NOTES on:

"An NJOY Processing Caution when Doppler Broadening"

1. **Some references about Doppler Broadening**

   - ❑ CIELO processing
   - ❑ Example of files in JEFF-3.2
   - ❑ Example of files in JENDL4.u

2. **NJOY versions**

   - ❑ Official versions NJOY 99 and NJOY2012.50: **Processing Caution!!**
   - ❑ Unofficial versions
   - ❑ Official NJOY2012.80 and NJOY2016

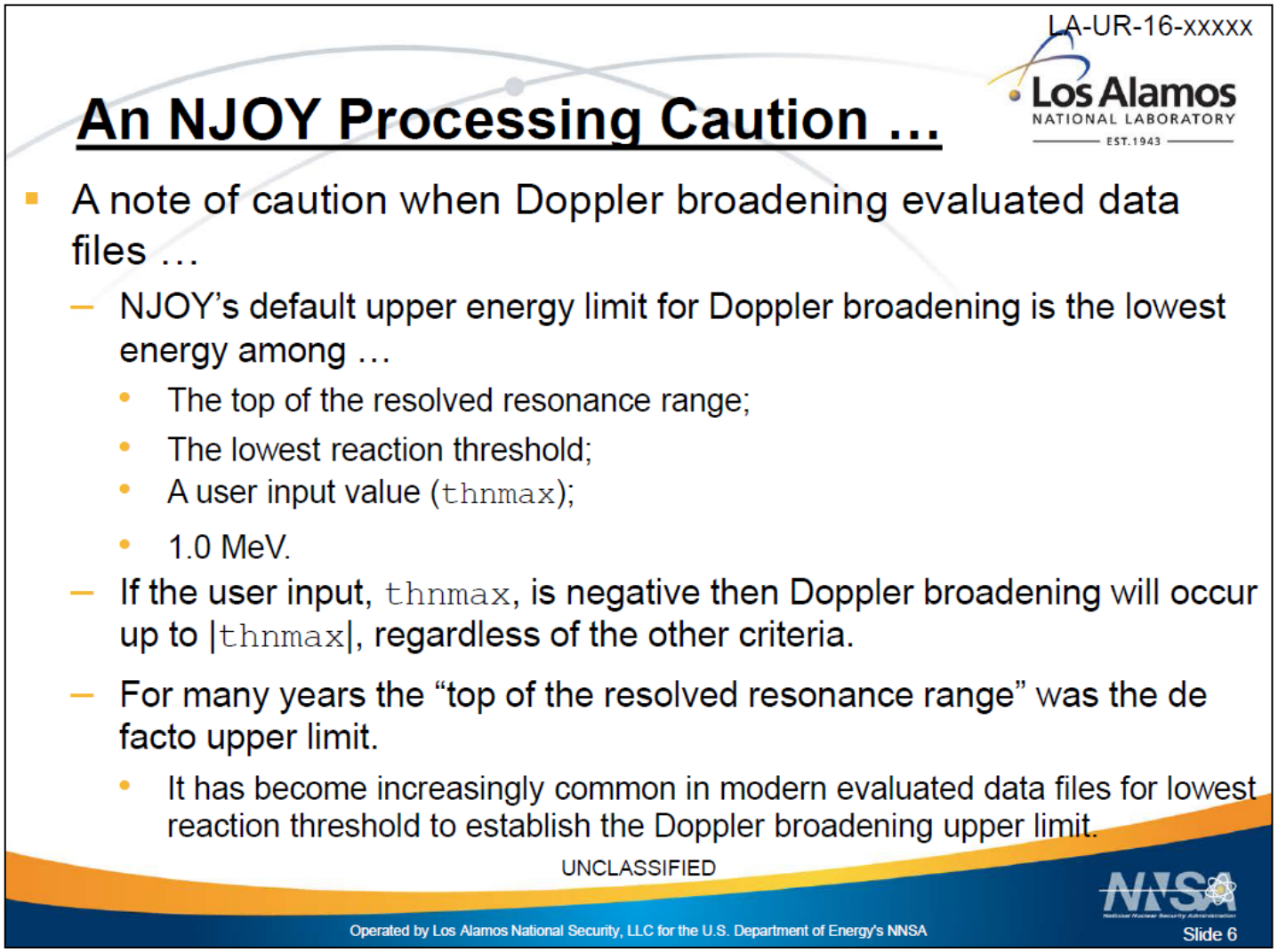
