ENDF/B-VII Beta 2 Covariance Data Testing

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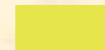# Create Covariance Matrices with PUFF-IV and ERRORJ

Using ENDF-VII-B2 library files containing File 31, 32 and/or File 33 we calculated all possible covariance matrices using PUFF-IV and NJOY/ERRORJ

Calculation was done at T=0 K for PUFF-IV and T=1.1 K for NJOY/ERRRORJ

Covariance matrices with equal MAT and MT values

	1	2	5	17	18	51	102	452	456	801	851	852	853	854	855
Au 197	■	■													
Bi 209	■	░	░	░	░	░	░	░	░	░	░	░	░	░	░
Th 232	■	■	■	■	■	■	■	■			■	■	■	■	■
U 235	░	░	░	░	░	░	░	■	■	░	░	░	░	░	░
U 238					■										

File 32 exists (yellow)

Matrix exists (blue ■)

Several explicit and implicit cross matrices are defined and are calculated by PUFF-IV and ERRORJ

Covariance matrices with equal MAT and MT values

	1	2	4	5	16	22	28	51	102	103	105	107	800	801
Li 6														
Li 7														
B 10														
C														
F 19														
Na 23														
Ti 48														
V														
Co 59														
Ni 58														
Nb 93														
Gd 152														
Gd 153														
Gd 154														
Gd 155														
Gd 156														
Gd 157														
Gd 158														
Gd 160														

File 32 exists

Matrix exists

^{7}Li File 33 content

$MT_1=1$, $MAT_1=328$

• • •

$MT_2=851$, $MAT_2=328$: 1 NI

NI: lb = 5, asymmetric

• • •

MT1=2, MAT1=328

MT2=851, MAT2=328:NI, NC

NC: lty = 0: 1, 4, 851

NI: lb = 6

$MT_1=4$, $MAT_1=328$

• • •

$MT_2=851$, $MAT_2=328$: 1 NI

NI: lb = 5, asymmetric

$MT_1=102$, $MAT_1=328$

• • •

$MT_2=851$, $MAT_2=328$: 1 NI

NI: lb = 5, asymmetric

^{7}Li, MAT=328

Missing lumped reaction covariance data referenced in evaluation

PUFF-IV

■Lists all possible covariance matrices

■Issues warning that some cross section data are not available

■Skips calculation of matrices that cannot be evaluated

ERRORJ

■Aborts since constituents of lumped reaction not found.

■Runs through if all references to lumped reaction 851 are deleted from ENDF file.

Missing, (present in ENDF/B-VI)

MT=16, MAT=328, component of MT=851

MT=24, MAT=328, component of MT=851

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^{232}Th, MAT=9040

^{232}Th File 31 content

MT$_1$=452, MAT$_1$=9040

MT$_2$=452, MAT$_2$=9040: 2 NI
NI: lb = 1
NI: lb = 5, asymmetric
MT$_2$=452, MAT$_2$=1380: 1 NI
NI: lb = 4
MT$_2$=452, MAT$_2$=1381: 1 NI
NI: lb = 3
MT$_2$=452, MAT$_2$=1395: 1 NI
NI: lb = 3
MT$_2$=456, MAT$_2$=1398: 1 NI
NI: lb = 3
MT$_2$=452, MAT$_2$=1399: 1 NI
NI: lb = 3

ENDF-V MAT ← MT$_2$=452, MAT$_2$=1380
ENDF-V MAT ← MT$_2$=452, MAT$_2$=1381
ENDF-V MAT ← MT$_2$=452, MAT$_2$=1395
ENDF-V MAT ← MT$_2$=456, MAT$_2$=1398
ENDF-V MAT ← MT$_2$=452, MAT$_2$=1399

PUFF-IV
- Lists all possible covariance matrices
- Issues warning that some cross section data are not available
- Skips calculation of matrices that cannot be evaluated

NJOY
- Fails to skip over File 6 while executing groupr.
- Runs through once File 6 is deleted (not used for File 31, 32 or File 33 covariance calculation)

ERRORJ
- Fails to skip over File 6 while executing groupr if processing File 31.
- Runs through once File 6 is deleted (not used for File 31 covariance calculation).
- Skips calculation of matrices that cannot be evaluated

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^{235}U, MAT=9228

^{235}U File 31 content

MT_1=452, MAT_1=9228
$\vdots$
MT_2=452, MAT_2=1380: 1 NI
NI: lb = 3
MT_2=452, MAT_2=1381: 1 NI
NI: lb = 2
MT_2=452, MAT_2=1390: 1 NI
NI: lb = 3
MT_2=456, MAT_2=1398: 1 NI
NI: lb = 3
MT_2=452, MAT_2=1399: 1 NI
NI: lb = 2
$\vdots$

ENDF-V MAT → (to MT_2=452, MAT_2=1380)

ENDF-V MAT → (to MT_2=452, MAT_2=1381)

ENDF-V MAT → (to MT_2=452, MAT_2=1390)

ENDF-V MAT → (to MT_2=456, MAT_2=1398)

ENDF-V MAT → (to MT_2=452, MAT_2=1399)

PUFF-IV
- Lists all possible covariance matrices
- Issues warning that some cross section data are not available
- Skips calculation of matrices that cannot be evaluated

ERRORJ
- Skips calculation of matrices that cannot be evaluated

ENDF-VII-B2 standard files

Standard files contain standard reaction covariance matrices. The same matrices are expected to be present in the neutron library files.

	Neutron library file	Standard file	
6Li	<MT=105;MT=105>	<MT=105;MT=105>	✓
C	-	<MT=2;MT=2>	✗
^{197}Au	<MT=1;MT=1>	<MT=102;MT=102>	✗
^{235}U	<MT=452; MT=452> <MT=456; MT=456>	<MT=18;MT=18>	✗
^{238}U	-	<MT=18;MT=18>	✗

ENDF MAT with problems in NJOY/ERRORJ

- ^{6}Li

ERRORJ constructs a union grid with too many energy boundaries and energy boundaries out of order.
This was fixed in ERRORR. If the same fix is applied in ERRORJ, the covariance data can be calculated

- C

NJOY fails to skip over File 12. The covariance matrices can be calculated if File 12 is deleted from the ENDF file.

- ^{23}Na

ENDF file contains only a File 32 and no File 33. ERRORJ only processes File 32 if a File 33 is present.