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**Precision of ENDF and ENDL**  
**Formatted Data Files**

by

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**Abstract**

**The purpose is to ensure that today's processing codes produce output to meet today's accuracy needs.** Since 1958 ENDL [1] and about 1965 ENDF [2] have each used a text format to define nuclear and atomic data in 11 columns for each data field. When these formats were initially released, they were judged to be adequate to reproduce the accuracy of data at the time and to meet the needs of our applications. When these formats originated, the dominant computer language of the day was FORTRAN and if written using an E11.4 format it would include only 4 or 5 digits of precision, e.g., 0.1234E-03 or 1.2345E-02, varying from one computer/system to another the result was not unique. In the case of ENDF the 4 digit precision was not even adequate to uniquely define the atomic weight of the target, e.g., U-238 = 92238 = 0.9224E+5 = WRONG!

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## First the Punchline: What is the Purpose of this report?

**The purpose is to ensure that today's processing codes produce output to meet today's accuracy needs.** Since 1958 ENDL [1] and about 1965 ENDF [2] have each used a text format to define nuclear and atomic data in 11 columns for each data field. When these formats were initially released, they were judged to be adequate to reproduce the accuracy of data at the time and to meet the needs of our applications. When these formats originated, the dominant computer language of the day was FORTRAN and if written using an E11.4 format it would include only 4 or 5 digits of precision, e.g., 0.1234E-03 or 1.2345E-02, varying from one computer/system to another the result was not unique. In the case of ENDF the 4 digit precision was not even adequate to uniquely define the atomic weight of the target, e.g., U-238 = 92238 = 0.9224E+5 = WRONG!

Since its inception, the ENDF format had a precision problem. Upon finishing graduate school and joining what later became the National Nuclear Data Center (NNDC) in 1967, one of my first tasks was to address this precision problem, by working with ENDF producers and users throughout the U.S. we verified,

- 1) E or D is not required to define FORTRAN readable numbers, e.g., E+4 or +4 are both o.k.
- 2) With ENDF energy eV and cross section in barns, 2 digit exponents are almost never required.
- 3) Since energy is never negative we could use the first of the 11 columns for a digit.

Knowing this allowed us to produce ENDF/B-II to 6 or 7 digit precision, e.g., blank, decimal point, 2 or 3 digit exponent, e.g., ^1.23456-12 or ^1.234567-3. Below is an example of the actual ENDF/B-II data released. Note, the date 1970 and the atomic weight, ZA, uniquely defined to 6 digit accuracy, ^9.22350+ 4

```
ENDF/B-II TAPE 201 REVISION 3 8-25-70                201 0 0 0
9.22350+ 4 2.33025+ 2                                421102 1451 1
0. + 0 0. + 0 1 1 93 01102 1451 2
U-235 CSEWG EVAL-SEP69 LEONARD,ALTER,LUBITZ (RE-EVAL) 1102 1451 3
AI-AEC-MEMO-12916 DIST-JAN70 REV-APR70 1102 1451 4
* * * * * 1102 1451 5
URANIUM-235 1102 1451 6
          VARIOUS INDIVIDUALS CONTRIBUTED TO TE EVALUATION OF 1102 1451 7
          THE CROSS SECTIONS FOR THIS MATERIAL 1102 1451 8
          1102 1451 9
          B.R..LEONARD (BNW) - CROSS SECTIONS BELOW 1.0 EV 1102 1451 10
```

From 1970 this format was adequate for decades until roughly 20 years ago, when,

- 1) ENDF evaluations were extended to high and higher resolved resonance energies.
- 2) Resonance peaks and width were defined to higher precision, i.e., to more digits.
- 3) Competition for FORTRAN, notably C and C++, where the above rules did not apply.

## Today's Precision Needs

This forced me to revisit the precision problem for both ENDF and ENDL. For ENDF the solution was fairly obvious. With energy in eV and resonances in the eV to keV range an exponent is seldom if ever needed. This allowed me to extend the precision of ENDF data from 7 to 9 or 10 digits of precision: a blank, decimal point and 9 digits, or a decimal point and 10 digits, e.g., ^1.23456789 or 1.234567891. This solved my ENDF format problem, but not my ENDL format; I use ENDL to prepare cross sections for input to my Monte Carlo transport code TART [3]. ENDF was designed for use with thermal fission systems, so energy is in eV. In contrast ENDL was designed for use with faster neutron systems, so energy is in MeV, so I could not ignore the exponent. I solved my ENDL program by defining the ENDLX format

(ENDL Extended), which extended the original 11 column ENDL data to 16 columns, so I could include an exponent and still maintain 10 digit precision, e.g., blank, decimal point, 4 column exponent and 10 digits,  $^1.234567891D-05$ .

## Precision Outside and Inside Computers

I also rethought how to define precision as uniquely as possible. The problem was that inside a computer our processing codes generally define energies and calculate cross sections to 64 bit accurately, roughly 16 digits. For almost 30 years, I addressed this problem only by rounding off the energy as **output** to the ENDF and ENDL format. This meant that the energy as **output** to the ENDF format was not always the same energy that was actually used to calculate the cross section **inside** the computer. Unfortunately, with today's nuclear data this round off can result in COMPLETE RUBBISH as output, as I illustrate here.

To translate ENDF data from the form originally distributed by evaluators to the form it is actually used in our applications' processing codes, use a simple interval halving method, i.e., they define the average energy as the midpoint between two endpoints, and see if they can accurately define the cross sections at this midpoint energy using ENDF-102 rules and linearly interpolation between the two endpoints, **OR** the width of the interval is zero. The problem in my approach to round the energy only on **output** was that inside computers the 64 bit, 16 digit energies, almost never result in zero length energy intervals. My current solution is to round the energies **inside** the computer to match the precision **output** to the ENDF format. This simple procedure **inside** a computer produces a dramatic difference in the **output** to the ENDF format, which I, in turn, copy to the ENDL format for use with TART. For example, if both INCORE and OUT round to the same precision it was then impossible to have duplicate energies during interval halving, e.g., with INCORE interval halving the difference between two ends of the interval would become zero at the defined precision to be later output to ENDF and halving would stop.

To make this as simple as possible I created FORTRAN subroutines named INCORE and OUT. For testing I created INCORE10, INCORE9, and INCORE7, to round off energies inside a computer to 10, 9, or 7 digits; I also, for testing, allowed no INCORE rounding. These routines have a single real\*8 argument to be rounded. I also created OU110, OUT9, and OUT7, to round off energies to be output from a computer to the ENDF format. These OUT routines have two arguments, a real\*8 argument to be rounded and a second argument of 11 characters that can be directly copied to ENDF format in 11A1 format.

## ENDF/B-VIII.1 U-238

In order to illustrate the problem in the precision of the ENDF 11 column format I will focus on the results for only one isotope; one of the most important and detailed evaluations, U-238. For this exercise I have calculated energy dependent cross sections to high precision, 0.01% allowable uncertainty. The resolved region extends up to 20 keV (20,000 eV). This includes over 3,300 resonances, and results in almost 4,000,000 tabulated linearly interpolate energy points. Notice this means almost 200 tabulated points per eV. If precision is not a problem 7, 9 and 10 digit results **MUST ALL** agree.