3. **NJOY input used in JEFF**

4. **Conclusion**

O. Cabellos, 8 February 2017

1. Some references about Doppler Broadening

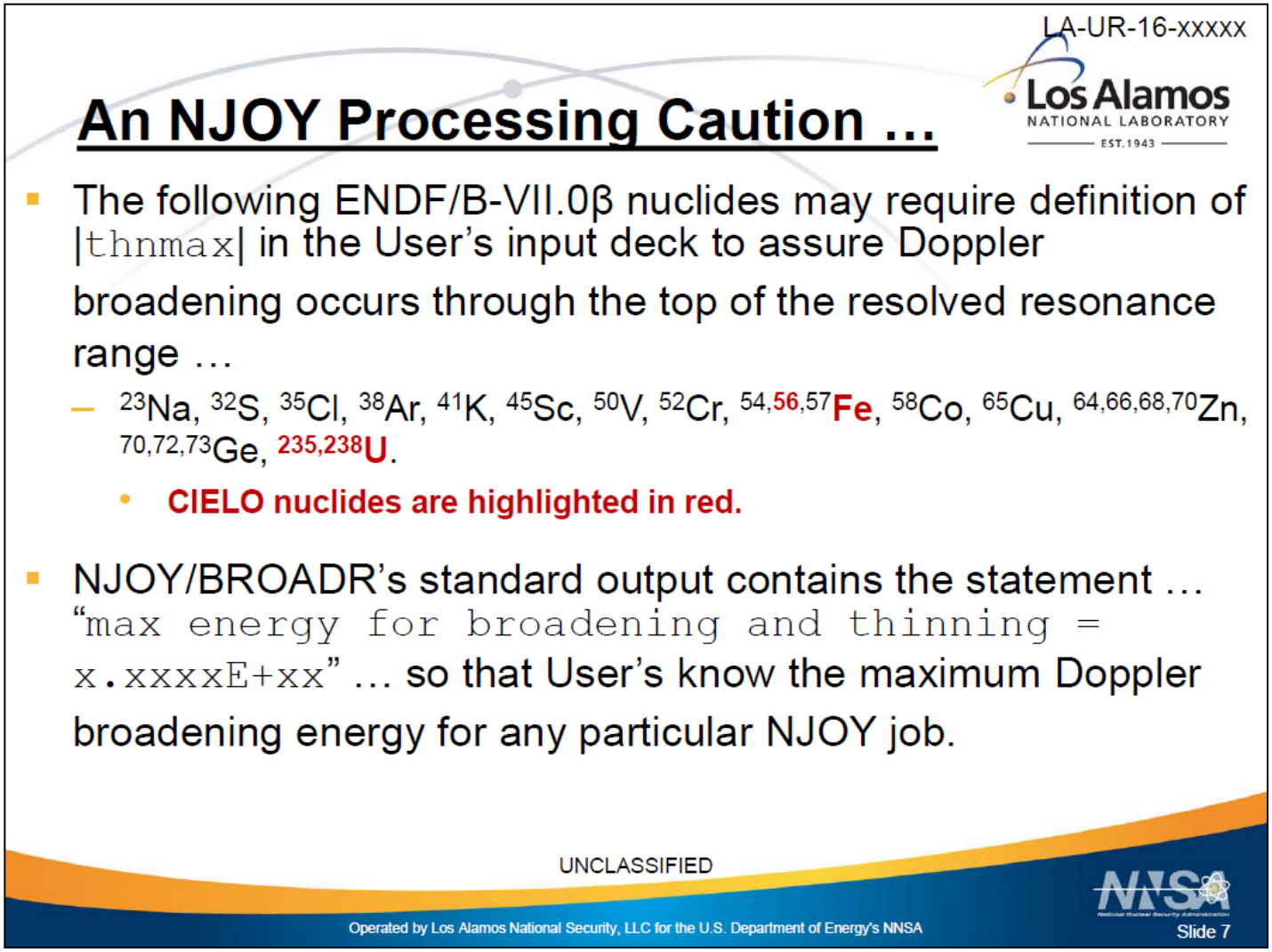
- **CIELO processing**



Testing ENDF/B-VIII.0b Data Files with ICSBEP Benchmarks, S. Kahler, CSEWG 2016.

1. Some references about Doppler Broadening

- **CIELO processing**



Testing ENDF/B-VIII.0b Data Files with ICSBEP Benchmarks, S. Kahler, CSEWG 2016.

