

LA-UR-22-30716

Approved for public release; distribution is unlimited.

Title: Utilization of a Nuclear Data Toolkit for Manual Perturbation of ACE Files

Author(s): Kleedtke, Noah Andrew
Haeck, Wim
Hutchinson, Jesson D.

Intended for: MCNP 2022 User Symposium, 2022-10-17/2022-10-20 (Los Alamos, New Mexico, United States)

Issued: 2022-10-13



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Utilization of a Nuclear Data Toolkit for Manual Perturbation of ACE Files

Noah Kleedtke*, Wim Haeck, Jesson Hutchinson

MCNP® 2022 User Symposium

LA-UR-22-XXXXX

*kleedtke@lanl.gov

Introduction

- MCNP® users interact with nuclear data in every input file
- Examples of user interaction with nuclear data:
 1. ZAID – the table identification number to be specified on the MT cards (e.g., ZAID for ENDF/B-VIII.0 Pu-239 is 94239.00c)
 2. XSDIR – data directory file (e.g., xsdir_mcnp6.2)
 3. XSn card - MCNP® card that can be used to load cross-section evaluations not listed in the XSDIR file
- The nuclear data is in **A Compact ENDF (ACE)** format[†]
- For novice MCNP® users, reading and interacting with ACE files is not trivial
- There are tools to help! → **ACEtk**

- Outline of this talk: (1) where can we obtain ACE files?, (2) how to read and interact with ACE files, (3) manual perturbation of an ACE file, (4) calculation of sensitivity coefficients from MCNP® output using perturbed and unperturbed ACE files

[†]J. Conlin and P. Romano, “A Compact ENDF (ACE) Format Specification,” Technical Report, LA-UR-19-29016
<https://doi.org/10.2172/1561065>

Where can we obtain ACE files?

Los Alamos NATIONAL LABORATORY

MISSION SCIENCE & INNOVATION COLLABORATION COMMUNITY ENVIRONMENT

News & Media Careers Quick Links

Search

NUCLEAR DATA HOME

DATA LIBRARIES

ACE LIBRARIES

- CP2020
- ENDF80SaB2
- Lib80x
- EPRData14
- ENDF71SaB
- EPRData12
- MCPLIB84
- MCPLIB63
- CP2011

Nuclear Data Libraries

Welcome to the LANL distribution site for nuclear data libraries. These libraries have been processed by the Nuclear Data Team at Los Alamos National Laboratory. Here you can download application libraries for use in your own applications.

LIBRARY TYPES

- ACE Continuous-energy data for use in codes like MCNP®.

For information on how to install the libraries, please see our [Installing ACE Libraries](#) page.

SUPPORT

If you have any questions regarding the nuclear data libraries found here or if there are problems with this site, please contact the Los Alamos National Laboratory, Nuclear Data Team, nuclldata@lanl.gov.

<https://nucleardata.lanl.gov/>

Where can we obtain ACE files?

The screenshot shows the Los Alamos National Laboratory website. The top navigation bar includes the logo and links for MISSION, SCIENCE & INNOVATION, COLLABORATION, COMMUNITY, and ENVIRONMENT. A search bar is located in the top right. The left sidebar contains a search bar and a list of data libraries under the heading 'NUCLEAR DATA HOME'. The 'ACE LIBRARIES' section is expanded, showing a list of libraries including CP2020, ENDF80SaB2, Lib80x (highlighted in blue), EPRData14, ENDF71SaB, EPRData12, MCPLIB84, MCPLIB63, and CP2011. The main content area displays the title 'Lib80x—Library based on ENDF/B-VIII.0' and its release date 'Released: 2018-06-29'. A paragraph explains that the library is based on ENDF/B-VIII.0 and contains ACE files for continuous-energy incident neutrons at various temperatures. A bulleted list of temperatures is provided: .00c (293.6 Kelvin), .01c (600 Kelvin), .02c (900 Kelvin), .03c (1200 Kelvin), .04c (2500 Kelvin), .05c (0.1 Kelvin), and .06c (250 kelvin). Below this, it states that full documentation is in the 'docs' directory. A 'DOCUMENTATION' section lists a reference: '1. "Release of ENDF/B-VIII.0-Based ACE Data Files," Conlin, J.L., Haeck, W., Neudecker, D., Parsons, D.K., White, M.C., (2018) LA-UR-18-24034'. A section titled 'Some additional information which may be of use for MCNP Users' lists: '3. F.B. Brown, M.E. Rising "Guide for Using ENDF/B-VIII.0 Nuclear Data with MCNP", LA-UR-20-30460 (2020)'.

