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Title: Processing of Nuclear Data for Applications

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Processing of Nuclear Data for Applications

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IAEA Workshop on Nuclear Reaction Data and Nuclear
Reactors: Physics, Design and Safety

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Overview of Lectures

- Creating a Validated Application Library
 - For use in a Monte Carlo code, e.g. MCNP or MCNPX
 - For use in an Sn code, e.g. ANISN or DANTSYS
- Discussion of Benchmarking Activities

Creating A Validated Application Library For Use With The MCNP Simulation Code

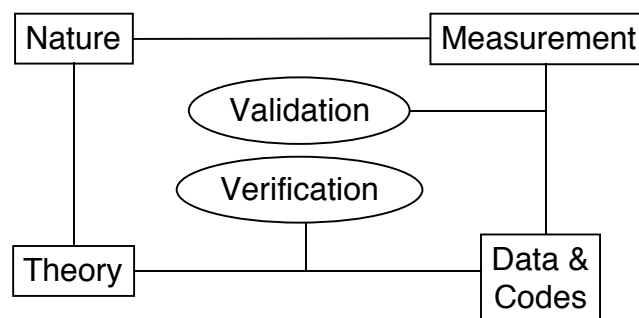
What is a Validated Application Library

- ENDF are raw data, unsuitable for use in an applications code
- NJOY is used to process ENDF evaluations into application libraries
- A validated application library has been through a quality assurance program that:
 - Verifies the data was processed correctly
 - Tests the data against standard benchmarks
 - Documents all aspects of the above

Why Create Validated Application Libraries

- A standard library provides a reference that is easily and quickly understood
- Everyone should not have to re-invent the wheel

Verification And Validation



Methodology to Create a Validated Library

- Selecting evaluated data
- Selecting library characteristics
- Selecting processing paths
- QA of NJOY
- Working procedures
- QA of processed data
- Benchmarking
- Documentation
- Distribution
- Maintenance

Priorities For Selecting Evaluated Data

- Target is essential for the specific application
- Prefer isotopic evaluations over elemental
- Target has been available in previous libraries
- Evaluation source
- Completeness of the evaluation

Evaluation Source

There are many sources of evaluated data

- Evaluated data comes from many sources
 - e.g. BNL, B3, CEA/Saclay, KAPL, LANL, LLNL, ORNL, CNDC, IPPE, JAERI, KAERI, MSU, Petten
- Peer reviewed evaluated data libraries
 - e.g. BROND, CENDL, ENDF/B, JEF, & JENDL
- Data centers that coordinate, maintain and disseminate these data files include
 - e.g. IAEA, JAERI, Obninsk, NNDC, NEA & RSICC

Completeness Of The Evaluation

The application dictates the level of detail necessary

- Activation/dosimetry applications
 - Requires only reaction cross-section data
- Transport applications
 - Requires interaction cross-section data
 - Requires emission data for secondary particles of interest
 - Must cover the energy range of interest
 - Some applications may require more sophisticated data

An Example: The Making of ENDF66

- General purpose, continuous-energy, Monte Carlo neutron transport library (i.e. ACE class 'c' library)
- Created from the ENDF/B-VI release 6 library (originally 325 evaluations)
 - 173 evaluations were judged complete and necessary
 - 129 evaluations will be considered again in 2nd pass
 - 15 evaluations were adequate only for activation/dosimetry
 - 8 evaluations not processed

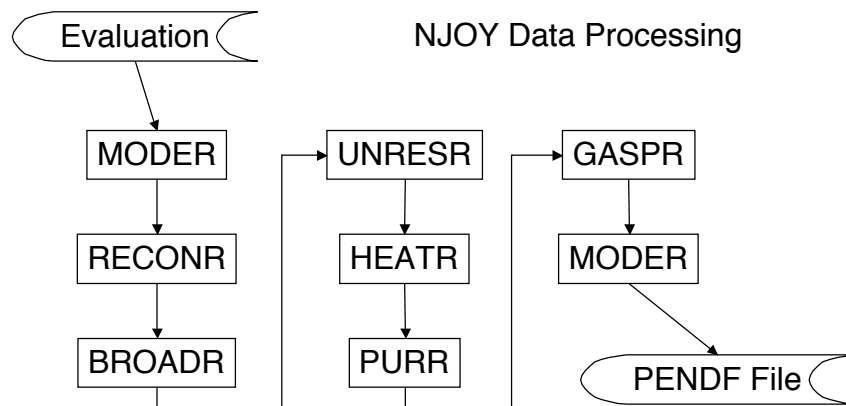
Library Characteristics

- Continuous-energy libraries may include
 - Input parameters to adjust
 - Tolerance for cross-section reconstruction
 - Temperature(s) for Doppler broadening of cross-sections
 - Which data to include
 - Enhanced delayed neutron emission data
 - Unresolved resonance probability tables
 - Equi-probable bin or tabular angular distributions
 - Photon production data
 - Charged particle production data

Library Characteristics (Continued)

- Multi-group libraries may include
 - Energy group structure
 - Temperature for Doppler broadening of cross-sections
 - Flux weighting for cross-section collapse to energy groups
 - Self-shielding parameters
 - Fission chi vectors or matrices
 - Up-scattering terms in transfer matrices
 - Transfer matrices for other particle production
 - Edit cross sections

Selecting A Processing Path



Example NJOY Input Deck

```

moder
20 -21
reconr
-21 -22
'pendf for endf/b-vi.5 92-u-235 njoy 99.50' /
9228 7 /
.001 /
'the following reaction types are added'/
' mt152 bondarenko unresolved'/
' mt153 unresolved probability tables'/
' mt20x gas production'/
' mt221 free thermal scattering'/
' mt301 total heating kerma factor'/
' mt444 total damage energy production'/
0 /

```

- RECONR is used to construct the point-wise cross sections
- Process mat 9228
- Add 7 lines of comments
- Construct the point-wise cross section data using a tolerance of 0.001

