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How Accurate Are Our Processed ENDF Cross Sections?

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May 2014

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May 2014

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Overview of the Problem

Let me start by reassuring you that **currently our nuclear data processing codes are very accurate** in the calculations that they perform **INSIDE COMNPUTERS**. However, most of them drop the ball in what should be a trivial final step to **output their results into the ENDF format** [1]. This is obviously a very important step, because without accurately outputting their results we would not be able to confidently use their results in our applications. This is indeed a very important step, but unfortunately it is one that is not given the attention it deserves; hence we come to the purpose of this paper.

Here I document first the state of a number of nuclear data processing codes as of February 2012, when this comparison began, and then the current state, November 2013, of the same codes. **I have delayed publishing results until now to give participants time to distribute updated codes and data.** The codes compared include, in alphabetical order: AMPX [2], NJOY [3], PREPRO [4], and SAMMY/SAMRML [5]. During this time we have seen considerable improvement in output results, and as a direct result of this study we now have four codes that produce high precision results, but this is still a long way from ensuring that all codes that handle nuclear data are maintaining the accuracy that we require today.

In the first part of this report I consider the precision of our tabulated energies; here we see obvious flaws when less-precise output is used. In the second part I consider the precision of our cross sections; here we see more subtle flaws. **The important point to stress is that once these flaws are recognized it is relatively easy to eliminate them and produce high precision energies and cross sections.**

Accuracy and Precision

Before discussing accuracy and precision I should first define what I mean by these terms. By ACCURACY I mean how uncertain the nuclear data is that we use, and by PRECISION I mean how many digits we use to represent our nuclear data. To understand the accuracy of our nuclear data, let me briefly discuss how we obtain and use them. I like to divide how we get the final answers from our application codes into four steps:

Measurement – we still cannot define nuclear data based strictly on theory, so we measure important nuclear data; that is, data that we can afford to measure.

Evaluation – here I include nuclear models — we cannot afford to measure everything we need, so the available measured data, nuclear model predictions, and yes, even best guesses are combined and used to completely define what we need — this is more of an art than a science.

Processing – there is a lot of work to do between having nuclear data in the ENDF format and the form we need them in for use in our application codes. Historically this step has been ignored or taken for granted. But it is very important if we are to preserve the accuracy of the evaluated data that is actually used in our applications.

Applications – Finally we come to "the proof of the pudding" where we use the nuclear data in our neutron transport codes [11, 12] to predict results for our systems of interest.

The results of our applications compared to measured results can be used in an attempt to "close the loop", by allowing us to change our evaluated data so that our calculated results better agree with measured results. But care must be used here to ensure that the changes in the evaluated data are really improved physics, and not just a "fit" to accommodate the

uncertainties in our nuclear data, processing and application codes. In order to accomplish this we must make every effort to control the accuracy of the nuclear data that we produce and use.

My general rule of thumb is that we do not know any cross section in any material at any temperature and neutron incident energy to better than roughly 1%; we may know some integral parameters more accurately, but not energy dependent cross sections. Each of the above steps adds its own uncertainty to the nuclear data, and these combine to define the overall uncertainty, or accuracy, of the data we end up using in our applications.

So PLEASE understand that in this paper when I state that our processing codes now attempt to achieve a target uncertainty of 0.1%, this does not mean that we claim to know the cross sections to within 0.1%;. **This 0.1% is the ADDITIONAL UNCERTAINTY introduced in processing the evaluated data.** In order to define the total uncertainty this MUST be added to the inherent uncertainty in the evaluated data; again, I assume at least 1%. If the uncertainties in these four steps are uncorrelated they will combine quadratically: $[E1^2+E2^2+E3^2+E4^2]^{1/2}$, and our objective is to ensure that the uncertainty introduced by processing is small compared to the uncertainty in the evaluation; our target 0.1% uncertainty due to processing meets this criteria.

Data Format

In this report I will be discussing data in the ENDF format [1]. But be aware that the conclusions I present here apply to nuclear data in any format. My conclusion is that today's nuclear data requires at least 9 digits of precision. It is IMPERATIVE that this precision be maintained all the way up until it is actually used in our applications. Currently some of our application-oriented formats, such as ACER for MCNP [12], and the extended ENDL format I use with TART [11], already include the required precision. So that the focus here is on ensuring that our processing codes produce results with enough precision to preserve the accuracy of the data we actually use in our applications.

My experience has been that it is all too easy to lose precision between the output from our processing codes and the actual use of the data in our applications. I will mention but a few actual examples.

First, as we will see in this report, the ENDF format is capable of accommodating 9 digit output from our processing codes, and the ACER format can accommodate even more digits of accuracy. However, I have seen people write computer codes to perform the seemingly trivial task of copying the data from ENDF to ACER format**, but they did it using 32 bit arithmetic**, thereby truncating the precision of the data in the ACER format.

A second example is with the ENDL format that I personally use as a bridge between ENDF and the input format for my TART Monte Carlo code [11]. The "standard" ENDL format is similar to ENDF in that it uses data fields 11 columns wide. But ENDL uses energy units of MeV, rather than eV, so ENDL cannot accommodate precise 9 digit energy output, which leads to truncation. As a result, many years ago I UNILATERALLY unofficially changed the "ENDL like" format that I use with TART, to include data fields 16 columns wide, so that using FORTRAN standard, formatted output 1PD16.9, I can accommodate 10 digits of accuracy; which is more than I need for the foreseeable future.

Hopefully these few examples will serve as a warning to all nuclear data producers, processors, and users that today's nuclear data requires 64 bit arithmetic. If you do not use it throughout you will obviously limit the precision of the data you are using, and in turn limit

the accuracy of your answers. Many years ago we always tried to avoid "double precision" 64 bit arithmetic because we thought it was too expensive. But today this is no longer true; today's computers are designed to handle 64 bit arithmetic, and trying to "economize", can actually lead to less efficient computer codes and obviously truncate the precision of your data, i.e., don't do it.

ENDF Character and Binary Formats

In the original documentation for ENDF/B, ENDF-102 two separate formats were described in detail: one using 80 characters per record, corresponding to the 80 column width of a computer card, and a more compact binary format. The intent was that the COMPUTER and LANGUAGE **INDEPENDENT CHARACTER** FORMAT be used to exchange nuclear data between users. It was assumed that each user would convert the character data to the COMPUTER and LANGUAGE **DEPENDENT BINARY** FORMAT to be used in-house

Somewhere along the way the details for the binary format have been lost from the ENDF/B documentation, ENDF-102. Indeed today when I search the entire ENDF102 report the word "binary" is only mentioned four times, in reference to a binary format, but there is no longer any detailed description of the ENDF/B binary format.

Personally I think this is a BIG loss, because if one was using the ENDF/B binary format the question of precision and standard formats do not arise, since the data is stored to the full precision of each computer without any truncation. In contrast when using the ENDF/B character format, precision and standard formats become extremely important. Indeed, if no one was using the ENDF character format there would be no reason for this document.

Of the processing codes compared here, only AMPX uses the ENDF binary format for all in-house (ORNL) processing, so that as long as it only uses the ENDF binary format, its calculated results are not subject to the precision truncation that occurs with all of the other codes compared here. **As far as precision, this is why I consider AMPX to be the Gold Standard**, since its binary results preserve the full precision of the computer used. The AMPX results presented here are based on ENDF character files sent to me from ORNL specifically for use in this code comparison; this allowed me to verify the accuracy of the results produced by AMPX, e.g. I was able to verify the accuracy of the energy dependent energy grid it produces.

We Have Come a Long Way

We have come a long way in being able to produce accurate processed nuclear data, compared to when I first started verifying nuclear data processing codes [6, 7, 8]. Back then we couldn't even get agreement between the outputs from our processing codes for even the simplest integral results, such as **unshielded, multi-group cross sections**. When I started these comparisons, roughly 20 years after ENDF/B started, I assumed this would merely confirm the then current excellent agreement between the results produced by our processing codes. So it came as a complete shock to me, and the other participants, to find that initially **NO TWO CODES AGREED**; remember: this was for the simplest possible quantity I could think of. Below is a copy of a table from Ref. [8], summarizing the initial and final results. Please remember that these results are from roughly 20 years after ENDF/B started; hopefully this will serve as a wakeup call to illustrate that nuclear data processing is not a trivial step between evaluation and use of the data in our applications.

