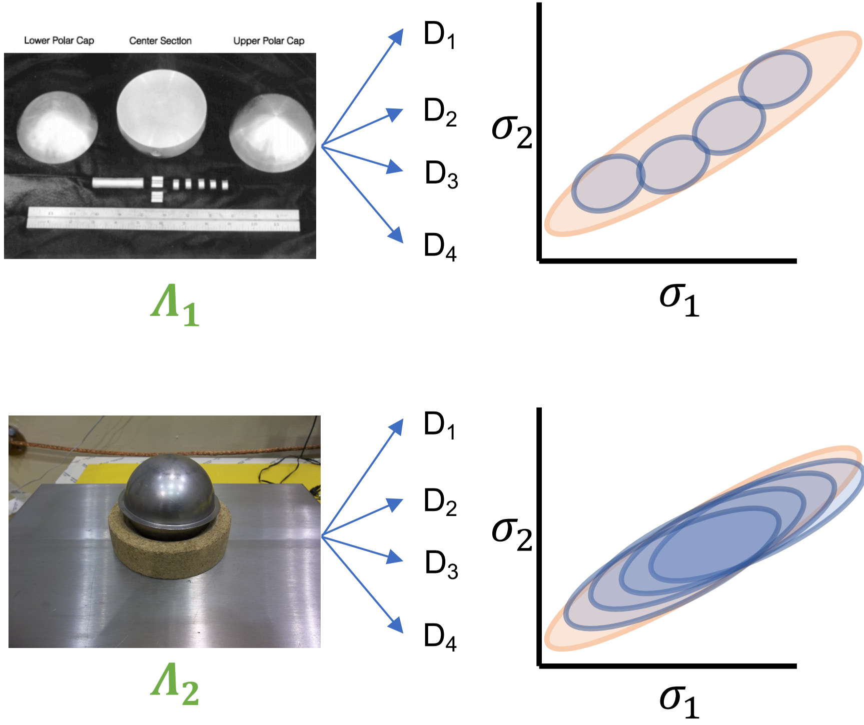






EUCLID also uses the sensitivities for experiment design.

- Goal: design integral experiment optimized to constrain nuclear data or application?
- Combining statistical design of experiments with ML-driven design optimization
- Sensitivities are used for
  - Incorporating all information from ENDF/B-VIII.0 and previous integral data into an optimization via adjustment,
  - Quantifying impact of proposed experiments on nuclear data adjustment/validation

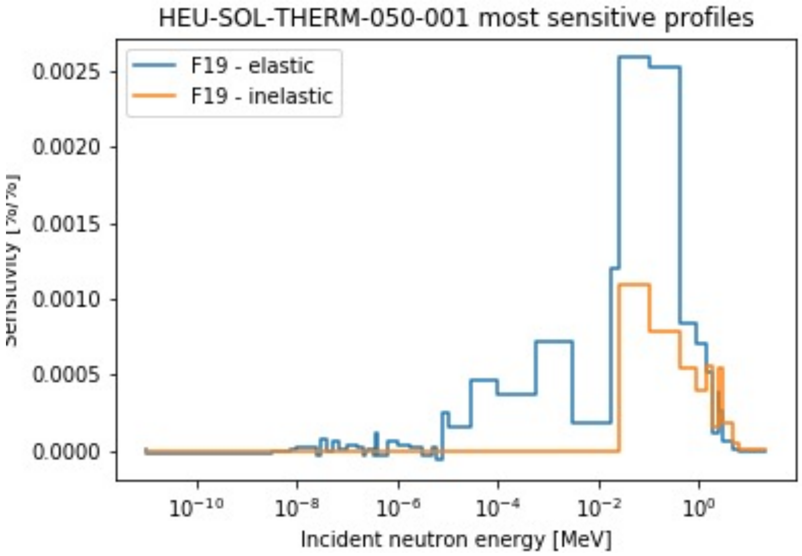


Sensitivities

Effective multiplication factor sensitivity profiles

- Sensitivity profiles for ~1100 ICSBEP benchmarks
  - Calculated using KSEN in MCNP6
  - Using the official ENDF/B-VIII.0 ACE library at 293.6 K

- Other available results
  - Values for k_{eff}, β_{eff} and Λ_{eff}
  - Three group spectra
  - Fission fractions
  - Average energy causing fission
  - Energy of the average lethargy causing fission



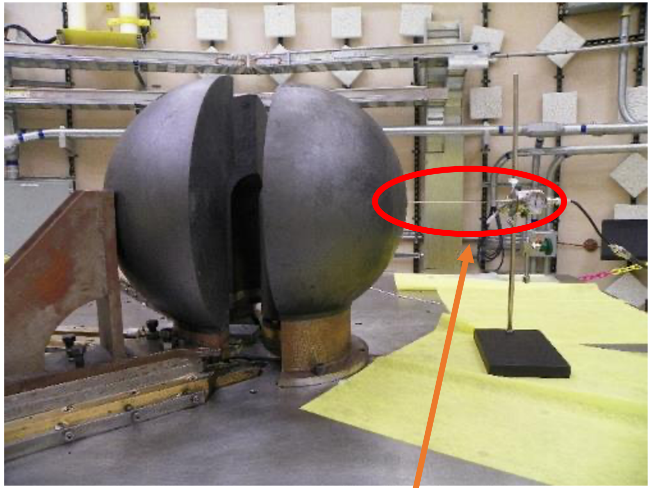
Reaction rate sensitivities: what is being measured?

Reaction rate ratios measure of spectrum, referred to as spectral index:

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

R … reaction rate ratio, V… problem volume
r … point within V, G … no. of energy groups,
$\Sigma_1^g(r), \Sigma_2^g(r)$ … reaction cross sections, and
$\phi^g(r)$ … scalar flux in g at r

We studied: ^{233}U(n,f)/^{235}U(n,f), ^{238}U(n,f)/^{235}U(n,f), ^{237}Np(n,f)/^{235}U(n,f), ^{239}Pu(n,f)/^{235}U(n,f) for HMF001, HMF028, PMF001, PMF006



Fission Chamber

Foils

Reaction rate sensitivities: How did we get sensitivities?