Example NJOY Input Deck (Continued)

```

broadr
-21 -22 -23
9228 3 /
.001 /
77. 293.6 3000. /
0 /

```

- RECONR creates point-wise data for a material temperature of 0 K
- BROADR is used to Doppler broaden the point-wise data to user input temperatures
- Process mat 9228 for three temperatures
- Add data for 77 K, 293.6 K and 3000 K
- Again, construct the point-wise cross section data using a tolerance of 0.001

DOPPLER Post-Processing Code

- The routines from the NJOY BROADR module have been extracted and used to create the stand-alone code DOPPLER
- DOPPLER works on ACE class 'c' neutron tables
- DOPPLER will broaden the point-wise cross sections in an ACE file to a user input temperature
- DOPPLER will interpret between two sets of unresolved resonance tables
- DOPPLER will also be able to work with S(σ_0) tables

Example NJOY Input Deck (Continued)

```
unresr
-21 -23 -24
9228 3 1 1
77. 293.6 3000. /
1e10 /
0 /
```

- UNRESR is used to create effective self-shielded cross sections for resonance reactions in the unresolved energy range
- Process mat 9228 for three temperatures and one sigma_0
- Process data for 77 K, 293.6 K and 3000 K all at a sigma_0 of 1e10

Example NJOY Input Deck (Continued)

```

heatr
-21 -24 -25 /
9228 7 /
302 303 304 318 402 443 444 /

```

- HEATR is used to generate point-wise heat and radiation damage energy production cross sections for specified reactions
- Process mat 9228 for seven reactions

Example NJOY Input Deck (Continued)

```

purr
-21 -25 -26
9228 3 1 20 64 /
77. 293.6 3000. /
1e10 /
0 /

```

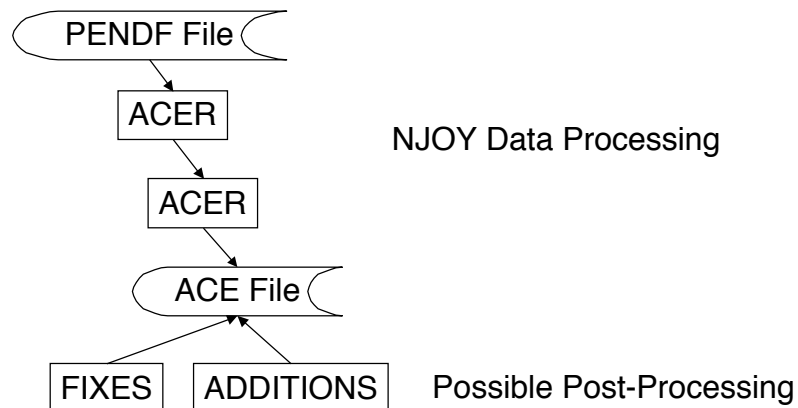
- PURR generates unresolved resonance probability tables and Bondarenko moments
- Process mat 9228 for three temperatures and one sigma_0
- Generate tables with 20 bins using 64 ladders

Example NJOY Input Deck (Continued)

```
gaspr
-21 -26 -27
moder
-27 30
stop
```

- GASPR is used to add total gas production cross sections (MT 203-207)
- MODER transforms the final PENDF tape back into ASCII format

Selecting A Processing Path (Continued)



Example NJOY Input Deck (Continued)

```

moder
20 -21
moder
30 -31
acer
-21 -31 0 50 51
1 0 1 0.66 /
'92-u-235 at 293.6K from endf/b-vi.5
  njoy99.50' /
9228 293.6 /
/
/

```

- ACER is used reformat the data from (P)ENDF into the MCNP ACE formats
- Load the original ENDF and process PENDF files
- Convert the data to the ACE class 'c' format and store them as a type 1 (ASCII) file using the library ID 66
- Get the data for mat 9228 at a temperature of 293.6

Example NJOY Input Deck (Continued)

```

acer
0 50 0 54 55
7 1 1 -1 /
'92-u-235 at 293.6K from endf/b-vi.5
  njoy99.50' /
stop

```

- ACER is also used to do consistency checks on the final ACE file
- Print as much information as possible
- Output a type 1 (possibly fixed) ACE file

Post Processing Additions To The ACE File

For ENDF66, the following code was used:

- ADD_DN – Add delayed neutron data

In past, other codes have been used:

- ADD_CP – Add charged particle emission data
- ADD_URES – Add unresolved resonance tables
- ADD_GP – Add gamma production data

Eventually these capabilities are added to NJOY

Fixes Used During the ENDF66 Processing

- Fixed the heating values in the unresolved probability tables
- Floored small values (to 1E-30) to ensure they would be non-zero if read as IEEE single precision real values

QA Of NJOY and Additional Codes

The quality assurance (QA) checks include two parts:

- Evaluations used to verify error checking
- Evaluations used to verify module performance

NJOY (No Really, It's Called NJOY)

Experience teaches you what went wrong last time; if you're smart, you'll check to make sure you don't do it twice

Corollary: If you were really smart, you would have checked for it the first time

Creating Bad Data To Test Error Checking (P)ENDF Checks

The following lists are examples of possible checks;
they are not comprehensive

- Missing Data
- Negative Cross-Section Values
- Inconsistent threshold energy & Q-value
- Inconsistent thresholds for multiple particles from the same reaction

Creating Bad Data To Test Error Checking ACER Checks

ACER has a number of consistency checks

- Do threshold values correspond to Q-values
- Is the energy grid monotonically increasing
- Check angular distributions for correct ref. frame
- Check angular distributions for unreasonable cosines
- Is the emission energy less than the incident energy
- Do summation cross sections match sums
- Ensure that PDF values are non-negative
- Are only appropriate interpolation values used
- Do threshold reactions start with a zero cross section

Verifying/Validating Correct Processing

- Miscellaneous energy grid tests
- Anisotropic photon production
- Summation of partial productions not equal total
- Charged-particle production with full data
- Charged-particle production with incomplete data
- Photon production from MF 6,12 & 15
- Unresolved resonance data
- Delayed neutron emission data

Working Procedures

- What scripts are used to automate the processing?
- What will be stored? Where? For how long?
- How to coordinate multiple people?
- What machine / code version was used?
- Will evaluations be processed one at a time? by element? by some other grouping?
- What will be checked in minute detail?
- What will be checked by eye? by other codes?
- What is required if code/evaluation errors are found?