One important thing we learned from this study is how conservative the nuclear data business really is, i.e., changes happen very slowly. What we found in this 1980s study was that even 20 years after the start of ENDF many of the major differences that we found was because some codes were still using 5 digit precision (1.2345D+03) instead of the 7 digit (1.234567+3) that I introduced to ENDF 15 years earlier. Today we continue to see this very slow change in that many codes are still using the 7 digit precision almost 15 years after I introduced 9 digit precision (1234.56789). As a direct result of this current comparison study we have at least four of our codes that have been brought up to date, as far as precision is concerned.

I mentioned how conservative the nuclear data business is, and one additional illustration of this point is that to a large degree we have not been able to implement changes because there are so many people who argue that change — any change — is not necessary. To them I say: It couldn't hurt. Certainly the changes needed to go from 5 digits to 7 digits and now to 9 digits was trivial, but **the improvement in the accuracy of the nuclear data we can now use in our applications is dramatic**; that's what makes these changes necessary.

Summary of Initial and Current Maximum Percent Differences for Each Code*

Code (Affiliation)	Initial Maximum Difference (%)	Current Maximum Difference or Status
RESEND (Brookhaven National Laboratory)	2018	Abandoned
ENTOSAN (Netherlands Energy Center, Petten)	2	Agreement
RECENT (IAEA)	6[a]	Agreement
FOURACES (European Nuclear Energy Agency, Bologna)	2692	Agreement
RESCAL (Argonne National Laboratory)	113	87%[a]
RESENDD (Japan Atomic Energy Research Institute)	5488	Agreement
FEDGROUP-3 (HUN, Budapest)	188[b]	16%[b]
FEDGROUP-C (IJS, Ljubljana)	2482[b]	Agreement
NJOY-CDC (Los Alamos National Laboratory)	19[a]	Agreement[a]
NJOY-IBM (Nuclear Energy Agency/Data Bank)	100[a]	19%[a]
AMPX [Oak Ridge National Laboratory (ORNL)]	24	1.7%
MINX (ORNL)	2018[b]	No additional results
GRUCON (CJD, Obninsk)	2.5[b]	No additional results

*Results are presented in chronological order according to initial date of receipt from code authors.
[a]Ignores large percent differences for small cross sections near thresholds.
[b]Comparison based on only a portion of the ENDF/B-V dosimetry library.

Today, almost 50 years after ENDF/B started, we at least like to think we can produce **highly accurate energy dependent cross sections,** and we have set a goal of producing such data to within a uncertainty of 0.1%, Be AWARE that here we are talking not about the absolute accuracy of the data, but about the ADDITIONAL UNCERTAINTY added by our processing codes – this is the 0.1% we are talking about; **PLEASE DO NOT make the mistake of thinking we are claiming to know cross sections to within an uncertainty of 0.1%; WE ARE NOT.**

What Differences Do We Expect?

With that as background I will merely state that although this 0.1% is our objective, and is often claimed in publications, we can see here that based on actual head-to-head processing code comparisons the ACTUAL differences are often over 10% – that's right, the actual differences **were** over 100 TIMES LARGER than the claimed accuracy of our processing code output. Here I will stress the word **WERE**, because thanks to our comparisons over the last few years we were able to locate and eliminate many sources of differences, so that TODAY we are close to meeting our uncertainty target of 0.1%.

If two codes independently attempt to produce energy dependent results to within an accuracy of 0.1%, at any given energy one code may be up to 0.1% above the correct answer and the other may be up to 0.1% below it, and yet both are within their target accuracy. So that when we compare the results from these two codes differences up to 0.2% indicate agreement to within their target accuracy. Use this as a guideline when viewing the comparison figures included here. I will merely mention that I have used my PREPRO code to produce energy dependent results with a much smaller allowable uncertainty (0.01%), and I used these data to verify that today all of the codes included in this study are now achieving their 0.1% goal.

What Are We Checking?

In this comparison study we are checking:

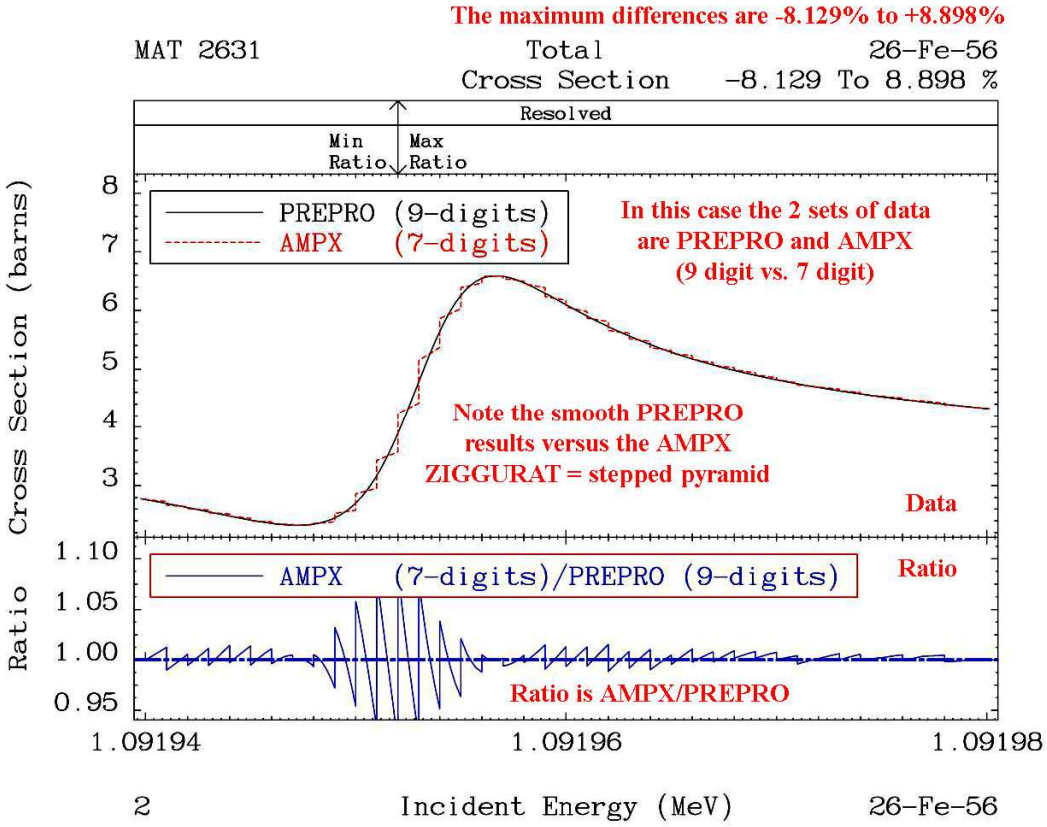
1) That our codes are producing accurate results INSIDE COMPUTERS.
2) That our codes are outputting results in the ENDF format to HIGH PRECISION.

In this report we will see that our codes are producing accurate results INSIDE COMPUTERS. Defining an energy grid to accurately reconstruct cross sections is much more difficult than it sounds. This study shows that AMPX, NJOY and PREPRO, that independently each defines its own energy grid to produce results that agree with each other to within 0.2%, as described above, and therefore meet our goal for a target accuracy. In contrast SAMRML does not define its own energy grid; it reads an energy grid as input. For this study I used the PREPRO energy grid. Here since both are using exactly the same energy grid we expect much closer agreement than 0.2%, which is exactly what we find.

