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# Distribution and Use of ACE Nuclear Data Files in MCNP<sup>®</sup>

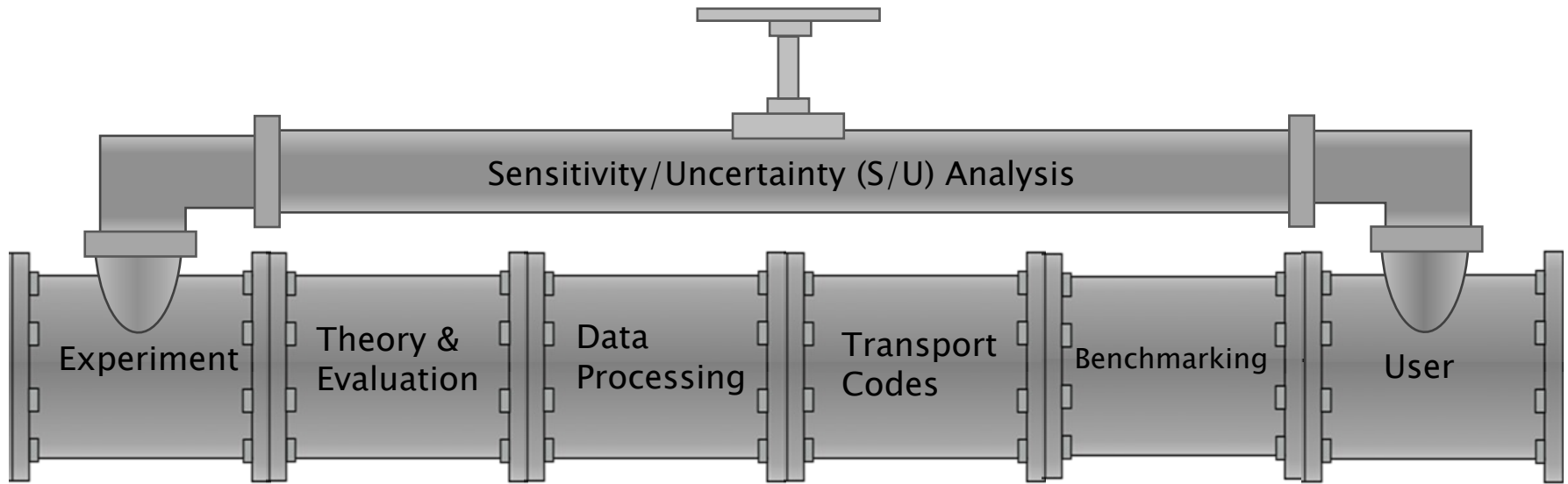
**Noah Kleedtke**

XCP-5, Materials and Physical Data Group

2023 MCNP<sup>®</sup> User Symposium

LA-UR-23-XXXXX

# Nuclear Data Pipeline



# Nuclear Data Pipeline

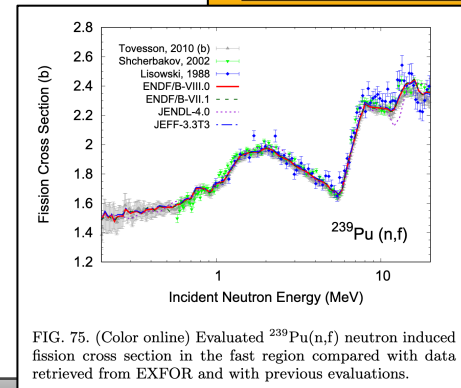
