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Los Alamos NATIONAL LABORATORY

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

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MCNP® 2022 User Symposium

LA-UR-22-XXXXX

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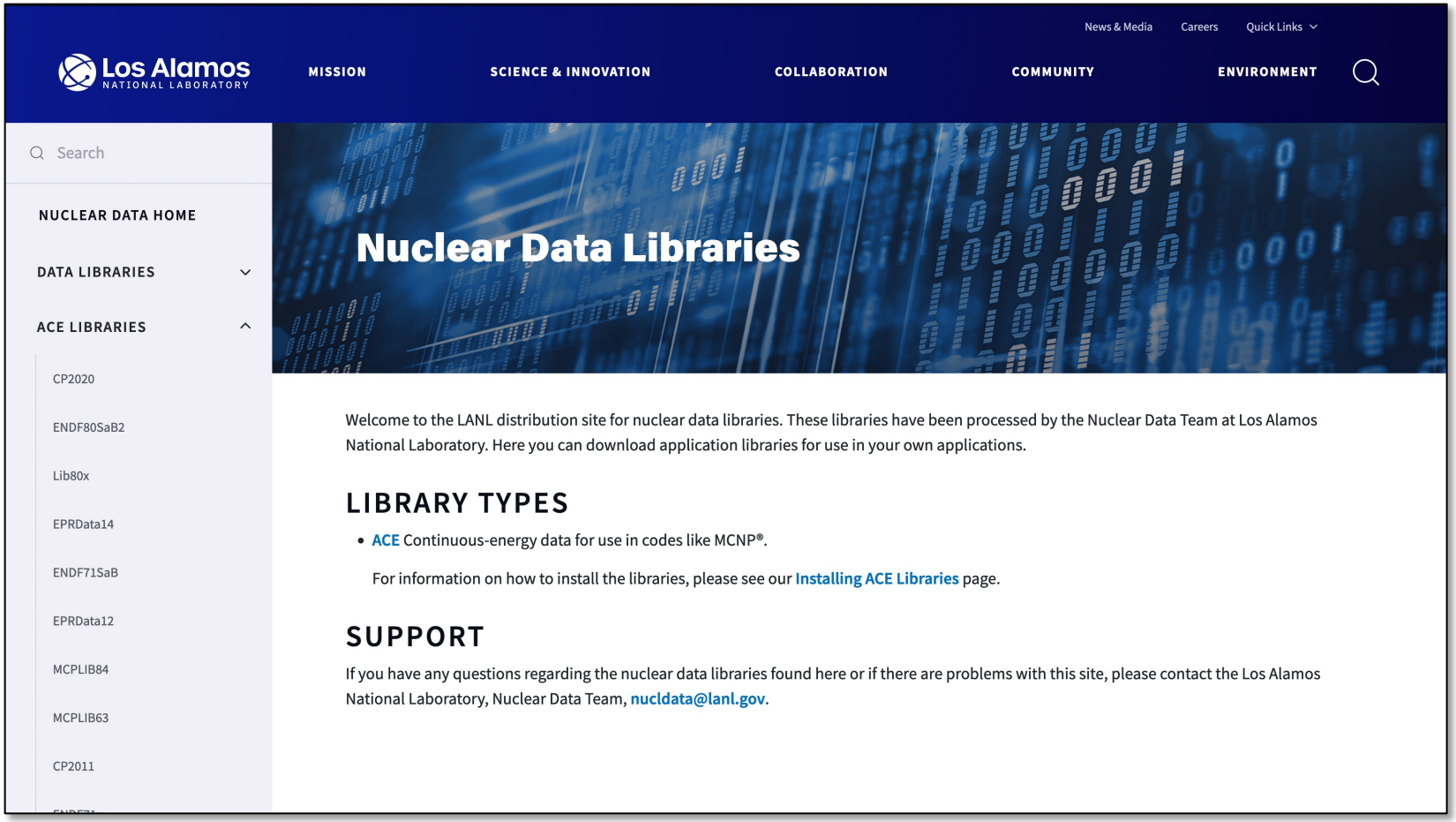
Introduction

- 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 C**ompact **E**NDF (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