1. Some references about Doppler Broadening

- **Example of files in JEFF-3.2**

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Task 9.4: NJOY input for ACE format

- **THNMAX PARAMETER IN BROADR**

The **thnmax parameter** sets the upper limit energy for Doppler broadening. No Doppler broadening is preformed above that energy.

This energy is the lowest between the following values:

- The input value (thnmax)
- The upper limit of the RRR
- The lowest reaction threshold

However, in some cases NJOY stops the Doppler broadening at a lower energy than the given value for thnmax. To avoid this problema and to force the Doppler broadening by setting **thnmax to a negative value**.

Table 1. List of materials affected by thnmax

Isotope	Max. energy for broadening and thinning (eV)	Max. resonance range information (eV)
Ag110M	3	125
Ar38	228102	300000
Ba132	68	100000
C13	4131500	6950000
Ce144	50	100000
Cr52	1233310	1430000
Cs137	1700	100000
Eu156	1	100000
Fe54	399996	700000
Fe57	14668.2	200000
I127	3502.12	5200
I130	100	560
I131	30	100000
K41	117386	887400
Mo95	995.19	2141
Mo99	24	100000
Nb95	25	100000
Ne20	713153	2201000
Ni58	399996	812000
Ni62	444520	600000
Pb205	2340.44	100000
Pb206	807025	900000
Pm148	1.1	100000
Pm149	2.6	100000
S32	957397	1660000
Sc45	12678.1	100000
Sn113	100	510
Xe133	80.5	100000
Zr95	125	100000

UPM contributions to CHANDA WP9, O. Cabellos, JEFF/DOC-1650, April 2015.

1. Some references about Doppler Broadening

❑ Example of files in JENDL4u

Isotope	E. Threshold	Emax. RRR	Isotope	E. Threshold	Emax. RRR	Isotope	E. Threshold	Emax. RRR	Isotope	E. Threshold	Emax. RRR
14-Si-29	1.00E+06	1.30E+06	32-Ge-72	1.00E+03	1.20E+04	50-Sn-123	5.00E+01	1.50E+05	57-La-140	5.70E+01	4.00E+04
15-P-31	5.44E+05	5.44E+05	32-Ge-73	9.95E+02	8.63E+03	50-Sn-126	6.80E+03	2.00E+05	58-Ce-143	6.50E+01	5.00E+05
16-S-32	9.57E+05	1.57E+06	34-Se-79	3.80E+01	5.00E+05	51-Sb-124	2.54E+00	1.00E+05	58-Ce-144	5.00E+01	2.00E+05
18-Ar-40	1.50E+06	1.50E+06	36-Kr-85	1.00E+03	1.00E+06	51-Sb-125	1.40E+01	3.00E+05	59-Pr-141	1.32E+04	1.32E+04
19-K-41	1.14E+05	1.25E+05	37-Rb-86	7.50E+01	3.80E+05	51-Sb-126	3.00E+01	1.00E+05	61-Pm-148	4.20E+00	1.00E+05
20-Ca-40	3.00E+05	5.00E+05	38-Sr-89	1.40E+03	1.00E+06	52-Te-120	6.80E+01	3.00E+05	61-Pm-149	2.70E+00	1.80E+05
20-Ca-43	1.00E+03	4.00E+04	38-Sr-90	6.00E+03	1.00E+06	52-Te-127m	3.00E+00	1.00E+05	61-Pm-151	2.40E+00	1.00E+05
21-Sc-45	1.27E+04	1.00E+05	39-Y-90	2.00E+02	2.00E+05	52-Te-129m	3.00E+00	1.00E+05	62-Sm-144	9.13E+02	1.00E+04
22-Ti-46	3.63E+05	3.63E+05	39-Y-91	3.00E+02	2.00E+05	52-Te-132	2.00E+03	1.00E+06	62-Sm-153	3.00E+00	1.00E+05
23-V-50	1.01E+04	4.25E+04	40-Zr-95	1.25E+02	5.00E+05	53-I-130	1.60E+01	4.00E+04	63-Eu-156	1.00E+01	1.00E+05
24-Cr-50	1.05E+05	6.00E+05	40-Zr-96	1.00E+05	1.00E+05	53-I-131	3.00E+01	1.60E+05	63-Eu-157	4.00E+00	1.70E+05
24-Cr-52	1.05E+05	1.43E+06	41-Nb-95	2.50E+01	5.00E+05	53-I-135	1.50E+04	5.00E+05	66-Dy-154	2.75E+00	1.00E+05
24-Cr-53	1.05E+05	5.64E+05	42-Mo-99	2.40E+01	3.00E+05	54-Xe-126	2.33E+03	2.33E+03	66-Dy-159	3.00E-01	1.00E+05
24-Cr-54	1.05E+05	7.50E+05	44-Ru-105	1.20E+01	1.20E+05	54-Xe-133	8.05E+01	2.50E+05	72-Hf-181	1.60E+01	1.60E+05
26-Fe-57	1.47E+04	2.00E+05	44-Ru-106	5.00E+02	2.00E+05	54-Xe-134	1.03E+04	1.03E+04	72-Hf-182	6.50E+01	6.50E+05
26-Fe-59	1.70E+03	2.00E+05	44-Ru-96	2.50E+02	3.00E+05	54-Xe-136	1.00E+05	4.90E+05	76-Os-184	1.00E+01	2.00E+05
28-Ni-58	9.00E+04	8.12E+05	44-Ru-98	1.40E+02	3.00E+05	55-Cs-135	2.18E+02	2.30E+02	80-Hg-196	1.03E+02	1.03E+02
28-Ni-60	1.00E+05	4.56E+05	46-Pd-104	2.23E+03	2.23E+03	55-Cs-136	2.90E+01	1.00E+05	80-Hg-198	4.59E+02	4.59E+02
29-Cu-63	5.00E+04	5.00E+04	46-Pd-105	2.05E+03	2.05E+03	55-Cs-137	6.40E+02	1.50E+05	80-Hg-202	4.52E+03	4.52E+03
30-Zn-64	7.64E+04	1.30E+05	46-Pd-106	2.02E+03	2.02E+03	56-Ba-132	6.80E+01	2.00E+05	80-Hg-204	1.00E+03	4.00E+05
30-Zn-65	1.40E+02	1.10E+05	47-Ag-107	7.01E+03	7.01E+03	56-Ba-134	1.06E+04	1.06E+04	82-Pb-206	1.50E+05	8.20E+05
30-Zn-66	1.05E+05	1.40E+05	47-Ag-109	7.01E+03	7.01E+03	56-Ba-137	1.19E+04	1.19E+04	82-Pb-207	1.50E+05	6.80E+05
30-Zn-68	1.05E+05	1.10E+05	47-Ag-111	1.00E+01	1.00E+05	56-Ba-138	1.00E+05	1.00E+05	82-Pb-208	1.50E+05	1.00E+06
30-Zn-70	1.05E+05	2.10E+05	50-Sn-116	3.28E+04	3.28E+04	56-Ba-140	1.40E+04	1.00E+05	**92-U-235**	**7.73E+01**	**5.00E+02**
32-Ge-70	9.92E+02	1.40E+04									