<https://nucleardata.lanl.gov/ace/lib80x>

Where can we obtain ACE files?

EPRData12	The full documentation for the Lib80x library can be found in the <code>docs</code> directory after decompressing the download.
MCPLIB84	<h2>DOCUMENTATION</h2> <ol style="list-style-type: none">"Release of ENDF/B-VIII.0-Based ACE Data Files," Conlin, J.L., Haeck, W., Neudecker, D., Parsons, D.K., White, M.C., (2018) LA-UR-18-24034
MCPLIB63	<h2>Some additional information which may be of use for MCNP Users</h2>
CP2011	<ol style="list-style-type: none">F.B. Brown, M.E. Rising "Guide for Using ENDF/B-VIII.0 Nuclear Data with MCNP"; LA-UR-20-30460 (2020).
ENDF71x	<ol style="list-style-type: none">xmdir file, with ENDF/B-VIII.0 defaults: xmdir_mcnp6.2_endf80,71.txt (download, then remove .txt extension)
ENDF7u	<ol style="list-style-type: none">xmdir file, with ENDF/B-VII.1 defaults: xmdir_mcnp6.2_endf71,80.txt (download, then remove .txt extension)
ENDF70SaB	<h2>DOWNLOADS</h2>
ENDF70PROT	Lib80x can be downloaded either as a zip file or as a compressed tarball
ENDF70	<ul style="list-style-type: none">lib80x.zip (sha512 801b9e5389ad75915cf6135d365f6684984c2aa0e990b74c40db29c5bd806daa417ee968ed71cbf6987bcbdb86895ca800788f8487004f862511df6b3be456f0b)lib80x.tgz (sha512 afa143e834eff02d8f535357dc2c3698e7565777849f5b8cfe225584541678acc702e41395706cb3e5e0d7a70e3fc25bf3f4428cad818062dbe0f36186b39d95)
TMCCS	<h2>ERRATA</h2>
T16_2003	Date: 2022-07-06
THERXS	Name: B-10 Lib80x
SaB2002	Description: After the release of ENDF/B-VIII.0 in February 2018, errors were discovered in the neutron on B-10 evaluation. A fix was provided for the errata; this update uses the fixed B-10 evaluation. For more information on the updated/fixed evaluation, please see: https://www.nndc.bnl.gov/endl-b8.0/errata.html .
MCPLIB04	<ul style="list-style-type: none">B-10-Lib80x.zip (sha512 7f2ba223bf1559dcf64201b2f9778b47ff83ad95325a6586d71a94739f785dcaa39f08ea2d675ddc2233d40ae5beb50d331022682489b89d260cba519b4ff5e2)B-10-Lib80x.tgz (sha512 d303dc2c4d213da690e6b14c6b29b9ef1716cafe137aad8c28e7e7578aeb8162f4ca824386ada8d4ab6f2a8de25b856790300f21fd55c9fe35a39734d51b9d3d)
MCPLIB03	
ACTIB	
EL03	<p>❓ If further information is required contact a member of the Data Team by e-mail at nuclldata@lanl.gov</p>

<https://nucleardata.lanl.gov/ace/lib80x>

How to read and interact with ACE files

The screenshot displays the GitHub repository page for `njoy/ACETk`. The repository is public and has 9 stars, 7 watchers, and 5 forks. The main content area shows the repository structure with a list of files and folders, including `.github/workflows`, `cmake`, `python`, `src`, `.gitignore`, `CMakeLists.txt`, `LICENSE`, and `README.md`. The `README.md` file is selected, showing the following content:

ACETk

Toolkit for reading and interacting with ACE nuclear data files. This toolkit provides a full C++ library along with python bindings.