QA of Processed Data

- Check the NJOY output from the PENDF run
- Check the NJOY output from the ACER runs
- Eyeball the plots
- Eyeball the numbers
- Stand-alone checking codes
- Ho-ho testing

An Example PENDF Output File

The following viewgraphs show examples of a PENDF output file created by processing U-235 following the prescription as previously described

NJOY Output: Header Information

```

1*****
*
*  $$  $$      $$  $$$$$$  $$  $$  *          *          *
*  $$$  $$      $$  $$$$$$$  $$  $$  * nuclear * site: lanl t-2 *
*  $$$$  $$      $$  $$  $$  $$$$  * data * mach: o2k-f90 *
*  $$  $$$$  $$  $$  $$  $$  $$  * processing * date: 08/13/01 *
*  $$  $$$  $$$$$$$$  $$$$$$$$  $$  * system * time: 21:24:10 *
*  $$  $$  $$$$$$  $$$$$$  $$  *          *          *
*          *          *
*****

```

- Note the version number, machine description and data & time

NJOY Output: MODER Module

```

moder...change the mode of an endf/b tape or njoy output tape          0.0s

input unit (+ for coded, - for bb) ...          20
output unit (+ for coded, - for bb) ..         -21

tape label
-----
ENDF/B-VI Release 5

using endf-6 format

0.5s

```

- Note the tape identifier and format are printed

NJOY Output: RECONR Module

```

reconr...reconstruct pointwise cross sections in pendf format      0.5s

unit for endf/b tape ..... -21
unit for pendf tape ..... -22

label for pendf tape
-----
pendf tape for endf/b-vi.5 92-u-235 njoy 99.50

tape label
-----
ENDF/B-VI Release 5

storage 17/100000

```

- Note, again, the tape identifier and format are printed
- Note the input label for the PENDF tape is printed

NJOY Output: RECONR Module (Cont.)

```

material to be processed ..... 9228
reconstruction tolerance ..... 0.001
reconstruction temperature ..... 0.k
resonance-integral-check tolerance ... 0.020
max resonance-integral error ..... 1.000E-07

```

descriptive cards for pendf tape

the following reaction types are added where available

```

mt152 bondarenko unresolved
mt153 unresolved probability tables
mt20x gas production
mt221 free thermal scattering
mt301 total heating kerma factor
mt444 total damage energy production

```

- Check the input parameters (mat, tolerance, etc.)
- Note the descriptive labels are printed

NJOY Output: RECONR Module (Cont.)

```
processing mat 9228 in endf-6 format
-----
92-U -235 ORNL,LANL,+EVAL-NOV89 WESTON, YOUNG, POENITZ, LUBITZ

changed threshold from 1.219440E+07 to 1.219442E+07 for mt 17.

changed threshold from 4.639801E+04 to 4.639828E+04 for mt 53.

...
```

- RECONR examines/corrects inconsistent energy thresholds and Q-values
- Note the evaluation target and source are printed

NJOY Output: RECONR Module (Cont.)

```
number of user and resonance nodes = 8602
points in initial unionized grid = 8982
points added by linearization = 269                                6.1s

...

points added by resonance reconstruction =201124
points affected by resonance integral check = 93862
points affected by significant figure reduction =      0
final number of resonance points =209972
number of points in final unionized grid =210375
```

- Note the number of points in the final unionized grid but remember that these are subject to thinning

NJOY Output: RECONR Module (Cont.)

estimated maximum error due to
resonance integral check (errmax,errint)
and significant figure truncation

upper energy	elastic integral	percent error res-int	percent error sig-fig	capture integral	percent error res-int	percent error sig-fig
1.00E-05						
1.00E-04	3.50E+01	0.000	0.000	8.15E+03	0.000	0.000
1.00E-03	3.50E+01	0.000	0.000	2.57E+03	0.000	0.000
...						
1.00E+03	8.28E+00	0.002	0.000	3.44E+00	0.019	0.000
2.00E+03	8.27E+00	0.007	0.000	2.54E+00	0.052	0.000

- Note the error induced due to resonance reconstruction

NJOY Output: BROADR Module

broadr...doppler broadening of endf/b data 3148.8s

```

...
material to be processed ..... 9228
number of final temperatures ..... 3
restart (0 no, 1 yes) ..... 0
bootstrap (0 no, 1 yes) ..... 1
starting material temperature ..... 0.0k
thinning tolerance ..... 0.001
max. energy ..... 1.000E+06
errmax for thinning ..... 2.000E-02
errint for thinning ..... 1.000E-07
final temperatures ..... 7.700E+01
                          2.936E+02
                          3.000E+03

```

- Check for expected input parameters
 - Note that this example uses bootstrapping during broadening

NJOY Output: BROADR Module (Cont)

```
files are in endf-6 format

max energy for broadening and thinning = 2.24998E+03          3160.8s

broadened mat9228 from 0.0000E+00 to 7.7000E+01 k
points in=210375 points out=111155
mt 2 18 102
```

- Note the maximum energy
- Check the requested final temperature
- Note the reduction in number of energy points
- Check for the expected MT values

NJOY Output: BROADR Module (Cont)

```
broadened mat9228 from 7.7000E+01 to 2.9360E+02 k
points in=111155 points out= 67410
mt 2 18 102
...
broadened mat9228 from 2.9360E+02 to 3.0000E+03 k
points in= 67410 points out= 24136
mt 2 18 102
```

- Note the reduction in the number of energy points as broadening continues to higher temperatures
 - The number of points can be dramatically different for broadening directly versus bootstrapping
 - E.g. From 0K to 77 K to 293.6 K : direct gives 74,843 points versus bootstrapping gives 67,410 (7% larger final file size)
 - No significant impact on the actual cross section values