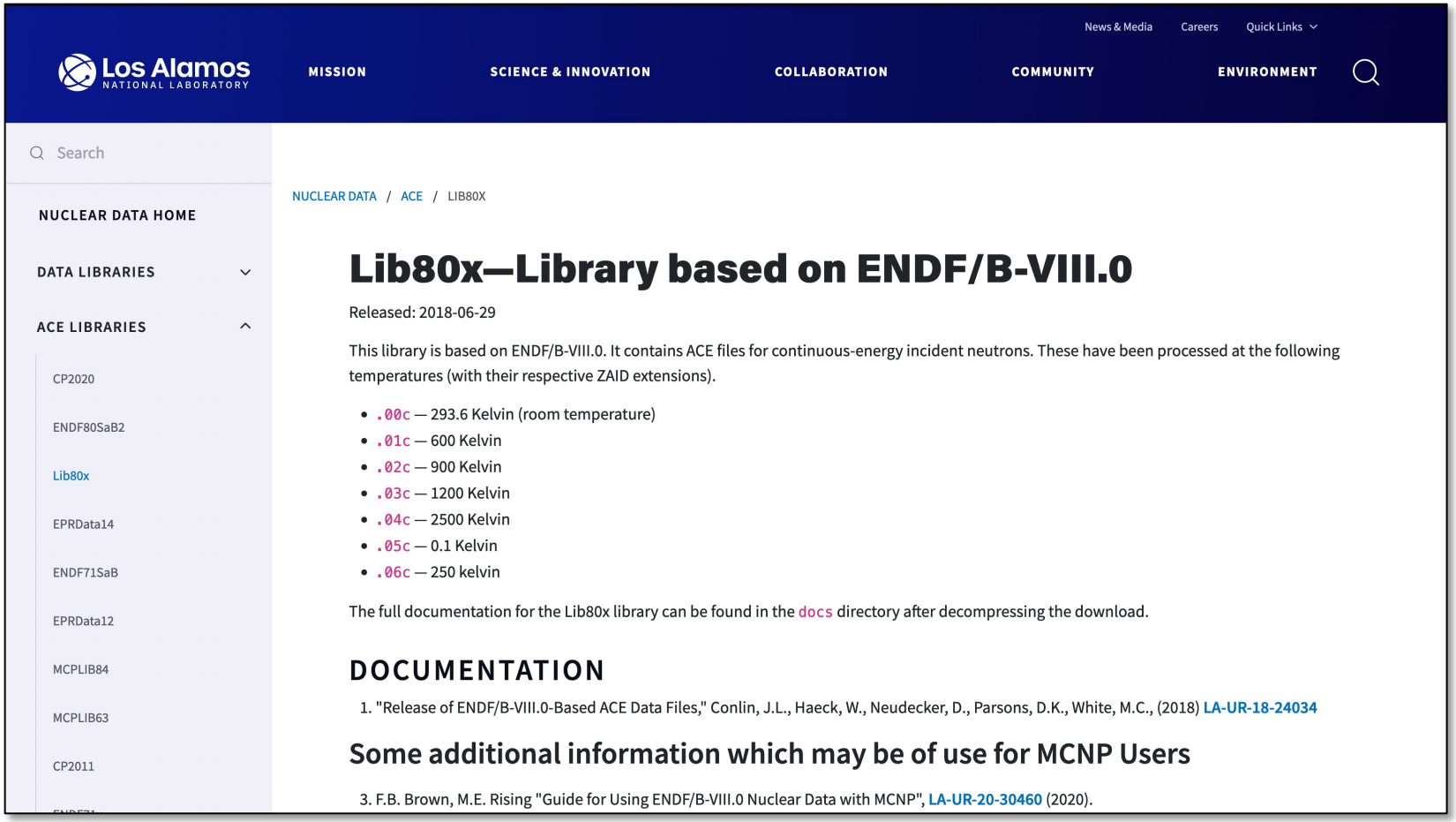
†J. Conlin and P. Romano, "A Compact ENDF (ACE) Format Specification," Technical Report, LA-UR-19-29016 https://doi.org/10.2172/1561065

Where can we obtain ACE files?



