

IRDF-2002 Dosimetry Cross-Section Library Covariance Processing Verification

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Introduction

The IRDF-2002 library containing cross sections for dosimetry has been released from the IAEA in 2005. Every effort was made that the library would conform strictly with the ENDF-6 rules, but unfortunately the status of the main cross-section processing system NJOY was not capable of handling covariances of partial cross-sections for the excitation of metastable states (i.e. the so-called File 40 in ENDF terminology). A set of updates is proposed to remove this deficiency of NJOY. The updates are listed in Appendix 2 and are available on the OECD/NEA server for the benefit of the broader users' community until the patches are reviewed and incorporated into the official distribution of NJOY by the author.

In addition, a few inconsistencies were encountered in the IRDF-2002 library. The ENDF-6 manual was deficient and did not specify IZAP in File 40 (analogously to the same parameter in File 10). A change to the manual was approved at the CSEWG Meeting in November 2009. Without this parameter it is impossible to match the cross sections with the covariances unambiguously when for example the data set under MT 5 is identified by the residual product IZAP and its final state LFS. In principle, the content of the IRDF-2002 library is not ambiguous because there is never more than one covariance set for MT 5, but for the sake of consistency, the necessary list of changes to the IRDF-2002 library is listed in Appendix 3.

Procedures

A batch procedure for Windows was prepared to generate NJOY inputs automatically. Group constant in four energy groups were generated with GROUPT for cross sections in File 3 and File 10 separately. The energy-group boundaries are given in Table 1. The same generic input was used for all materials, only the MAT number was changed as necessary. Sample input is shown in Appendix 4.

Table 1: Energy-group boundaries

Energy	E_{low}	E_{high}
Thermal	10^{-5} eV	5.5 eV
Resonance	5.5 eV	0.1 MeV
Fission	0.1 MeV	10 MeV
Fusion	10 MeV	20 MeV

The four-group covariance matrices were generated with the ERRORR module for covariance data in File 33 and File 40 separately. A small local code GNTOKEN for converting ERRORR output into ENDF-6 format was executed. The MERGER code of the Pre-Pro series was used

to combine the two parts together. The so-produced ENDF files were merged into a single file. An ad-hoc code ENDDX was used to tabulate the cross sections with relative uncertainties for all reactions. The results are given in Appendix 1.

For verification purposes the same procedure was employed, but the source IRDF-2002 file was processed with the SUMF10 code from the ENDVER package to convert File 10 into File 3 equivalent (neglecting the fact that the cross-sections are only partial cross-sections). Similarly, covariances in File 40 were converted into File 33 equivalent with another ad-hoc code MF40TO33. The resulting file could be processed without the new features in the ERRORR module of NJOY. By comparing the summary table to that in Appendix 1 it was confirmed that the results were identical.

Conclusions

A patch for the NJOY data processing system was prepared to enable processing of the covariances in ENDF File-40. This is needed for processing the dosimetry libraries such as IRDF-2002 and activation libraries that may include covariance information. Extensive testing confirmed that the IRDF-2002 dosimetry library can be processed correctly.

The patch is available from <http://www.nea.fr/html/dbprog/njoy-links.html> and can be used with the official patches up304.

Additional testing of the patches might be necessary when more elaborate evaluated data files become available.