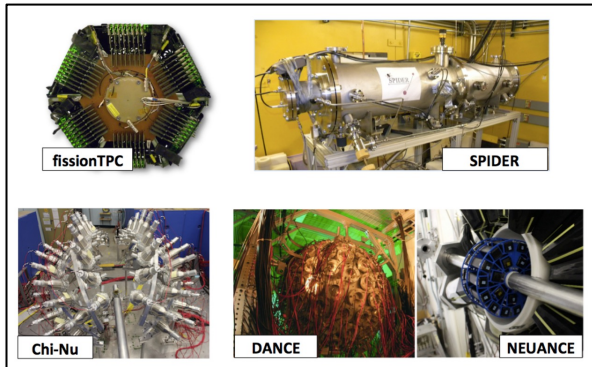
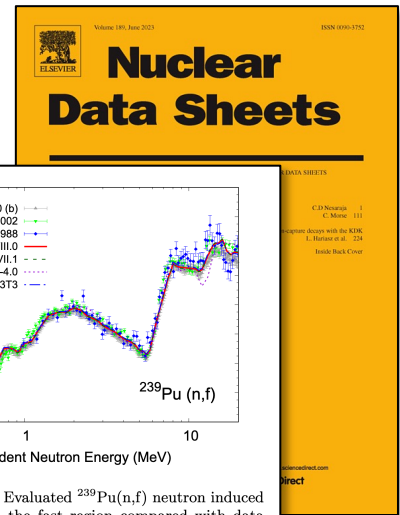
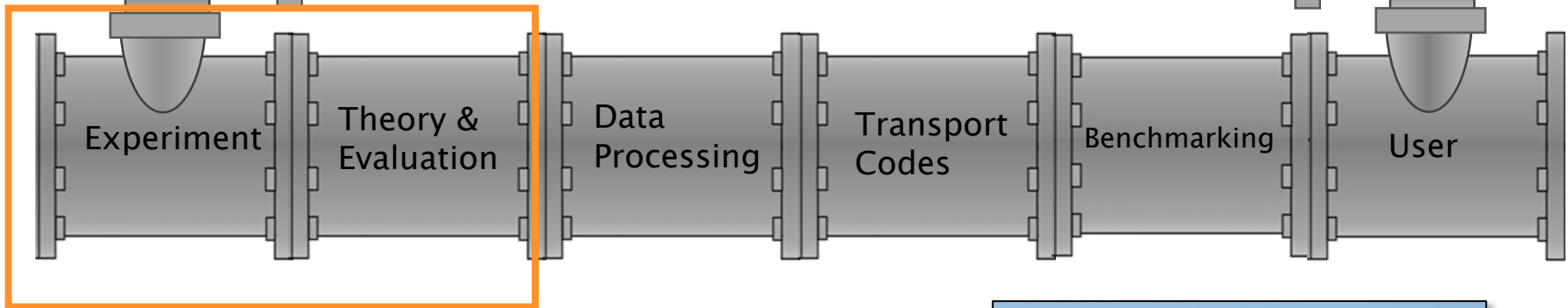


FIG. 75. (Color online) Evaluated  $^{239}\text{Pu}(n,f)$  neutron induced fission cross section in the fast region compared with data retrieved from EXFOR and with previous evaluations.