Below I show just one of the thousands of resolved resonances included in this U-238 evaluation. Based on the tabulated resonance peak energy and elastic and capture widths, it would require 12 and 13 digits to exactly reproduce just both the resonance peak and an energy point 1 width above the peak. Truncated to 10 digits we are still including 3 digits, whereas to 7 digits there are almost no digits to define the shape of a resonance. Please remember this is

only for 2 points separated by 1 total resonance width. To define the actual shape of a resonance to 0.01% precision requires many tabulated energy points. As we will see in the following plots, the 7 digit output cannot reproduce the 10 digit results to within the 0.01 % allowable uncertainty. The difference grows with each increase in decade of energy, as the digits needed to define the resonance peak energy increases, and the remaining digits available to define the resonance shape decreases. By the last decade above 10,000 eV here is what one typical resonance looks like.

<b>Example</b>	<b>Elastic</b>	<b>Capture</b>	
Digits	12345.6789012	12345.67890123	
Peak	11172.79	11172.79	
Width	0.1697223	0.03592838	
ALL Digits	11172.9597223	11172.82592838	= E+width 13 digits
10 Digits	11172.95972	11072.82593	= rounded 10 output
7 Digits	11172.96	11072.86	= rounded 7 output

### What Effect do these options make?

To illustrate the difference between the results using these INCORE and OUT options, I have used an obviously important and difficult evaluation, namely U-238, ENDF/B-VIII.1. I used ONLY my PREPRO [4] code varying the INCORE and OUT rounding, in each case starting from the original evaluation using the PREPRO codes,

- 1) LINEAR – linearize all tabulated MF=3 cross sections,
- 2) RECENT – add the resonance, MF=2, data,
- 3) SIGMA1 – Doppler broaden from 0 Kelvin and room temperature, 293.6 Kevlin.

Each of these codes reads and writes ENDF formatted data, i.e., precision affects all of them.

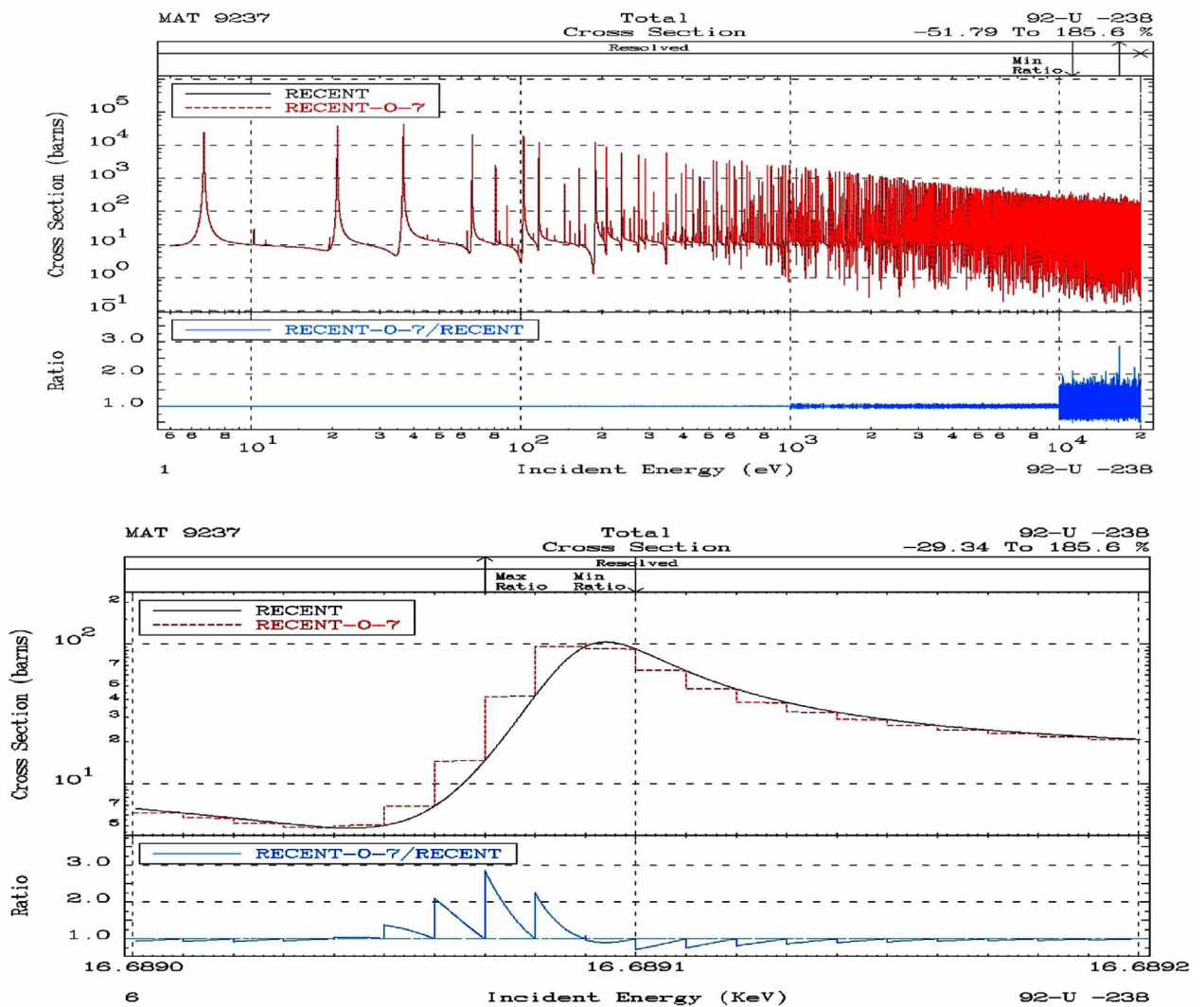
All of these calculations were performed using an allowable uncertainty of 0.01%, 4 digits, well beyond our ability to measure this data; this was done in an attempt to ensure that processing does not add any significant additional uncertainty – repeat, add uncertainty – ENDF data is not perfect.

OUT	INCORE	Energies Output	Total Cross Section Difference	Comments
10	0	3,784,661	0.05%	No INCORE round Output energy count Independent of OUT
9	0	3,784,661	0.52%	
7	0	3,784,661	185.6%	
10	10	3,755,278	-----	PREPRO Standard
9	9	3,702,770	0.01%	
7	7	1,963,044	17.1%	

## U-238 Total 7 digit OUT – no INCORE (50 year old format)

The resolved resonance region extends up to 20 keV. From the below plot we can see that the ERROR increases with each decade in energy; another digit is needed to define the resonance peak, so one less digit is available to define the shape of the resonance. Above 10 keV at least 5 digits are required to define the peak leaving little room to define the shape. **The result as we can see is COMPLETE RUBBISH. Rather than the resonance shape we see a Ziggurat (a stepped pyramid).**

In the below zoomed plot the resonance peak is defined to 6 digits, 16.6891 eV, and the entire width of the plot is from 16.6890 to 16.6892. With no INCORE rounding to limit interval halving the result is many, many repeated energies when the actual **INSIDE** 16 digit energies used in the calculation are rounded for output to the ENDF format. We can see this in the following table: 75 identical output energies; identical due solely to **output** rounding to 7 digits.