Appendix 1: Four-group average cross sections with uncertainties from IRDF-2002

ENDDX - Calculate group-uncertainties

=====

Material	MT	ZAP/LFS	Thermal [barns]	[%]	Resonance [barns]	[%]	Fission [barns]	[%]	Fusion [barns]	[%]
Material 3006										
105	0		4.722E+02	0.14	3.328E+01	0.19	6.533E-01	6.46	2.660E-02	14.36
Material 5010										
107	0		1.927E+03	0.16	1.356E+02	0.27	7.517E-01	7.99	4.341E-02	9.40
Material 9019										
16	0		0.000E+00	0.00	0.000E+00	0.00	0.000E+00	0.00	3.339E-02	2.69
Material 11023										
16	0		0.000E+00	0.00	0.000E+00	0.00	0.000E+00	0.00	2.333E-02	1.66
102	0		2.650E-01	2.00	2.506E-02	9.94	4.707E-04	15.56	2.105E-04	25.00
Material 12024										
103	0		0.000E+00	0.00	0.000E+00	0.00	1.009E-03	3.24	1.836E-01	1.22
Material 13027										
103	0		0.000E+00	0.00	0.000E+00	0.00	2.606E-03	3.29	7.767E-02	1.89
107	0		0.000E+00	0.00	0.000E+00	0.00	4.510E-04	2.98	1.145E-01	0.96
Material 15031										
103	0		0.000E+00	0.00	0.000E+00	0.00	1.659E-02	4.92	9.692E-02	3.12
Material 16032										
103	0		0.000E+00	0.00	0.000E+00	0.00	3.785E-02	4.87	2.659E-01	4.95
Material 21045										
102	0		1.365E+01	6.15	9.319E-01	4.97	9.360E-03	11.53	7.083E-04	13.42
Material 22046										
16	0		0.000E+00	0.00	0.000E+00	0.00	0.000E+00	0.00	3.054E-02	3.08
103	0		0.000E+00	0.00	0.000E+00	0.00	7.333E-03	4.68	2.539E-01	3.17
Material 22047										
5	210460		0.000E+00	0.00	0.000E+00	0.00	4.568E-09	14.66	4.361E-02	19.64
103	0		0.000E+00	0.00	0.000E+00	0.00	1.051E-02	5.11	1.132E-01	6.36
Material 22048										
5	210470		0.000E+00	0.00	0.000E+00	0.00	1.052E-09	4.16	9.218E-03	22.06
103	0		0.000E+00	0.00	0.000E+00	0.00	1.854E-04	4.72	5.758E-02	3.93
Material 22049										
5	210480		0.000E+00	0.00	0.000E+00	0.00	8.401E-12	0.09	5.560E-03	9.15
Material 23051										
107	0		0.000E+00	0.00	0.000E+00	0.00	1.131E-05	5.33	1.431E-02	1.76
Material 24052										
16	0		0.000E+00	0.00	0.000E+00	0.00	0.000E+00	0.00	2.502E-01	2.24
Material 25055										
102	0		6.734E+00	12.08	9.468E-01	7.57	4.579E-03	11.93	6.621E-04	23.55
Material 26054										
16	0		0.000E+00	0.00	0.000E+00	0.00	0.000E+00	0.00	7.590E-03	3.69
103	0		0.000E+00	0.00	0.000E+00	0.00	4.767E-02	2.42	3.435E-01	4.49
107	0		0.000E+00	0.00	0.000E+00	0.00	5.451E-04	4.62	8.319E-02	2.56
Material 26056										
103	0		0.000E+00	0.00	0.000E+00	0.00	7.104E-04	2.53	1.053E-01	1.32

102	0	1.063E+01	3.00	5.441E+01	4.38	1.380E-01	7.81	3.795E-07	21.21
Material	74186								
102	0	1.950E+01	2.68	3.931E+01	4.72	4.452E-02	10.48	1.132E-03	16.52
Material	79197								
1	0	5.832E+01	0.00	1.597E+02	0.70	5.785E+00	0.35	4.673E+00	0.40
16	0	0.000E+00	0.00	0.000E+00	0.00	1.083E-03	2.15	2.045E+00	1.92
102	0	5.159E+01	0.15	1.288E+02	0.70	1.311E-01	16.04	1.281E-03	25.00
Material	80199								
4	801990	0.000E+00	0.00	0.000E+00	0.00	1.393E-01	8.15	1.827E-01	12.32
Material	82204								
4	802040	0.000E+00	0.00	0.000E+00	0.00	0.000E+00	0.00	0.000E+00	0.00
Material	90232								
18	0	0.000E+00	0.00	0.000E+00	0.00	4.300E-02	5.87	3.614E-01	10.77
102	0	3.634E+00	7.56	7.048E+00	11.18	1.228E-01	18.88	1.571E-03	20.62
Material	92235								
18	0	2.686E+02	0.20	2.159E+01	0.36	1.248E+00	0.40	1.983E+00	0.58
Material	92238								
18	0	5.964E-06	25.04	1.564E-04	28.84	1.756E-01	2.14	1.110E+00	4.23
102	0	1.387E+00	1.35	2.292E+01	0.90	9.360E-02	13.95	1.073E-03	30.00
Material	93237								
18	0	1.301E-02	10.00	5.301E-02	23.54	8.873E-01	1.79	2.151E+00	2.15
Material	94239								
18	0	8.810E+02	1.01	2.286E+01	5.58	1.680E+00	2.07	2.328E+00	5.15
Material	95241								
18	0	4.428E+00	2.00	5.819E-01	4.47	8.424E-01	3.13	2.572E+00	3.15