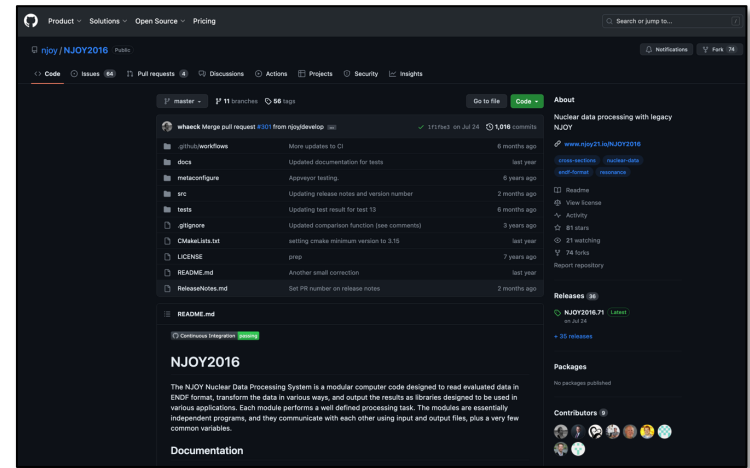
Sensitivity/Uncertainty (S/U) Analysis



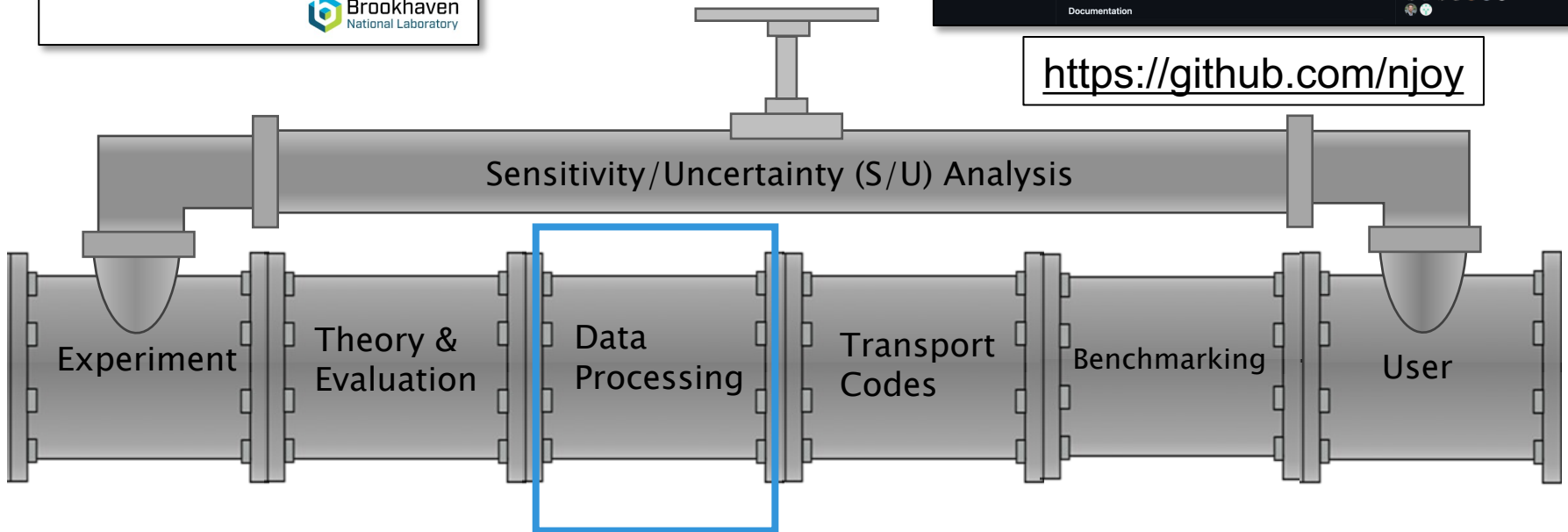
D. Neudecker, "What is nuclear data evaluation?"