## 1 step of the Ziggurat

Here we can see what is causing the steps of the Ziggurat (stepped pyramid). Below is a short part of the ENDF output rounded to 7 digits for **output** and **NO INCORE** rounding, i.e., what we used for decades in ENDF and ENDL. Here all 75 energies are identical 1.668907E+4 eV. But the cross sections differ, proving that the exact energy used **inside** the computer has been moved/rounded for **output**. The result is the COMPLETE RUBBISH Ziggurat. **There are differences up to: Total 185%, Elastic 595%, Fission 101%, and Capture 133%**. Remember, we ask for and assume our processing codes will produce reconstructed energy dependent ENDF data to within 0.01% differences. You might ask how many of these hundreds/thousands of resonances are affected: the answer is above 10 keV almost ALL of the more than 1,000 resonances are output as COMPLETE RUBBISH, similar to the table shown below.

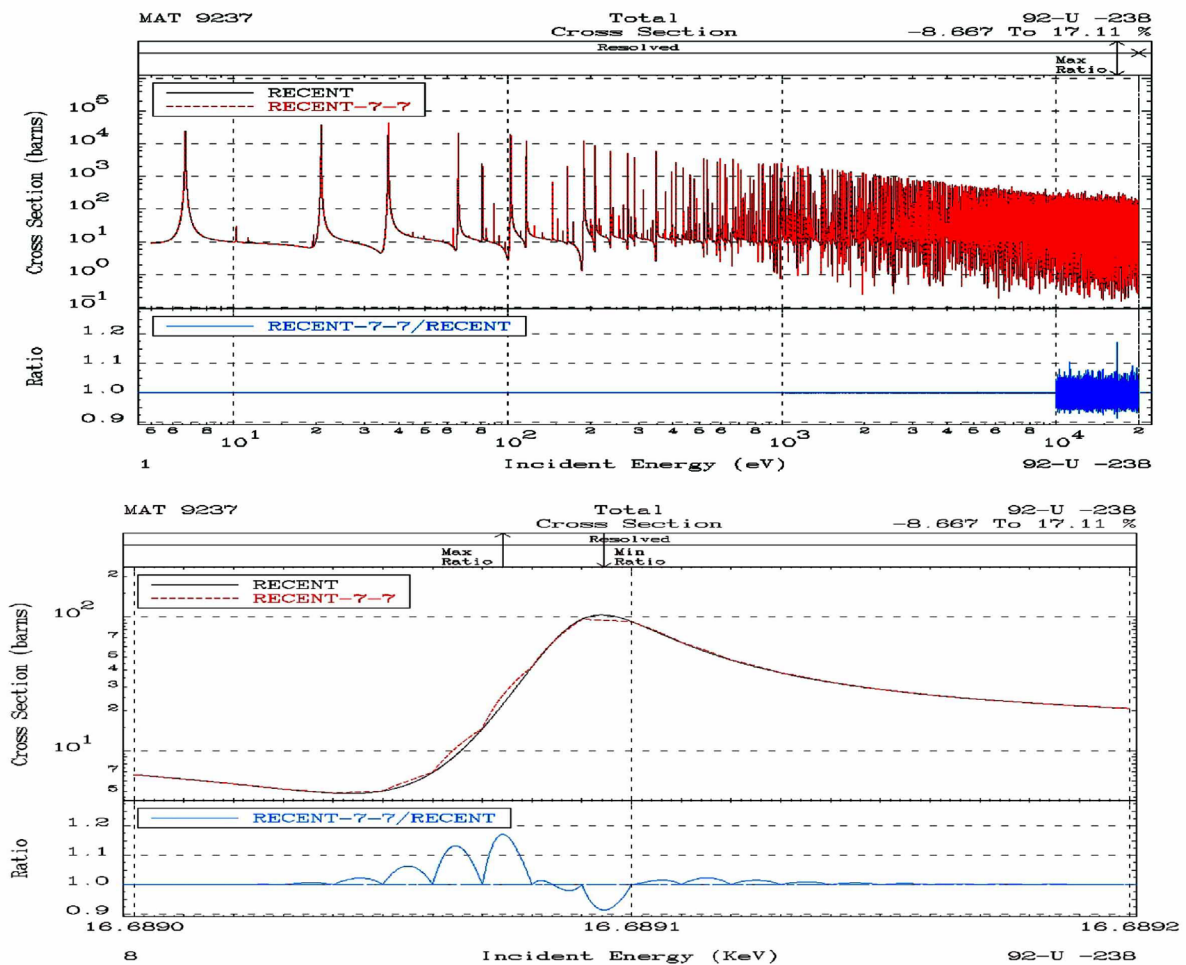
### ALL ENDF Output Energies are Identical 7 Digits: 1.668907E+4

1.668907E+4	14.79720331.668907E+4	14.89607421.668907E+4	14.99584669237	3	1
1.668907E+4	15.09652831.668907E+4	15.19812731.668907E+4	15.30065149237	3	1
1.668907E+4	15.40410851.668907E+4	15.50850691.668907E+4	15.61385459237	3	1
1.668907E+4	15.72015951.668907E+4	15.82743021.668907E+4	15.93567489237	3	1
1.668907E+4	16.15511901.668907E+4	16.37855961.668907E+4	16.60606469237	3	1
1.668907E+4	16.83770331.668907E+4	17.07354551.668907E+4	17.31366239237	3	1
1.668907E+4	17.55812521.668907E+4	17.80700701.668907E+4	18.06038119237	3	1
1.668907E+4	18.31832171.668907E+4	18.58090401.668907E+4	18.84820399237	3	1
1.668907E+4	19.12029801.668907E+4	19.39726371.668907E+4	19.67917949237	3	1
1.668907E+4	19.96612381.668907E+4	20.25817641.668907E+4	20.55541769237	3	1
1.668907E+4	20.85792801.668907E+4	21.16578911.668907E+4	21.47908279237	3	1
1.668907E+4	21.79789141.668907E+4	22.12229781.668907E+4	22.45238529237	3	1
1.668907E+4	22.78823721.668907E+4	23.12993761.668907E+4	23.47757059237	3	1
1.668907E+4	23.83122001.668907E+4	24.19097041.668907E+4	24.55690609237	3	1
1.668907E+4	24.92911111.668907E+4	25.30766951.668907E+4	25.69266529237	3	1
1.668907E+4	26.08418151.668907E+4	26.48230151.668907E+4	26.88710779237	3	1
1.668907E+4	27.29868171.668907E+4	27.71710461.668907E+4	28.14245659237	3	1
1.668907E+4	28.57481661.668907E+4	29.01426271.668907E+4	29.46087149237	3	1
1.668907E+4	29.91471791.668907E+4	30.37587581.668907E+4	30.84441679237	3	1
1.668907E+4	31.32041061.668907E+4	31.80392521.668907E+4	32.29502599237	3	1
1.668907E+4	32.79377551.668907E+4	33.30023431.668907E+4	33.81445979237	3	1
1.668907E+4	34.33650581.668907E+4	34.86642351.668907E+4	35.40426029237	3	1
1.668907E+4	35.95005931.668907E+4	36.50386031.668907E+4	37.06569849237	3	1
1.668907E+4	37.63560411.668907E+4	38.21360331.668907E+4	38.79971679237	3	1
1.668907E+4	39.39395961.668907E+4	39.99634151.668907E+4	40.60686639237	3	1