Appendix 2: Updates for NJOY compatible with NJOY99.304

```
*/
*ident upnea062
*/ errorr A. Trkov, Jan-2010
*/      1. Add MF40 processing capability
*/      WARNING:
*/      The coding was tested on the IRDF-2002 dosimetry library.
*/      If mfcov=40, the GENDF file must contain processed mf=10 data.
*/      The procedure was tested a single LFS state in MF10
*/      and a single covariance set for that state in MF40.
*/      There may be more final states (e.g. in an activation library)
*/      but there are no suitable examples for testing.
*/      2. Change of convention in GENDF files generated by ERRORR
*/      Originally the C1 and C3 records were zero. For consistency
*/      with GENDF files produced by groupr, C1 was set to ZA and C2
*/      to 10*ZAP+LFS. This allows picking proper group data for MF40
*/      covariance processing.
*/      3. Correction of a trivial typing error correction in up307
*/      (statement beyond column 72)
*/
*/      NOTE: All testing was done with group data on ngout present.
*/      Further modifications might be needed if group data are
*/      to be generated internally.
*/
*d errorj.122
c      * mfcov      endf covariance file (31, 33, 34, 35 or 40) to be      *
*i up272.28
      & ,mzap(80),lfs
*i up272.37
      & ,mzap(80),lfs
*i up272.50
      & ,mzap(80),lfs
*i up272.69
      & ,mzap(80),lfs
*i up272.73
      & ,mzap(80),lfs
*i up272.102
      & ,mzap(80),lfs
*i up272.108
      & ,mzap(80),lfs
*i up272.110
      & ,mzap(80),lfs
      common/temper/tempin
*i up272.141
      & ,mzap(80),lfs
*i up272.178
      & ,mzap(80),lfs
*i up272.181
      & ,mzap(80),lfs
*i up272.185
      & ,mzap(80),lfs
*i up272.187
      & ,mzap(80),lfs
*i up272.189
      & ,mzap(80),lfs
*i up272.191
      & ,mzap(80),lfs
*i up272.193
      & ,mzap(80),lfs
*i up272.216
```

```

        & ,mzap(80),lfs
*i up272.222
        & ,mzap(80),lfs
*i up272.230
        & ,mzap(80),lfs
*i up272.236
        & ,mzap(80),lfs
*d errorj.424,425
        if(mfcov.ne.31.and.mfcov.ne.33.and.
        &      mfcov.ne.34.and.mfcov.ne.35.and.
        &      mfcov.ne.40) then
*i errorj.620
c
c      *** check if relevant covariance data are available
        nd=nw/6
        icov=0
        do i=1,nd
            mfi=nint(a(idict+2+(i-1)*6))
            if(mfcov.eq.30 .and. (mfi.ge.30 .and. mfi.le.33)) icov=icov+1
            if(mfcov.eq.31 .and. mfi.eq.31) icov=icov+1
            if(mfcov.eq.32 .and. mfi.eq.32) icov=icov+1
            if(mfcov.eq.33 .and. (mfi.eq.32 .or. mfi.eq.33)) icov=icov+1
            if(mfcov.eq.34 .and. mfi.eq.34) icov=icov+1
            if(mfcov.eq.35 .and. mfi.eq.35) icov=icov+1
            if(mfcov.eq.40 .and. mfi.eq.40) icov=icov+1
        end do
        if(icov.eq.0) then
            write(strng, '('no data on file for mfcov='',i3)') mfcov
            call mess('errorr',strng,'processing terminated')
c          -- skip remaining errorr input (if any)
            if (ign.eq.1.or.ign.eq.19) then
                read(nsysi,*) ng
                ngp=ng+1
                read(nsysi,*) (dmy,i=1,ngp)
            end if
            go to 330
        end if
*i errorj.685
        330 continue
*i errorj.816
        if (iverf.eq.4) then
            nl=l2h
        else
            nl=n2h
        end if
        izap=0
*d errorj.821,824
        elseif (mfcov.eq.40) then
            za=c1h
            awr=c2h
            nl=n1h
            call contio(nendf,0,0,a(iscr),nb,nw)
            izap=10*11h+12h
*i errorj.1480
            else if (mfcov.eq.40) then
                call sigc(ngn,a(isum),a(icflx),a(iscr),a(iun),a(iflx),a(isig))
*i errorj.1566
            izap=mzap(ix)
*d errorj.1576
            a(iscr+1)=izap
*d errorj.1590