Use SENSMG to calculated sensitivities:

- 1st order sensitivities using Generalized Perturbation Theory using PARTISN multigroup discrete-ordinates code.
- 1-D spherical or slab & 2-D cylindrical geometries

Used MCNP6.2 to calculate flux in central region of assembly

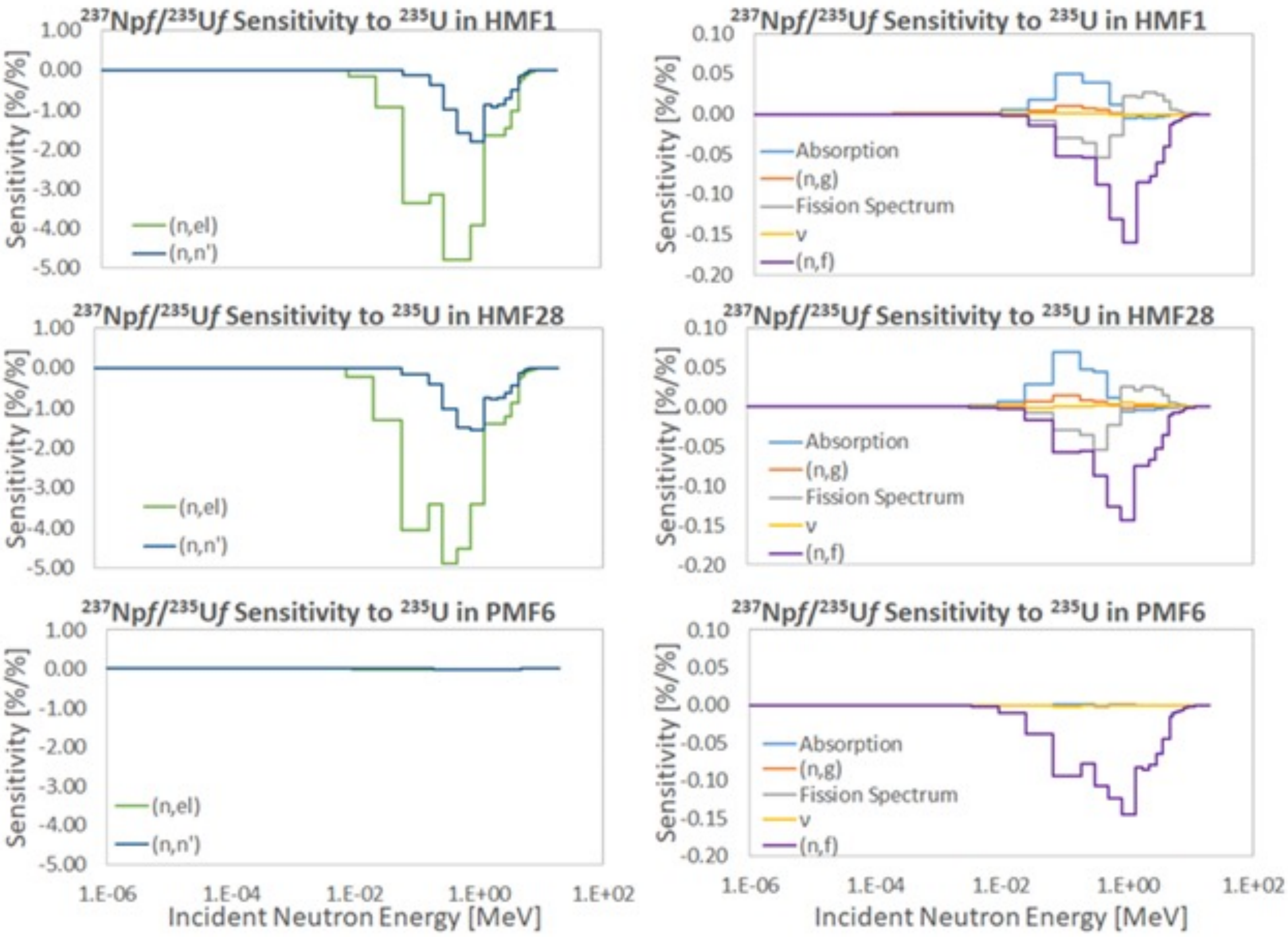
$S_{R,x}$ … total 1st order sensitivity of R to reaction x = sum of the relative sensitivity over energy groups

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

$$S_{R,x}^{g} = \frac{\sigma_{x,0}^{g}}{R_0} \frac{\partial R}{\partial \sigma_x^g} \Big|_{\sigma_x^g = \sigma_{x,0}^g}$$

Reaction rate sensitivities: Example

- $^{237}Np/^{235}U$ spectral index sensitivities to ^{235}U
- ^{235}U not present in PMF6 fuel only reflector



Beta-eff sensitivities: what is beta-eff?

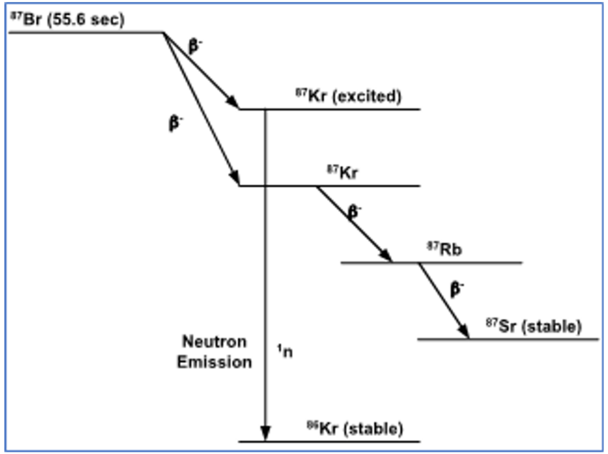
- The effective delayed neutron fraction (β_{eff}) is the effective number of delayed neutrons (neutrons born through fission product decay after fission).
- The "effectiveness" refers to delayed neutrons being born at different energies than prompt neutrons.
- Important for reactor operations.

- One way to simulate β_{eff}

$$\beta_{\text{eff}} = 1 - \frac{k_p}{k}$$

k_p ← Simulation without delayed neutrons

k ← Simulation with delayed neutrons



Beta-eff sensitivities: How did we get sensitivities?