NJOY Output: BROADR Module (Cont)

```

thermal quantities at 293.6 K = 0.0253 eV
-----
thermal fission xsec:  5.8493E+02
thermal fission nubar: 2.4367E+00
thermal capture xsec:  9.8672E+01
thermal capture integral: 8.6645E+01
thermal capture g-factor: 9.9086E-01
capture resonance integral: 1.4047E+02
thermal fission integral: 5.0608E+02
thermal fission g-factor: 9.7629E-01
thermal alpha integral: 1.6828E-01
thermal eta integral: 2.0859E+00
thermal k1 integral: 6.4044E+02
equivalent k1: 7.2266E+02
fission resonance integral: 2.7602E+02
-----

```

- If 293.6 K is requested, NJOY prints some common numbers; these can be checked against standard references
 - E.g. Glasstone & Sesonske list 99 & 582 b for β_a & β_f

NJOY Output: UNRESR Module

```

unresr...calculation of unresolved resonance cross sections      3778.0s

                                                                storage  8/ 20000

unit for input endf/b tape ..... -21
unit for input pendf tape ..... -23
unit for output pendf tape ..... -24

temperatures ..... 7.700E+01
                               2.936E+02
                               3.000E+03
sigma zero values ..... 1.000E+10

print option (0 min., 1 max.) ..... 1

```

- Check input parameters

NJOY Output: UNRESR Module (Cont)

```

mat = 9228      temp = 7.700E+01                3778.1s
energy = 2.2500E+03
  1.965E+01
  1.194E+01
  5.676E+00
  2.038E+00
  1.965E+01
...
energy = 2.5000E+04
  1.411E+01
  1.118E+01
  2.193E+00
  7.334E-01
  1.411E+01
generated cross sections at 14 points                3781.6s

```

- Note unresolved cross section reconstructions

NJOY Output: HEATR Module

```

heatr...prompt kerma                                3786.4s
...
mat to be processed ..... 9228
no. temperatures (0=all) ..... 0
gamma heat (0 nonlocal, 1 local) ..... 0
print option (0 min, 1 more, 2 chk) .. 0
damage displacement energy ..... default
partial kerma mt-s desired .....
                                     302
                                     303
                                     304
                                     318
                                     402
                                     443
                                     444

default damage energy = 25.0 ev

```

- Check input parameters

NJOY Output: HEATR Module (Cont)

```

q correction for delayed fission energy
  delayed gammas:    6.3300E+06
  delayed betas:     6.5000E+06
  total correction:  1.2830E+07
...
---message from nheat---changed q from  1.9372E+08 to  1.8089E+08
                           for mt  18

```

- Note that NJOY does not include energy from delayed emissions (gammas and betas) in its calculation of the prompt heating
- Prompt gammas are accounted for explicitly in the calculation of the gamma heating values

NJOY Output: HEATR Module (Cont)

```

---message from hinit---mf6, mt 16 does not give recoil za=92234
                           one-particle recoil approx. used.

---message from hinit---mf6, mt 17 does not give recoil za=92233
                           one-particle recoil approx. used.

...

generating recoil with one-particle approx.

```

- Example of missing data in the evaluation
 - NJOY needs energy distributions for all secondary particles from a reaction to compute the energy deposition
 - In this case, NJOY is able to make assumptions and generate an approximate to the data needed

NJOY Output: HEATR Module (Cont)

```

photon energy production check
      e      ev-barns      min      max
1.0000E-05  2.4951E+11  5.5649E+12  5.5649E+12  ----
1.0000E-04  7.8871E+10  1.7591E+12  1.7590E+12  ----
1.0000E-03  2.4841E+10  5.5399E+11  5.5398E+11  ----
1.0000E-02  7.5846E+09  1.6997E+11  1.6997E+11  ----
...
1.8000E+07  2.4966E+07  3.3350E+08  3.5847E+08  ----
1.9000E+07  2.5596E+07  3.2613E+08  3.5173E+08  ----
2.0000E+07  2.6226E+07  3.2616E+08  3.5239E+08  ----

```

- Note the energy carried away by gamma production

NJOY Output: PURR Module

```

purrr...probabalistic unresolved calculation          3965.4s
                                                    storage 24/ 70000

unit for input endf/b tape ..... -21
unit for input pendf tape ..... -25
unit for output pendf tape ..... -26
temperatures ..... 7.700E+01
                               2.936E+02
                               3.000E+03
sigma zero values ..... infinity
number of probability bins ..... 20
number of resonance ladders ..... 64
print option (0=min, 1=max) ..... 1
no. of energy points (0=all) ..... 0

```

- Check the input parameters

NJOY Output: PURR Module (Cont)

```

e= 2.2500E+03  spot= 1.1663E+01  dbar= 1.4860E-01  sigx=-3.9991E-05
      total      elastic      fission      capture
1  2.0329E+01  1.1989E+01  6.1668E+00  2.1733E+00
2  1.9634E+01  1.1809E+01  5.7079E+00  2.1172E+00
...
64  1.9478E+01  1.1861E+01  5.7334E+00  1.8835E+00
bkgd -3.9991E-05  0.0000E+00  0.0000E+00  0.0000E+00
infd  1.9654E+01  1.1940E+01  5.6761E+00  2.0378E+00
aver  1.9602E+01  1.1907E+01  5.6650E+00  2.0301E+00
pcsd  2.03      0.52      4.78      6.75
nres  3675

```

- Spot check the infinitely dilute (infd) versus UNRESR
- Note the difference between the infinitely dilute and the average