## U-238 Total - 7 digit OUT - 7 digit INCORE

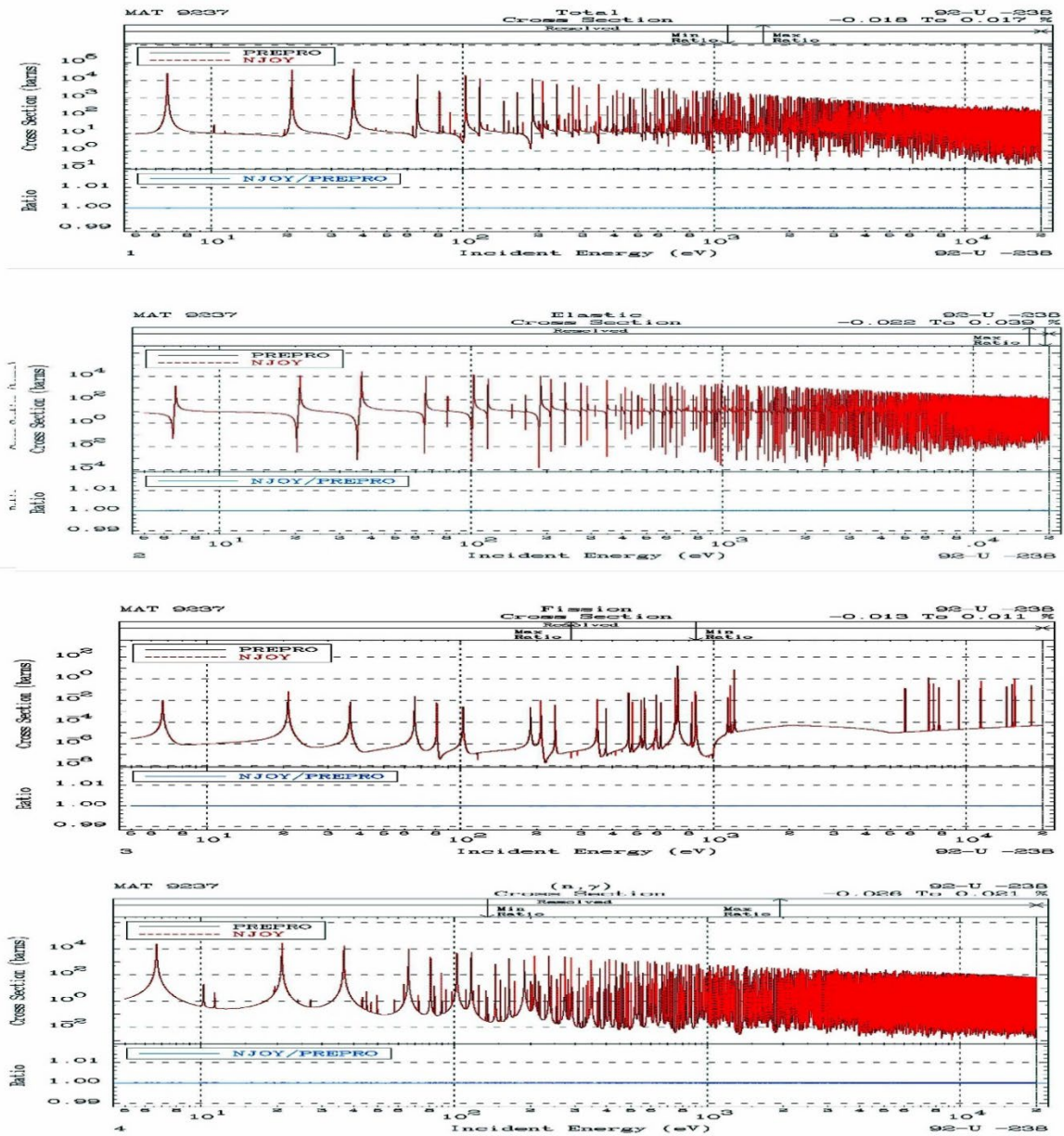
Can we still use 7 digit precision OUT rounding if we add 7 digit precision INCORE rounding? Adding the INCORE rounding prevents repeated energies, so we do not expect any more RUBBISH Ziggurats, and it reduces the number of energies output by about 2. But is 7 digits accurate enough for today's ENDF data? The below plots show that it does decrease the ERROR and eliminate Ziggurats, e.g., now we can see the resonance shape, not the Ziggurat RUBBISH. But 7 digits is simply not enough to reproduce U-238 to within the 0.01% allowable difference. What we see here is differences of: **Total 17%, Elastic 106%, Fission 7%, and Capture 12%.**

From the below zoomed plot we can see that the tabulated output energies are unique and differ by 7 digits; so, we cannot force or expect more using data with 7 digit precision output. **Sorry to say that my original idea circa 1970 served us well for many years, but it simply cannot produce accurate tabulated linearly interpolable data from today's ENDF evaluations.** I should mention that this is also true of data in the ENDL format. I use the LLNL ENDL in-house format with my unpublished TARTMAKER code that I use to prepare cross sections for use by my TART Monte Carlo code. **Today I use ENDLX to supply 10 digit accuracy for TART.**



## U-238 NJOY vs. PREPRO Agree

The NJOY and PREPRO MF=2 resonance reconstructions were developed independently. So, the following is an excellent example of true code verification. The following results are for ENDF/B2212–VIII.1 U-238 MF=2 resolved resonance parameters, which extend up to 20 keV. Both codes independently reconstructed MF=3 tabulated cross sections to within an allowable accuracy of 0.01 % (4 digits; beyond experimental accuracy). The lowest energy resonance is near 7 eV, so for maximum clarity the below plots are from slightly below this up to 20 keV. Allowing for each code’s reconstructed data to differ from the exact value by 0.01% in different directions, 0.02 % differences we see are in complete agreement. **Bottom Line: Today NJOY and PREPRO agree.**