# Nuclear Data Pipeline

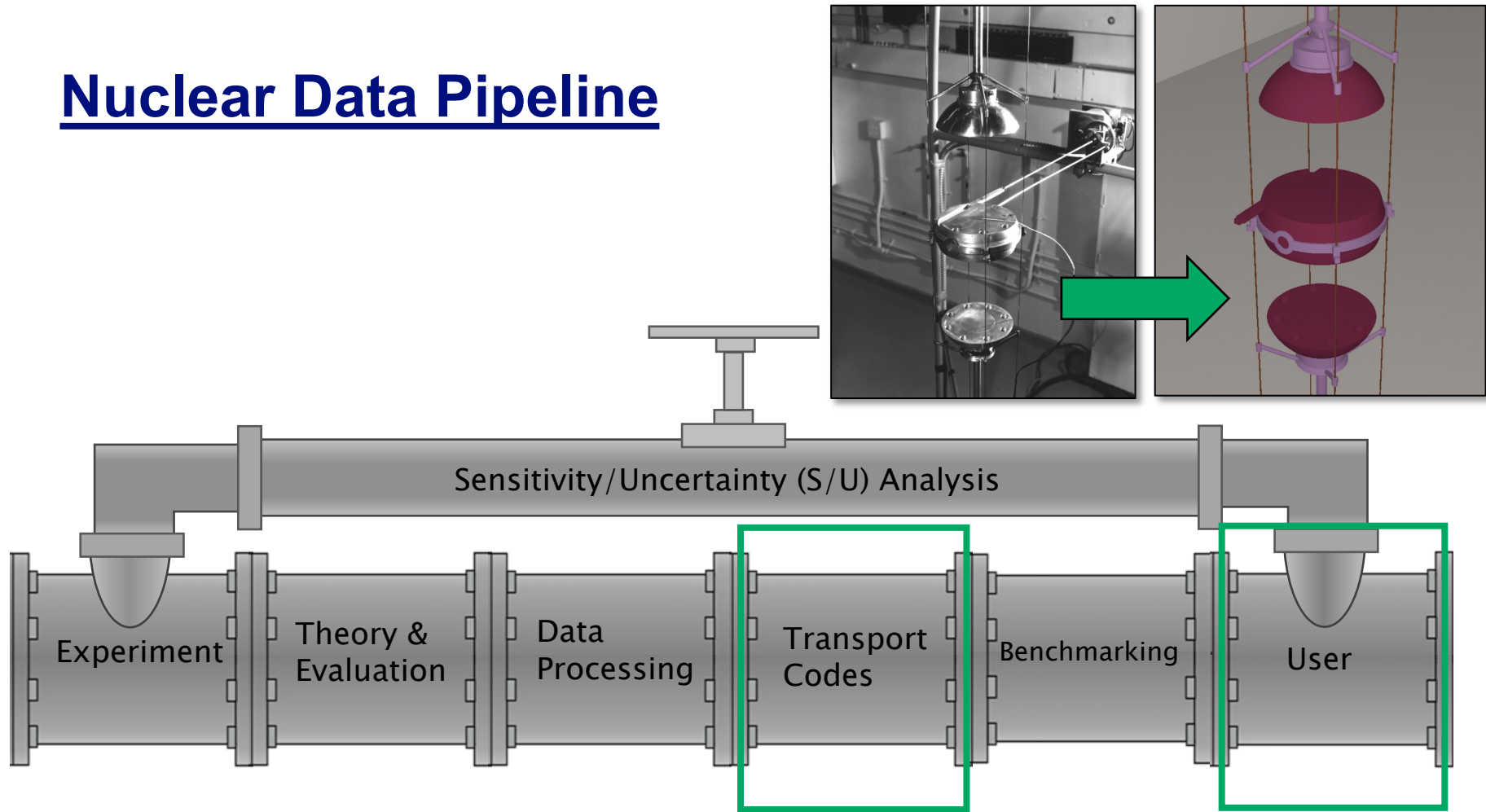


<https://github.com/njoy>



W. Haeck, B. Riedel, "Processing MCNP libraries with NJOY and the road to a modern data processing system"

# Nuclear Data Pipeline



Current Presentation



# Distribution of ACE Nuclear Data Files

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## Nuclear Data Libraries

### OVERVIEW

Welcome to the Los Alamos National Laboratory (LANL) distribution site for nuclear data libraries. These libraries contain A Compact ENDF (ACE) files that have been processed using the nuclear data processing code NJOY (<https://github.com/njoy>). Compressed folders with each nuclear data library are downloadable for use in your own applications.

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



# Latest Distribution of ACE Nuclear Data Files: ENDF/B-VIII.0 (Lib80x)

The screenshot shows the Los Alamos National Laboratory website. The top navigation bar includes links for Careers, News & Media, and Quick Links. The main navigation bar features the Los Alamos logo and links for MISSION, SCIENCE & INNOVATION, COLLABORATION, COMMUNITY, and ENVIRONMENT. A search icon is also present. On the left side, there is a search bar and a sidebar menu with categories: HOME, DATA LIBRARIES, and ACE LIBRARIES. Under ACE LIBRARIES, several libraries are listed, with Lib80x highlighted in blue. The main content area displays the title "Lib80x—Library based on ENDF/B-VIII.0" and the release date "Released: 2018-06-29". Below this, 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 K), .01c (600 K), .02c (900 K), .03c (1200 K), .04c (2500 K), .05c (0.1 K), and .06c (250 K). A note indicates that full documentation is in the docs directory. A "DOCUMENTATION" section includes a reference to a 2018 report (LA-UR-18-24034). At the bottom, a heading reads "Some additional information which may be of use for MCNP Users".

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**Lib80x**

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NUCLEAR DATA / ACE / LIB80X

## Lib80x—Library based on ENDF/B-VIII.0

Released: 2018-06-29

This library is based on ENDF/B-VIII.0. It contains ACE files for continuous-energy incident neutrons. These have been processed at the following temperatures (with their respective ZAID extensions).

- **.00c** — 293.6 Kelvin (Room Temperature)
- **.01c** — 600 Kelvin
- **.02c** — 900 Kelvin
- **.03c** — 1200 Kelvin
- **.04c** — 2500 Kelvin
- **.05c** — 0.1 Kelvin
- **.06c** — 250 Kelvin

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

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

# 3 Ways to Specify ACE Files in MCNP

1. Using ZAID extensions
2. Modifying the XSDIR file
3. Implementing XS<sub>n</sub> card in the input file

F.B. Brown, M.E. Rising, “Guide for Using ENDF/B-VIII.0 Nuclear Data with MCNP,” LA-UR-20-30460 (2020)