ACETk in python

The python bindings for ACETk are still work in progress and should be used accordingly. Please report any

The right sidebar contains information about the repository, including the description "Toolkit for working with ACE-formatted data files", the repository type "ace nuclear-data", and the number of stars, watchers, and forks. It also shows the "Releases" and "Packages" sections, both of which are currently empty.

<https://github.com/njoy/ACETk>

How to read and interact with ACE files

- ACETk in Python

1. Import ACETk

```
# add ACETk build path to the python path $PYTHONPATH environmental variable
acetek_build_path = r"/usr/projects/data/nuclear/special/opt/ACETk/bin"
sys.path.append( acetk_build_path )
import ACETk
```

- Toolkit includes C++ library with Python bindings

2. Open continuous energy ACE file

```
table = ACETk.ContinuousEnergyTable.from_file( file_name )
```

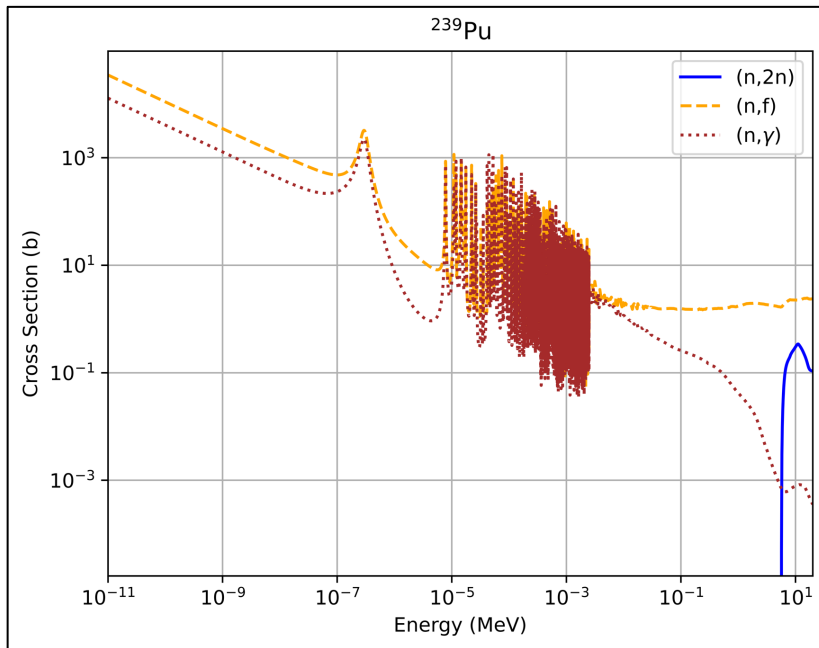
3. Read cross section values from SIG block and energy values from ESZ block

```
index = table.MTR.index( mt_number )
mt_xs_data = table.SIG.cross_section_data( index )
mt_xs_data_values = mt_xs_data.cross_sections.to_list()
energy_grid = table.ESZ.energies.to_list()
```