## U-238 Doppler Broadened: 0 Kelvin vs. 293.6 Kelvin

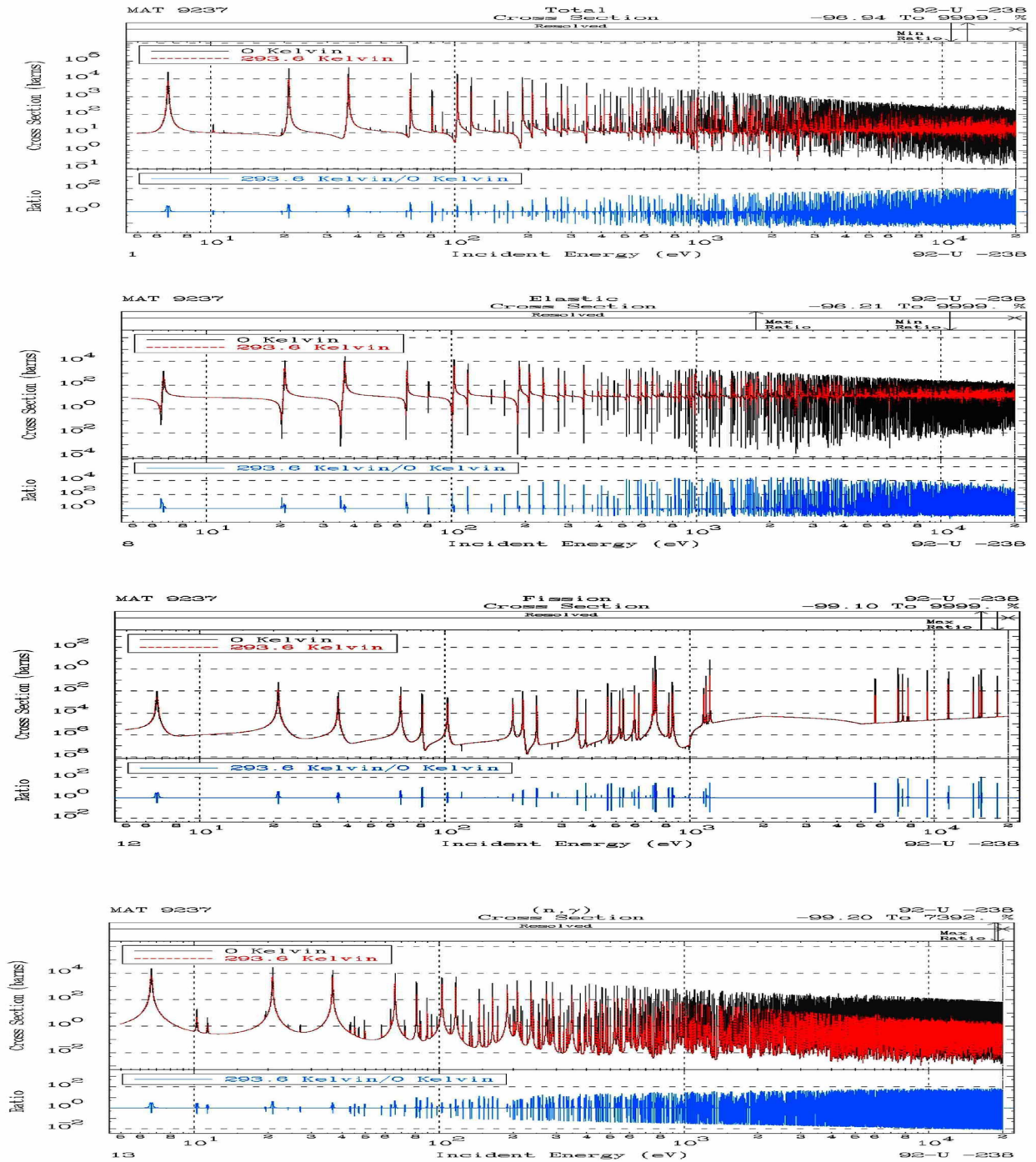
Calculating the cold (0 Kelvin) ENDF cross sections is merely one step toward defining the cross sections that we need for use in our actual applications; unless you are only interested in very cold refrigerators. Compared to the complications of resonance reconstruction, with its many different resonance models Doppler broadening is relatively simple, with our three codes, AMPX, NJOY and PREPRO all using the same SIGMA1 [5] model, which I supplied almost 50 years ago. I only recently described Doppler broadening in detail [6], so here I will present results to illustrate how important it is.

ENDF/B-VIII.1 U-238 includes resolved resonances from about 7 eV up to 20 keV; for clarity only this energy range is shown in the below figures. There are over 3,000 resolved resonances included in this evaluation; roughly half (1/2) up to 10 keV, and the other half up to 20 keV. For this comparison I have reconstructed cross sections to within an allowable uncertainty of 0.01 %, i.e., to within four (4) digits of accuracy, well beyond the resolution to which we can measure this data. This accuracy was used in this example to ensure that processing introduces little if any additional uncertainty to the evaluation defined data. The 0 Kelvin data required almost 4,000,000 tabulated energy points (in 20,000 eV, this means about 200 energy points per eV). **In contrast the 293.6 Kelvin data required roughly 200,000 data points; only 5 % of the cold (0 Kelvin) data.**

Note the range of the U-238 cross sections. The 0 Kelvin data extends from minima between resonances to peaks over a range of almost 1,000,000, i.e., roughly 0.01 barns to 10,000 barns. In contrast Doppler broadened fills in minima (less neutron streaming; flux) and reduces peaks (lower local reaction rates). Broadened minima can be over 100 higher than the cold minima, and peaks can be reduced to almost 100 times less than the cold values, i.e., enormous differences, that hopefully illustrate that the **cold 0 Kelvin) data cannot – or at least should not – be used if you expect accurate results when this data is used in our real world temperature dependent applications.**