2. NJOY versions

- **Official versions NJOY 99 and NJOY2012.50: <u>Processing Caution!!</u>**

NJOY input

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-235 from jendl4ut'/ Comment line about file
20 9228 /
0/
reconr / Reconstruct XS from resonance parameters
21 22
'92-U-235 PENDF from jendl4ut'/
9228 2 /  ncards = 2, two comment lines added to the new MF1
0.005 0.0 0.005/ err tempr errmax
'Reconstructed 92-U-235 PENDF from jendl4ut'/
'Processed with NJOY2012.50 NEA modified, at NEA 2017-02-02'/
0/
broadr / Perform Doppler-broadening
21 22 23
9228 1 0 0 0./  IMAT, #temps, restart?, bootstrap?, restart from?
0.005 2.0e+6 0.005/ errthn thnmax errmax
293.6 / Description of temperatures
0/
```

Thnmax=+2.0MeV

2. NJOY versions

- **Official versions NJOY 99 and NJOY2012.50: <u>Processing Caution!!</u>**

NJOY output

```
1*************************************************************************
 *                                          *              *              *
 *   $$   $$       $$   $$$$$   $$    $$   *              *  vers: 2012.50   *
...
...
reconr...reconstruct pointwise cross sections in pendf format          10.6s
...
...
resonance range information
 ---------------------------------
 ier     energy-range     lru lrf  method
  1  1.000E-05 5.000E+02   1   3   normal
  2  5.000E+02 3.000E+04   2   2   normal
...
...
 broadr...doppler broadening of endf data                              35.8s

