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Los Alamos NATIONAL LABORATORY

Distribution and Use of ACE Nuclear Data Files in MCNP®

Noah Kleedtke

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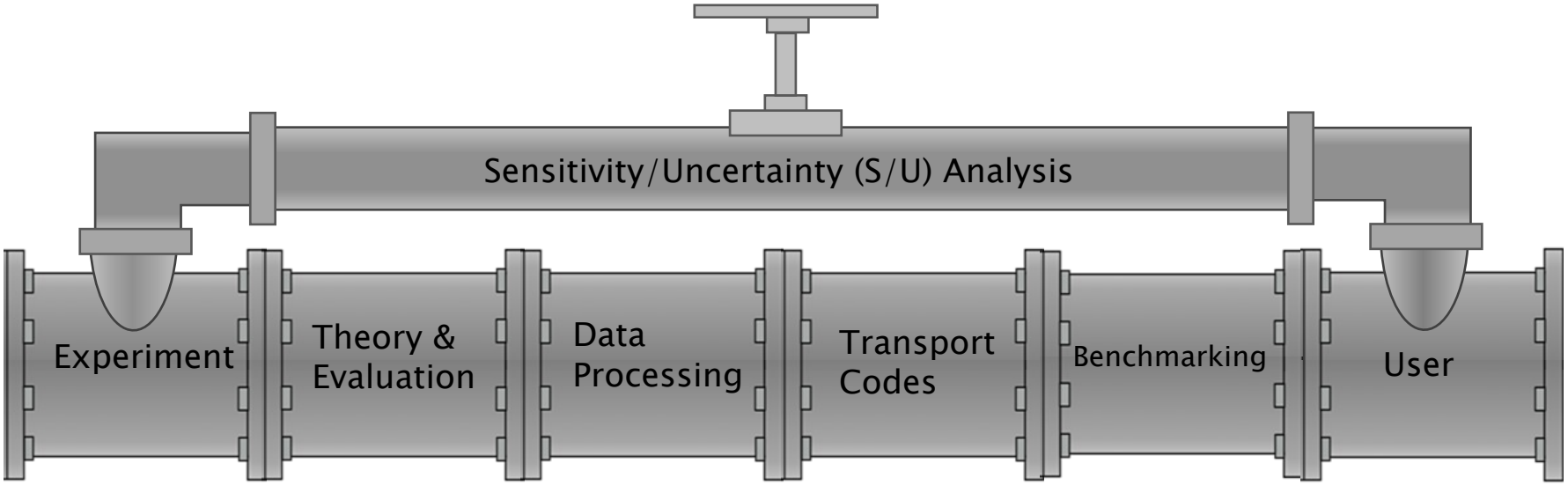
2023 MCNP® User Symposium

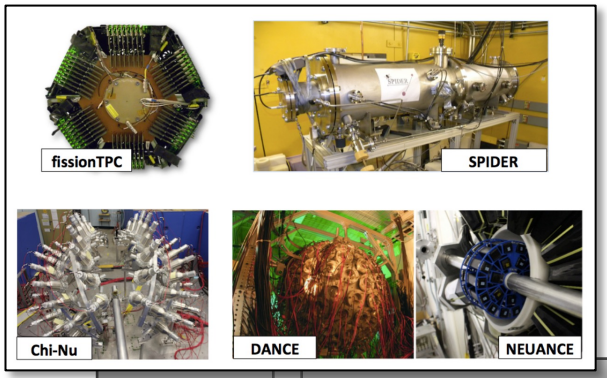
LA-UR-23-XXXXX

Nuclear Data Pipeline



D. Brown, "Nuclear Data Pipeline," *Workshop for Applied Nuclear Data Activities* (2023)

Nuclear Data Pipeline



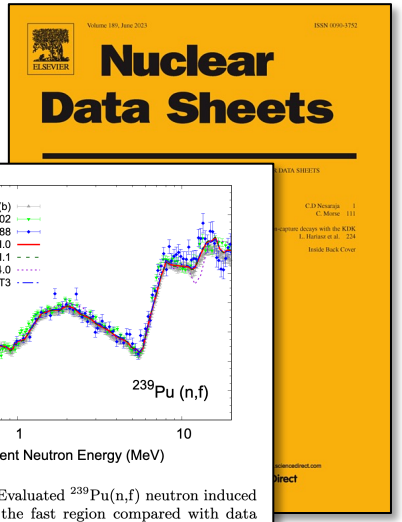


FIG. 75. (Color online) Evaluated ^{239}Pu(n,f) neutron induced fission cross section in the fast region compared with data retrieved from EXFOR and with previous evaluations.