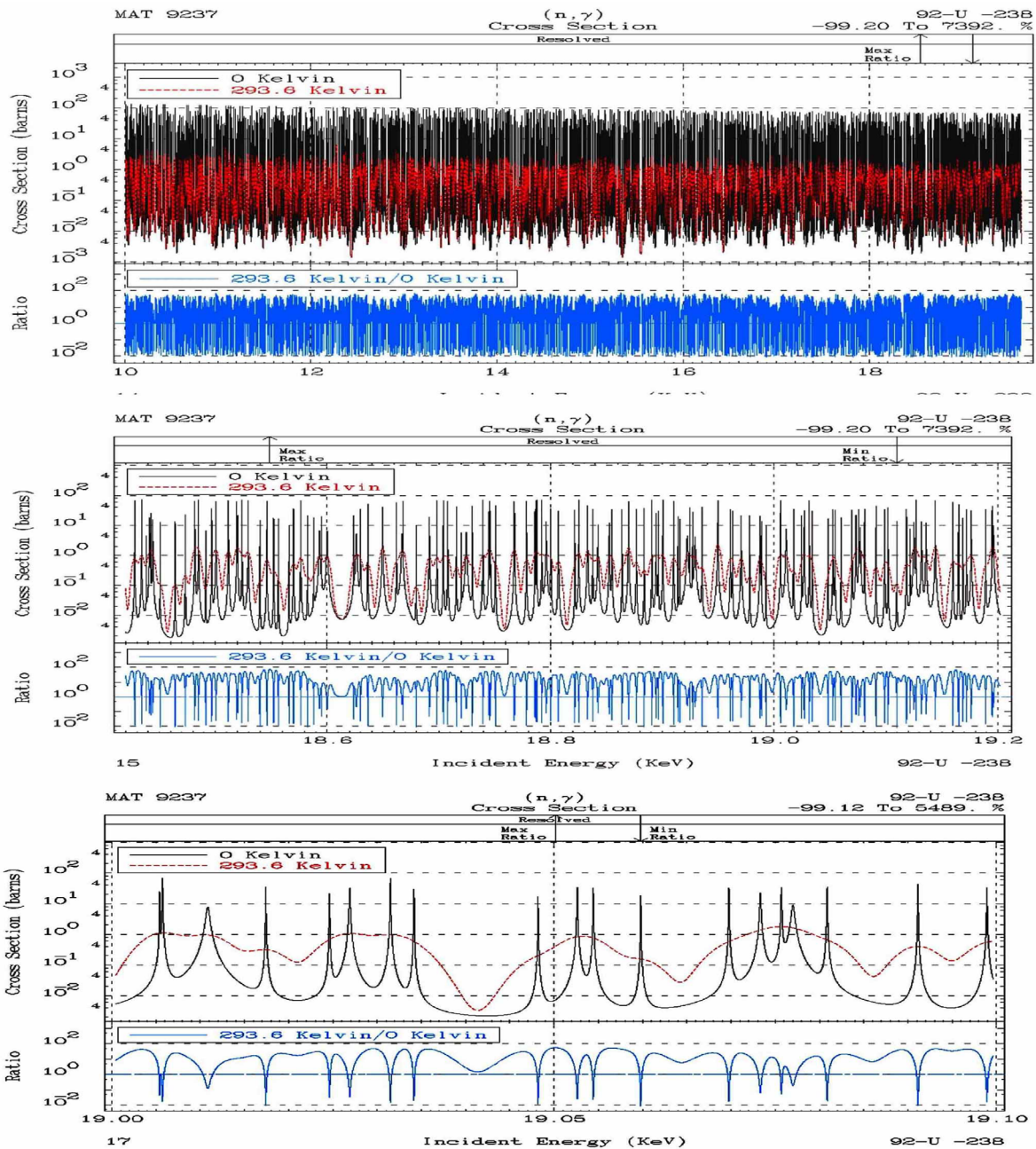
## U-238 Overview: ALL 4 reactions

Note the enormous differences between the cold, 0 Kelvin, and room temperature, 293.6 Kelvin, data. At higher energies, the very narrow, separated resonances, almost disappear, particularly the important capture resonances that result in important isotope production. Here the “hot” peaks and valleys can differ from the “cold” data by a factor of 100, i.e., the “hot” data has little resemblance to the “cold” data, proving that the “cold” data cannot be used in our real world applications.



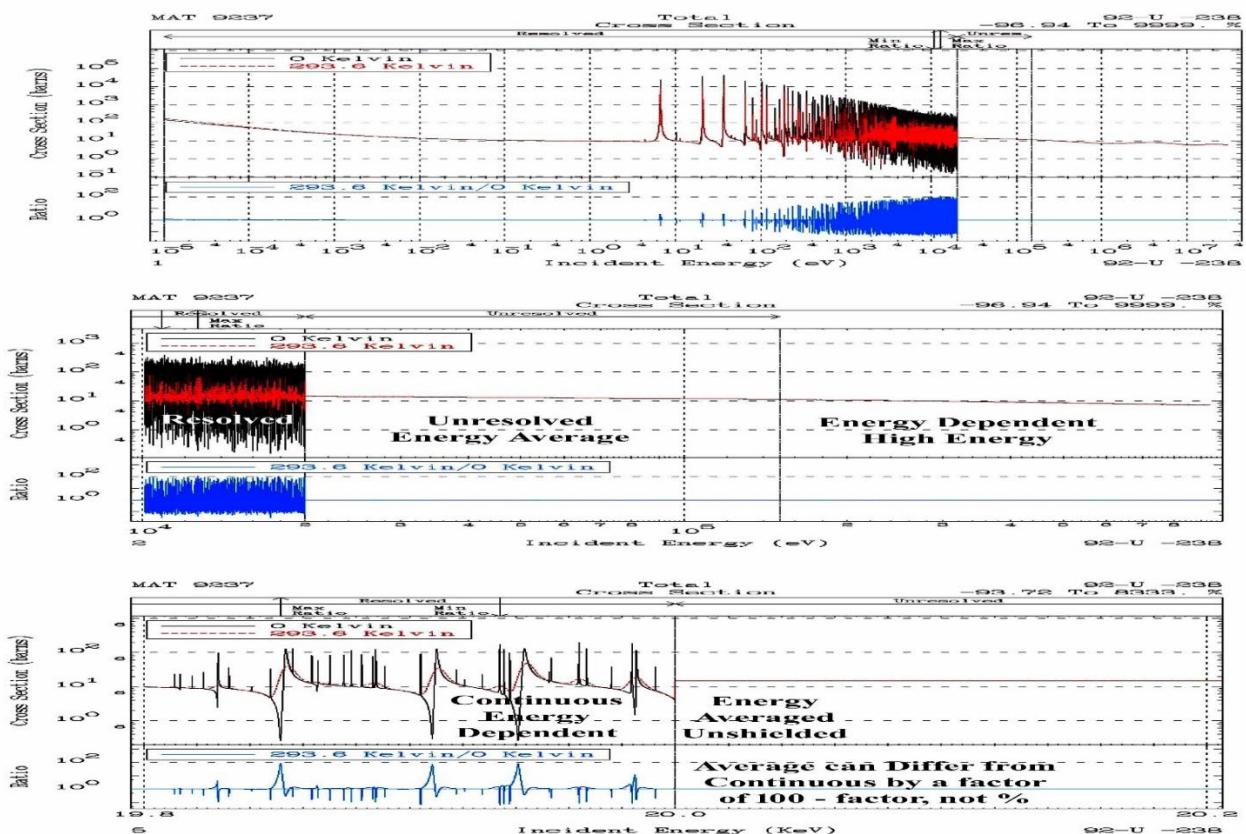
## U-238 Capture Details: 0 vs. 293.6 Kelvin

Below are three plots of the Capture cross section starting with 10 to 20 keV in progressively smaller energy ranges to illustrate both the overall and detailed changes due to Doppler broadening from 0 to 293.6 Kelvin. Even over this relatively small temperature range (0 to 293.6 K) isolated narrow capture resonances virtually disappear over this entire energy range. Note the reconstructed to 0.01 % allowable uncertainty 0 Kelvin data over this energy range required almost 2,000,000 tabulated energy points, almost all of them disappear due to Doppler broadening. In my humble opinion this looks like a perfect example of where the ENDF-102 unresolved resonance definition could have been used to both simplify and more accurately represent the distribution of resonances.



## The ENDF Unresolved Resonance Region

In the ENDF-102 defined Unresolved Resonance Region by definition we do not uniquely know the energy dependent cross sections; if we did, they would be in the resolved region. Based on the ENDF-102 definition of evaluated unresolved parameters we only know the distribution of cross sections; we do not uniquely know the energy dependent cross section. The actual energy averaged cross sections are application dependent. This presented a problem when we first decided to publish the ENDF data in graphic form circa 1972, ENDF/B-III [7]. We decided in the unresolved region to only show the unshielded, energy average cross section; this is unique but may not apply to any specific application due to self-shielding. This decision has been widely accepted and seems to be still used by all our processing codes today. I have discussed ENDF Unresolved Resonance self-shielding in detail elsewhere; see my website [8]. **I mention it here only as a WARNING to readers that what you see in our plots of ENDF data in the unresolved region may be very different from the actual energy averaged, self-shielded cross section in your applications and the unresolved region may be more important than it appears compared to the resolved range.** The plots of ENDF/B-III.1 U-238 that we see below illustrate properly defined ENDF-102 data, with resonances ONLY in the resolved resonance region, a smooth unshielded, energy average in the unresolved, and smooth tabulated high energy cross sections.