 unit for input endf tape .............        21
 unit for input pendf tape ............        22
 unit for output pendf tape ...........        23
 material to be processed .............      9228
 number of final temperatures .........         1
 restart (0 no, 1 yes) ................         0
 bootstrap (0 no, 1 yes) ..............         0
 starting material temperature ........       0.0k
 thinning tolerance ...................     0.005
 max. energy ..........................  2.000E+06
 errmax for thinning ..................  5.000E-03
 errint for thinning ..................  2.500E-07
 final temperatures ...................  2.936E+02

 files are in endf-6 format
 max energy for broadening and thinning =    7.73297E+01
...
```

top of the RRR energy

Value given in the input: Thnmax=+2.0MeV

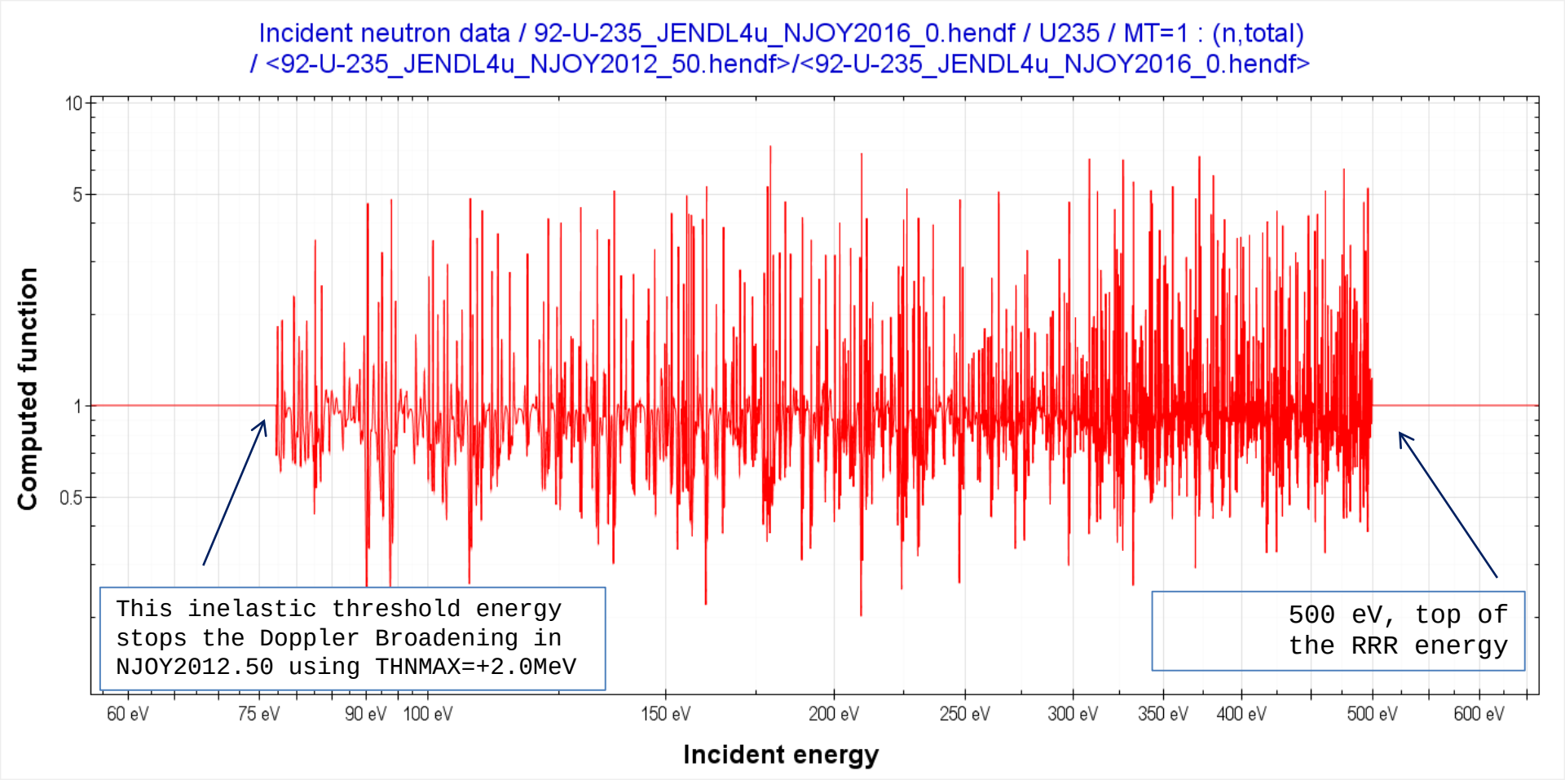
This inelastic threshold energy stops the Doppler Broadening.
It's the max Doppler Broadening energy used in NJOY

2. NJOY versions

- **Official versions NJOY 99 and NJOY2012.50: <u>Processing Caution!!</u>**

Ratio of MT1 (total cross-section) with two different NJOY versions
Using the same input with THNMAX = +2.0MeV in ^{235}U-JENDL4u

⇒ Caution!!! Doppler Broadening up to `7.73297E+01` eV !!



2. NJOY versions

- **Unofficial versions Upnea111_NJOY99 (October 2012)**