```

```

        a(iscr+1)=izap
*d errorj.1873
        if (mfcov.eq.31.or.mfcov.eq.33.or.mfcov.eq.35.or.
&
        mfcov.eq.40) then
*i errorj.3793
        nfs =1
*i errorj.3795
        nfs =1
        if(mfcov.eq.40) then
            nfs=nlh
            nsub=1
            call contio(nendf,0,0,a(iscr),nb,nw)
            lfs=12h
            izap=10*11h+12h
        end if
*i errorj.3815
        mzap(nmt)=izap
*i errorj.3831
        do 310 ilfs=1,nfs
*i errorj.3978
        310 continue
*i errorj.1875
            if (mfcov.eq.40) write(nsyso,38)lfs
c...
            if (mfcov.eq.40) write(nsyso,38)lfs/10,lfs-10*(lfs/10)
*i errorj.2126
        38 format(' final metastable state lfs',i3/)
c..38 format(' final metastable state zap,lfs',i6,i3/)
*/
*/ search gout tape by product identifier
*d errorj.2985
        subroutine rdgout(ngout,matd,mfd,mti,izap,b,sig)
*i errorj.3076
        jzap=0
        if(izap.ne.0) jzap=c2h+0.01
*d errorj.3078
        if (mf.eq.mfd.and.mt.eq.mtd.and.jzap.eq.izap) go to 230
*d errorj.5320
        subroutine rdsig(mat,mt,izap,b,sig)
*i errorj.5329
        izero=0
*d errorj.5342
        call rdgout(ngout,matrd,mfri,mtri,izero,b,sig)
*d errorj.5345
        call rdgout(ngout,matrd,mfrd,mtrd,izap,b,sig)
*i errorj.734
        izero=0
*d errorj.752
        call rdgout(ngout,matd,mfd,mtd,izero,a(ib),a(iegt))
*d errorj.784
        call rdgout(ngout,matd,mfd,mtd,izero,a(ib),a(iflx))
*d errorj.786
        call rdsig(matd,izero,izero,a(ib),a(iscr))
*d errorj.874
        call rdsig(mat,mt,izap,a(ib),a(isig))
*d errorj.986
        if (mt1.lt.851) call rdsig(mat1,mt1,izero,a(ib),a(isig1))
*i errorj.3142
        izero=0
*d errorj.3220
        call rdsig(mats(ix),mtd,izero,b,a(isg))
*d errorj.3226

```

```

250    call rdsig(mats(ix),mts(ix),mzap(ix),b,sig)
*d errorj.3243,3244
      b(1)=za
      b(2)=mzap(ix)
*i errorj.5217
      izero=0
*d errorj.5246
      call rdsig(matd,mtd,izero,a(ib),a(iscr2))
*i errorj.7604
      izero=0
*d errorj.7617
      200 call rdsig(matd,mt1,izero,b,sig)
*d errorj.7628
      call rdsig(matd,mt2,izero,b,sig)
*i errorj.7782
      izero=0
*d errorj.7841
      call rdsig(mat,mt,izero,b,sig)
*/
*/ add tmeperature to the output tape
*i errorj.3134
      common/temper/tempin
*d errorj.3163
      b(1)=tempin
*i errorj.3520
      tempin=clh
*/
*/ prevent printing "undefined" cross sections and covariances
*d errorj.1921
*i errorj.1922,1924
      if(denom.gt.zero) then
          denom=max(denom,eps)
          a(iscr+ibase+ip-1)=a(iscr+ibase+ip-1)/denom*
&          (egn(ig+1)-egn(ig)) * (egn(igp+1)-egn(igp))
      else
          a(iscr+ibase+ip-1)=0
      end if
*d errorj.1926
      if(denom.gt.zero) then
          denom=max(denom,eps)
          a(iscr+ibase+ip-1)=a(iscr+ibase+ip-1)/denom
      else
          a(iscr+ibase+ip-1)=0
      end if
*d errorj.3235
      ff=cflx(ig)
      if(ff.gt.0) then
          csig(ig,ix)=csig(ig,ix)/ff
      else
          csig(ig,ix)=0
      end if
*/
*/ fix record overflow beyond column-72
/**d up307.6,7
*/          if(irelco.eq.0)write(nsyso,40)mt,mats(ixp),mts(ixp),time
*/          if(irelco.eq.1)write(nsyso,45)mt,mats(ixp),mts(ixp),time
*/
*ident upnea063
*/ reconr A. Trkov, November 2009
*/          When no MF3 data present (e.g. dosimetry library with MF10)
*/          make sure that the group structure (MF3 MT1)