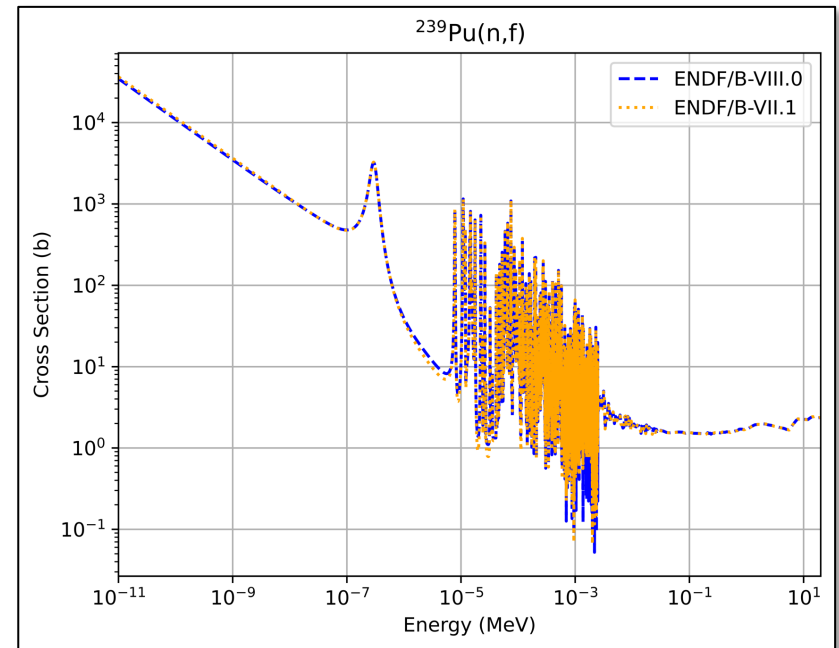
How to read and interact with ACE files

- More information at Nuclear Data & Physics Session (1:00pm – 4:00pm)
- Wim Haeck will be giving a demonstration on how to use ACETk

Multiple Reactions



Multiple Nuclear Data Libraries



Manual Perturbation of ACE File

1. Follow steps outlined in previous slide to obtain cross section values and energy grid information
2. Perturb cross section values by some amount *perturbation_fraction*

```
for k in perturbed_energy_indices:
    a = mt_xs_data_values[k]
    b = mt_xs_data_values[k] * perturbation_fraction
    difference = b - a
    mt_xs_data_values[k] = b
    disap_xs_data_values[k + energy_index] = disap_xs_data_values[k + energy_index] + difference
    total_xs_data_values[k + energy_index] = total_xs_data_values[k + energy_index] + difference
```

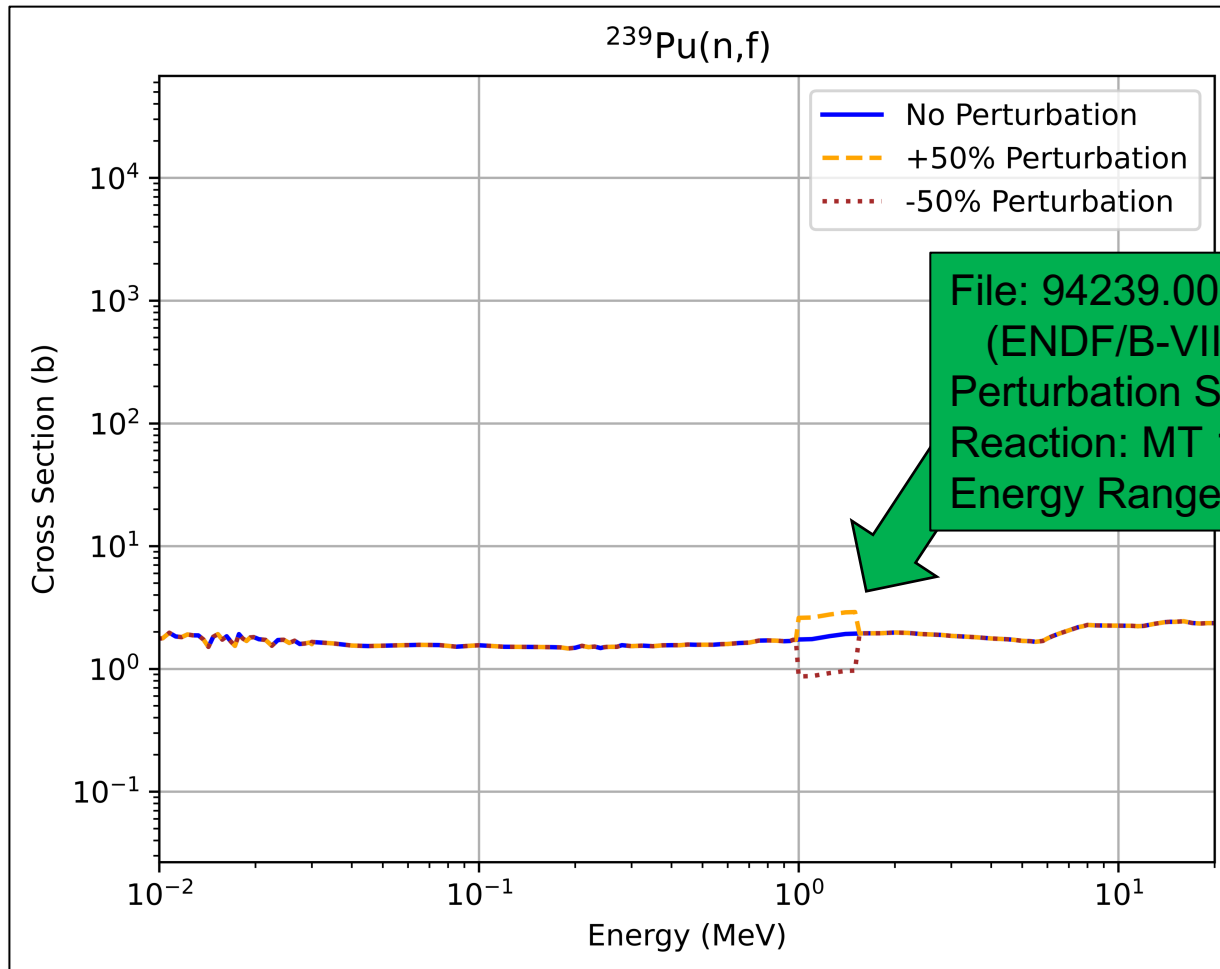
3. Create a new SIG block and ESZ block with perturbed values

```
new_xs_data = ACEtk.CrossSectionData( mt_xs_data.energy_index, mt_xs_data_values )
old_SIG = [ table.SIG.cross_section_data(i) for i in range( 1, table.NTR + 1 ) ]
old_SIG[table.MTR.index( mt_number ) - 1] = new_xs_data
new_SIG = ACEtk.CrossSectionBlock( old_SIG )
new_ESZ = ACEtk.PrincipalCrossSectionBlock( energies = table.ESZ.energies.to_list(), total = total_xs_data_values, disappearance = disap_xs_data_values, elastic = table.ESZ.elastic.to_list(), heating = table.ESZ.heating.to_list() )
```