```
*ident upnea111
*/ broadr -- A. Trkov, October 2012
*/           Optionally deactivate lowering the energy range for Doppler
*/           broadening to the lowest threshold (e.g. the original option
*/           suppresses Doppler broadening of the cross sections above 80 eV
*/           in some U-235 evaluations that have non-zero inelastic cross
*/           section specified in the resonance range).
*d broadr.88,98
c     * thnmax     the upper limit for broadening and thinning is the
c     *            lowest of the input value of thnmax, the start of
c     *            the unresolved range or the lowest threshold.
c     *            If there is resolved-unresolved overlap, the overlap
c     *            region is included in the broadening. A zero value
c     *            of thnmax will override the lowest threshold limit;
c     *            a negative value will override also the resolved
c     *            resonance limits and set the new limit to the
c     *            absolute value of thnmax. The magnitude of thnmax
c     *            must be chosen to keep the number of broadenable
c     *            reactions less than or equal to the  maximum of
c     *            ntt (current limit=160).
*d broadr.283
            if (mth.eq.152) then
              errr=20.e6
              call stounx(nin,no,nscr1,a,errr)
              write(nsyso,'(/
     &        '' upper resolved resonance energy range  ='',1p,e14.5)')
     &        errr
              if(thnmx.gt.zero) thnmax=min(errr,thnmx)
              if(thnmx.eq.zero) thnmax=errr
            end if
*d broadr.300
c* conditionally lower energy range for Doppler broadening to threshold
      if (thnmx.gt.zero .and. c2h.lt.thnmax) thnmax=c2h
*d broadr.338
c* conditionally lower energy range for Doppler broadening to threshold
      if (thnmx.gt.zero .and. fact*enext.lt.thnmax) thnmax=fact*enext
*/
```

2. NJOY versions

- **Upnea111_NJO2012.50 (February 2014)**

```
*ident upnea111
*/ broadr -- A. Trkov, Converted from NJOY99 of October 2012
*/           Optionally deactivate lowering the energy range for Doppler
*/           broadening to the lowest threshold (e.g. the original option
*/           suppresses Doppler broadening of the cross sections above 80 eV
*/           in some U-235 evaluations that have non-zero inelastic cross
*/           section specified in the resonance range).
*/*d broadr.112,114
*/   !            A zero value of thnmax overrides the lowest threshold
*/   !            limit; a negative value overrides also the resolved
*/   !            resonance limits and set the new limit to the
*/   !            absolute value of thnmax.
*i broadr.147
   real(kr)::errr
*i broadr.159
   real(kr),parameter::sixmev=6.e6_kr
*d broadr.197
!  thnmx=onemev
   thnmx=sixmev
*i broadr.329
      write(nsyso,'(/&
        &'' upper resolved resonance energy range  =''&
        &,1p,e14.5,'' eV'')') eresh
      if(thnmx.gt.zero) thnmax=min(eresh,thnmx)
      if(thnmx.eq.zero) thnmax=eresh
      if(thnmx.eq.zero) emin  =eresh
*d broadr.351
   if (thnmx.gt.zero .and. c2h.lt.thnmax) thnmax=c2h
*d broadr.423
   if (thnmx.gt.zero .and. fact*enext.lt.thnmax) thnmax=fact*enext
*i broadr.459
   if (thnmax.eq.0 .and. thnmx.eq.0) thnmax=sixmev
*/ Add units to the printed energy
*d broadr.462,463
     &'' max energy for broadening and thinning =''&
     &,1p,e14.5,'' eV'')') thnmax
*/
```

2. NJOY versions

- **NJOY2012.82 (Release 7 February, 2017)**

  - Up75: revised logic in broadr to assure Doppler broadening always occurs to the top of the RRR. This is a significant change in philosophy and user's legacy input decks may produce different answers with this update. Refer to the manual and use of the thnmax input variable.

- **NJOY2016.0 (Release 2 February, 2017)**

  - Revised logic in broadr to assure Doppler broadening.

3. NJOY input used in JEFF