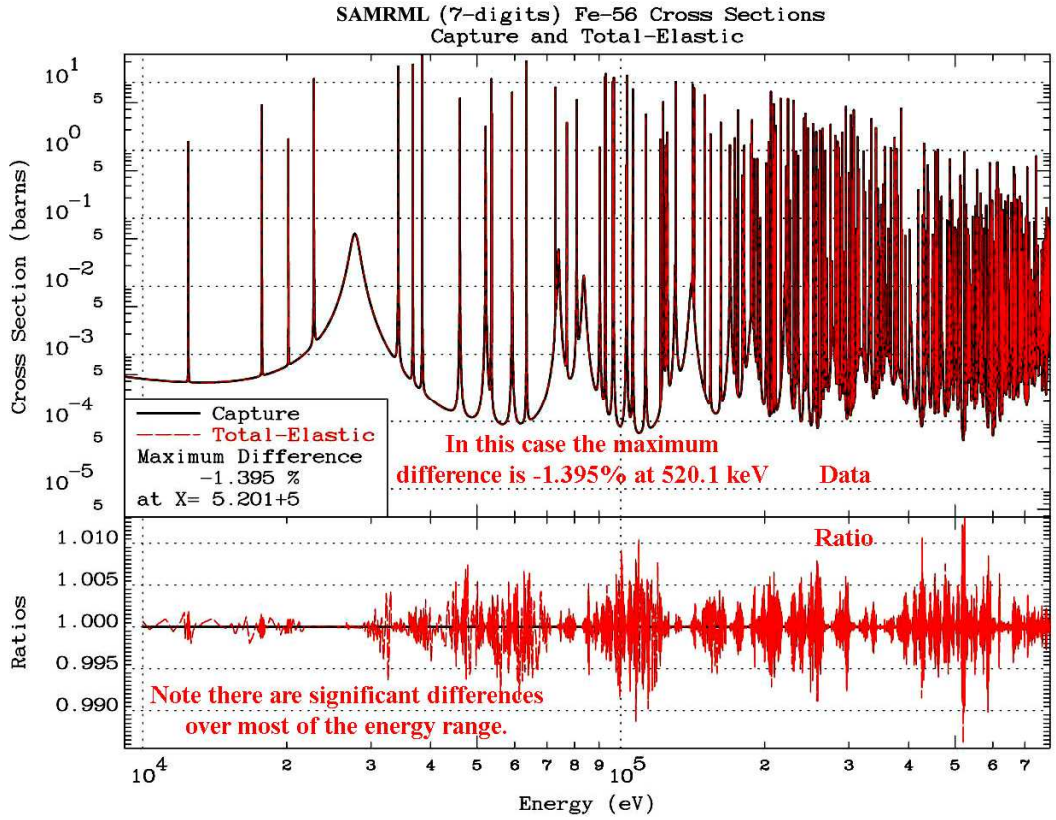
The major problem that this report focuses on is that at the beginning of this study although ALL of these codes were producing accurate results INSIDE COMPUTERS, they had a design flaw in that they were ALL **TRUNCATING** and outputting their results into the ENDF format using a lower precision than we require to accurately handle today's evaluations. As a result of this study this design flaw was found and corrected by the end of this study.

A Guide to Interpretation of the Following Figures

In the first section where we investigate the **energy precision**, each of the figures (plotted with COMPLOT [9]) is divided into two sections: the upper two-thirds shows a comparison of two sets of data and the lower one-third shows the ratio of the second set of data divided by the first set. Near the upper right hand corner the figure shows the maximum % differences between the two sets of data; for example, in the below figure the two sets differ by -8.129% to +8.898% = up to 80 times our 0.1% target — let me repeat that — up to 80 times (8000%) of our target accuracy.



In the next section where we investigate the **cross section precision**, each of the figures (plotted with PLOTTAB [10]) is also divided into two sections: the upper two-thirds shows a comparison of two sets of data and the lower one-third shows the ratio of the second set of data divided by the first set. In this case the maximum % difference is shown in the legend box, in the below figure near the lower left hand corner of the figure; for example, in the below figure the two sets differ by -1.395% = up to almost 14 times our 0.1% target — let me repeat that — up to 14 times (1400%) of our target accuracy.



Energies: 9 digits versus 7 digits

Since our objective is to reproduce the cross sections to within 0.1%, one might assume we only need to know any energy to an accuracy of 3 or 4 digits. However, this does not allow for the fact that energies that define the shape of cross sections, particularly narrow resonances and minima, often have exactly the same leading digits, and it is actually the **difference in energies** that we must accurately define. For example, consider a narrow capture resonance in the high keV or even MeV energy range. In the example tabulated and plotted below we have a resonance, whose entire shape is between:

1.09194 MeV
1.09196 MeV

This is an example where the first 5 digits of the energy tell us nothing about the shape of this resonance. Even the 9 digit energy output defines the shape to an accuracy of only 4 digits, and 7 digit output to only 2 digits.

The below comparisons of tabulated and plotted data illustrates the results of representing this resonance using either 7 digit or 9 digit output. The 7 digit output completely fails and

produces what I call '**ZIGGURATS',** which are **stepped pyramids,** where EXACTLY the same 7 digit energy is repeated, often many times. But we can also clearly see this problem did not occur INSIDE the computer, but is actually strictly due to OUTPUT TRUNCATION. We can see this because where the energies are EXACTLY repeated the cross section at each energy point is DIFFERENT, i.e., clearly the energy points used INSIDE the computer were not EXACTLY the same, because if they were the output for BOTH energy and cross section would be identical at the repeated energy points.

Here are a few actual tabulated output energy points, first using 7 digit output, where EXACTLY the same 7 digit **energy** is repeated 11 times!

```
1.091946+6 2.385267+0 1.091946+6 2.378021+0 1.091946+6 2.371612+0
1.091946+6 2.368007+0 1.091946+6 2.365001+0 1.091946+6 2.359234+0
1.091946+6 2.356032+0 1.091946+6 2.353387+0 1.091946+6 2.348391+0
1.091946+6 2.345669+0 1.091946+6 2.343455+0
```

Next, output from EXACTLY the same code, doing EXACTLY the same calculations INSIDE the computer, but now outputting the results using a combination of 7 digit and 9 digit output for the same energy range. Here we can see the changes in the energy, beyond 7 digits. Note that the cross section is still output only to 7 digits.

```
1.091946+6 2.357910+0 1091946.25 2.347066+0 1091946.50 2.338049+0
1091946.75 2.331196+0 1.091947+6 2.326890+0
```

Finally, I show results from a different code using 9 digit output for both energy and cross section over the same energy range.

```
                                                1091946.01 2.35744465
1091946.34 2.34359345 1091946.67 2.33313163 1091946.99 2.32700824
```

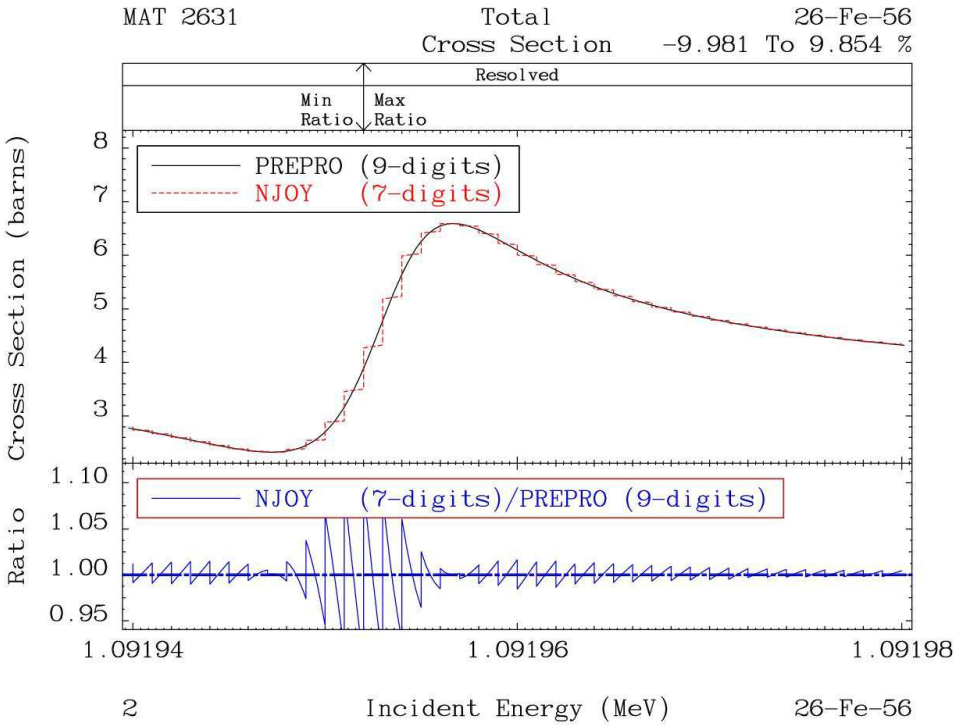
This simple example clearly illustrates that 7 digits of accuracy in tabulated energies is not adequate to define the shape of a narrow resonance, and even 9 digits only gives us about 4 digits to actually define the resonance shape.