NJOY Output: PURR Module (Cont)

```

bondarenko cross sections by direct sampling
temp      sig0      p0 total      elastic      fission      capture      p1 total
7.700E+01  1.000E+10  1.9602E+01  1.1907E+01  5.6650E+00  2.0301E+00  1.9602E+01
2.936E+02  1.000E+10  1.9634E+01  1.1915E+01  5.6813E+00  2.0376E+00  1.9634E+01
3.000E+03  1.000E+10  1.9678E+01  1.1925E+01  5.7049E+00  2.0480E+00  1.9678E+01
...
bondarenko cross sections from probability table
temp      sig0      p0 total      elastic      fission      capture      p1 total
7.700E+01  1.000E+10  1.9602E+01  1.1907E+01  5.6650E+00  2.0301E+00  1.9602E+01
2.936E+02  1.000E+10  1.9634E+01  1.1915E+01  5.6813E+00  2.0376E+00  1.9634E+01
3.000E+03  1.000E+10  1.9678E+01  1.1925E+01  5.7049E+00  2.0480E+00  1.9678E+01

```

- Cross check the Bondarenko values

NJOY Output: PURR Module (Cont)

```

probability table
tmin      1.035E+01
tmax      1.250E+01  1.351E+01  1.459E+01  1.577E+01  1.704E+01  1.841E+01 ...
          2.712E+01  2.930E+01  3.166E+01  3.421E+01  3.696E+01  3.994E+01 ...
          2.250E-02  7.773E-02  1.207E-01  1.270E-01  1.172E-01  1.033E-01 ...
prob      3.922E-02  3.022E-02  2.441E-02  1.830E-02  1.417E-02  1.038E-02 ...
          3.922E-02  3.022E-02  2.441E-02  1.830E-02  1.417E-02  1.038E-02 ...
tot 7.700E+01  1.211E+01  1.306E+01  1.406E+01  1.517E+01  1.639E+01  1.769E+01 ...
          2.606E+01  2.816E+01  3.043E+01  3.285E+01  3.552E+01  3.838E+01 ...
          2.606E+01  2.816E+01  3.043E+01  3.285E+01  3.552E+01  3.838E+01 ...
els 7.700E+01  1.056E+01  1.112E+01  1.136E+01  1.157E+01  1.164E+01  1.175E+01 ...
          1.242E+01  1.258E+01  1.288E+01  1.314E+01  1.357E+01  1.393E+01 ...
          1.242E+01  1.258E+01  1.288E+01  1.314E+01  1.357E+01  1.393E+01 ...
fis 7.700E+01  1.192E+00  1.524E+00  2.119E+00  2.828E+00  3.694E+00  4.603E+00 ...
          9.966E+00  1.130E+01  1.257E+01  1.391E+01  1.549E+01  1.710E+01 ...
          9.966E+00  1.130E+01  1.257E+01  1.391E+01  1.549E+01  1.710E+01 ...
cap 7.700E+01  3.578E-01  4.216E-01  5.800E-01  7.741E-01  1.051E+00  1.345E+00 ...
          3.680E+00  4.283E+00  4.981E+00  5.804E+00  6.457E+00  7.342E+00 ...
          3.680E+00  4.283E+00  4.981E+00  5.804E+00  6.457E+00  7.342E+00 ...

```

- Note the probability table values
- Spot check the average against the average from the ladder calculation

NJOY Output: GASPR Module (Example is from Fe-56)

```

gaspr...add gas production cross sections          221.4s
mf6,mt5 found
the gas production threshold is 8.6227E+05 ev
found 2871 points
pendf mt  mt203  mt204  mt205  mt206  mt207
-----
  5      ***    ***    ***    0.0    ***
 22      0.0    0.0    0.0    0.0    1.0
 28      1.0    0.0    0.0    0.0    0.0
103      1.0    0.0    0.0    0.0    0.0
104      0.0    1.0    0.0    0.0    0.0
105      0.0    0.0    1.0    0.0    0.0
106      0.0    0.0    0.0    1.0    0.0
107      0.0    0.0    0.0    0.0    1.0

```

*** means that the yield is energy dependent

Examples Of Other NJOY Messages

Now that we have seen what a typical NJOY PENDF print output looks like, lets go on to examine some sections that show “interesting” output

It is worth commenting that most “interesting” output is a result of poor, incomplete or incorrect evaluations

“Interesting” NJOY Output Message – calc. ang. dist. not installed

```
---message from rdf2bw---calculation of angular distribution not installed.
```

- RECONR message while processing Fe-56
- This message can be ignored
 - This is a reminder to the NJOY author that there is still more to do

“Interesting” NJOY Output Message – changed threshold

changed threshold from 7.747200E+06 to 7.747232E+06 for mt 22.

- RECONR message while processing Fe-56
- NJOY finds and corrects inconsistencies between threshold energy values and Q-values
 - For a negative Q-value $threshold \geq \frac{A+1}{A}Q$
 - The threshold is adjusted upwards as necessary
 - The warning is printed if the change exceeds 0.1%
- This message should be noted
 - Again, the only solution is to find a better evaluation

“Interesting” NJOY Output Message – nonpositive elastic cross section

---message from emerge---nonpositive elastic cross sections found.

number of nonpositive cross sections removed = 383
number of points in final unionized grid = 7000

- RECONR message while processing Pu-238
- Evaluation uses old single-level Britt-Wigner resonance parameters
 - This representation occasionally goes negative
 - NJOY fixes this by setting the cross section to a small positive value
- This message should be noted
 - The only solution is to find a better evaluation

“Interesting” NJOY Output Message – No Resonance Parameters

```
---message from unresr---mat 425 has no resonance parameters
```

- URESR message while processing Be-9
- Evaluation does not contain resonance parameters
 - RECONR still constructs unionized grid
 - BROADR thins grid but does not broaden
 - URESR has nothing to do, so it complains (i.e. message)
- Note that the absence of resonance (resolved and unresolved) parameters is also reported in RECONR
- This message can be ignored
 - The only solution is to find a better, i.e. more complete, evaluation

“Interesting” NJOY Output Message – missing fission spectrum

```
---message from hinit---mt19 has no spectrum
      mt18 spectrum will be used.
```