- Start with a basic definition $S_{\beta_{\text{eff}},x} = \frac{\partial \beta_{\text{eff}}}{\beta_{\text{eff}}} \frac{x}{\partial x}$
- This becomes $S_{\beta_{\text{eff}},x} = \frac{k_p}{k - k_p}\left[S_{k,x} - S_{k_p,x}\right]$
- Which means we can solve for the sensitivity as a function of the *k* and k_p sensitivities

$$\sigma_{S_{\beta_{\text{eff}},x}} = \left[\sum_i \left(\frac{\partial S_{\beta_{\text{eff}},x}}{\partial p_i}\right)^2 \text{Var}(p_i) + \sum_i \sum_{j \neq i} \left(\frac{\partial S_{\beta_{\text{eff}},x}}{\partial p_i} \frac{\partial S_{\beta_{\text{eff}},x}}{\partial p_j}\right) \text{Cov}(p_i, p_j)\right]^{\frac{1}{2}}$$

$$\frac{\partial S_{\beta,x}}{\partial k} = \frac{k_p(S_{k_p,x} - S_{k,x})}{(k - k_p)^2} = \frac{k_p(S_{k_p,x} - S_{k,x})}{k^2\beta^2}$$

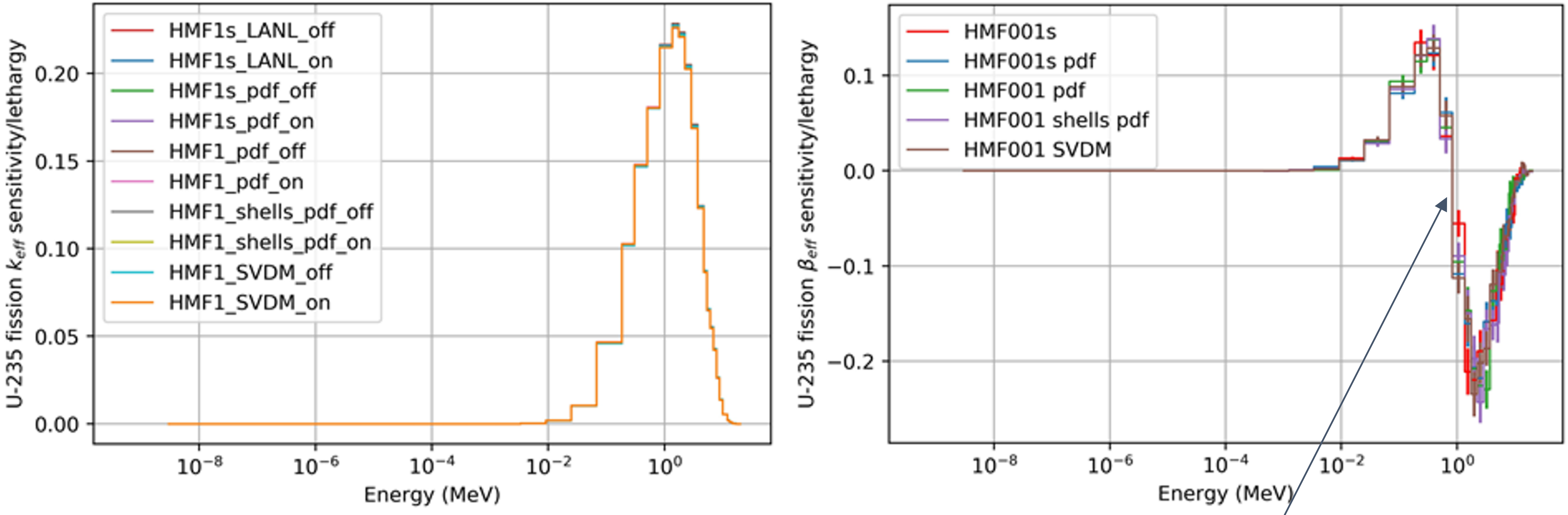
$$\frac{\partial S_{\beta,x}}{\partial k_p} = \frac{S_{k,x} - S_{k_p,x}}{k\beta^2}$$

$$\frac{\partial S_{\beta,x}}{\partial S_{k,x}} = \frac{k_p}{k - k_p} = \frac{k_p}{k\beta}$$

$$\frac{\partial S_{\beta,x}}{\partial S_{k_p,x}} = \frac{k_p}{k_p - k} = -\frac{k_p}{k\beta}$$

Given that k and kp are typically ~1, this is just $1/\beta_{\text{eff}}$. Since β_{eff} is very small, this results in a large number. This term will dominate the total uncertainty.

Beta-eff sensitivities: Example

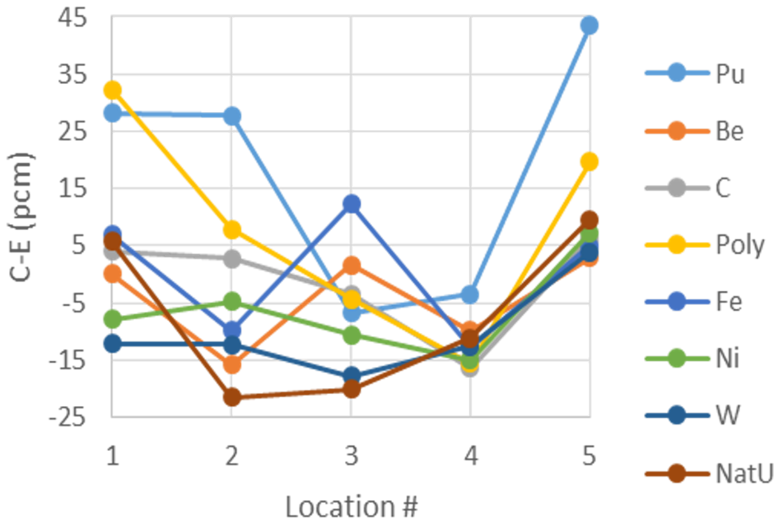


- This graph goes drops steeply between 500 keV to 1.35 MeV
- 500 keV is where the number of delayed neutrons dramatically decreases

Reactivity coefficient sensitivities: what is being measured?

- comparison of reactivity (or delta-keff) at two different states
  - difference between void and small sample in the same location
- small perturbation is localized and thus does not affect the spectra or flux of the entire assembly
- Key aspect: removes some systematic uncertainties

Jezebel r.c. by radial position



Reactivity coefficient sensitivities: How did we get sensitivities?

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

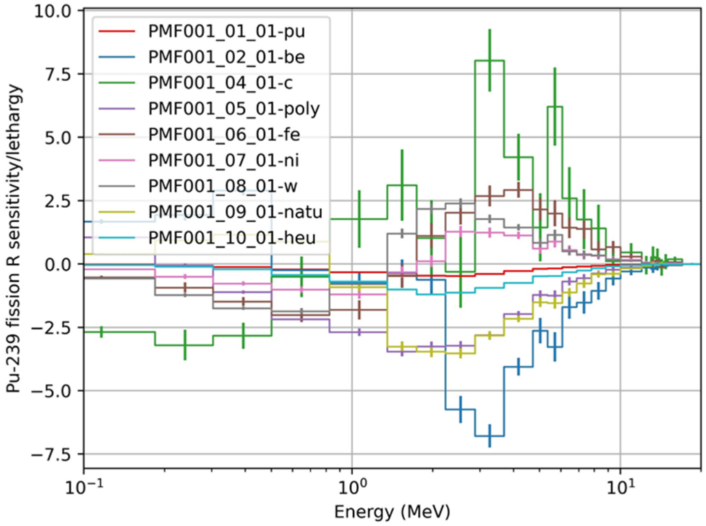
simulated measured

- Sensitivity simulation
  - requires two separate simulations, one with void and one with sample
- Analysis method
  - Faust (new portion)
- Testing and validation
  - Jezebel
  - Lady Godiva