Below is an actual example of data that is accurately calculated within NJOY [3] (that is to say the data are highly accurate within the computer), but are then output to the ENDF format to a lower precision, i.e., 7 digits. The below first table is from NJOY when this study started; this is followed by NJOY results by the time this study was completed. Here we see a marked improvement: Initially all of the other codes, including NJOY, were producing ZIGGURATS – stepped pyramids. But by the end of this study all of the codes were producing high precision, 9 digit output, and the ziggurats have disappeared.

First the original results, showing a ziggurat, due to 9 repeated energies (to 7 digits):

NJOY (7 digit energies) 1.091943 to 1.091948 MeV

```
1.091943+6 2.537448+0 1.091943+6 2.528038+0 1.091944+6 2.519367+02631 3  186263
1.091944+6 2.509997+0 1.091944+6 2.501377+0 1.091944+6 2.492080+02631 3  186264
1.091944+6 2.483543+0 1.091944+6 2.474358+0 1.091944+6 2.465946+02631 3  186265
1.091944+6 2.456919+0 1.091945+6 2.448676+0 1.091945+6 2.439860+02631 3  186266
1.091945+6 2.431839+0 1.091945+6 2.423296+0 1.091945+6 2.415560+02631 3  186267
1.091945+6 2.407361+0 1.091945+6 2.399981+0 1.091945+6 2.392210+02631 3  186268
1.091946+6 2.385267+0 1.091946+6 2.378021+0 1.091946+6 2.371612+02631 3  186269
1.091946+6 2.368007+0 1.091946+6 2.365001+0 1.091946+6 2.359234+02631 3  186270
1.091946+6 2.356032+0 1.091946+6 2.353387+0 1.091946+6 2.348391+02631 3  186271
1.091946+6 2.345669+0 1.091946+6 2.343455+0 1.091947+6 2.339374+02631 3  186272
1.091947+6 2.337222+0 1.091947+6 2.335518+0 1.091947+6 2.332521+02631 3  186273
1.091947+6 2.331041+0 1.091947+6 2.329938+0 1.091947+6 2.328215+02631 3  186274
1.091947+6 2.327525+0 1.091947+6 2.327126+0 1.091947+6 2.326896+02631 3  186275
1.091947+6 2.327128+0 1.091947+6 2.327555+0 1.091948+6 2.329064+02631 3  186276
```



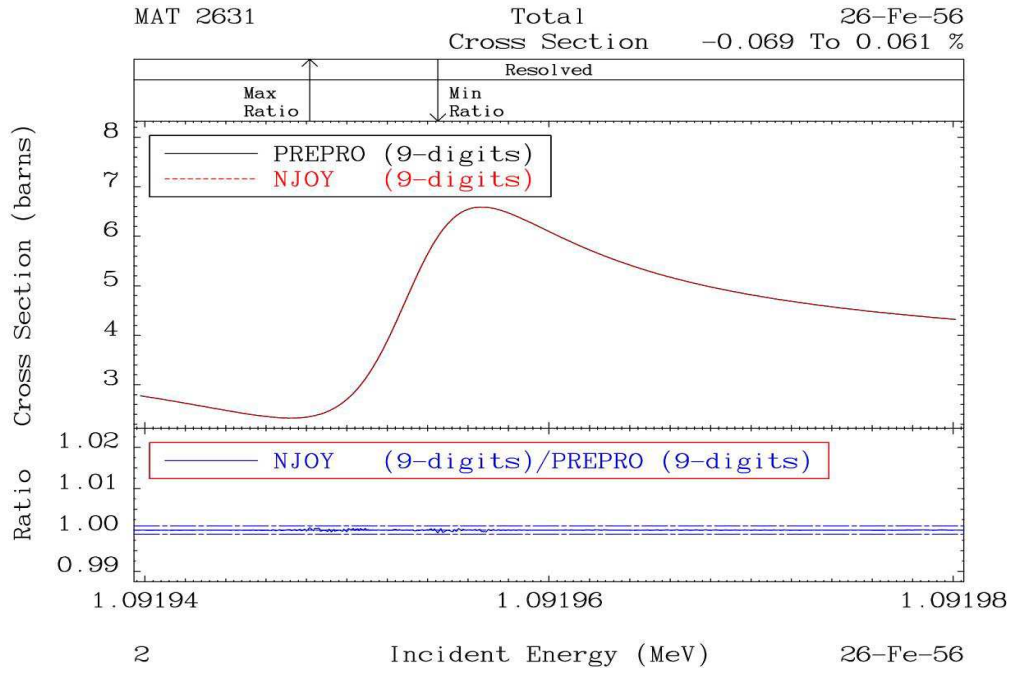
Next, the current results, showing smooth 9 digit results, and agreement:

NJOY (mixed 7 and 9 digit energies) 1.091943 to 1.091948 MeV

```
1.091943+6 2.554237+0 1091943.25 2.536123+0 1091943.50 2.518042+02631 3  127176
1091943.75 2.500052+0 1.091944+6 2.482219+0 1091944.25 2.464621+02631 3  127177
1091944.50 2.447351+0 1091944.75 2.430514+0 1.091945+6 2.414235+02631 3  127178
1091945.25 2.398656+0 1091945.50 2.383942+0 1091945.75 2.370287+02631 3  127179
1.091946+6 2.357910+0 1091946.25 2.347066+0 1091946.50 2.338049+02631 3  127180
1091946.75 2.331196+0 1.091947+6 2.326890+0 1091947.25 2.325572+02631 3  127181
1091947.50 2.327739+0 1091947.75 2.333960+0 1.091948+6 2.344872+02631 3  127182
1091948.35 2.369408+0 1091948.70 2.406785+0 1091948.88 2.431825+02631 3  127183
```