Sensitivity/Uncertainty (S/U) Analysis

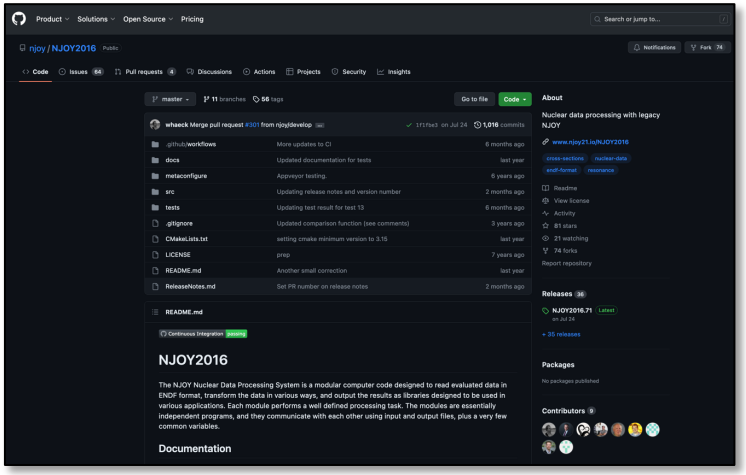
Experiment | Theory & Evaluation | Data Processing | Transport Codes | Benchmarking | User

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

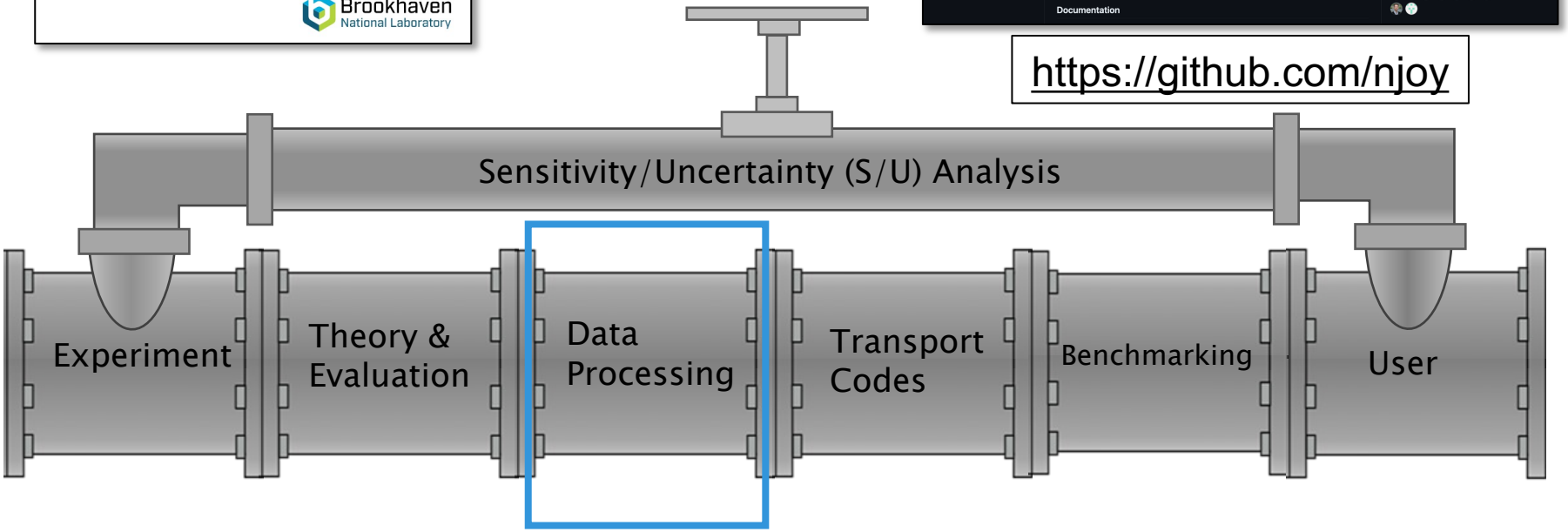
D. Brown et al., "ENDF/B-VIII.0: The 8th Major Release of the Nuclear Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data," *Nuclear Data Sheets* **148** (2018) 1-142