4. Save perturbed ACE information to *my_new_file.ace*

```
new_Table = ACEtk.ContinuousEnergyTable( z = table.Z, a = table.A, header = table.header, esz = new_ESZ, nu = table.NU, dnu = table.DNU, mtr = table.MTR, lqr = table.LQR, sig = new_SIG, ang = table.AND, dlw = table.DLW, bdd = table.BDD, dned = table.DNED )
new_Table.to_file( "my_new_file.ace" )
```

Manual Perturbation of ACE File



Sensitivity Coefficient Calculation

- Sensitivity coefficient:

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

k = neutron multiplication factor

σ = nuclear data

- Sensitivity coefficient calculation with *Central Difference* approximation:

$$S_{k,\sigma} = \frac{k_+ - k_-}{2k_0 p}$$

k_+ = k from simulation with positively perturbed nuclear data

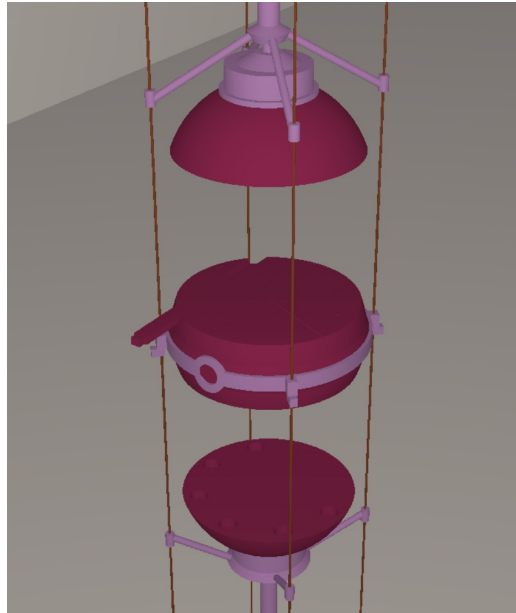
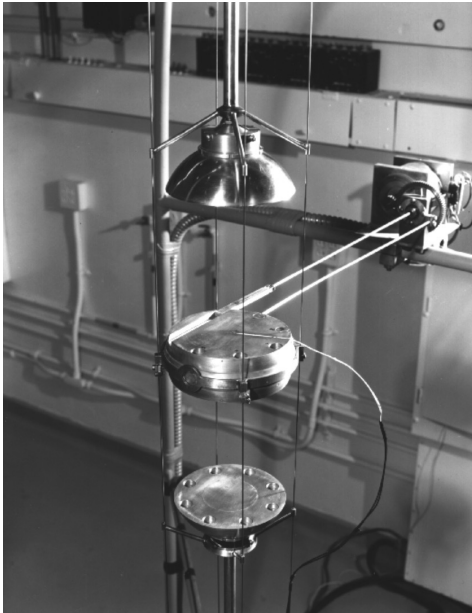
k_- = k from simulation with negatively perturbed nuclear data