PREPRO (9 digit energies) 1.091943 to 1.091948 MeV

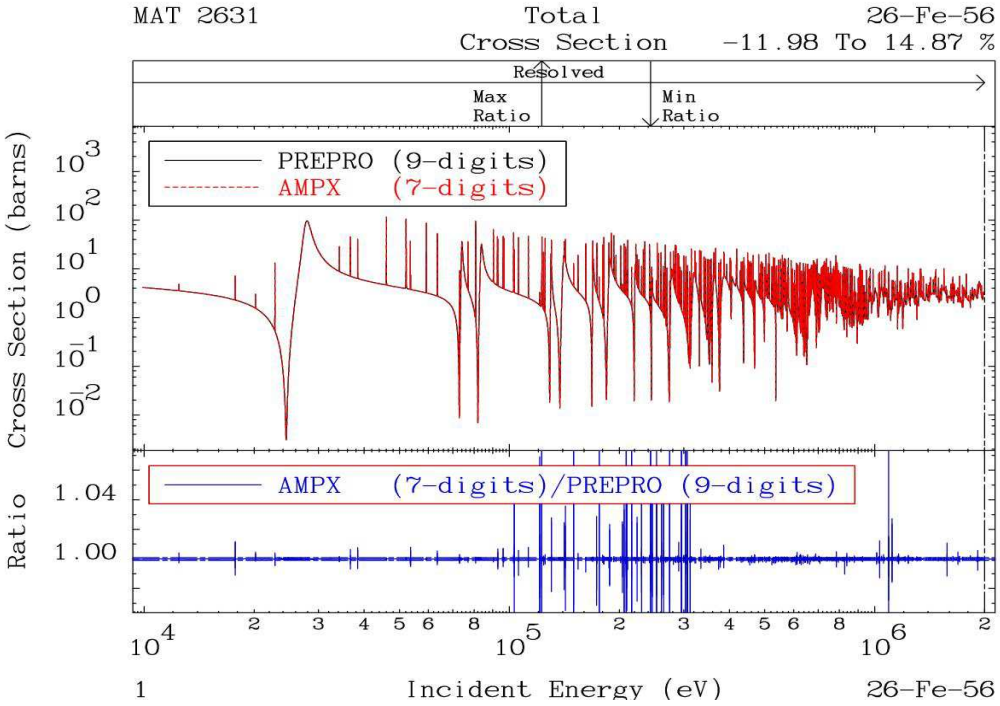
```
1091942.40 2.59756586 1091942.73 2.57377957 1091943.06 2.549888682631 3  128618
1091943.39 2.52599003 1091943.72 2.50220364 1091944.05 2.478677582631 3  128619
1091944.37 2.45628467 1091944.70 2.43384158 1091945.03 2.412325452631 3  128620
1091945.36 2.39206433 1091945.68 2.37399130 1091946.01 2.357444652631 3  128621
1091946.34 2.34359345 1091946.67 2.33313163 1091946.99 2.327008242631 3  128622
1091947.20 2.32557308 1091947.44 2.32687174 1091947.68 2.331774002631 3  128623
1091947.92 2.34082753 1091948.16 2.35464449 1091948.40 2.373904892631 3  128624
```