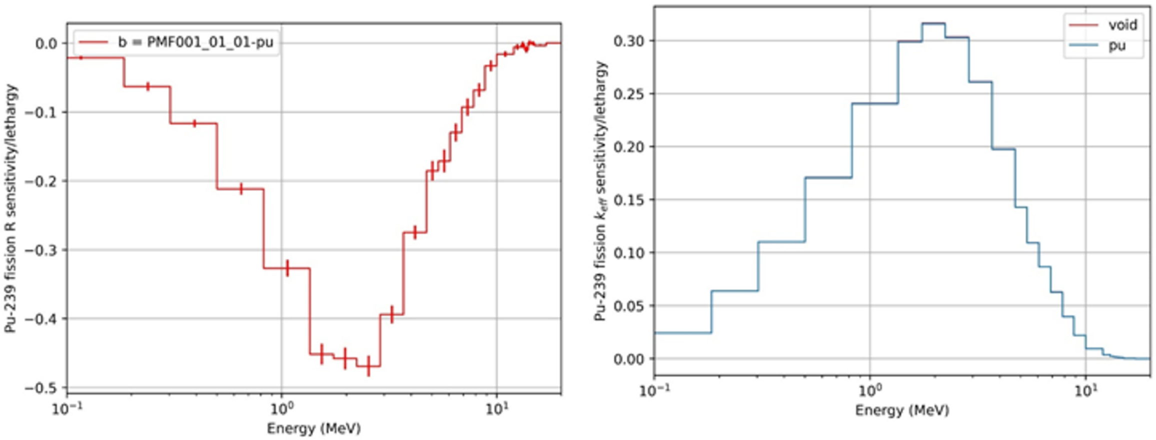
$$S_{k,x} = \frac{\frac{\Delta k}{k}}{\frac{\Delta x}{x}}$$

$$S_{\Delta\rho_{a-b},x} = \frac{\frac{S_{k_a,x}}{k_a} - \frac{S_{k_b,x}}{k_b}}{\Delta\rho_{a-b}}$$

Reactivity coefficient sensitivities: Example



Sensitivity to Pu239, Fission xs, Center



Pu239 sample, reactivity coefficient sensitivity vs keff sensitivity

Prompt Neutron Decay Constant Sensitivity: What is being measured?

Objective: Simulate Experimental Uncertainty in Prompt Neutron Decay Constant

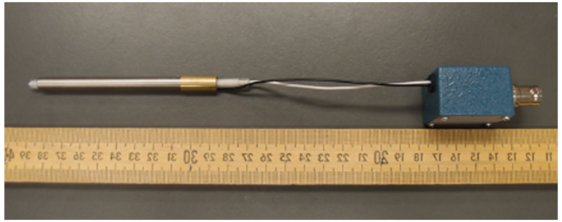
Validation: Rossi-α Measurement

Theory: Prompt Neutron Decay Constant

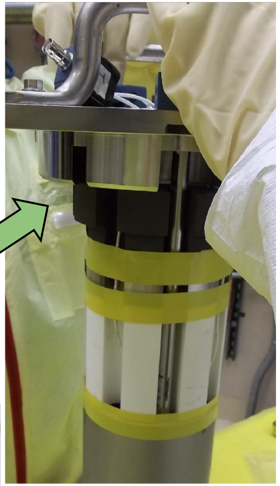
$$\alpha = \frac{k_p - 1}{l}$$

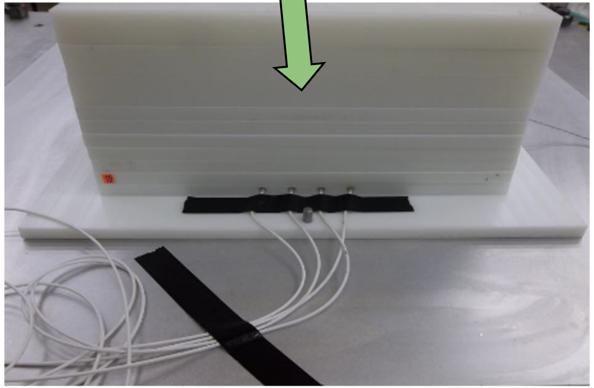
k_p = Prompt Neutron Multiplication Factor, l = Mean Neutron Lifetime

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



Experimental Capability:
He-3 detectors
Organic Scintillators





Prompt Neutron Decay Constant Sensitivity: How did we calculate sensitivity?

Relative Sensitivity Coefficient of Prompt Neutron Decay Constant α to Cross Section Data σ can be written as

$$S_{\alpha,\sigma} = \frac{\partial\alpha}{\alpha}\frac{\sigma}{\partial\sigma}$$

$$S_{\alpha,\sigma} = \rho_p^{-1} S_{k_p,\sigma} - S_{l,\sigma}$$

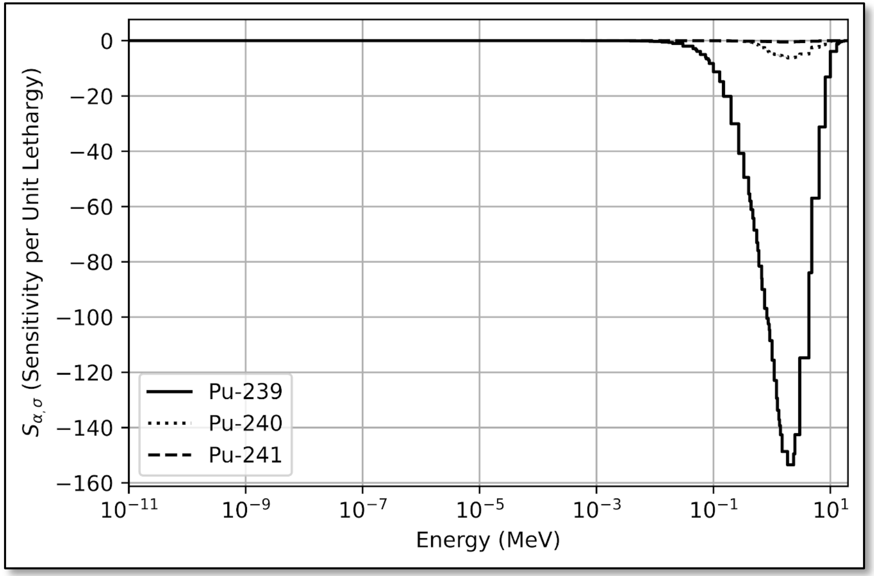
$\rho_p = \frac{k_p - 1}{k_p}$ Prompt Reactivity