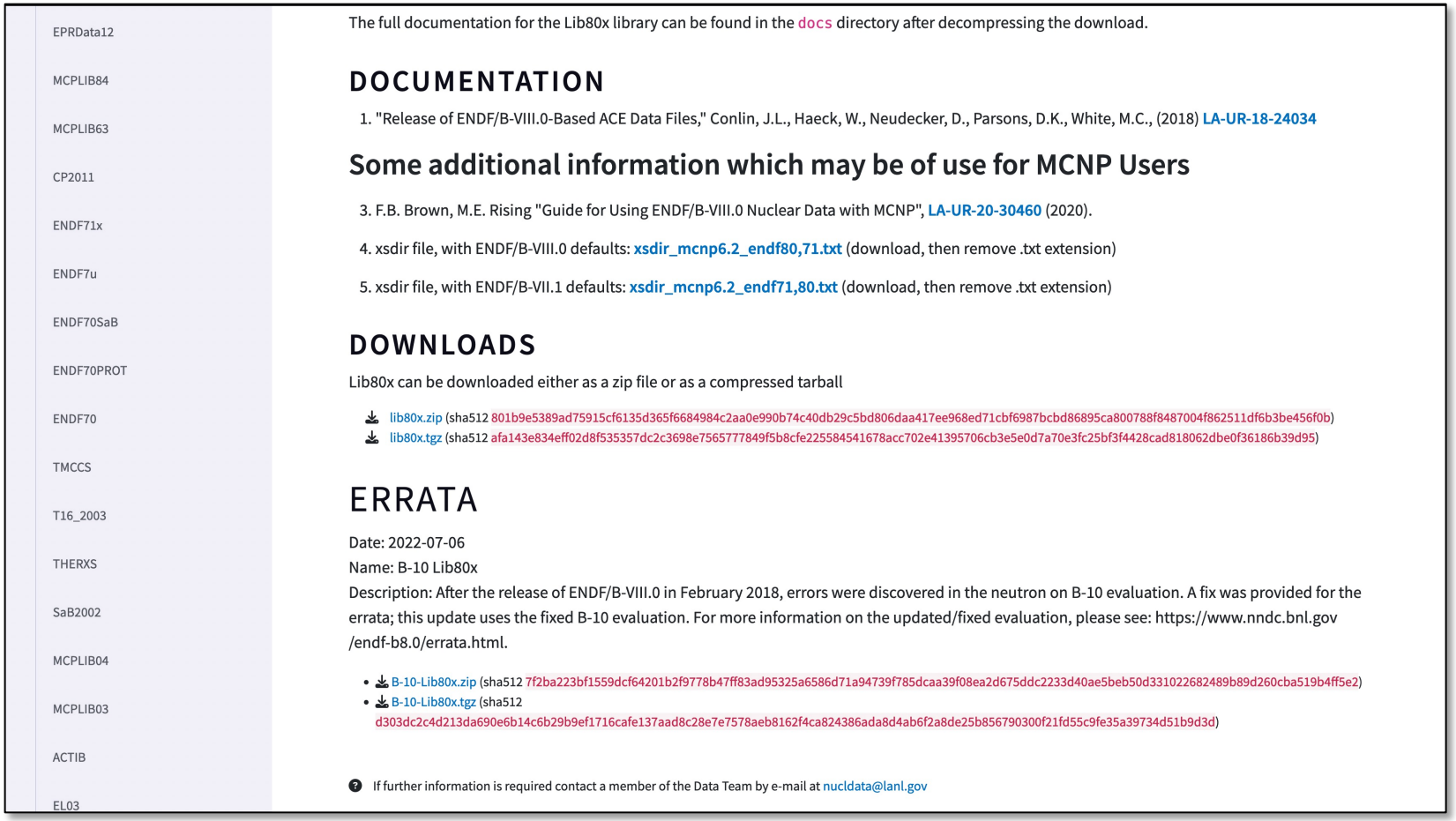
https://nucleardata.lanl.gov/

Where can we obtain ACE files?



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

Where can we obtain ACE files?



EPRData12
MCPLIB84
MCPLIB63
CP2011
ENDF71x
ENDF7u
ENDF70SaB
ENDF70PROT
ENDF70
TMCCS
T16_2003
THERXS
SaB2002
MCPLIB04
MCPLIB03
ACTIB
EL03

The full documentation for the Lib80x library can be found in the docs directory after decompressing the download.

DOCUMENTATION

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

Some additional information which may be of use for MCNP Users

3. F.B. Brown, M.E. Rising "Guide for Using ENDF/B-VIII.0 Nuclear Data with MCNP", LA-UR-20-30460 (2020).
4. xsdir file, with ENDF/B-VIII.0 defaults: xsdir_mcnp6.2_endf80,71.txt (download, then remove .txt extension)
5. xsdir file, with ENDF/B-VII.1 defaults: xsdir_mcnp6.2_endf71,80.txt (download, then remove .txt extension)

DOWNLOADS

Lib80x can be downloaded either as a zip file or as a compressed tarball

lib80x.zip (sha512 801b9e5389ad75915cf6135d365f6684984c2aa0e990b74c40db29c5bd806daa417ee968ed71cbf6987bcbd86895ca800788f8487004f862511df6b3be456f0b)
lib80x.tgz (sha512 afa143e834eff02d8f535357dc2c3698e7565777849f5b8cfe225584541678acc702e41395706cb3e5e0d7a70e3fc25bf3f4428cad818062dbe0f36186b39d95)