Unfortunately, my impression is that today both evaluators and users do not seem to understand the ENDF-102 definition of Unresolved Resonance Region. Fewer and fewer new ENDF evaluations include an unresolved region. Those that do seem to treat it as an unimportant add on to the Resolved range; i.e., it is just a smooth energy range for a decade or so above the resolved. The above plot of U-238 shows a log energy plot which makes the unresolved range seem insignificant, but in fact **the added decade of energy makes the unresolved range 90 % of the resonance range (resolved and unresolved).** These plots show that in the resolved

range we have uniquely defined energy dependent cross sections; in contrast in the unresolved we only “show” unshielded, energy average cross sections. Also, from these plots we can see that the two differ by a factor of up to 100 – a factor of 100 = 10.000 %, abruptly at the Resolved/Unresolved resonance boundary at 20 keV. Please remember that these are two completely different types of data. In the resolved range we have energy dependent linearly interpolable cross sections, and in the unresolved range we only show **unshielded, energy average** data – we would not expect continuity between these two very different types of data = energy dependent and energy averaged data.

## Processing Code Verification

Almost from the start of ENDF we realized that the processing and application codes required to accurately calculate fission reactor related problems were far too complicated to assume any one set of codes would be perfect. The solution was to verify code results by comparing ENDF output from a variety of independently developed codes. For almost 50 years we have compared output from 3 U.S. developed codes: AMPX, MINX (later named NJOY), and PREPRO. Today we have confidence that the results produced by these codes agree **inside** computers. But we faced the task to carefully output the results to a simple text format **outside** computers that we could verify and then use in our applications, namely the ENDF format – and in my case ENDL with TART.

A problem was “incest” – the methods used by these codes for ENDF formatted output are not completely independent. For decades, the output that we compared was based on my 7 digit format that I developed over 50 years ago. This was adequate for decades, but not today, where ENDF data has been extended to higher and higher incident neutron energies, and resonance was defined to more digits. In order to demonstrate that the problems I see today are based solely on limitations of the 11 column ENDF format, not on problems in calculated energy dependent cross sections inside our computers, here I have used one ENDF processing code, my own PREPRO/RECENT, that starts from ENDF resonance parameters (MF=2) and produces energy dependent tabulated cross sections (MF=3). I have modified my code to perform exactly the same calculations inside a computer and produce EXACTLY the same 64 bit results **inside** my computer, and **output** 3 complete sets of ENDF formatted results using both my earlier 7 digit and newer 9 and 10 digit results. These results prove that 7 digit precision is no longer adequate, but 9 or 10 digit precision is.

## ENDF versus In-House Formats

ENDF was designed as a simple text-based computer independent format to allow us to exchange evaluated nuclear and atomic data between data evaluators and users. Over the past 60 years it has been very successful in meeting this goal. But please be aware that in many cases once the data arrives at a site it may be translated for ENDF to an in-house format that better meets the needs of users. In our case we have been attempting to verify results between AMPX, NJOY and PREPRO ENDF users as well as ENDL users, such as myself. One problem we faced is that each of these codes uses an in-house format that differs from ENDF. AMPX used an in-house binary system that in principle should make it immune to the precision problem I have discussed here; in binary everything is defined to roughly 16 digits. NJOY processes ENDF data and outputs it into its in-house PENDL format. In my case I process ENDF data using my PREPRO codes to ENDF output and then translate it into our LLNL in-house ENDLX format for use by my TARTMAKER code, to prepare data for use by my TART Monte Carlo code.

There is one important thing that is missing from the three codes, AMPX, NJOY, and TARTMAKER. None of them include any information defining the ENDF resonance region. This is not a problem I have directly addressed here since this does not affect the ability of these codes to start from ENDF formatted data and process it into tabulated energy dependent cross sections at 0 Kelvin. But once translated to their in-house formats, these codes have no idea where the resonance region is, particularly the ENDF unresolved resonance region, needed for Doppler broadening.

This was not a problem when I originally developed my SIGMA1 method to Doppler broaden cross sections that are tabulated and linearly interpolable in the ENDF format, which I gave to my friends Maurice Greene for use in AMPX and Chuck Weisbin to use in MINX which became NJOY developed by Bob MacFarlane. I also developed the SIGMAL [11] code to use my SIGMA1 method using the ENDL format. To my knowledge all of these codes are still using my SIGMA1 method to define Doppler broadened cross sections in their in-house systems.

This became a problem when my good friend S. Ganesan pointed out that my SIGMA1 method does not work in the unresolved resonance region, since we do not uniquely know the unresolved energy dependent cross sections; again, I will mention we only know a distribution, and what we usually show in plots is only the unshielded, energy average cross section. Fortunately, we were lucky because resonance theory predicts resonance approach regular spacing and width with increasing neutron energy, and the unshielded, energy averaged cross section we show in plots varies as  $1/v$  (neutron speed). This means the unresolved, unshielded energy average reaction rate ( $v$ \*cross section) is constant, making **the unresolved resonance region independent of temperature** (see my detailed report on Doppler broadening my website) [6]. Since working with my PREPRO codes using the ENDF format, including MF=2 resonance data, I know the energy range of the unresolved resonance region, so it was easy for me to simply copy the unresolved unshielded, energy averaged data. **I know of no code except PREPRO/SIGMA1 that today correctly handles the ENDF-102 defined Unresolved Region unshielded, energy average data as temperature independent.**

However, this was not a simple fix for anyone using an in-house format that does not include the original ENDF resonance region data. **In my case this put my SIGMAL code using the ENDL format out of business and I abandoned it.** Today I simply use my PREPRO/SIGMA1 code and translate its output from ENDF to ENDLX for my in-house use at LLNL. I will merely mention that I do not know how AMPX and NJOY deal with this unresolved region. For example, in the above NJOY vs. PREPRO comparison I only compared 0 Kelvin data in the resolved region below 20 keV. Nowhere have I compared to AMPX/SAMRML results because I was unable to obtain any. With that I will conclude my discussion of ENDF and ENDL production to create 0 Kelvin data and leave the question of a detailed discussion of the unresolved region for another day; I suggest you see [8].

## Conclusions

Since 1958 ENDL and about 1965 ENDF have each used a text format to define nuclear and atomic data in 11 columns for each data field. When these formats originated this was judged to be adequate to reproduce the accuracy of data at the time and to meet the needs of our applications. When these formats originated the dominant computer language of the day was FORTRAN and if written using an E11.4 format it would include only 4 or 5 digits of precision, e.g., 0.1234E-03 or 1.2345E-02, varying from one computer/system to another the result was

not unique. In the case of ENDF the 4 digit precision was not even adequate to uniquely define the atomic weight of the target, e.g.,  $U238 = 92238 = 0.9224E+5 = \text{WRONG!}$

Today my circa 1970 7 digit precision ENDF output is no longer adequate to accurately define the ENDF 11 column data for use in our applications. Fortunately, there is a fairly simple solution, Our ENDF processing codes have been verified to be very accurate to define cross sections **inside** computers, where they use real\*8, 64 bit, about 16 digit accuracy; they are not the problem. The problem is how can we – must we – accurately translate this data to the ENDF 11 column data format **outside** a computer. This is similar to the three little bears problem: the internal 16 digits is too BIG (not physically possible); 7 digit is too SMALL (used for many years by our codes, but not adequate today); 10 digits works today (the maximum possible to uniquely define in 11 columns; for uniqueness we must include a decimal point).