k_0 = k from simulation with no perturbed nuclear data

p = perturbation fraction (e.g., 50% perturbation, $p = 0.5$)

Jezebel Sensitivity Profiles

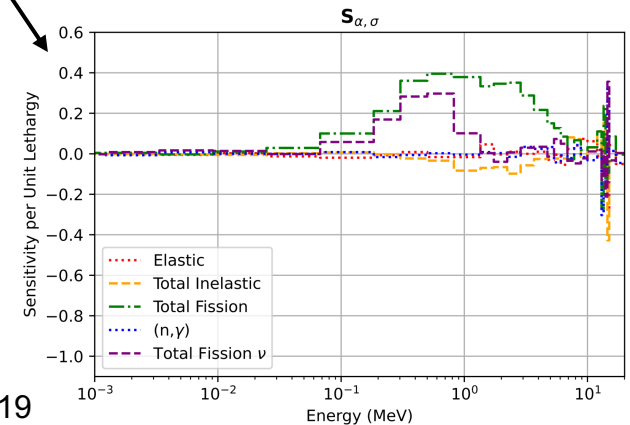
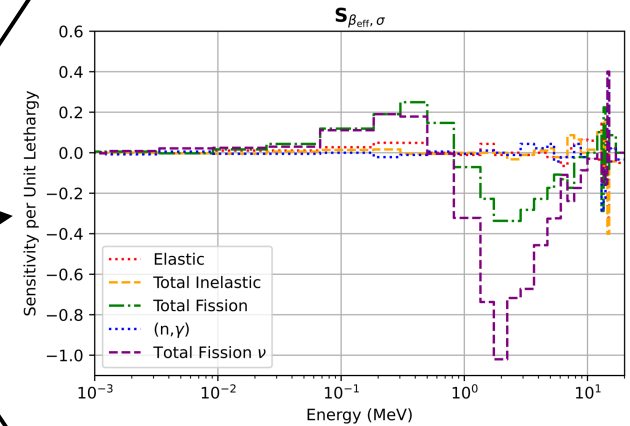
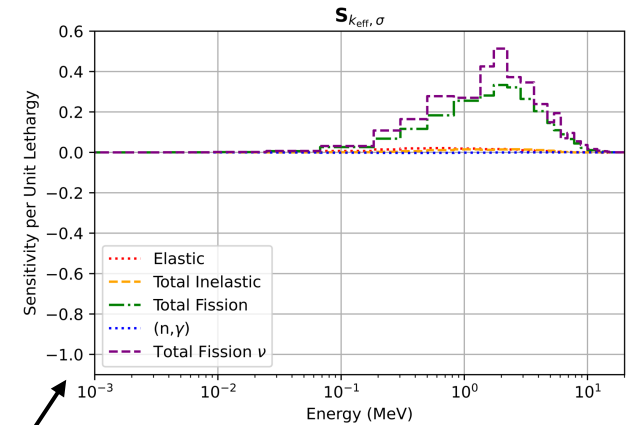
- Jezebel – ICSBEP Benchmark PU-MET-FAST-001