- HEATR message while processing U-235
 - There has been debate over what representation is appropriate for the fission cross sections representation
 - MT 18 versus MT 19, 20, 21 & 38
 - As a consequence, the current evaluations are inconsistent in which representation to use
 - NJOY tries to do something reasonable
- This message can be ignored

“Interesting” NJOY Output Message – missing angular distributions

```
---message from hinit---mf4 and 6 missing, isotropy assumed for mt 800  
---message from hinit---mf4 and 6 missing, isotropy assumed for mt 801  
...
```

- HEATR message while processing O-16
- No angular distribution is given for the secondary alpha in the evaluation
 - HEATR assumes isotropic distribution and goes on
- This message can be ignored
 - The only solution is to find a better evaluation

“Interesting” NJOY Output Message – missing MT 458

```
---message from hinit---mt458 is missing for this mat
```

- HEATR message while processing Pu-243
- No partial components of the fission energy released are given in the evaluation
- This message can be ignored
 - The only solution is to find a better evaluation

Examples From ACER Output Files

The following viewgraphs show examples from the ACER output files created by processing Be-9 following the prescription as previously described

NJOY Output: ACER Module

- Produces two output files:
 - Run-time output with consistency checks
 - This includes NJOY messages and error checking
 - Interpreted output
 - These are the actual numbers in the final ACE library file
 - They are printed in a readable format
 - They can be checked by hand/eye

NJOY Output: ACER Module (Cont)

```

acer...monte carlo neutron and photon data                               39.9s

input endf/b unit ..... -21
input pendf unit ..... -31
input gendf unit ..... 0
output ace format unit ..... 50
output directory unit ..... 51

run type option ..... 1
print option (0 min, 1 max) ..... 0
type of ace file ..... 1
mat to be processed ..... 9228
temperature ..... 2.936E+02
thermal name .....
new formats ..... 1
photon option ..... 1

```

- Check input parameters

“Interesting” NJOY Output Message – energy discontinuities

```

energy discontinuities found in gamma files
1.30960E+04
1.09000E+06

```

- ACER message while processing U-235
- The gamma production data often contains “jumps” in the production cross section as reactions open and close
 - This comes from trying to estimate where the gamma’s came from
 - Newer evaluations from model codes can properly sort out the gamma production
- This message can be ignored

“Interesting” NJOY Output Message – found probability tables

```
found mt=153 with unresolved-range probability tables
energy range: 2.2500E+03 - 2.5000E+04 ev
tables are factors
inelastic competition = 4
absorption competition = 0
```

- ACER message while processing U-235
- This message is a reminder that probability tables will be included in the final ACE table
 - It should match what we learned from the PURR output
 - i.e. that (n,n') competes with the unresolved-range of energies and those energies are 2.25 to 25 keV

“Interesting” NJOY Output Message – negative probs found

```
---message from ptleg2---negative probs found
      1 for mt= 73 e= 1.600E+07

---message from ptleg2---negative probs found
      1 for mt= 77 e= 1.600E+07

...
```

- ACER message while processing U-235
- This message indicates that a negative pdf value was found and fixed
 - When ACER encounters a negative PDF value, it sets the value to zero and renormalizes the distribution

NJOY Output: ACER Module (Cont)

```

acer...monte carlo neutron and photon data                               77.4s

input endf/b unit ..... 0
input pendf unit ..... 50
input gendf unit ..... 0
output ace format unit ..... 54
output directory unit ..... 55

run type option ..... 7
print option (0 min, 1 max) ..... 1
type of ace file ..... 1

```

- Check input parameters for 2nd pass

NJOY Output: ACER Module (Cont)

```

ace consistency checks
-----
check reaction thresholds against q values

check that main energy grid is monotonic

check angular distributions for correct reference frame

check angular distributions for unreasonable cosine values

check energy distributions

check photon production sum

check photon distributions

no problems found

```

- “no problems found” – isn’t life good

“Interesting” NJOY Output Message – ep.gt.epmax

```

check energy distributions
consis: ep.gt.epmax 8.701311E-12 with q.lt.0 for (n,x) at e 1.000000E-11 ->
1.000000E-11
consis:   awr.lt.180---this is probably an error.
consis: shifting eprimes greater than epmax and renorming the distribution
consis: ep.gt.epmax 2.001301E+01 with q.lt.0 for (n,x) at e 2.300000E+01 ->
2.005538E+01
consis:   awr.lt.180---this is probably an error.
consis: shifting eprimes greater than epmax and renorming the distribution
...

```

- ACER message while processing N-14
- This message indicates that a $E' > E$ incident could occur; NJOY will shift the errant E' and renormalize the distribution

Eyeball The Plots

The human eye is a wonderfully complex tool, able to spot inconsistency and error with amazing precision

- Look for unexpected discontinuities in cross sections
- Examine secondary distributions
- Examine threshold regions
- Examine resonance regions

Plots from t2.lanl.gov

- Go to <http://t2.lanl.gov>
- Click on “Data”
- Click on “ENDF/B-VI Neutron Data”
- Click on the @@ signs in “@@ 9228 92-U -235 r4”
 - Note that this is the plots for U-235 release 4, not release 5 which has been used in the examples so far
 - Updates from release 4 to 5 were

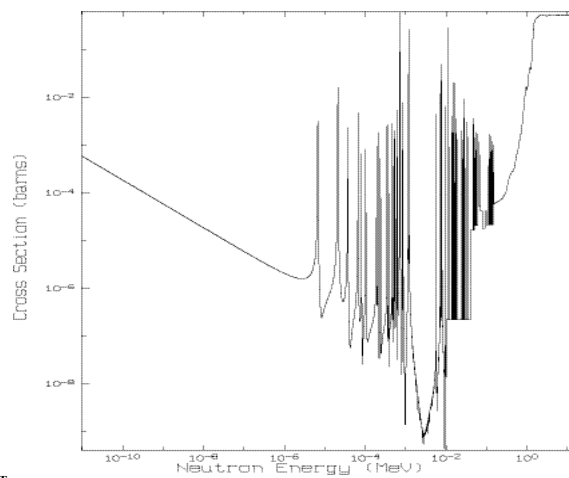
ENDF/B-VI MOD 6 Revision, October 1997, L.C. Leal, H. Derrien,
N.M. Larson, and R.Q. Wright (ORNL)

1. New resonance parameter analysis; File 2, MT=151.
2. Total and prompt-nubar revised below 2 eV; File 1, MT=451, 452,456.