ERRATA

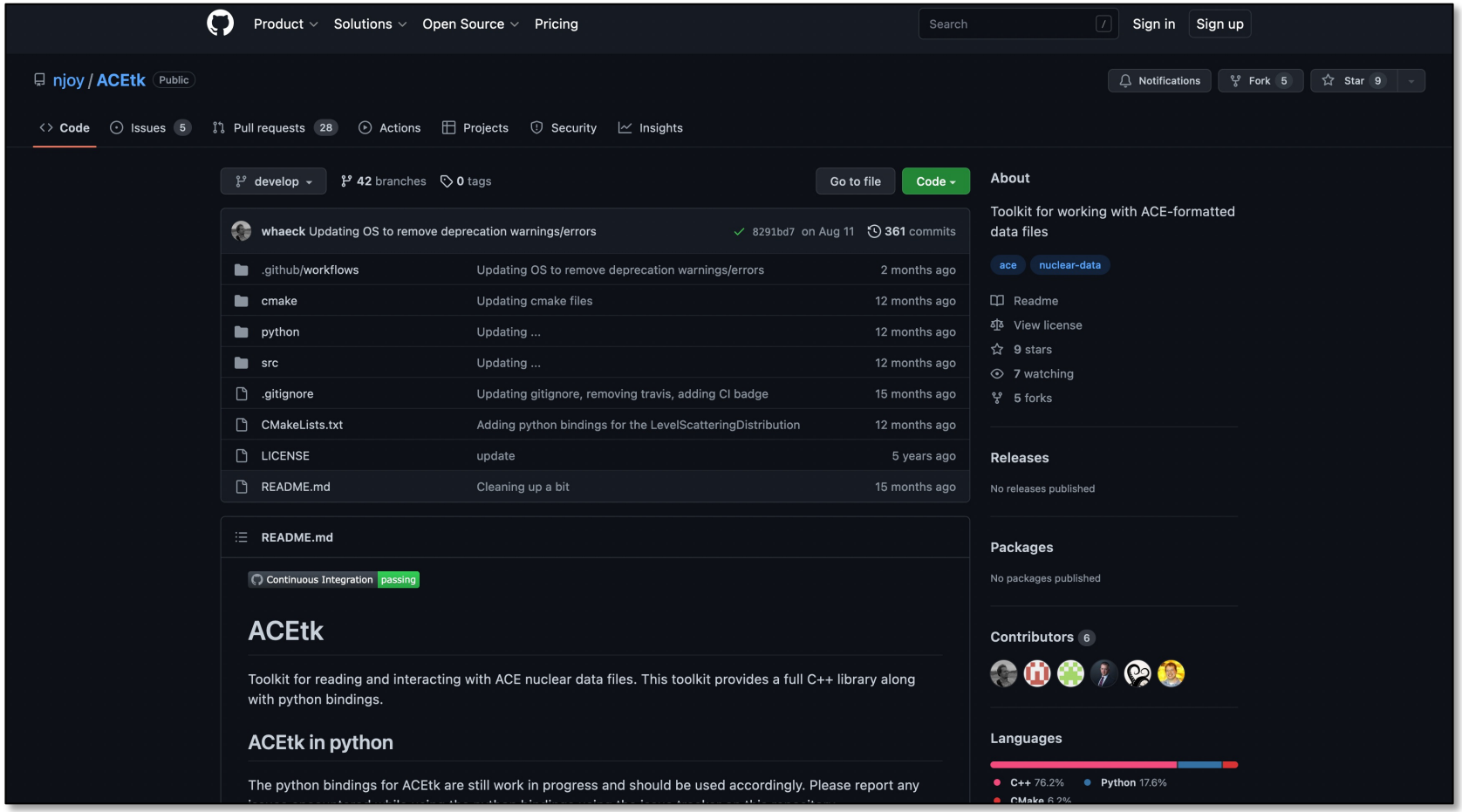
Date: 2022-07-06
Name: B-10 Lib80x
Description: After the release of ENDF/B-VIII.0 in February 2018, errors were discovered in the neutron on B-10 evaluation. A fix was provided for the errata; this update uses the fixed B-10 evaluation. For more information on the updated/fixed evaluation, please see: https://www.nndc.bnl.gov /endf-b8.0/errata.html.