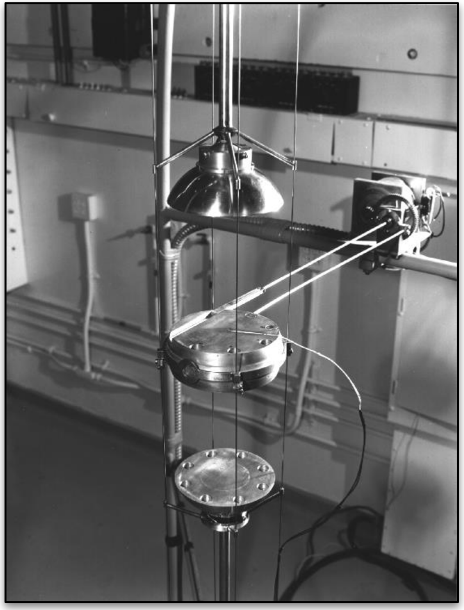
$S_{k_p,\sigma}$ Relative Sensitivity Coefficient of Prompt Neutron Multiplication Factor to Cross Section Data

$S_{l,\sigma}$ Relative Sensitivity Coefficient of Mean Neutron Lifetime to Cross Section Data

Prompt Neutron Decay Constant Sensitivity: Jezebel (PU-MET-FAST-001) Example

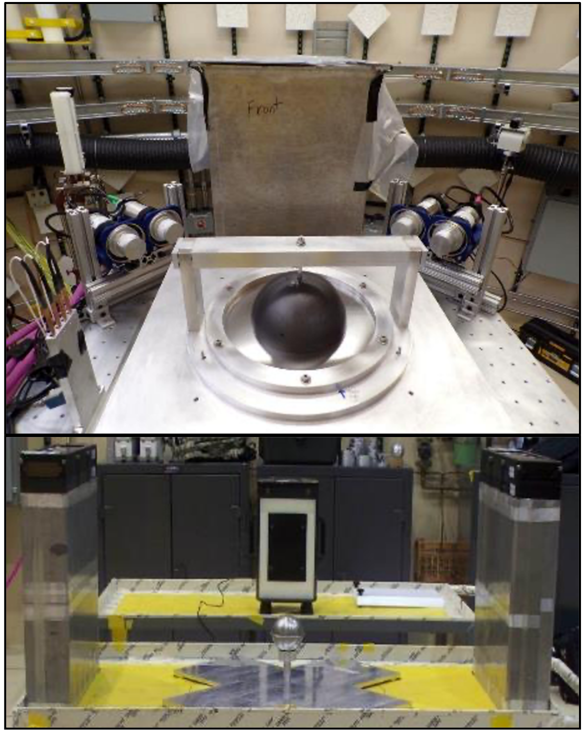
Relative Sensitivity Coefficients of Prompt Neutron Decay Constant to Pu (n,f) Cross Section (52-group Energy Structure)





Sub-crit sensitivities: what is being measured?

- Description
  - Use non-destructive analysis to infer integral properties of SNM (M_L, S_F, (α, n))
    - Gross neutron counting
    - Neutron multiplicity counting
    - Gamma spectroscopy
  - Compare to critical benchmarks
    - Small scale
    - Fissile core surrounded by reflector/moderator material
    - Fission chains initiate but die away (keff < 1)
- Experiment capabilities
  - NoMAD neutron multiplicity counters
  - Organic scintillators



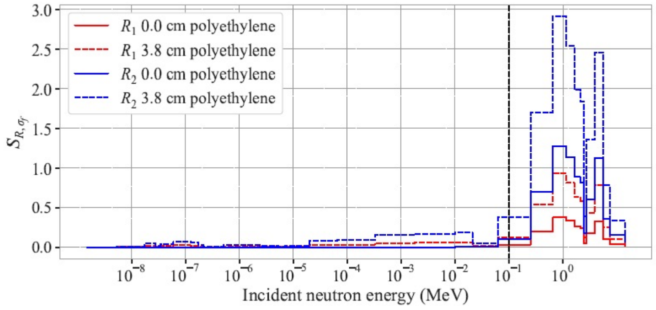
MUSiC experiment (top) and FUND-NCERC-PU-HE3-MULT-001 (BeRP-nickel) benchmark (bottom).

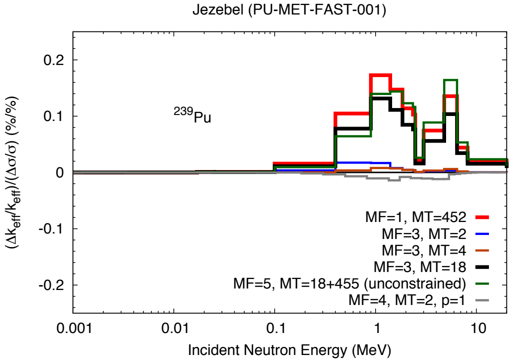
Sub-crit sensitivities: How did we get sensitivities?

- Compute R_1 (mean neutron count rate) using standard forward/adjoint Boltzmann neutron transport equations
  - $L\psi = Q$
  - $L^*\psi_1^* = Q_1^*$
  - $R_1 = \langle\psi, Q_1^*\rangle = \langle\psi, \sigma_d\rangle$
- Compute R_2 (related to NMC distribution variance) using second moment of solution to Muñoz-Cobo's stochastic transport equation
  - $L^*\psi_2^* = Q_2^*$
  - $R_2 = \langle\psi, Q_2^*\rangle + \left\langle S, Q_{2,sf}^*\right\rangle$
- Compute sensitivities via adjoint-based approach
  - $\frac{\partial R_1}{\partial\alpha} = \left\langle\frac{\partial Q_1^*}{\partial\alpha}, \psi\right\rangle + \left\langle\psi_1^*, \frac{\partial Q}{\partial\alpha} - \frac{\partial L}{\partial\alpha}\psi\right\rangle$
  - $\frac{\partial R_2}{\partial\alpha} = \left\langle\psi_2^*, \frac{\partial Q}{\partial\alpha} - \frac{\partial L}{\partial\alpha}\psi\right\rangle + 2\left\langle\Phi, \frac{\partial Q_1^*}{\partial\alpha} - \frac{\partial L^*}{\partial\alpha}\psi_1^*\right\rangle + \left\langle\frac{\partial Q_2^*}{\partial\beta}, \psi\right\rangle + \left\langle\frac{\partial Q_{2,sf}^*}{\partial\beta}, S\right\rangle + \left\langle Q_{2,sf}^*, \frac{\partial S}{\partial\alpha}\right\rangle$