```
moder / Extract/convert neutron evaluated data
1 -21
'92-U-235 from JEFF33T1'/ Comment line about file
20 9228 /
0/
reconr / Reconstruct XS from resonance parameters
-21 -22
'92-U-235 PENDF from JEFF33T1'/
9228 2 /  ncards = 2, two comment lines added to the new MF1
0.001 0.0 / err tempr errmax (default = err*10)
'Reconstructed 92-U-235 PENDF from JEFF33T1'/
'Processed with NJOY2012.050, at NEA 2016-06-24'/
0/
broadr / Perform Doppler-broadening
-21 -22 -23
9228 1 0 0 0./  IMAT, #temps, restart?, bootstrap?, restart from?
0.001 / errthn thnmax errmax
293.6 / Description of temperatures
0/
unresr
-21 -23 -24
9228 1 1  1 /
293.6 /
1.E10 /
0/
heatr / Add heating kerma
-21 -24 -25 /
9228  7 0 0 0 2 / (7) Add 7 partial KERMAS (302, 303, 318, 402, 442, 443)
302 303 304 318 402 442 443/
heatr / Add damage energy
-21 -25 -26 /
9228  4 0 0 0 2 / (7) Add 4 partial DPA (444 445 446 447)
444 445 446 447/
gaspr / Add gas production
-21 -26 -27
```

3. NJOY input used in JEFF

```
thermr / Add thermal scattering data free-gass
0 -27 -61 /
0 9228  20 1 1 0 0 1 221 1 / Add free-gas model(mt=221), 20 equi-probable angles, MF6 law (E-mu-
E'), output exteded
293.6 /
0.001 10.0 / tolerance emax (max energy for thermal treatment in eV)
purr / Process Unresolved Resonance Region (URR) if any -> Generate PTables for MCNP
-21 -61 -30
9228 1 1 20 64 / 20 bins and 64 ladders for generating XS in URR
293.6 /
1.E10 /
0/
moder
-30 28
acer / Prepare ACE files
-21 -30 0 31 32 /
1 0 1 .03 / Create fast data (for neutrons), if change to 2 for TSL. Add suffix for ACE file
'92-U-235 ACE from JEFF33T1,NJOY2012.050,at NEA 2016-06-24'/
9228 293.6
1 1/
/
acer / Check ACE files
0 31 0 33 34 /
7 1 1 -1 /
''/
stop
```

3. NJOY input used in JEFF