- B-10-Lib80x.zip (sha512 7f2ba223bf1559dcf64201b2f9778b47ff83ad95325a6586d71a94739f785dcaa39f08ea2d675ddc2233d40ae5beb50d331022682489b89d260cba519b4ff5e2)
- B-10-Lib80x.tgz (sha512 d303dc2c4d213da690e6b14c6b29b9ef1716cafe137aad8c28e7e7578aeb8162f4ca824386ada8d4ab6f2a8de25b856790300f21fd55c9fe35a39734d51b9d3d)

If further information is required contact a member of the Data Team by e-mail at nucldata@lanl.gov

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

How to read and interact with ACE files



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
acetk_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 )
```

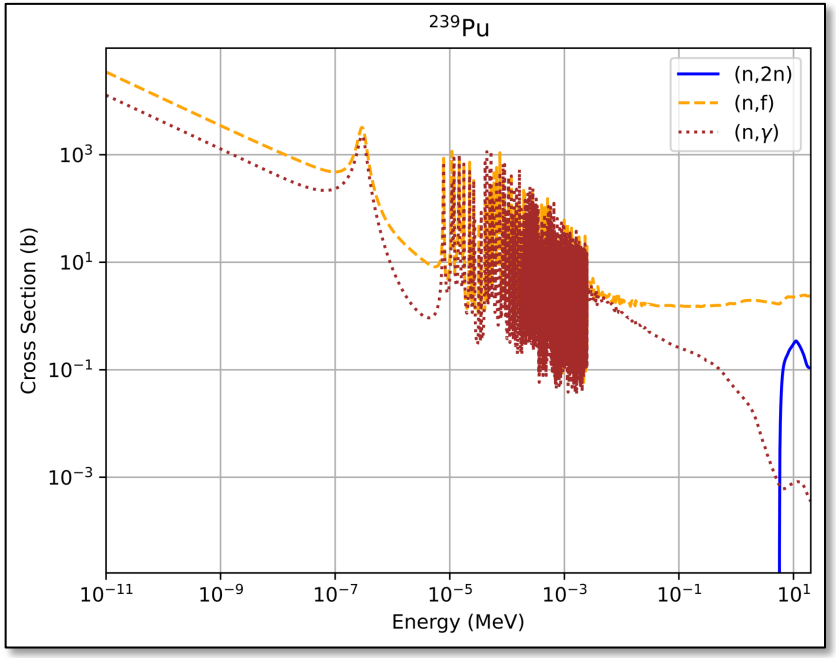
3. Read cross section values from SIG block and energy values from ESZ block

```
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()
```

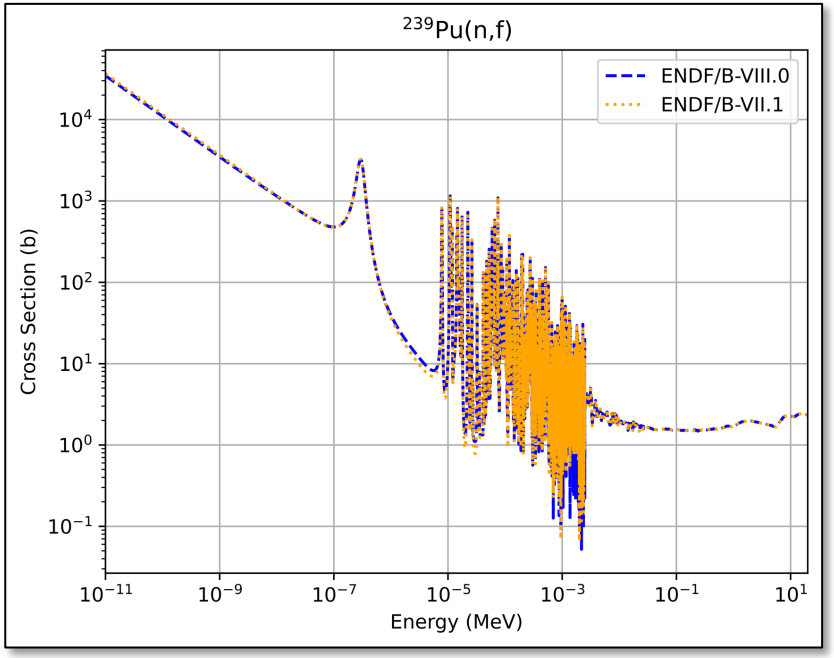
How to read and interact with ACE files

- 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
```