Nuclear Data Pipeline

National Nuclear Data Center
A DOE PuRe Data Resource Facility
Brookhaven National Laboratory

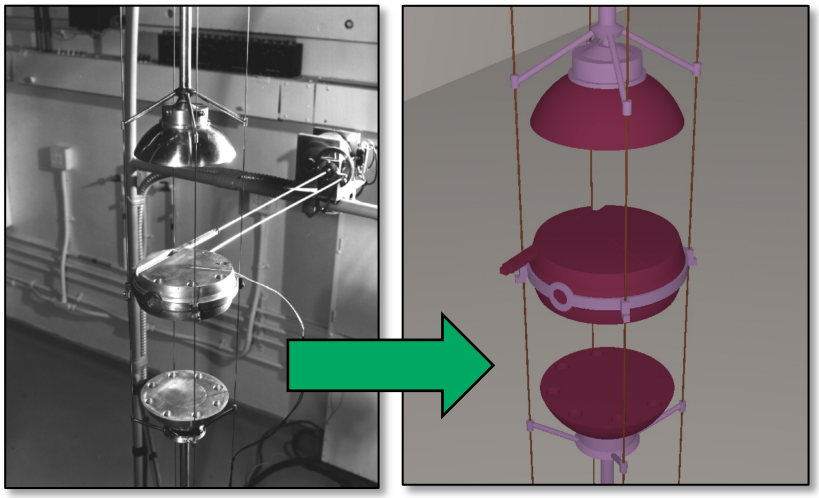


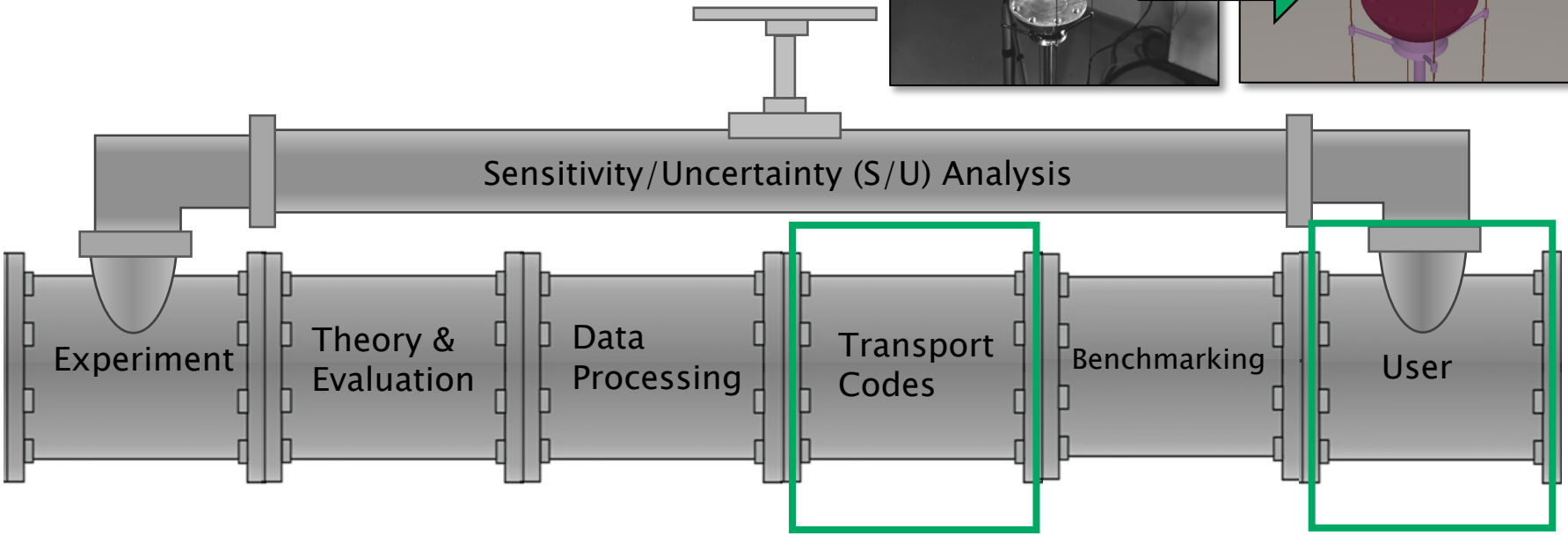