```
groupr / Generate multigroup cross section data
-21 -30 0 35/
9228 1 0 2 6 1 1 1 /
'92-U-235 GENDF 238 JEFF33T1,NJOY2012.050, at NEA 2016-06-24'/
293.6
1.E10
238 /
   1.000E-05, 1.000E-04, 5.000E-04, 7.500E-04, 1.000E-03,
   1.200E-03, 1.500E-03, 2.000E-03, 2.500E-03, 3.000E-03,
   4.000E-03, 5.000E-03, 7.500E-03, 1.000E-02, 2.530E-02,
   3.000E-02, 4.000E-02, 5.000E-02, 6.000E-02, 7.000E-02,
   8.000E-02, 9.000E-02, 1.000E-01, 1.250E-01, 1.500E-01,
   1.750E-01, 2.000E-01, 2.250E-01, 2.500E-01, 2.750E-01,
   3.000E-01, 3.250E-01, 3.500E-01, 3.750E-01, 4.000E-01,
   4.500E-01, 5.000E-01, 5.500E-01, 6.000E-01, 6.250E-01,
   6.500E-01, 7.000E-01, 7.500E-01, 8.000E-01, 8.500E-01,
   9.000E-01, 9.250E-01, 9.500E-01, 9.750E-01, 1.000E+00,
   1.010E+00, 1.020E+00, 1.030E+00, 1.040E+00, 1.050E+00,
   1.060E+00, 1.070E+00, 1.080E+00, 1.090E+00, 1.100E+00,
   1.110E+00, 1.120E+00, 1.130E+00, 1.140E+00, 1.150E+00,
   1.175E+00, 1.200E+00, 1.225E+00, 1.250E+00, 1.300E+00,
   1.350E+00, 1.400E+00, 1.450E+00, 1.500E+00, 1.590E+00,
   1.680E+00, 1.770E+00, 1.860E+00, 1.940E+00, 2.080E+00,
   2.120E+00, 2.210E+00, 2.300E+00, 2.380E+00, 2.470E+00,
   2.570E+00, 2.670E+00, 2.770E+00, 2.870E+00, 2.970E+00,
   3.000E+00, 3.050E+00, 3.150E+00, 3.500E+00, 3.730E+00,
   4.000E+00, 4.750E+00, 5.000E+00, 5.400E+00, 6.000E+00,
   6.250E+00, 6.500E+00, 6.750E+00, 7.000E+00, 7.150E+00,
   8.100E+00, 9.100E+00, 1.000E+01, 1.150E+01, 1.190E+01,
   1.290E+01, 1.375E+01, 1.440E+01, 1.510E+01, 1.600E+01,
   1.700E+01, 1.850E+01, 1.900E+01, 2.000E+01, 2.100E+01,
   2.250E+01, 2.500E+01, 2.750E+01, 3.000E+01, 3.125E+01,
   3.175E+01, 3.325E+01, 3.375E+01, 3.460E+01, 3.550E+01,
   3.700E+01, 3.800E+01, 3.910E+01, 3.960E+01, 4.100E+01,
   4.240E+01, 4.400E+01, 4.520E+01, 4.700E+01, 4.830E+01,
   4.920E+01, 5.060E+01, 5.200E+01, 5.340E+01, 5.900E+01,
   6.100E+01, 6.500E+01, 6.750E+01, 7.200E+01, 7.600E+01,
   8.000E+01, 8.200E+01, 9.000E+01, 1.000E+02, 1.080E+02,
   1.150E+02, 1.190E+02, 1.220E+02, 1.860E+02, 1.925E+02,
   2.075E+02, 2.100E+02, 2.400E+02, 2.850E+02, 3.050E+02,
   5.500E+02, 6.700E+02, 6.830E+02, 9.500E+02, 1.150E+03,
   1.500E+03, 1.550E+03, 1.800E+03, 2.200E+03, 2.290E+03,
   2.580E+03, 3.000E+03, 3.740E+03, 3.900E+03, 6.000E+03,
   8.030E+03, 9.500E+03, 1.300E+04, 1.700E+04, 2.500E+04,
   3.000E+04, 4.500E+04, 5.000E+04, 5.200E+04, 6.000E+04,
   7.300E+04, 7.500E+04, 8.200E+04, 8.500E+04, 1.000E+05,
   1.283E+05, 1.500E+05, 2.000E+05, 2.700E+05, 3.300E+05,
   4.000E+05, 4.200E+05, 4.400E+05, 4.700E+05, 4.995E+05,
   5.500E+05, 5.730E+05, 6.000E+05, 6.700E+05, 6.790E+05,
   7.500E+05, 8.200E+05, 8.611E+05, 8.750E+05, 9.000E+05,
   9.200E+05, 1.010E+06, 1.100E+06, 1.200E+06, 1.250E+06,
   1.317E+06, 1.356E+06, 1.400E+06, 1.500E+06, 1.850E+06,
   2.354E+06, 2.479E+06, 3.000E+06, 4.304E+06, 4.800E+06,
   6.434E+06, 8.187E+06, 1.000E+07, 1.284E+07, 1.384E+07,
   1.455E+07, 1.568E+07, 1.733E+07, 2.000E+07/
3/
3  221 Free Gas/
3  251 mubar/
3  252 xi/
3  253 gamma/
3  259 1/v /
3 452 nubar_t/
3 455 nubar_d/
3 456 nubar_p/
5 455 nubar_spc/
6/
6 221 Free Gas /
0/
0/
stop
```

4. Conclusion

- **Running Official versions NJOY 99 and NJOY2012.50, processing Caution!!**
  - It also applies to NJOY2012 up to 2012.75

- **To avoid Doppler Broadening problem:**

1. If you still use NJOY99 or NJOY2012, please …
   - Check your NJOY input/output to ensure right Doppler Broadening
   - If needed, change THNMAX = - (max. energy RRR)

2. or, update your NJOY code
   - NJOY99+upnea111

     See at: https://www.oecd-nea.org/dbprog/njoy-links.html
   - NJOY2016 (free open source) **(Release 2 February, 2017)**

     The initial release of NJOY2016.0 is equivalent to NJOY2012.80

     See at: https://njoy.github.io/NJOY2016/
   - NJOY2012.82 **(Release 7 February, 2017)**

     NJOY2012.82 is equivalent to NJOY2016.3

     See at: http://t2.lanl.gov/nis/codes/NJOY12/index.html