Sub-crit sensitivities: Example

- More sensitive to nuclear data compared to critical benchmarks
- Have sensitivity to higher-order $P(\nu, E)$ moments ($\overline{\nu} = \sum_{\nu=1}^{\nu_{max}} \nu P(\nu, E)$)
- Sensitivity capability
  - SENSMG
  - Faust (post-processing)

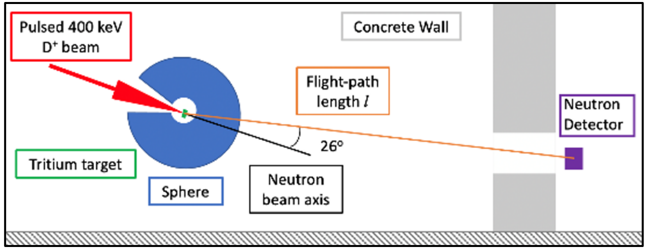


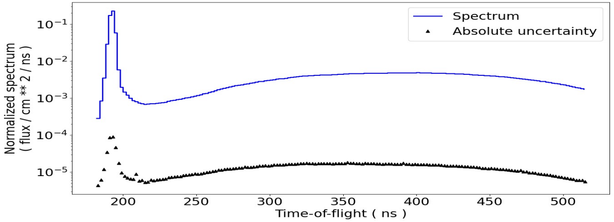


Sensitivity of (top) NMC distribution moments from PU-MET-FAST-038 (BeRP-polyethylene) to the Pu-239 fission cross section and (bottom) keff from PU-MET-FAST-001 (Jezebel) to various Pu-239 nuclear data.

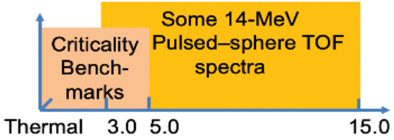
LLNL pulsed sphere sensitivities: what is being measured?

- Description
  - Measured neutron TOF leakage spectra are useful for nuclear data validation
  - D-T reaction produces 14-MeV neutrons that propagate through pulsed sphere
  - Detectors placed at angles w.r.t. the deuteron beam observe varied TOF spectra
  - Spectra are highly sensitivity to scattering angular distributions and PFNS
  - Composed entirely of fissile or non-fissile material
- Experimental Capability
  - D-T generator
  - Organic scintillator detectors





Schematic of LLNL pulsed sphere measurement (top) and neutron TOF leakage spectra from plutonium pulsed sphere measurement (bottom; pu0.7b)



Nuclear-data energy range simulations are sensitive to (MeV)

LLNL pulsed sphere sensitivities: How did we get sensitivities?

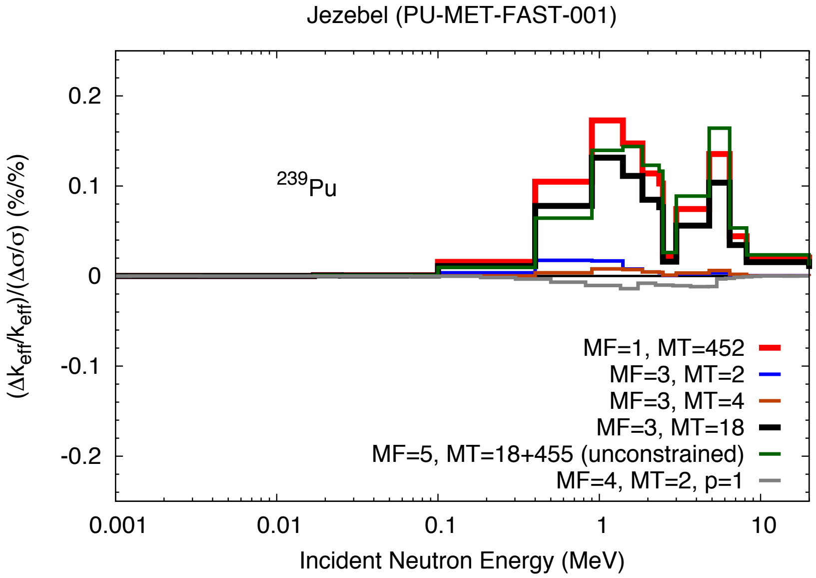
- Sensitivity of pulsed-sphere TOF spectrum to group-wise nuclear data is defined as

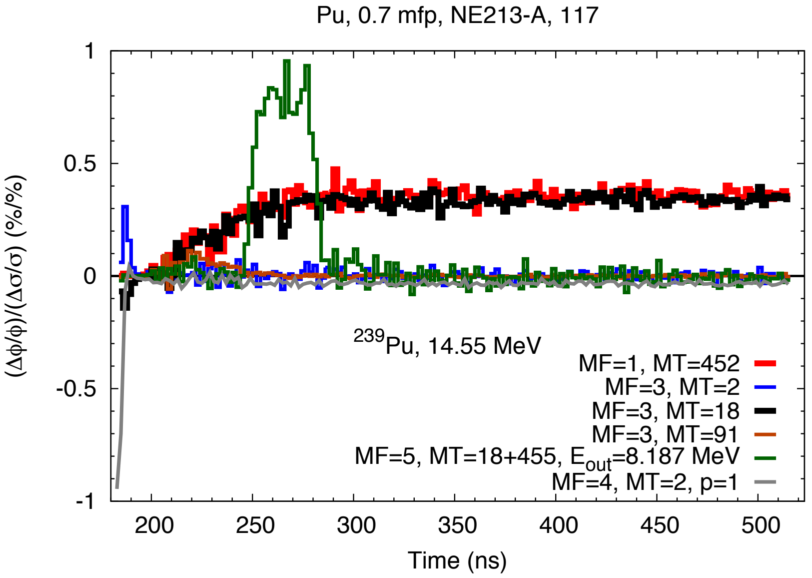
$$S_{R_t,\alpha_g} = \frac{\alpha_{g,0}}{R_t|_{\alpha=\alpha_{g,0}}} \frac{\partial R_t}{\partial \alpha_g}\Big|_{\alpha=\alpha_{g,0}}$$

  - $R_t =$ Time-of-flight spectrum at time bin t
  - $\alpha_g =$ Nuclear data parameter at group g
- Sensitivity can be numerically estimated to second-order in perturbation size with central-differences

$$S_{R_t,\alpha_g} = \frac{\alpha_{g,0}}{R_t|_{\alpha=\alpha_{g,0}}} \frac{R_t|_{\alpha=\alpha_{g,0}+\Delta\alpha_g} - R_t|_{\alpha=\alpha_{g,0}-\Delta\alpha_g}}{2\Delta\alpha_g} + \mathcal{O}(\Delta\alpha^2)$$