https://github.com/njoy



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

Nuclear Data Pipeline





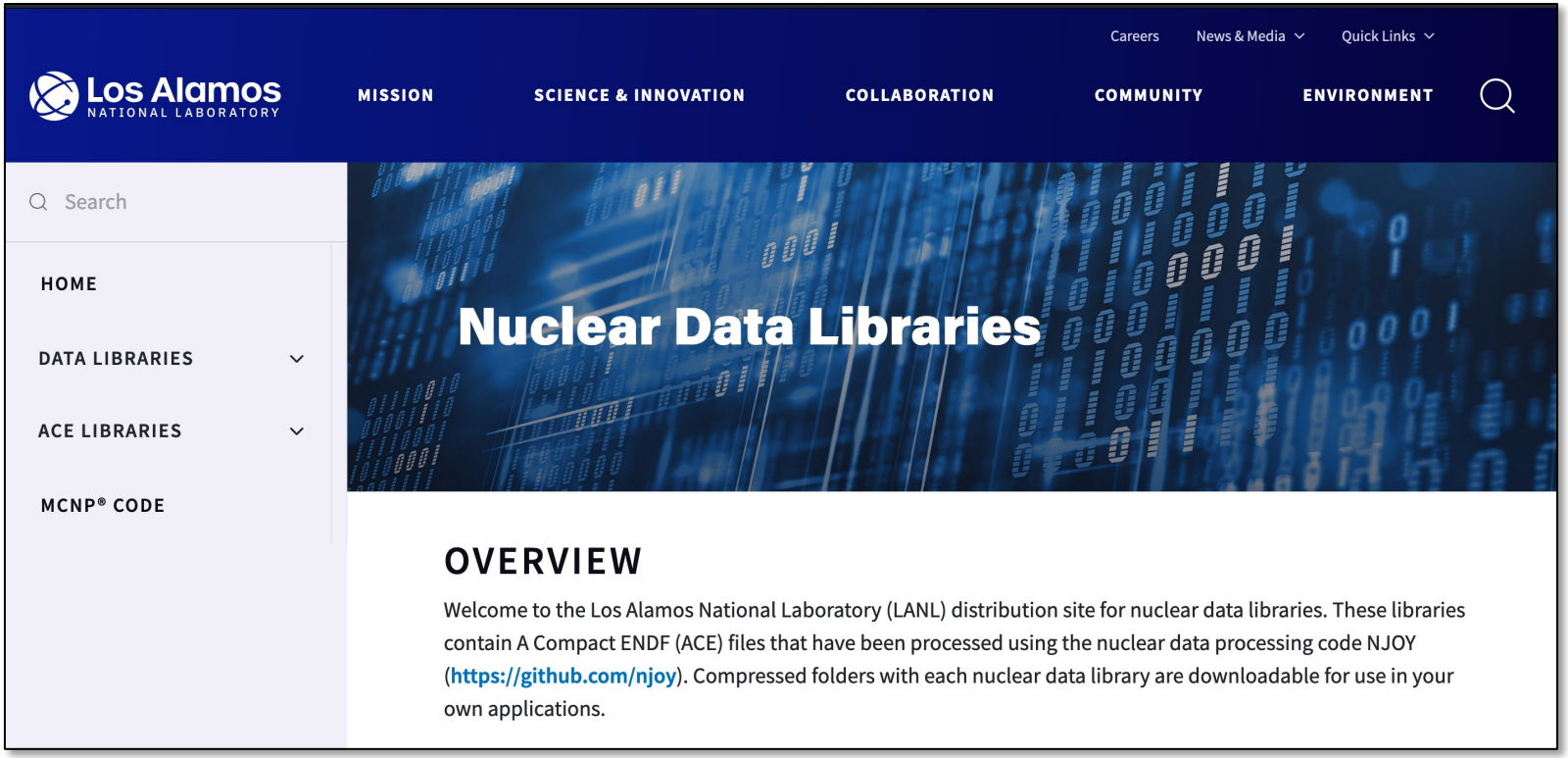
Current Presentation

MCNP® MONTE CARLO N-PARTICLE