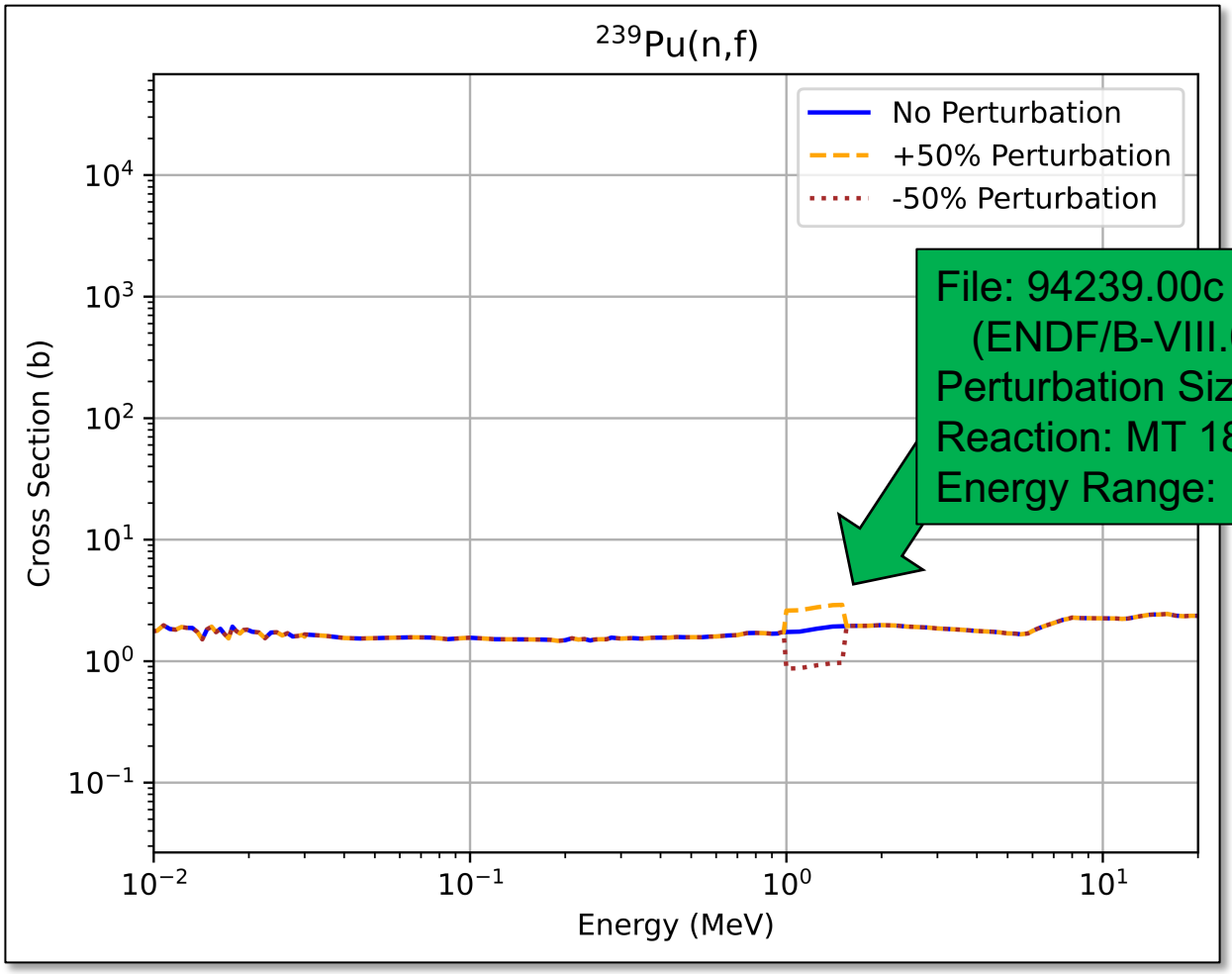
3. Create a new SIG block and ESZ block with perturbed values

```
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, disappe
arance = 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, dn
u = 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

$\sigma =$ 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

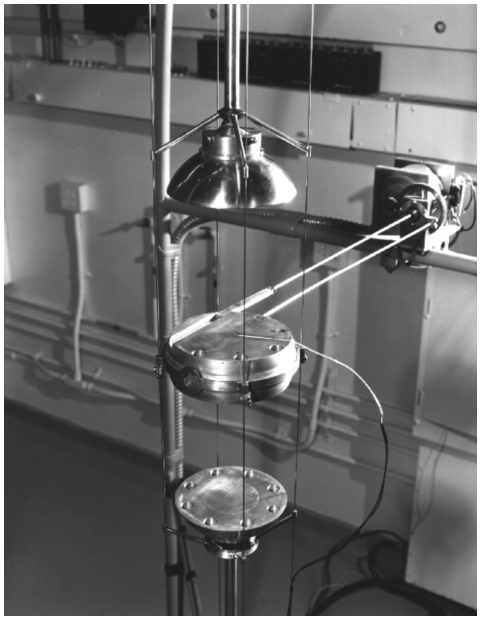
$k_- =$ k from simulation with negatively perturbed nuclear data

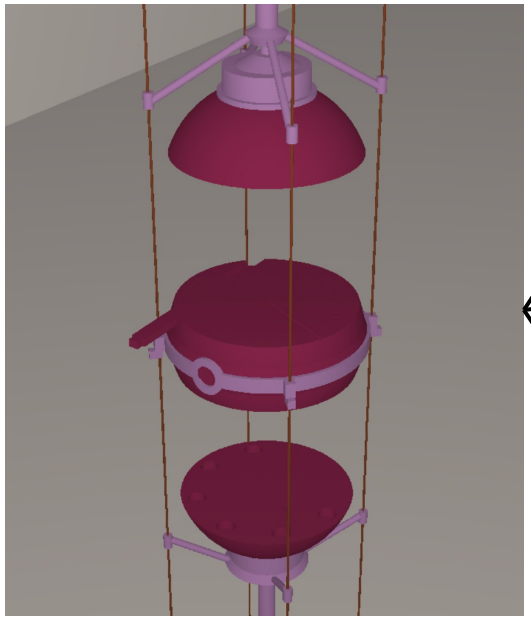
$k_0 =$ k from simulation with no perturbed nuclear data

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

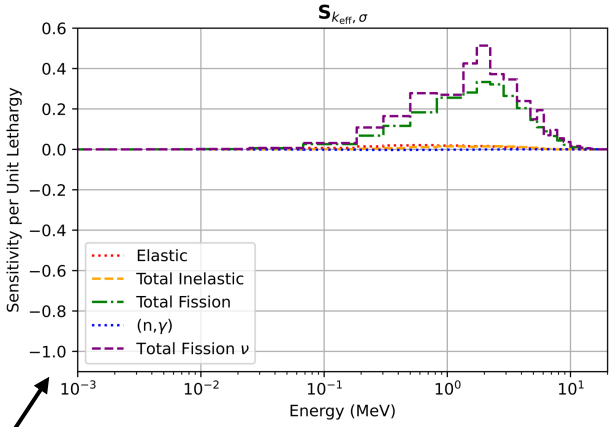
Jezebel Sensitivity Profiles