LLNL pulsed sphere sensitivities: Example





1. D. Neudecker, O. Cabellos, A. R. Clark et al, "Which nuclear data can be validated with LLNL pulsed-sphere experiments?," Ann. Nuc. En. (2021)

Format and Database

Calculation and experimental results

- A calculation result consists of two distinct components
  - Attributes (or metadata) that give information about the result
    - What type of result is it?
    - What nuclide and reaction is it for (if it is a reaction rate)?
    - What volume is it for (if it is a particle spectrum)?
    - Which code and version produced the result?
    - Which nuclear data library was used to produce the result?
    - <u>This is what we will want to search and filter on</u>
  - The actual calculation result
    - Values for the result: a single value, an array of values, an array of arrays of values, etc.
    - Optional uncertainties: in the same form as the values for the result
    - The structure of the result: a histogram of flux values as a function of incident energy, etc.
    - Optional units for the values and uncertainties
    - <u>This is what we will want to compare, store, exchange, plot, etc.</u>

A simple json format

```
[ { 'type' : 'effectiveMultiplicationFactor',
    'data' : { 'values' : [ 1.0000 ],
               'uncertainties' : [ 0.0001 ] } },
  { 'type' : 'sensitivityProfile',
    'response' : 'effectiveMultiplicationFactor',
    'parameter' : 'crossSection',
    'particleId' : 'neutron',
    'nuclide' : 'U235',
    'reaction' : 'fission',
    'material' : 'total',
    'data' : { 'values' : [ -1.7129e-17, 1.4106e-09 ],
               'uncertainties' : [ 0.0034, 0.0033 ],
               'structure' : [ { 'name' : 'energy-in',
                                 'type' : 'histogram',
                                 'limits' : [ 1e-11, 10.0, 20.0 ],
                                 'unit' : 'MeV'} ],
               'units' : { 'value' : '%/%', 'uncertainty' : 'relative' } } }
```

Attributes describe the data

The actual data for the result

Attributes

- `type` is an essential attribute and should be always be present
  - Indicate the type of result we're storing
  - Possible values that are currently identified:

    `effectiveMultiplicationFactor`, `effectiveDelayedNeutronFraction`, `effectiveNeutronGenerationTime`, `thermalFissionFraction`, `aboveThermalFissionFraction`, `averageEnergyCausingFission`, `energyAverageLethargyFission`, `particleSpectrum`, `particleFlux`, `particleCurrent`, `reactionRate`, `sensitivityProfile`
- Some attributes will appear based on the value of type
  - For example, for `sensitivityProfile` :
    - `response` : for which "response function" we have a sensitivity $\partial r/\partial p$, e.g. keff
    - `parameter` : the sensitivity of the response is given with respect to a parameter
    - `nuclide` : the nuclide for which a sensitivity profile is given
    - `reaction` : the reaction for which the sensitivity profile is given, e.g. fission, n,gamma
    - `material` : the material in the model for which the sensitivity is given

Attributes

- Some attributes could appear based on the application but should be independent of the value of type
  - For example:
    - `code` : which calculation code generated the result, e.g. `mcnp`, `cog`, `partisan`, `ardra`
    - `date` : the calculation date
    - `library` : the nuclear data library, e.g. `endf/b-viii.0`
    - `temperature` : the temperature of the material for which the result is given

- The way attributes are stored and defined makes it flexible enough for extension
  - Retrieving a non-existent attribute is NOT an error, it is simply undefined
  - This allows for filters to function properly

Data

- As indicated earlier, a calculation result consists of the following:
  - A one dimensional array of `values`, this is always present
  - An optional one dimensional array of `uncertainties`
  - The `structure` of the `values` and `uncertainties`
    - This is a list of dimensions that defines how to interpret the the `values` and `uncertainties`
    - This is not required if the `values` array contains a single value
  - An optional set of `units`, one for a `value` and another one for an `uncertainty`

- `values` and `uncertainties` are always an array
  - This even applies to a single value (every result needs to look like another one)

Dimensions and the structure of the result

- The structure of a result is made up of dimensions, defined by:
  - `name` : the name for the dimension, e.g. `energy-in`
  - `type` : the type of the dimension, either `histogram` or `points`
  - `limits` : the bins or points for which we have data in the current dimension
  - `unit` : an optional unit for the dimension
- A one dimensional result will have only one dimension, and so on
  - A particle spectrum integrated over a given number of energy bins has one dimension
  - A 2D sensitivity profile will have an incident and outgoing energy dimension
  - The order of the dimensions determines the order of the values (obviously)
- The number of values and uncertainties is directly linked to the dimension
  - Dimensions must be present as soon as there is more than 1 value in the arrays
- The dimension type can be mixed over multiple dimensions

Python interface

```
# retrieve attribute information with the 'attributes' property on Result
type = result.attributes.type            # 'sensitivityProfile'
nuclide = result.attributes.nuclide      # '92235'
reaction = result.attributes.reaction    # 'fission’
date = result.attributes.date            # None, 'date' attribute is not present

# retrieve the data
values = result.values                   # result.data.values also works here
groups = result.structure[0].limits
valueUnit = result.units.value

# data can also be retrieved through its own property
data = result.data
values = data.values
groups = data.structure[0].limits
valueUnit = data.units.value
```

Formal description of the format

- 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

New Capabilities for Sensitivities

Developing New Sensitivity Capabilities within the MCNP6 Code

- From experience with the k-effective adjoint-weighted sensitivity method (KSEN) and the differential operator sensitivity method (PERT) in MCNP, inline sensitivity/perturbation capabilities typically have distinct differences with external methods
  - More efficient to calculate
  - Less prone to Monte Carlo statistical noise issues
  - More complicated and obviously more intrusive

- With the success of the KSEN adjoint-weighted capability, we are developing a new methodology that will be useful for more general tallies of MCNP
  - **FSEN** will be used for computing sensitivities to general (F) tallies

The development of new MCNP6 sensitivity capabilities

One of the project goals is to create a **NEW** capability in the MCNP6 code

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**

Comparison of various fixed-source sensitivity methodologies to motivate this new effort