```

```
*/          is written with zero cross sections and that N1, N2
*/          parameters from the CONT record are transferred consistently.
*i reconr.4560
    ns1=n1h
    nr1=n2h
*i reconr.4561
    mf1=mfh
    mfh=3
*i reconr.4623
    mfh=mf1
*i reconr.4635
    ns1=n1h
    nr1=n2h
    mf1=mfh
*i reconr.4617
    if(mfh.ne.mf1) call afend(nout,0)
*d reconr.4655,4656
    a(iscr+4)=ns1
    a(iscr+5)=nr1
    mfh=mf1
```

Appendix 3: Errata for the IRDF-2002 library

22-Ti-047

MF40 MT 5 NS2 should be: IZAP=21046, LFS=0

22-Ti-048

MF40 MT 5 NS2 should be: IZAP=21047, LFS=0

22-Ti-049

MF40 MT 5 NS2 should be: IZAP=21048, LFS=0

41-Nb-093

MF40 MT 4 NS2 should be: IZAP=41093, LFS=0

45-Rh-103

MF40 MT 4 NS2 should be: IZAP=45103, LFS=0

47-Ag-109

MF40 MT 102 NS2 should be: IZAP=47110, LFS=2

49-In-115

MF40 MT 4 NS2 should be: IZAP=49115, LFS=0

MF40 MT 16 NS2 should be: IZAP=49114, LFS=1

MF40 MT 102 NS2 should be: IZAP=49116, LFS=1

80-Hg-199

MF40 MT 4 NS2 should be: IZAP=80199, LFS=0

82-Pb-204

MF40 MT 4 NS2 should be: IZAP=82204, LFS=0

Appendix 4: Sample NJOY input

```
moder / Extract/convert neutron evaluated data
1 -21
'95-Am-241 from IRDF-2002'/
20 9543
0/
moder / Make an ASCII copy for test purposed
-21 41 /
reconr / Reconstruct XS for neutrons
41 42
'PENDF for 95-Am-241'/
9543 2/
0.001 0. 0.003/
'95-Am-241 from IRDF-2002'/
'Processed with NJOY99.304+ on 31/01/2010 15:37:22.40'/
0/
broadr / Doppler broaden XS
41 42 43
9543 1 0 0 0./
0.001 2.0e6 0.003/
300.
0/
groupr / Thermal average and resonance integral
41 43 0 38 /
9543 1 0 6 0 1 1 1 /
'95-Am-241 from IRDF-2002 with NJOY99.304+ on 31/01/2010'/
300. /
1.e10 /
4 /
1.e-5 0.55 0.1e6 10.e6 20.e6 /
3 /
0/
0/
errorr / Thermal and resonance covariance matrix
41 43 38 48/
9543 1 6 1 1 /
0 33 /
4 /
1.e-5 0.55 0.1e6 10.e6 20.e6 /
groupr / Thermal average and resonance integral
41 43 0 39 /
9543 1 0 6 0 1 1 1 /
'95-Am-241 from IRDF-2002 with NJOY99.304+ on 31/01/2010'/
300. /
1.e10 /
4 /
1.e-5 0.55 0.1e6 10.e6 20.e6 /
10 /
0/
0/
errorr / Thermal and resonance covariance matrix
41 43 39 49/
9543 1 6 1 1 /
0 40 /
4 /
1.e-5 0.55 0.1e6 10.e6 20.e6 /
stop
```