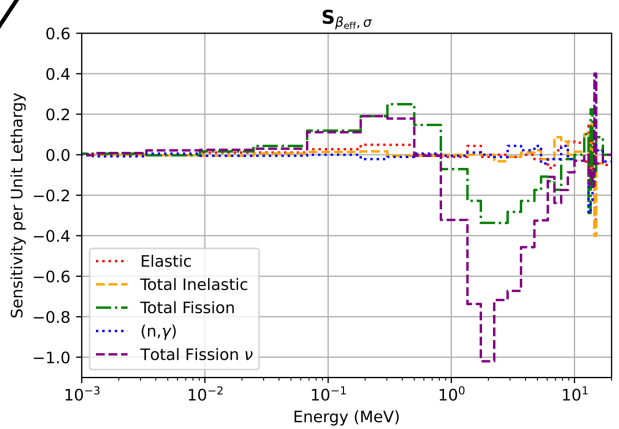
- Jezebel – ICSBEP Benchmark PU-MET-FAST-001

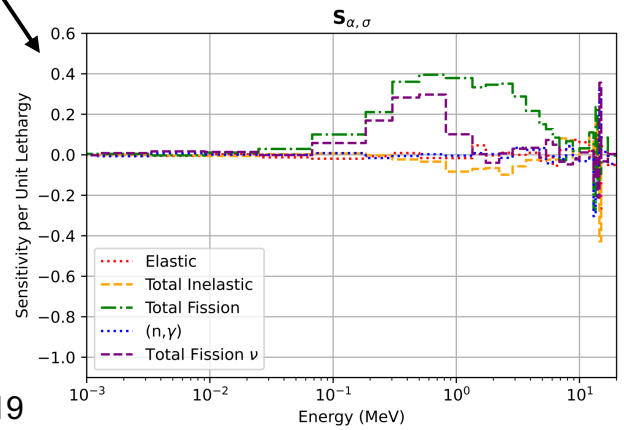




- Sphere of plutonium metal (4.5 at.% ^{240}Pu, 1.02 wt.% Ga)

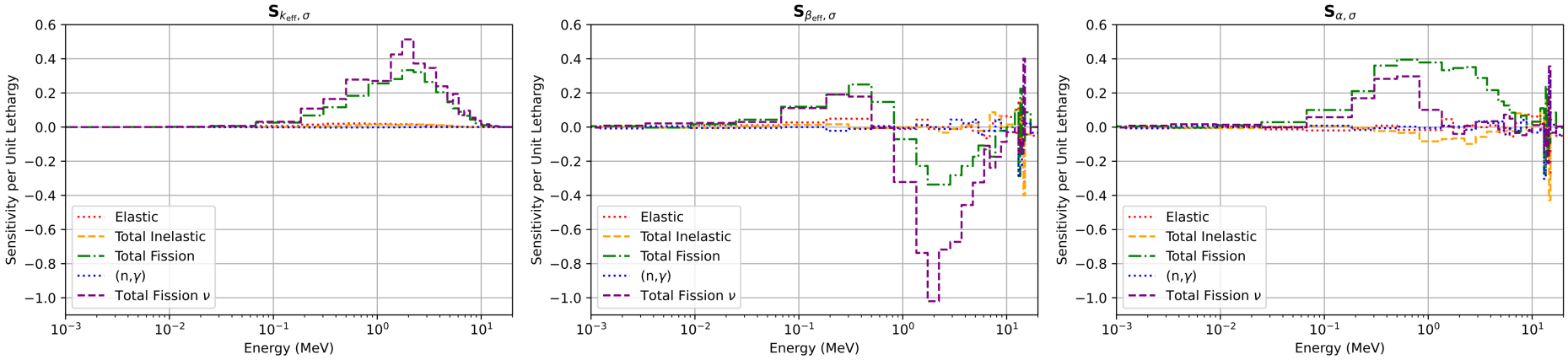






Images from J. D. Bess et al., "The 2019 Edition of the ICSBEP Handbook," *Transactions of the American Nuclear Society*, **121**, 901-904 (2019).
Sensitivity profiles from N. Kleedtke et al., "Data Assimilation Using Non-invasive Monte Carlo Sensitivity Analysis of Reactor Kinetics Parameters," LA-UR-22-30019

Jezebel Sensitivity Profiles



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

k_{eff} = effective neutron multiplication factor