# 3 Ways to Specify ACE Files in MCNP

## 1. Using ZAID extensions

2. Modifying the XSDIR file

3. Implementing XS<sub>n</sub> card in the input file

- ZA identifiers (ZAID) are used by MCNP input files to associate data files with nuclide specifications
- The first several digits of the ZAID follow a convention related to the atomic number  $Z$ , mass number  $A$ , and excited state  $S$ :

$$\text{ZAID} = Z * 1000 + A + S * 400$$

# (1) Using ZAID Extensions

Input File: Jezebel Benchmark  
(PU-MET-FAST-001) (J. Favorite)

```
Pu239 Jezebel 17,065.5 g Pu-alloy (4.5 at% 240Pu, 1.02 wt% Ga)
1 94 0.0402901 -1 imp:n=1
2 0 1 imp:n=0

1 so 6.39061

mode n
rand gen=2 seed=2901000001
prtmp j 500
kcode 2400000 1.0 50 1050
totnu
sdef pos=0. 0. 0. rad=d1 erg=d2
si1 0. 6.39061
sp1 -21 2
sp2 -3 0.966 2.842
m94 94239.00c 3.7047E-02
94240.00c 1.7512E-03
94241.00c 1.1674E-04
31069.00c 8.2663E-04
31071.00c 5.4857E-04
print
```

```
m94 nlib=80c
94239 3.7047E-02
94240 1.7512E-03
94241 1.1674E-04
31069 8.2663E-04
31071 5.4857E-04
```

## Specification Examples:

“.XXc” → continuous-energy neutron  
“.XXp” → continuous-energy photoatomic  
“.XXe” → continuous-energy electron  
“.XXu” → continuous-energy photonuclear  
“.XXt” → thermal  $S(\alpha, \beta)$   
XX is the evaluation identifier

## Options:

- (1) NLIB (neutron)
- (2) PLIB (photoatomic)
- (3) ELIB (electron)
- (4) PNLIB (photonuclear)
- (5) HLIB (proton)

# 3 Ways to Specify ACE Files in MCNP

1. Using ZAID extensions
  - 2. Modifying the XSDIR file**
  3. Implementing XS<sub>n</sub> card in the input file
- XSDIR File = data directory file
  - The XSDIR file will have two major sections: (1) Atomic Weight Ratios and (2) Directory
  - XSDIR File for MCNP 6.3 is called “xmdir\_mcnp6.3”

## (2) Modifying the XSDIR File

The data directory file will have 7-11 entries for each table:

1. Name of the Table
2. Atomic Weight Ratio
3. File name
4. Access Route
5. File Type
6. Address
7. Table Length
8. Record Length
9. Number of Entries per Record
10. Temperature
11. Probability Table Flag

### <sup>239</sup>Pu in XSDIR File xsdir\_mcnp6.3

```

94239.00c 236.9986 Lib80x/Pu/94239.800nc 0 1 3 1039943 0 0 2.530100E-08 +
ptable
94239.01c 236.9986 Lib80x/Pu/94239.801nc 0 1 3 931925 0 0 5.170400E-08 +
ptable
94239.02c 236.9986 Lib80x/Pu/94239.802nc 0 1 3 873452 0 0 7.755600E-08 +
ptable
94239.03c 236.9986 Lib80x/Pu/94239.803nc 0 1 3 835490 0 0 1.034100E-07 +
ptable
94239.04c 236.9986 Lib80x/Pu/94239.804nc 0 1 3 743915 0 0 2.154300E-07 +
ptable
94239.05c 236.9986 Lib80x/Pu/94239.805nc 0 1 3 1670591 0 0 8.617400E-12 +
ptable
94239.06c 236.9986 Lib80x/Pu/94239.806nc 0 1 3 1064261 0 0 2.154300E-08 +
ptable
    
```