## WARNING to ENDL Users

Today's ENDF data, where energy is in eV, cannot be adequately defined in the traditional ENDL 11 column format where energy is in MeV. You **MUST** use the ENDLX, ENDL Extended, 16 column format. Failure to heed this WARNING will result in creating and using the RUBBISH results I have shown above. This will be putting the results of your application codes in what we describe as the “Garbage In = Garbage Out’ situation; **no matter how perfect your application codes may be results can be no better than the data they use.**

## Advice to ENDF Evaluators

ENDF has come a long way since 1965 toward meeting the goal it was designed for: namely to supply accurate nuclear and atomic data for use in thermal fission related applications. By roughly ENDF/B-VI to VII it had met almost all our needs. Beyond that point I had hoped to see improvements in the data itself without trying to extend ENDF in directions it was never intended to be used. Unfortunately, what I see is evaluations moving in different directions; sometimes at odds with our needs. One direction is continuing to move the resolved resonance region to ever higher energy limits, and at least as important, totally ignoring the ENDF-102 defined Unresolved Resonance Region. These extensions may be of personal interest to the evaluators, but today they contribute little toward improving the accuracy of our thermal fission-related systems. Indeed, as I hope I have demonstrated here, extending resolved resonances to higher energies may directly lead to decreased precision of the data actually being used by our application codes. Also, I will add that in my case using ENDF data extended to higher energy in my TART code does not significantly change TART answers, it merely makes it run significantly longer because it is forced to sample more cross sections.

My advice to evaluators is to concentrate on improving the resolved resonances and define the upper energy limit of the resolved range no higher than you can define ALL resonances in ALL sequences; not just the L=0 sequence. Today in too many ENDF evaluations L > 0 sequences end far below the upper limit of the resolved range. These missing, generally narrow, unmeasurable, resonances lead to incorrect Doppler broadening and resonance self-shielding.

Also PLEASE learn and use the ENDF-102 definition of the Unresolved Region [2]. I repeat, above the Resolved Range ENDF-102 does not uniquely define ANY individual resonances. It only allows Unresolved parameters to define the distribution of resonance parameters. By definition, any individual resonances that you try to define above the Resolved range are: 1) obviously not resolved, and 2) also obviously not allowed in any properly ENDF-102 defined evaluation. Clusters of resonances above the resolved range may look impressive, but again, any missing, usually narrow resonances, will lead to incorrect Doppler broadening and

resonance self-shielding [6, 8, 9, 10]. Finally, I will stress that the ENDF-102 defined tabulated energy dependent smooth MF=3 cross sections above the resonance regions are intended to be just that = SMOOTH. Too many evaluations look like they merely copied measured data, including resonance structure, to the ENDF format and call that evaluation. Need I repeat that this data if missing any, usually narrow, resonances will lead to incorrect Doppler broadening and resonance self-shielding.

ENDF evaluators have done a GREAT job over 60 years to get us this far and I am confident they will continue to do a GREAT job if they: 1) Concentrate on our thermal fission application needs, and 2) Continue to learn and work within ENDF-102 guidelines. **The safety of our systems relies on accurate Doppler broadening [5, 6] and self-shielding [8, 9, 10]. Get my point?**

## Advice to ENDF Processing Code Designers

Usually, the evaluators who create the evaluated data and the application code users who perform and publish results get the headlines. But the processing codes serve such an important purpose and yet they are often overlooked. I can only hope that this report demonstrates what an important role the ENDF and ENDL processing play. I must start by apologizing since a major source of the precision problems I describe in this report originated with me. My circa 1970 7 digit precision method has been so widely accepted over the decades that hardly anyone questions it today. It has gotten to the point where users no longer question the ENDF processed data they are given. Users assume that if it comes from a given processing code it MUST be correct. I keep adding checks and WARNINGS to my PREPRO codes, but today nobody seems to look at the output reports from these codes; they assume the data MUST be correct, so my WARNINGS go unheeded.

This report is aimed primarily at processing code designers and maintainers to make them aware of the precision problem they face. Of equal if not even GREATER importance is to make them aware of how easy it is to correct/avoid precision problems. I supply both INCORE and OUT routines through my website; you can use them from my website or ask me directly and I will email them to you. Let me congratulate the NJOY designers who based on the comparison shown above independently – let me repeat – INDEPENDENTLY - recognized and solved the problem: the NJOY results use 9 digits of precision. If you as a processing code developer do not know what precision you are now using look at your ENDF formatted output at MF/MT=3/1, Total Cross Section, in the eV range how many digits do you see? If not 9 or more, PLEASE UPDATE your ENDF format. Again, this should be simple, based on and using our decades of experience addressing this precision problem.

## Advice to ENDF Data Users

I hate to, but I MUST admit, that it can be so easy for codes to fall into the “incest” trap, where two or more perfectly good codes use the same input data, and get the same or very similar answers and therefore they assume they must be right. In fact, in far too many cases over the last 60 years I have found that the answers were actually WRONG!!! because the data they all used was wrong. I will mention one case. In the pre-ENDF years the ENDL format developed at LLNL was used by both what became MCNP at LLNL and TART at LLNL. ENDL never included any models, and since it was only designed for fast fission systems, included only a limited energy range. There was no thermal interactions or thermal scattering. For years comparisons of results from MCNP and TART agreed using the same ENDL data = INCEST!!! It was not until after ENDF came along and provided accurate data particularly to lower energies that ENDL was extended down to below thermal energies and thermal scattering was

added. After these two format developments, MCNP and TART again agreed, but they agreed on completely different answers from what they both had calculated earlier. To my knowledge until I wrote this here nobody has spoken up and admitted to this problem which was solved decades ago. Hopefully, we can learn from this experience and try to avoid it today and in the future.

My point is: As a user of **ENDF** formatted data PLEASE do not make the mistake of assuming that the data handed to you by any processing code is correct, as far as precision. With ENDF formatted data files it is so easy to open and examine the data. Search for the tabulated energy dependent data in the section of ENDF MF/MT=3/1 (total cross section). Energy is in eV. Pan down in the ENDF data to the 1 eV or more range. How many digits of precision are energies listed to? **If not 9 or 10, DO NOT USE.** Even worse if there is no decimal point, **DO NOT USE** = without a decimal point the data may not (usually will not) be interpreted correctly.

At LLNL **ENDL** format users can open the ENDL text file. **If the data is in the old 11 column format DO NOT USE.** Today you MUST use ENDLX, ENDL Extended, with 16 column data. Finally let me stress that my SIGMAL [11] code to Doppler broaden ENDL formatted data was never updated and MUST never for usage today. Use my PREPRO/SIGMA1 to Doppler broaden ENDF formatted data and translate it to ENDLX format. That is what I do to supply Doppler broadened data to my TART Monte Carlo code.

## References

Many of these reference reports can be found on my website.

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