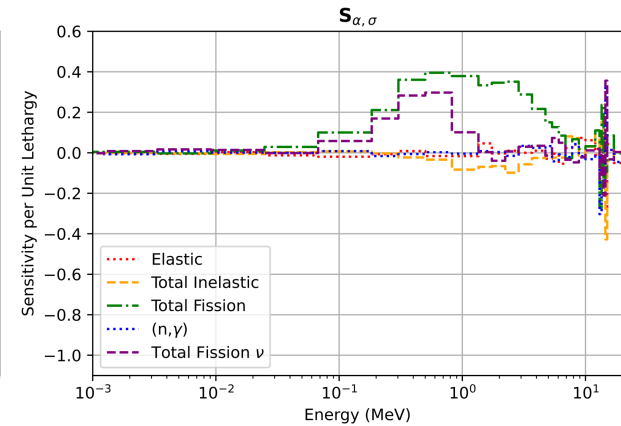
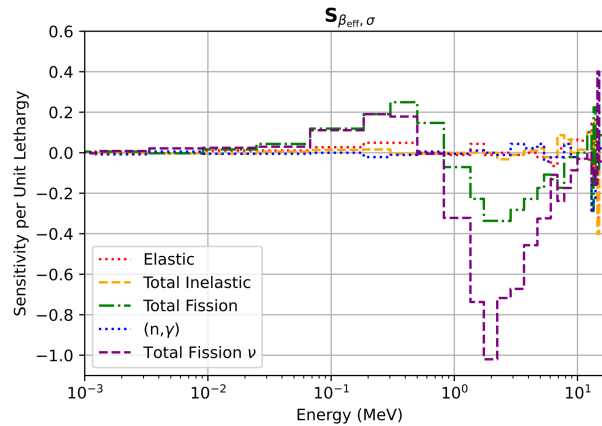
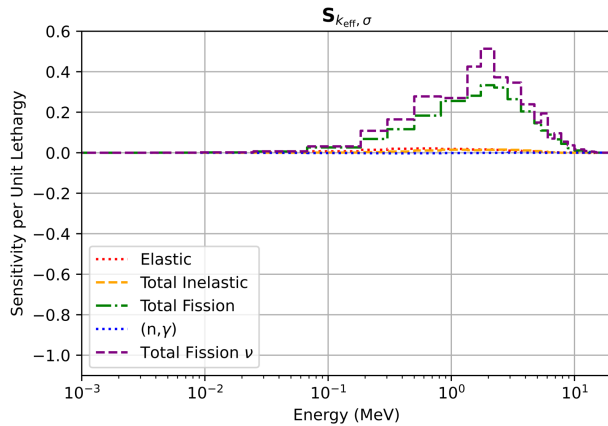
- Sphere of plutonium metal (4.5 at.% ^{240}Pu , 1.02 wt.% Ga)

Images from J. D. Bess et al., “The 2019 Edition of the ICSBEP Handbook,” *Transactions of the American Nuclear Society*, **121**, 901-904 (2019).

Sensitivity profiles from N. Kleedtke et al., “Data Assimilation Using Non-invasive Monte Carlo Sensitivity Analysis of Reactor Kinetics Parameters,” LA-UR-22-30019