Los Alamos NATIONAL LABORATORY

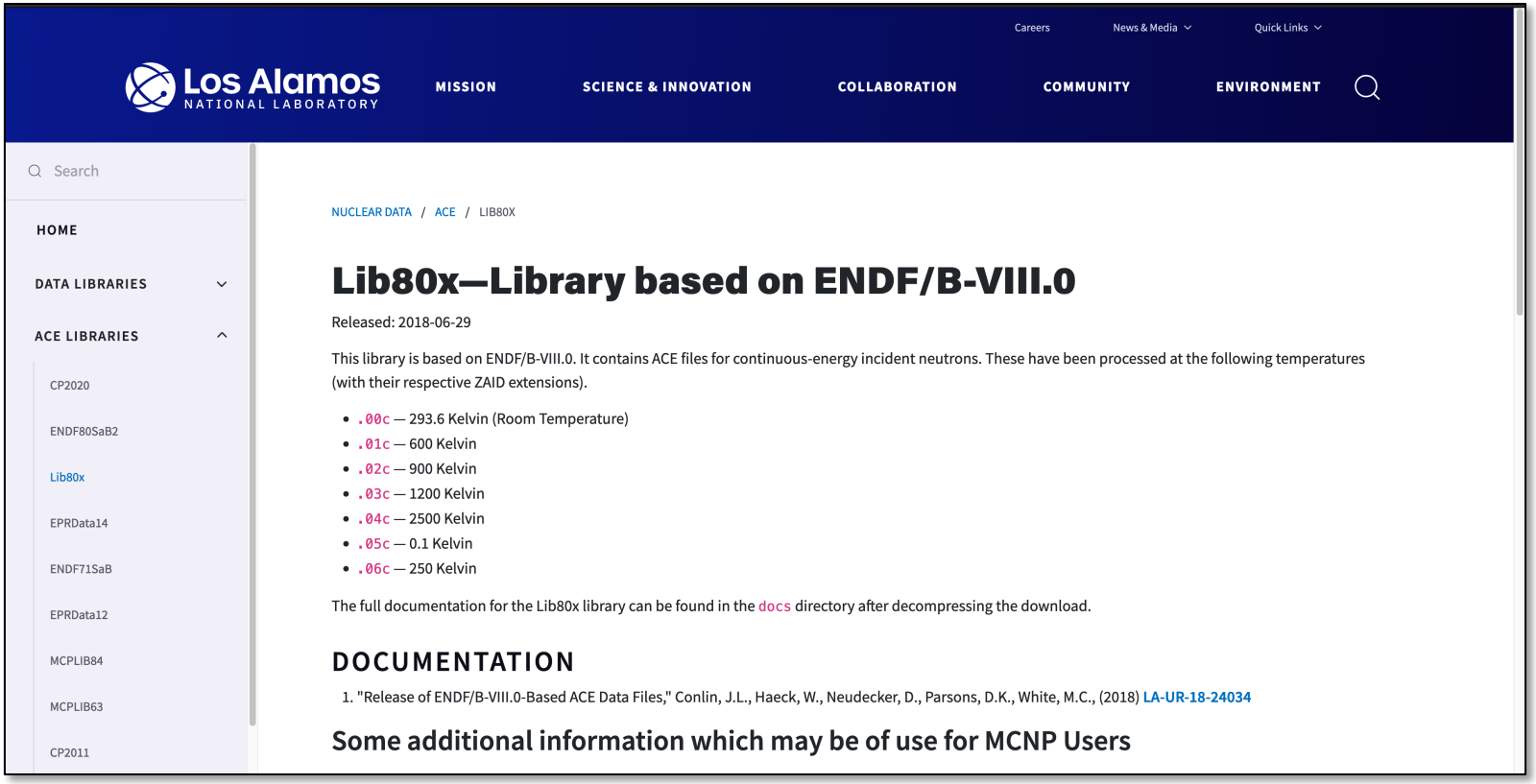
OECD/NEA. International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)03. Paris (France): OECD/NEA; 2021.