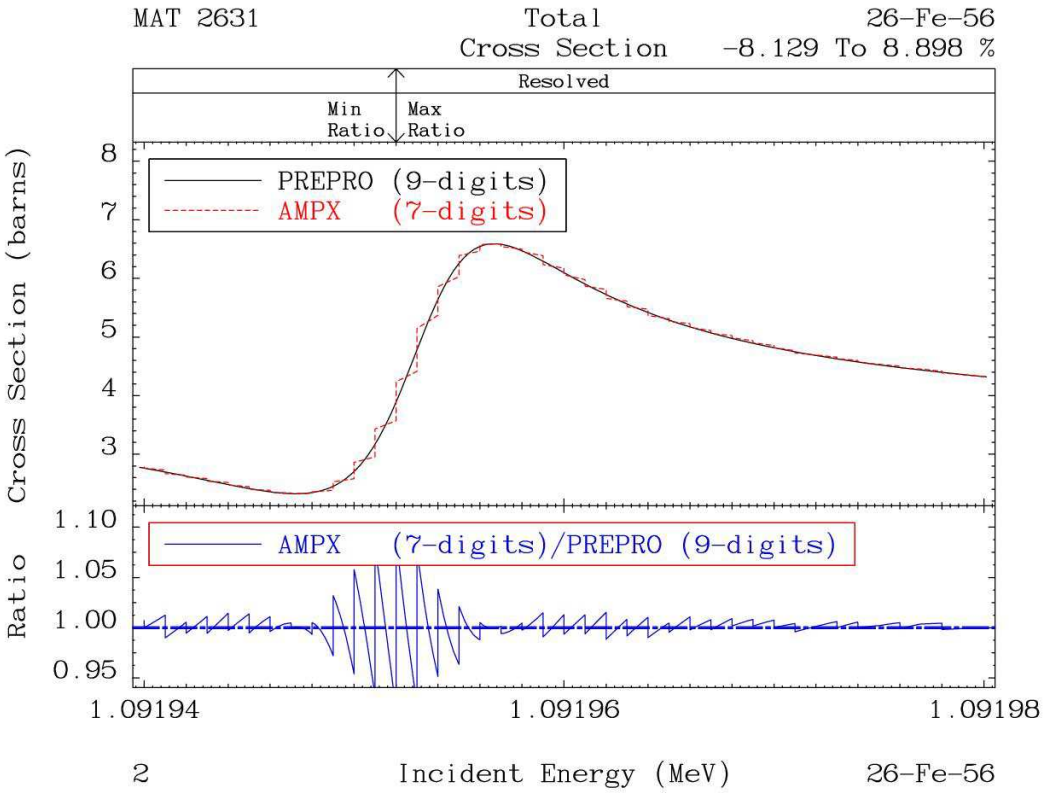


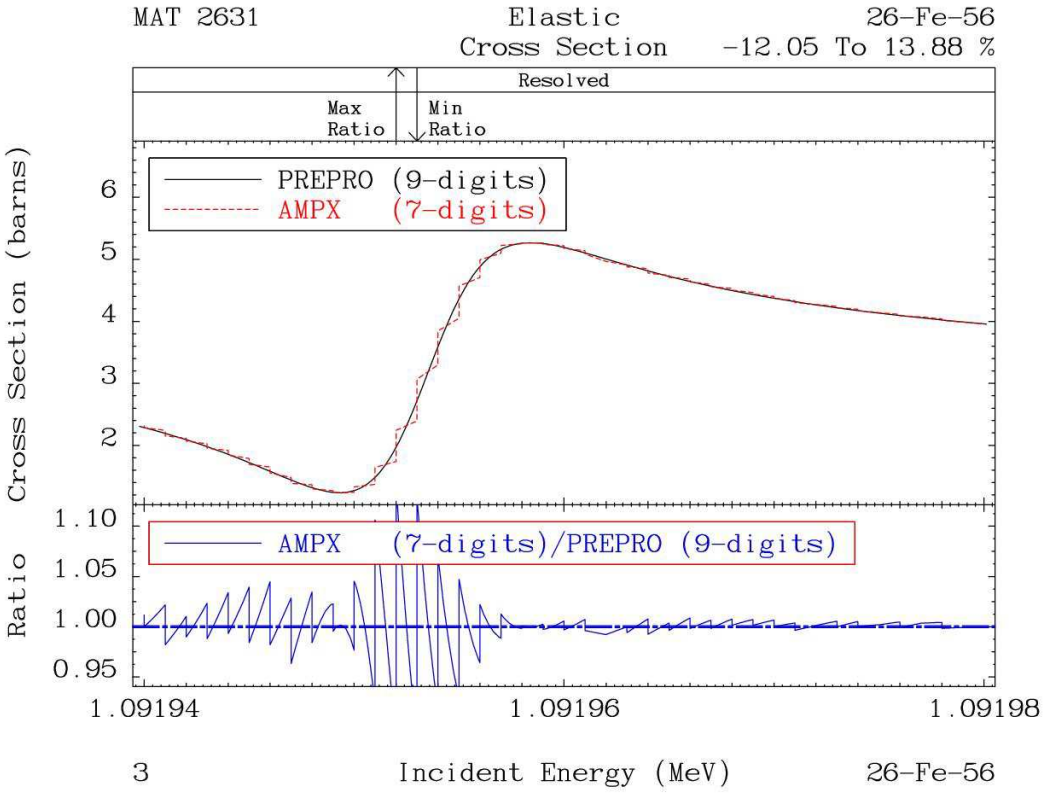
Comparison Figures for Energy Precision

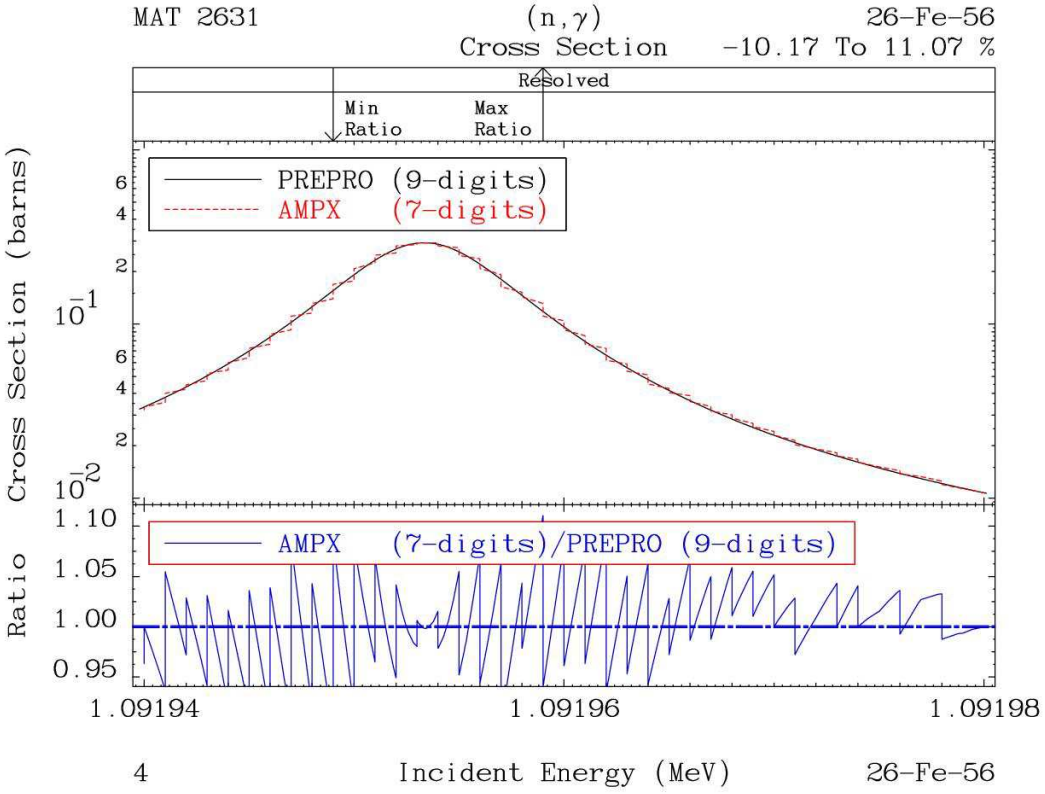
In the firm belief that one picture is worth a thousand words, the remainder of this section of this report presents results for ALL codes: first when this comparison started (7 digit) and then by the end of our comparisons (9 digit), for AMPX [2], NJOY [3], and SAMRML [5]. I believe that these figures speak for themselves and do not require any explanatory text. **PLEASE do not overlook the following section, showing similar results for 7 and 9 digit cross sections.**