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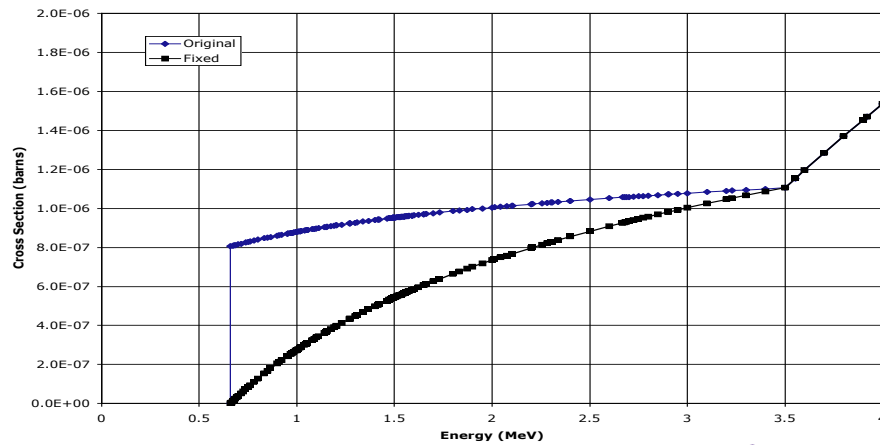
Plot Of Direct Fission Cross Section (MT 19) For U-238



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Plot Of (n,n'_{α}) (MT 22) For Gd-158



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Poor Gd-158 (n,n'_{α}) Cross Section

Interpreted ENDF file for Gd-158

(n,na) cross section

QM = -6.56950E+05 eV

QI = -6.56950E+05 eV

Interpolation table:

35 3

Cross section table:

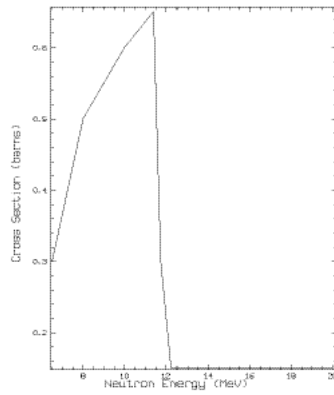
eV	barns	eV	barns	eV	barns
6.611460+5	8.054000-7	3.500000+6	1.105900-6	4.000000+6	1.536100-6
4.500000+6	2.154200-6	5.000000+6	3.043700-6	5.500000+6	4.324500-6

- The first energy value is non-zero
- The energy grid is widely spaced (i.e. poor resolution)

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Poor Cf-252 (n,2n) Cross Section



Eyeball The Numbers

- Spot check known trouble areas
 - This is where experience counts
- Skim through output and “look” for areas where things don’t make sense
 - This is where luck counts

Examples of Stand-alone Checking Codes

- Check for non-zero starting value in threshold reaction
- Check that the summation cross sections are equal to the sum of the partials at energy grid points and mid-points
- Check that the infinitely dilute cross section matches the average cross section in the unresolved probability table
- Check for unrealistic physical values, e.g. heating values > 220
- Check for negative PDF values and that CDF values are monotonically increasing
- Check the discrete lines in emission spectra
- Check that the maximum emission energy for threshold reactions is less than the incident energy

Some Examples of Things We Have Changed

- Correct evaluation to use consistent thresholds
- Correct negative PDF values

B-11 Release 1 Has Inconsistent Thresholds For (n,n') Continuum Reaction (MT 91)

Interpreted ENDF file for B-11

(n,n_cont) cross section

QM = 0.00000E+00 eV

QI = -9.18500E+06 eV

Interpolation table:

16 2

Cross section table:

eV	barns	eV	barns	eV	barns
1.002700+7	0.000000+0	1.050000+7	2.689800-4	1.100000+7	4.538780-4

- File 3 Cross Section data gives threshold as 10.027 MeV
 - Note that 10.027 threshold > 10.0265 by Q-value

Change B-11 Energy Distribution

Particle: neutron

AWP: 1.000000+0

Law 1: Continuum Energy-Angle Distribution

Interpolation:

2 2

Particle yield vs incident energy:

eV	yield	eV	yield	eV	yield
1.050000+7	1.000000+0	2.000000+7	1.000000+0		

- The first energy value 1.050000+7 was changed to 1.002700+7 to provide consistency with cross section value
- The starting energy for the photon yield was similarly changed

F-19 Has Negative PDF Values In Two Energy Distributions

Interpreted ENDF file for F-19
 MT 107 (n,alpha) cross section
 neutron energy distributions
 Energy: 1.650000+7

eV	prob	eV	prob	eV	prob
0.000000+0	0.000000+0	4.000000+5	1.90000-14	8.000000+5	2.72230-13
...					
1.320000+7	2.447700-7	1.360000+7	1.137100-7	1.400000+7	-1.326300-7
1.440000+7	0.000000+0				

- File 6 energy distribution data gives negative PDF value
 - For lack of something better, just changed sign
- Similar change in MF6 MT28 (n,np) energy distribution

Corrected Capture Photon Energy For H-1

Interpreted ENDF file for H-1f

capture photon production yields

1. Discrete photon:
 EG= 2.2246E+06
 ES= 0.0000E+00
 LP=2 Primary photon. Energy is $EG+AWR*E/(AWR+1)$

- The correct EG value is 2.2233E+06 not 2.2246E+06
- This has since been corrected in ENDF/VI release 8

Corrected Atomic Weight Ratio For He-4

Interpreted ENDF file for He-4

ZA= 2004.
 AWR= 4.00150
 MAT= 228
 incident particle= 1

- The correct AWR value is 3.968219 not 4.00150
- This has a large impact on simple photon production where E_{out} is $E_{G} + AWR/(AWR+1) * E_{incident}$