Jezebel Sensitivity Profiles



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

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

k_{eff} = effective neutron multiplication factor

β_{eff} = effective delayed neutron fraction

α = prompt neutron decay constant

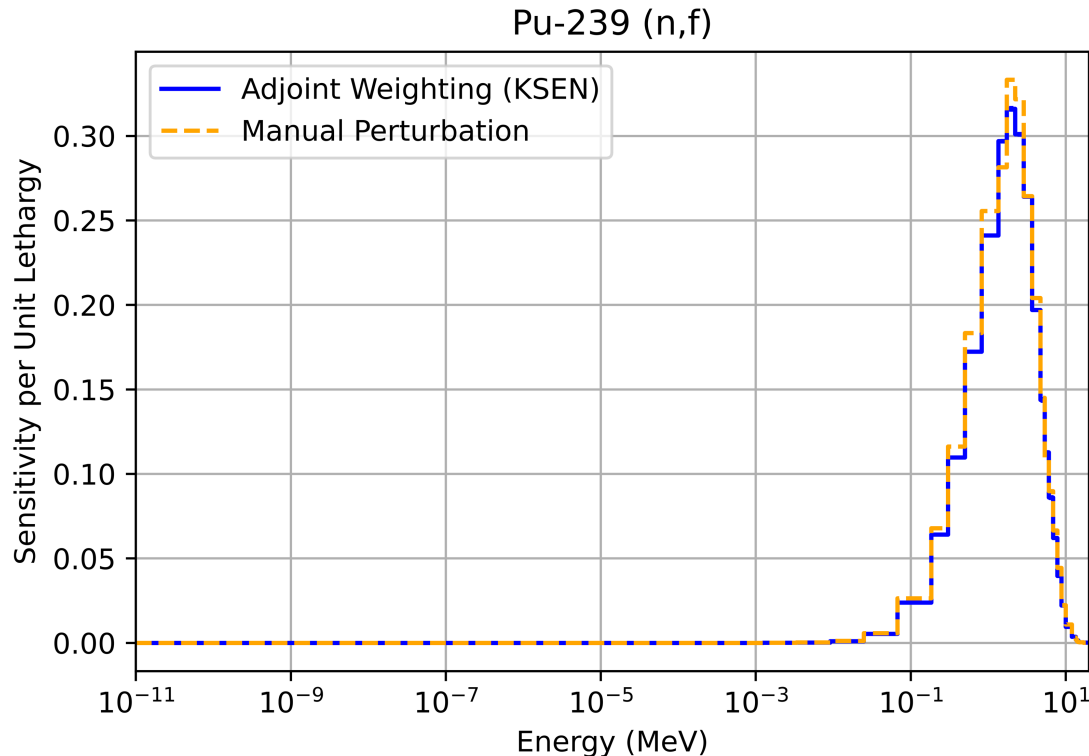
k_p = prompt neutron multiplication factor

l = mean neutron lifetime

Sensitivity profiles from N. Kleedtko et al., "Data Assimilation Using Non-invasive Monte Carlo Sensitivity Analysis of Reactor Kinetics Parameters," LA-UR-22-30019

Comparison to adjoint-weighted sensitivity coefficients

- Currently, adjoint-based k -eigenvalue sensitivity coefficients to nuclear data can be calculated in MCNP® Code Version 6.2 using the KSEN card^{1,2}



¹B. C. KIEDROWSKI, F. B. BROWN, "Adjoint-Based k -Eigenvalue Sensitivity Coefficients to Nuclear Data Using Continuous-Energy Monte Carlo," *Nuclear Science and Engineering*, **174**, 227-244 (2017).

²J. A. Kulesza et al., "MCNP® Code Version 6.3.0 Theory & User Manual," Technical Report, LA-UR-22-30006

Nuclear Data-Induced Uncertainty Calculation

- Nuclear data-induced uncertainty of neutron multiplication factor ($\Delta_{k_{\text{eff}}}$):

$$\Delta_{k_{\text{eff}}} = \sqrt{\mathbf{S}_{k_{\text{eff}},\sigma} \mathbf{C}_{\sigma,\sigma} \mathbf{S}_{k_{\text{eff}},\sigma}^T}$$

$\mathbf{C}_{\sigma,\sigma}$ = covariance matrix of nuclear data σ

$\mathbf{S}_{k_{\text{eff}},\sigma}$ = vector of sensitivity coefficients over multiple energies for nuclear data σ

- Nuclear data-induced uncertainty calculations can be performed for specific nuclides, reactions, and energy groups
- The sensitivity and uncertainty (S/U) methods are important for determining sources of computational bias and informing nuclear data evaluators of areas where possible nuclear data adjustments might be necessary

Summary

- In this talk we went through
 1. Where can we obtain ACE files?
Nuclear Data Website (<https://nucleardata.lanl.gov/>)
 2. How to read and interact with ACE files
Nuclear Data Toolkit **ACEtk** (<https://github.com/njoy/ACEtk>)
More information at Nuclear Data & Physics Session (1:00pm – 4:00pm)
 3. Manual perturbation of an ACE file
Positive/Negative/Unperturbed ACE files for Nuclide/Reaction/Energy Range
 4. Calculation of sensitivity coefficients from MCNP® output
Sensitivity coefficient calculation with central difference approximation
- Results shown for sensitivity coefficients of effective neutron multiplication factor (k_{eff}), effective delayed neutron fraction (β_{eff}), and prompt neutron decay constant (α) to Pu-239 elastic, total inelastic, total fission, radiative capture (n,γ), and total fission multiplicity (ν) nuclear data