- 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
```

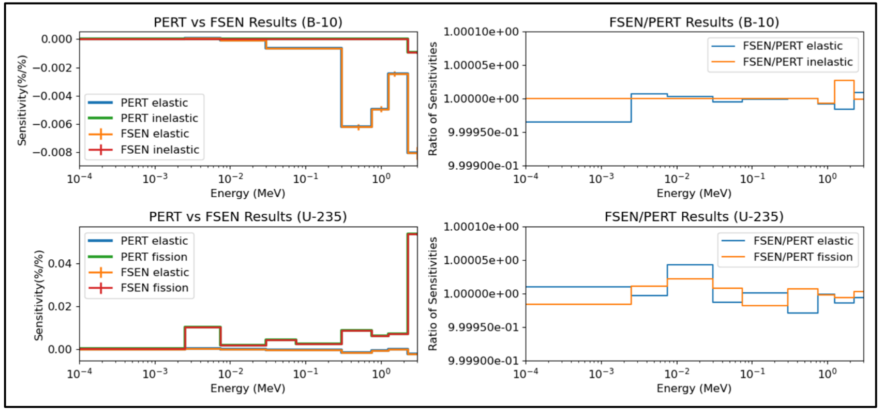
- **Adjoint-weighting (new FSEN card)**
  - **Easy to use with accurate results (like KSEN)**
  - **Reactions, multiplicity, and energy / angular distributions all available**

```
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
```

FSEN will be useful for a broad range of applications outside of EUCLID

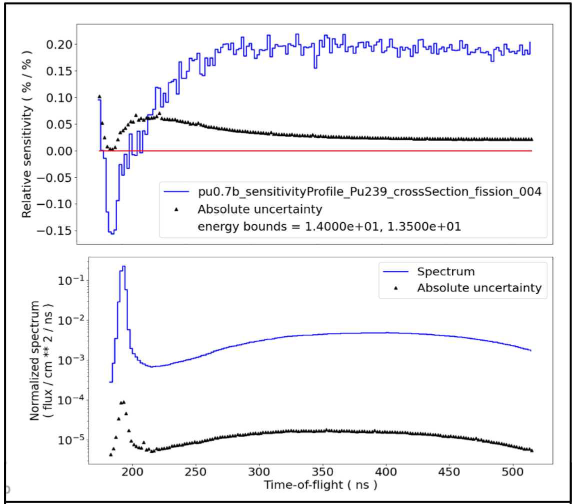
Verification of the new sensitivity methodology is extremely important

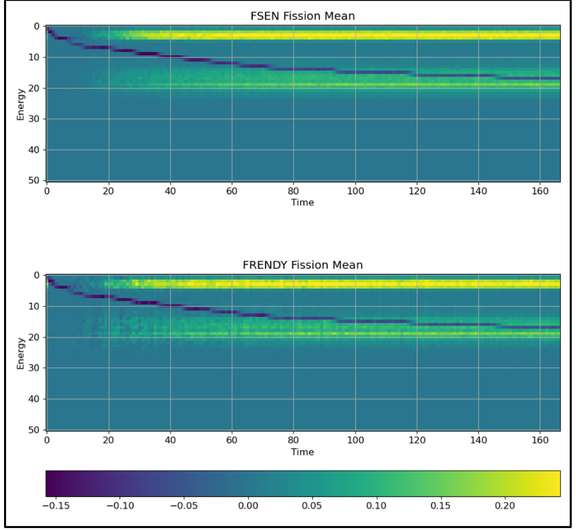
- Performing extensive verification to provide a robust and accurate capability
  - Comparison between FSEN and PERT



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

LLNL Pulsed Sphere of 0.7 MFP Pu



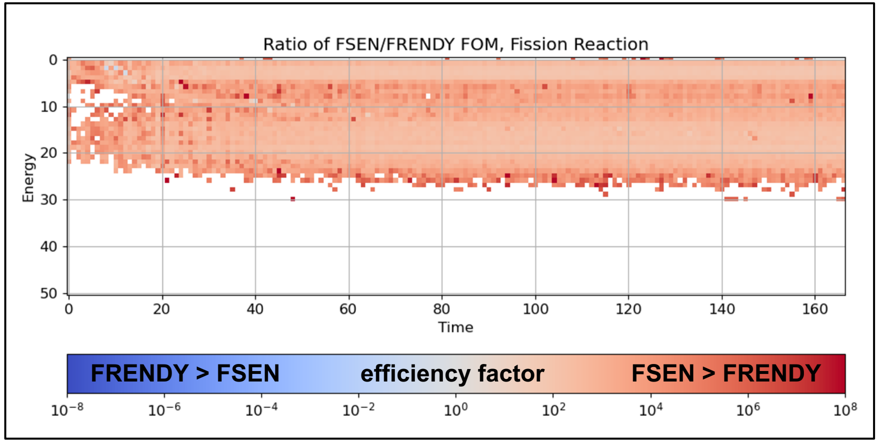


Computational benefits of the new MCNP6 sensitivity methodology are promising

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

$7.3 \cdot 10^5$ 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

Current Progress and Ultimate Goals for the FSEN Capability in the MCNP6 Code

Fixed-Source Calculations

- Neutron Tallies
- Current / Flux / Energy Deposition / Reaction Rates
- Next-event Estimators (point detectors)
- Subcritical Multiplication (through PTRAC)
- Pulse-height Tallies
- Photon Tallies

K-eigenvalue Calculations

- Neutron Tallies
- Current / Flux / Energy Deposition / Reaction Rates
- Next-event Estimators (point detectors)
- Other tallies, like the prompt kinetics parameters Beta-effective and neutron lifetime, and perturbation quantities like reactivity coefficients

- Done or In Progress
- Next To Do
- Stretch Goal / Open Questions

Summary

Summary: EUCLID has a sensitivity library for many different responses. How can we share them with the NEA?

We can deliver to the NEA the EUCLID sensitivity library in a common format for the same observables and on the same grid.

We have a document (LA-UR-22-21534) describing this work for further information.

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	✓		✓	

<u>Main questions:</u>

- Is there interest from the NEA/ WPEC SG-46 to have the EUCLID sensitivity library?
- What would you like to discuss, see, etc., before the data can be adopted by the NEA?

Team

Experiments
Underpinned by
Computational
Learning for
Improvements in nuclear
Data

Thank you for letting us present!!!

Nuclear Data


Wim Haeck


Michal Herman


Robert Little


Denise Neudecker

Simulations


Jennifer Alwin


Alexander Clark

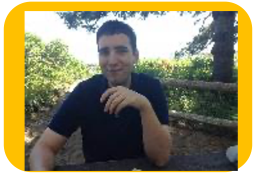

Juliann Lamproe


Michael Rising

Machine Learning


Michael Grosskopf


Noah Kleedtke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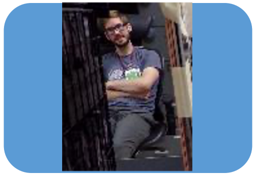
Theresa Cutler


Jesson Hutchinson


Travis Smith


Nicholas Thompson

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