AMPX: 7 digit energies

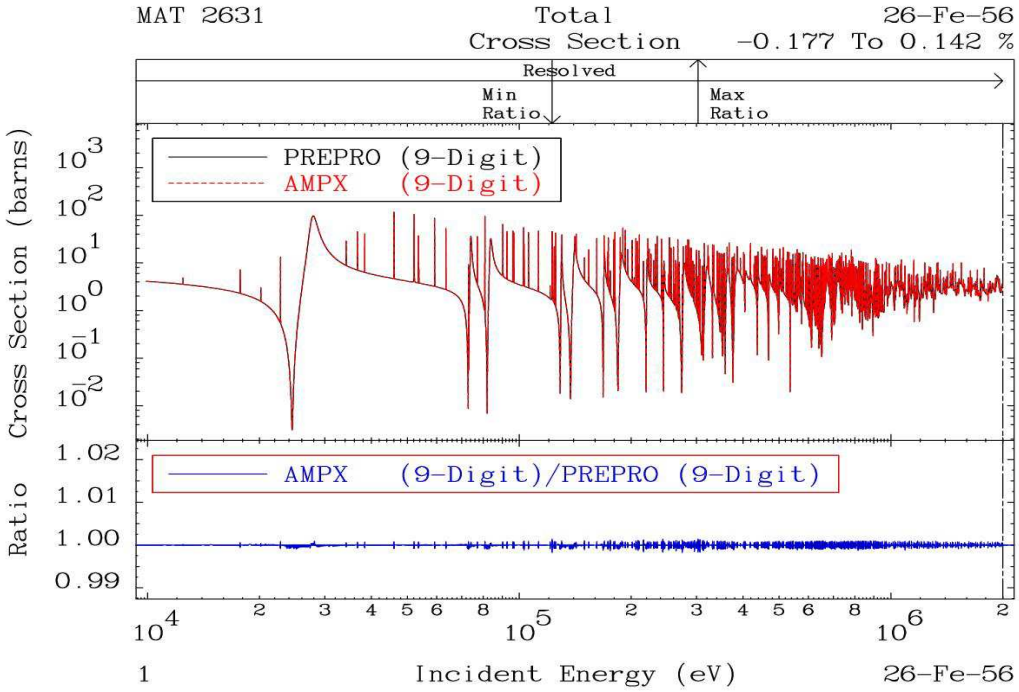


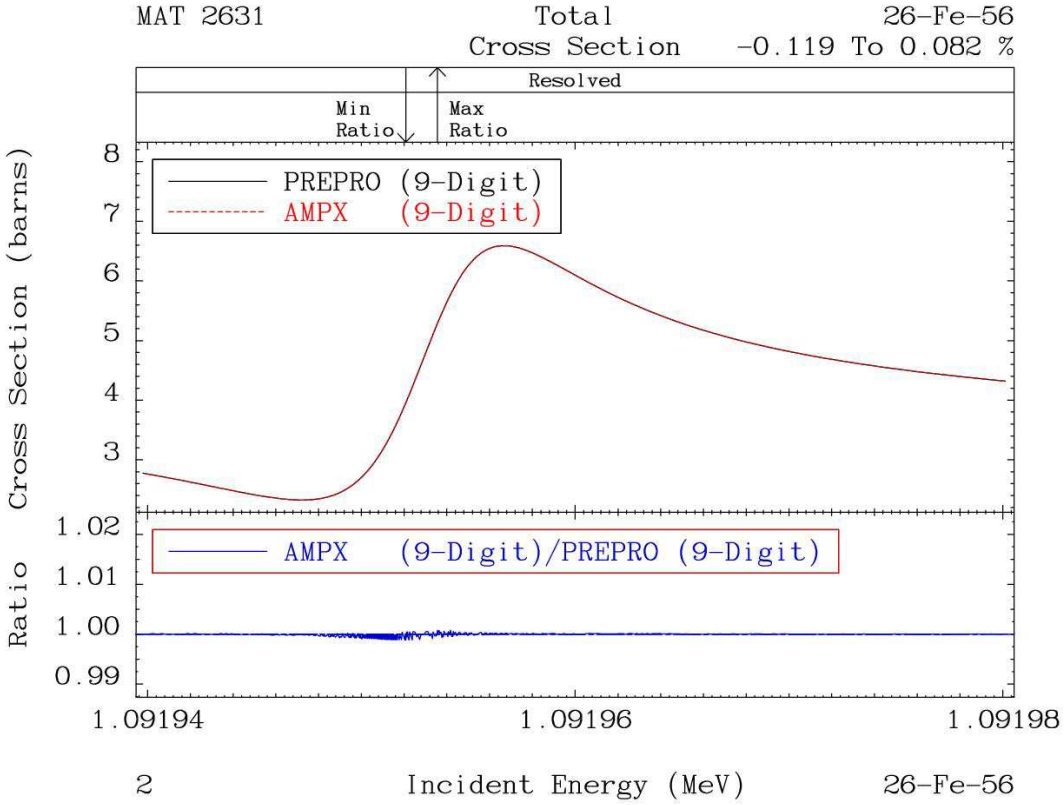


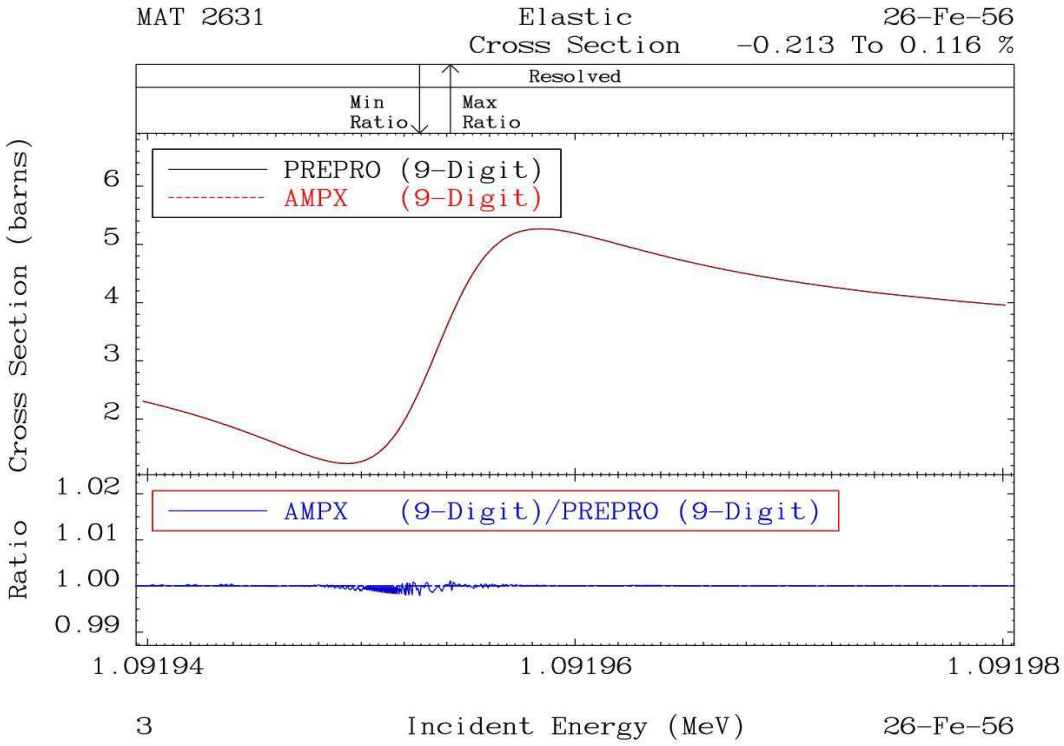

MAT 2631
Elastic
Cross Section
26-Fe-56
-12.05 To 13.88 %
Resolved
Max Ratio
Min Ratio
PREPRO (9-digits)
AMPX (7-digits)
AMPX (7-digits)/PREPRO (9-digits)
Cross Section (barns)
Ratio
1.09194
1.09196
1.09198
3
Incident Energy (MeV)
26-Fe-56

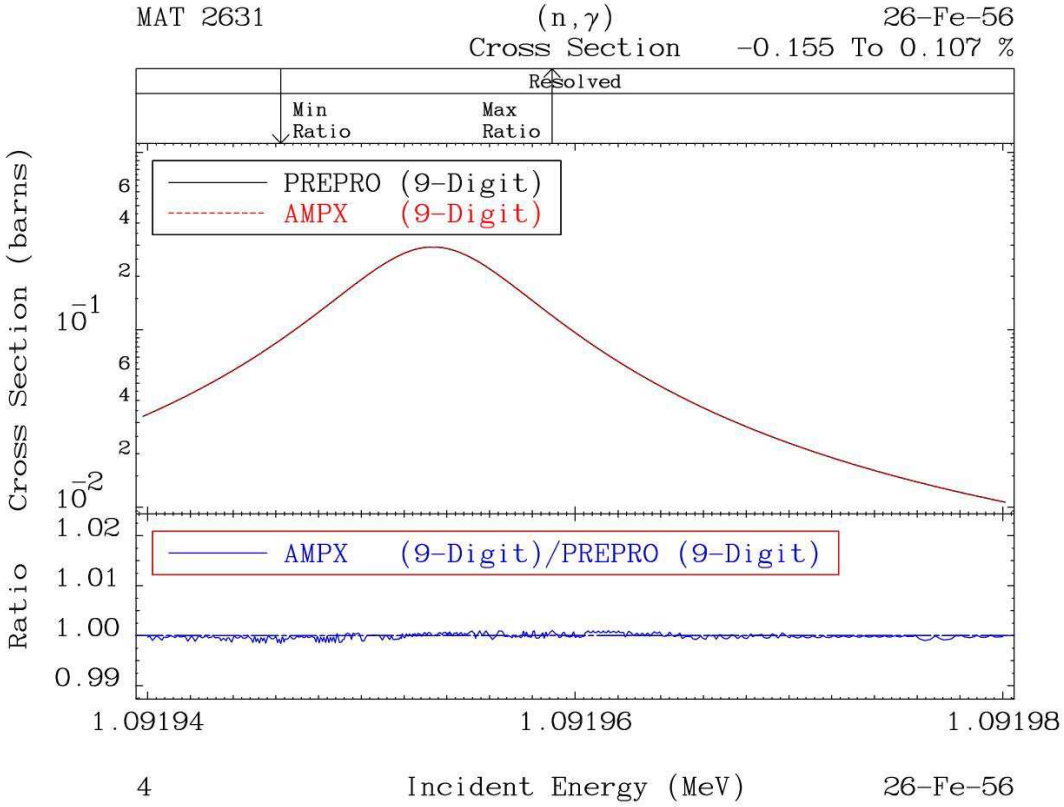

MAT 2631
(n,γ)
Cross Section
26-Fe-56
-10.17 To 11.07 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-digits)
AMPX (7-digits)
AMPX (7-digits)/PREPRO (9-digits)
Cross Section (barns)
Ratio
1.09194
1.09196
1.09198
4
Incident Energy (MeV)
26-Fe-56