Distribution of ACE Nuclear Data Files



https://nucleardata.lanl.gov/

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



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 XSn 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 XSn 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
prdmp 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(α, β)

XX is the evaluation identifier

Options:

(1) NLIB (neutron)

(2) PLIB (photoatomic)

(3) ELIB (electron)

(4) PNLIB (photonuclear)

(5) HLIB (proton)

OECD/NEA. International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)03. Paris (France): OECD/NEA; 2021.

3 Ways to Specify ACE Files in MCNP

1. Using ZAID extensions
2. **Modifying the XSDIR file**
3. Implementing XSn 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 “xsdir_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

^{239}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
```

^{239}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 Lib80x (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.      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        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 XSn card in the input file**

- XSn 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

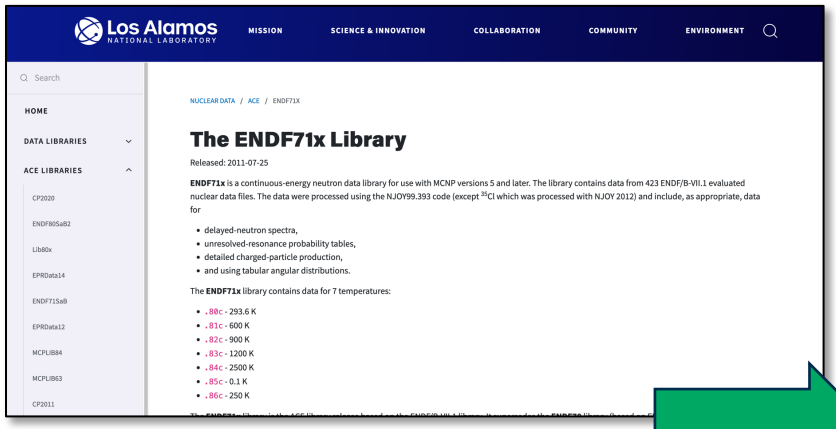
J. Kulesza et al., "MCNP® Code Version 6.3.0 Theory & User Manual," LA-UR-22-30006, Rev. 1 (2022)

(3) Implementing XSn card in the input file

Data-card Form: `XSn z1 a1 z2 a2 ...`

n	Arbitrary cross-section identification number. Restriction: $1 \leq n \leq 99,999,999$.
zk	Nuclide identifier (ZZZAAA.*abx*) used on the `M` material card.
ak	Atomic weight ratio associated with nuclide k.
...	Remaining **xsdir** 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
prdmp 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
print
XS1 94239.710nc 236.9986 endf71x/Pu/94239.710nc 0 1 1 811599 0 0 2.530100E-08 ptable
```


J. Kulesza et al., "MCNP® Code Version 6.3.0 Theory & User Manual," LA-UR-22-30006, Rev. 1 (2022)

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 XSn 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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Wim Haeck


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Donald Kent Parsons


Thomas Saller


Patrick Talou


Martin Frank Staley


Noah Andrew Kleedtke


Ajeeta Khatiwada


Bobbi Riedel


Miriam Anne Kreher


Albert Comstock Kahler III