β_{eff} = effective delayed neutron fraction

α = prompt neutron decay constant

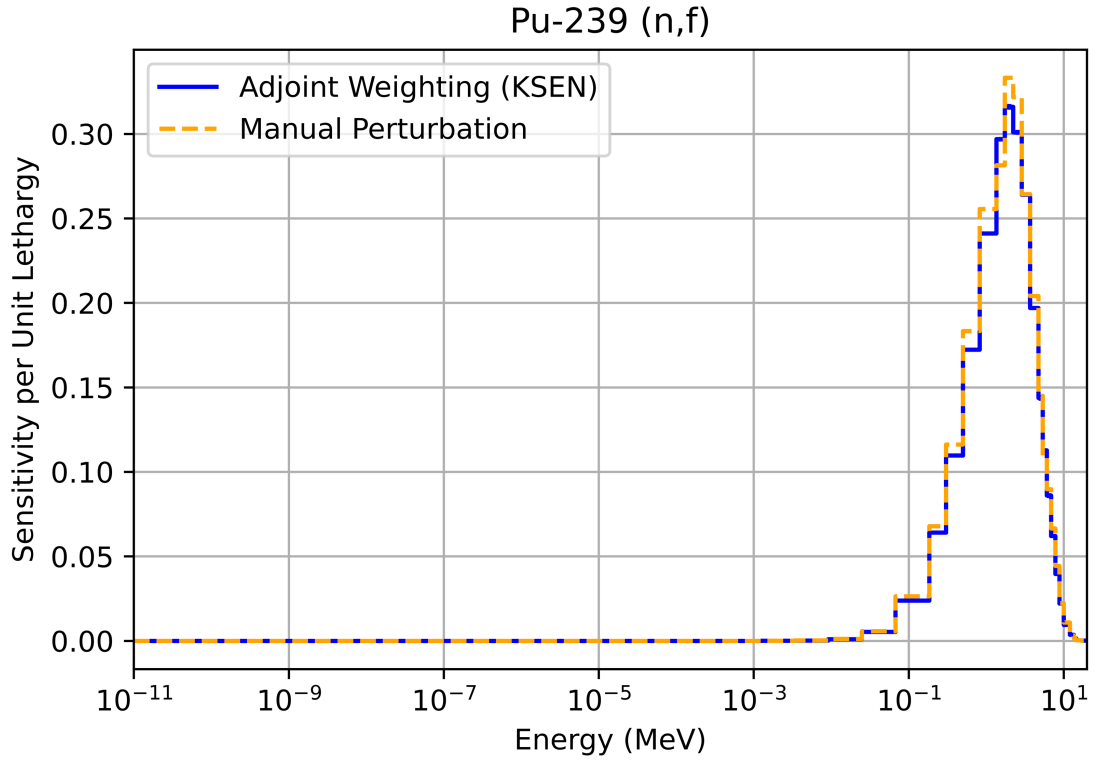
k_p = prompt neutron multiplication factor

l = mean neutron lifetime

Sensitivity profiles from N. Kleedtke 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]



[1]B. 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).
[2]J. 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 ($\Delta_{k_{\text{eff}}}$):

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

$\boldsymbol{C}_{\sigma,\sigma}$ = covariance matrix of nuclear data σ
$\boldsymbol{S}_{k_{\text{eff}},\sigma}$ = 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