Corrected Restriction Energy For Zirconium Isotopes

4.009000+4	8.913200+1	0	0	1	04025 5 91 1057
2.871000+6	0.000000+0	0	9	1	24025 5 91 1058
4.009000+4	8.913200+1	0	0	1	04025 5 91 1
2.821000+6	0.000000+0	0	9	1	24025 5 91 2

- First discovered (and corrected in release 1) when ENDF/B-V natural Zr was translated to ENDF/B-VI
 - Problem can cause LF=9 evaporation spectrum to sample negative energy causing some programs (MCNP) to fail
- The isotopic zirconium evaluations have never been corrected
 - Corrections were made locally during the ENDF66 processing

Ho-Ho Tests (Think Oh-Oh)

- Use a single cell geometry of reasonable size
- Define the material to use only one ACE table
- Use a reasonable material density
- Ask for simple tallies
- Use a white (i.e. broad-spectrum) energy distribution
- Run a lot of particles

- Check for reported errors and “strange” output

Example MCNP Input Deck For Ho-Ho Test

```

Test ACE Cross Section Table
1  1 -20.0 -1 imp:n,p=1
2  0      +1 imp:n,p=0

1  so  2.0

mode n p
sdef  erg=d1
sil   1e-11 20 $ replace upper energy with max in table
spl   0      1
ctme  120 $ Replace with a LONG TIME
f14:n 1      $ test general neutron physics
f26:n 1      $ test neutron heating numbers
f34:p 1      $ test photon creation
phys:p j 1   $ turn off electron physics
m1    92235.66c -1.00 $ replace with appropriate table zaid

```

- Simple test problem to “exercise” all data sampling options

Benchmarking

- Examples of testing regimes
 - Critical assemblies
 - Pulsed assemblies
 - Shielding assemblies
 - Other reaction rate / flux measurements
- Some sources of benchmarks
 - CSEWG Benchmarks
 - RSICC/NEA SINBAD
 - OECD/NEA International Criticality Safety Benchmark Evaluation Project (ICSBEP)
 - New ANS M&C/RPSD/Reactor Physics Project
 - Literature

Documentation

What needs to be documented and for what audience?

- Internal documentation
 - A complete description of everything to this point
- Library documentation
 - External report describing library contents
 - Evaluation sources
 - Processing methodology
 - QA process
 - Exceptions / corrections
- Benchmark documentation
 - Analysis of benchmark results

Distribution

Who will use this library?

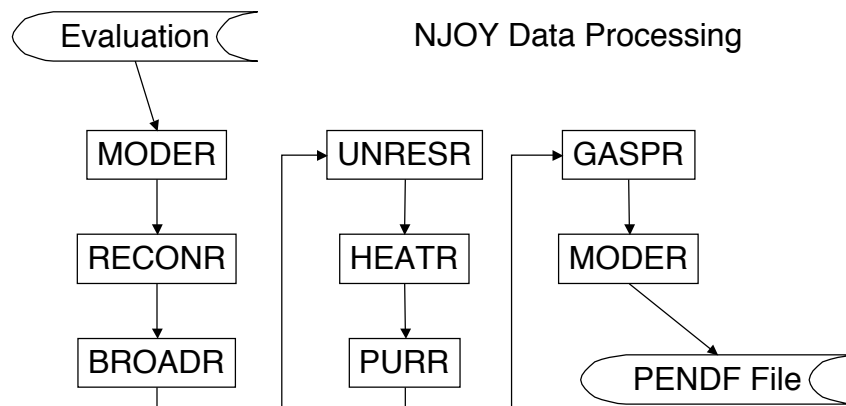
- Internal users
 - Typically to a standard location
 - Must include appropriate documentation
 - Announcements
- External users
 - Distribution through RSICC/NEA? or via web-site?
 - How packaged?
 - Including what documentation?
 - Announcements

Maintenance (What next?)

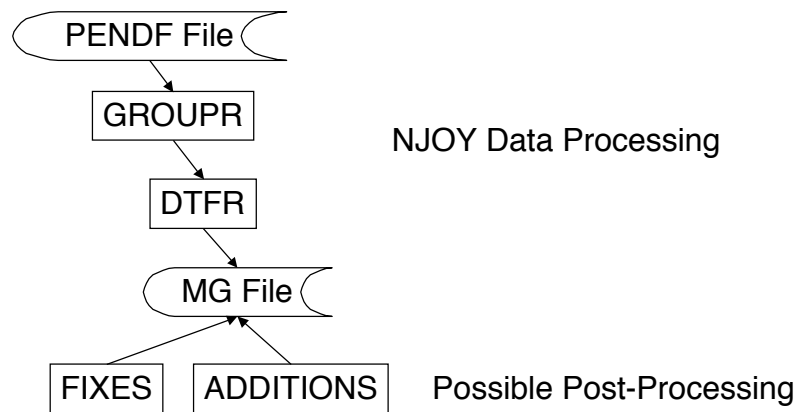
- What do you do if you find an error?
 - Errors in a few or one processed data file may be corrected
 - Make sure to provide appropriate documentation
 - Rename/renumber library/files to indicate the change
 - The big oops: what if everything is wrong?
 - A good reason to retire a library
- When to retire a library?
 - Upon discovery of error(s) in the library
 - Upon creation of a final library incorporating new features
 - When the original evaluations are no longer current

What Is Different in the Approach to Create a Validated Application Library For Use In a a Multigroup Simulation Code

Selecting A Processing Path For Multigroup



Selecting A Processing Path (Continued)



Nuclear Data Team Web Page

<http://www-xdiv.lanl.gov/PROJECTS/DATA/nuclear/nuclear.html>

- Available Documentation
- Discussion of Current Library Releases
- Discussion of Special Libraries
- Future Projects
- Miscellaneous
- FAQ (Frequently Asked Questions)