### <sup>239</sup>Pu ACE File "94239.800nc" ZAID: 94239

```

2.0.1          94239.800nc          ENDF/B-VIII.0
236.998600    2.5301e-08 2018-05-02    2
94239.00c    236.998600 2.5301E-08    05/02/18
Pu239 Lib80 (jlconlin) Reference LA-UR-18-24034 by Conlin, J.L., et al.mat9437
0 0 0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0
1039943 94239 72095 47 45 155 0 6
0 94 239 0 0 0 0 0
1 360476 373151 373198 373245 373292 373339 600148
600194 727862 727907 918604 990699 990854 991009 992427
992582 992582 992737 1039919 373526 1039943 900912 907805
907816 907858 907864 0 0 0 0
1.00000000000E-11 1.03125000000E-11 1.06250000000E-11 1.09375000000E-11
1.12500000000E-11 1.15625000000E-11 1.18750000000E-11 1.21875000000E-11
1.25000000000E-11 1.28125000000E-11 1.31250000000E-11 1.34375000000E-11
1.37500000000E-11 1.43750000000E-11 1.50000000000E-11 1.56250000000E-11
    
```

# 3 Ways to Specify ACE Files in MCNP

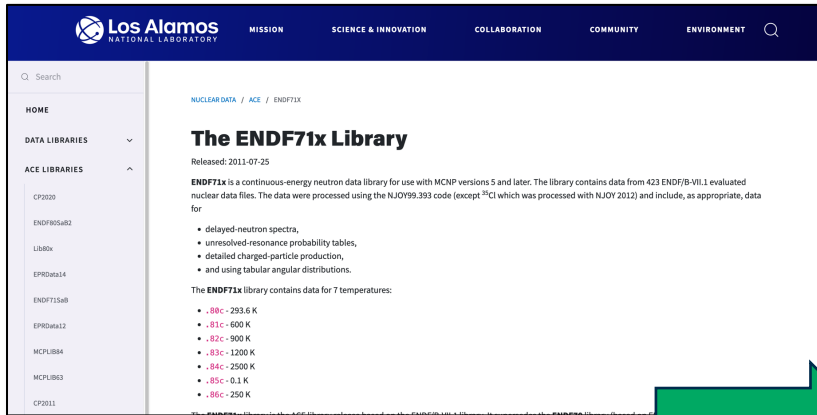
1. Using ZAID extensions
2. Modifying the XSDIR file
- 3. Implementing XS<sub>n</sub> card in the input file**
  - XS<sub>n</sub> Card: Cross Section File Card
  - Information on this card can be found on page 316 of the latest MCNP Code Version 6.3.0 Theory & User Manual
  - This card can be used to load ACE files not listed in the XSDIR file

# (3) Implementing XS<sub>n</sub> card in the input file

Data-card Form: **XS<sub>n</sub>** *z1 a1 z2 a2 ...*

<i>n</i>	Arbitrary cross-section identification number. Restriction: $1 \leq n \leq 99,999,999$ .
<i>zk</i>	Nuclide identifier (ZZZAAA. <i>abx</i> ) used on the <b>M</b> material card.
<i>ak</i>	Atomic weight ratio associated with nuclide <i>k</i> .
...	Remaining <b>xsd<sub>ir</sub></b> file entries for the user-provided cross-section table as described in Appendix B.

## ENDF71x Example:



```
Pu239 Jezebel 17,065.5 g Pu-alloy (4.5 at% 240Pu, 1.02 wt% Ga)
1 94 0.0402901 -1 imp:n=1
2 0 1 imp:n=0

1 so 6.39061

mode n
rand gen=2 seed=2901000001
prmdp j 500
kcode 2400000 1.0 50 1050
totnu
sdef pos=0. 0. 0. rad=d1 erg=d2
si1 0. 6.39061
sp1 -21 2
sp2 -3 0.966 2.842
m94 94239.710nc 3.7047E-02
94240 1.7512E-03
94241 1.1674E-04
31069 8.2663E-04
31071 5.4857E-04

XS1 94239.710nc 236.9986 endf71x/Pu/94239.710nc 0 1 1 811599 0 0 2.530100E-08 ptable
```



# Summary

- Nuclear data is evaluated and analyzed by experimentalists and theoretical physicists, which gets compiled by the Cross Section Evaluation Working Group (CSEWG)
- The LANL Nuclear Data Team processes the ENDF-6 formatted files into ACE files and distributes these files on <https://nucleardata.lanl.gov>
- 3 different ways of using these processed files in MCNP were presented: (1) using ZAID extensions, (2) modifying the XSDIR file, and (3) implementing XS<sub>n</sub> card in the input file
- ENDF/B-VIII.1 nuclear data files will be publicly available soon!

# Questions?

Contact the Los Alamos National Laboratory  
Nuclear Data Team by email at [nucldata@lanl.gov](mailto:nucldata@lanl.gov)



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