AMPX: 9 digit energies

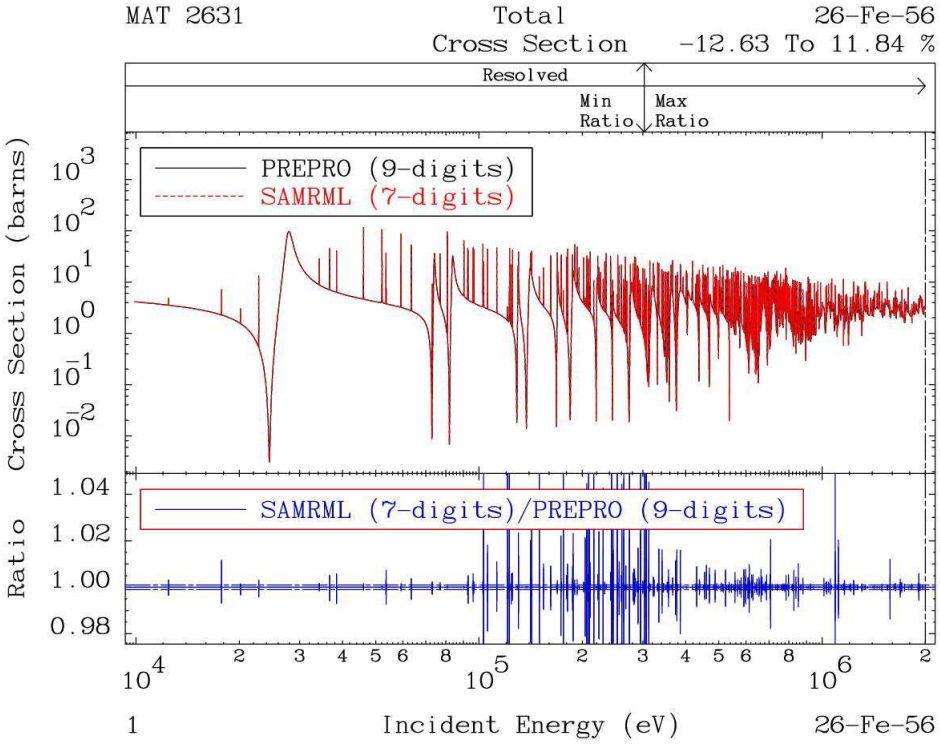


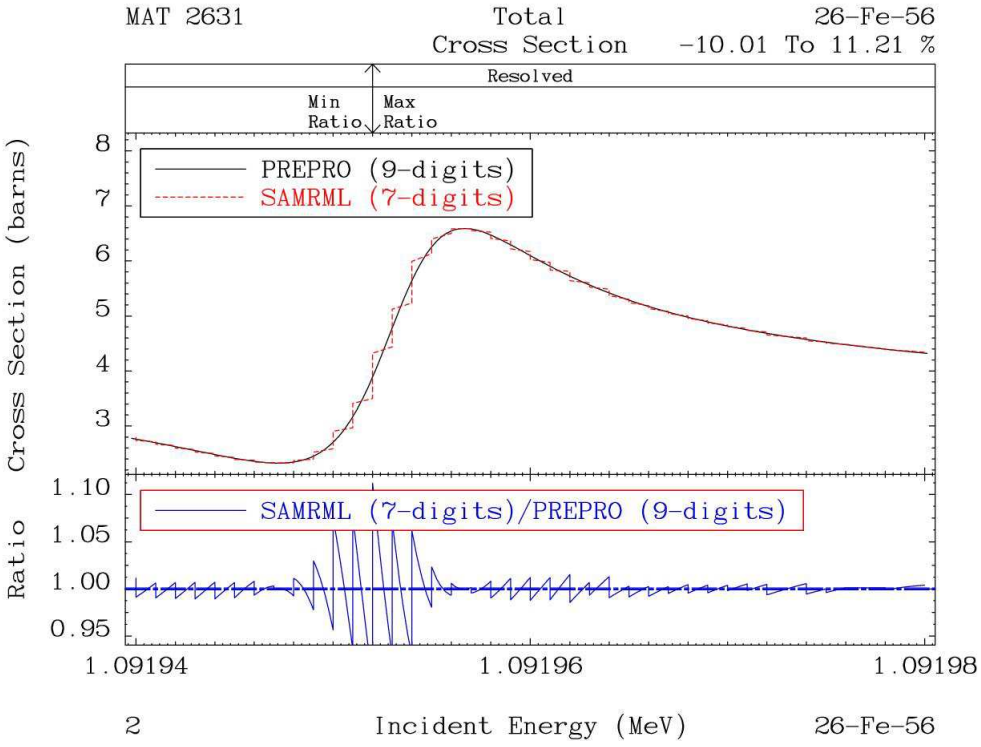


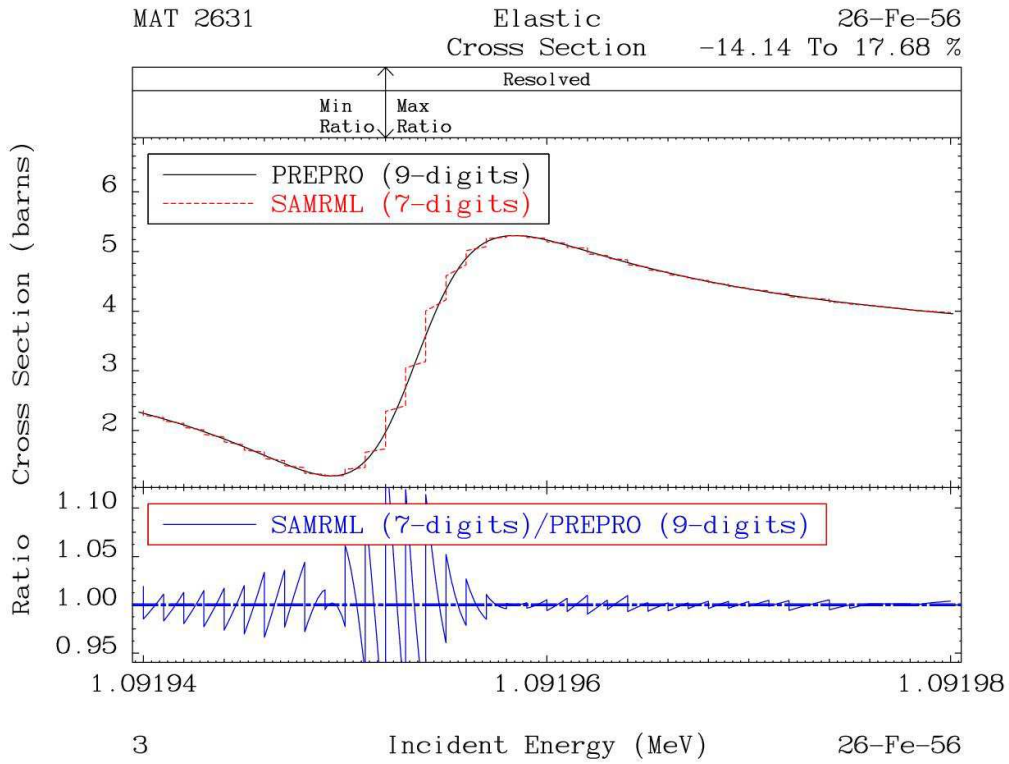

MAT 2631
Elastic
Cross Section
26-Fe-56
-0.213 To 0.116 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-Digit)
AMPX (9-Digit)
Cross Section (barns)
6
5
4
3
2
AMPX (9-Digit)/PREPRO (9-Digit)
Ratio
1.02
1.01
1.00
0.99
1.09194
1.09196
1.09198
3
Incident Energy (MeV)
26-Fe-56

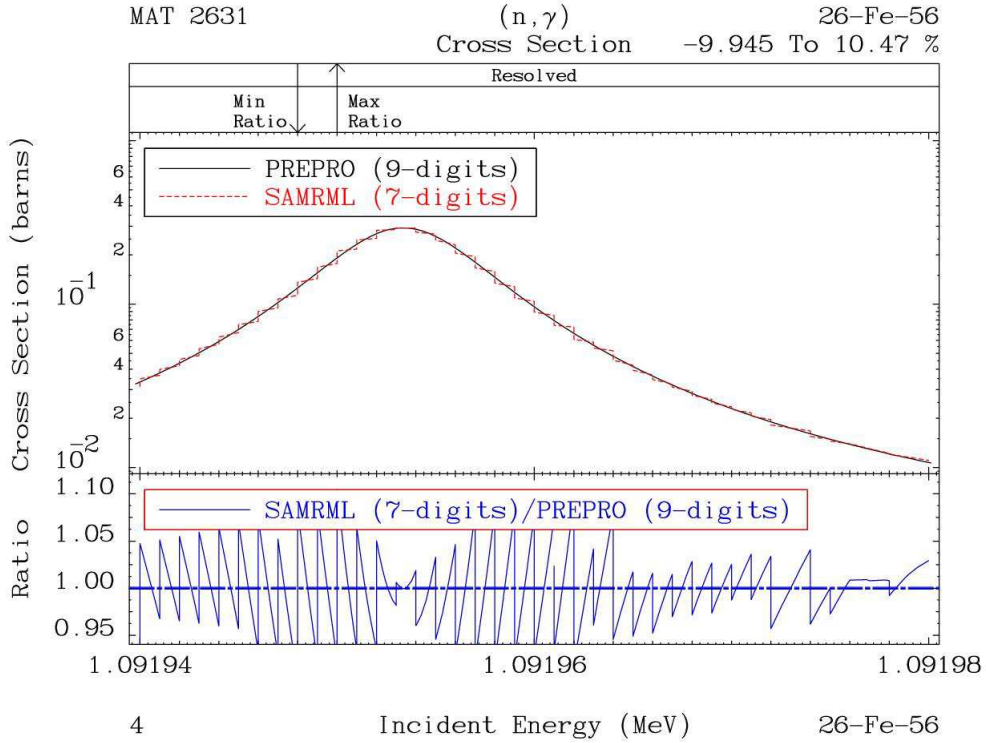

MAT 2631
(n,γ)
Cross Section
26-Fe-56
-0.155 To 0.107 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-Digit)
AMPX (9-Digit)
Cross Section (barns)
6
4
2
10-1
6
4
2
10-2
AMPX (9-Digit)/PREPRO (9-Digit)
Ratio
1.02
1.01
1.00
0.99
1.09194
1.09196
1.09198
4
Incident Energy (MeV)
26-Fe-56

SAMRML: 7 digit energies

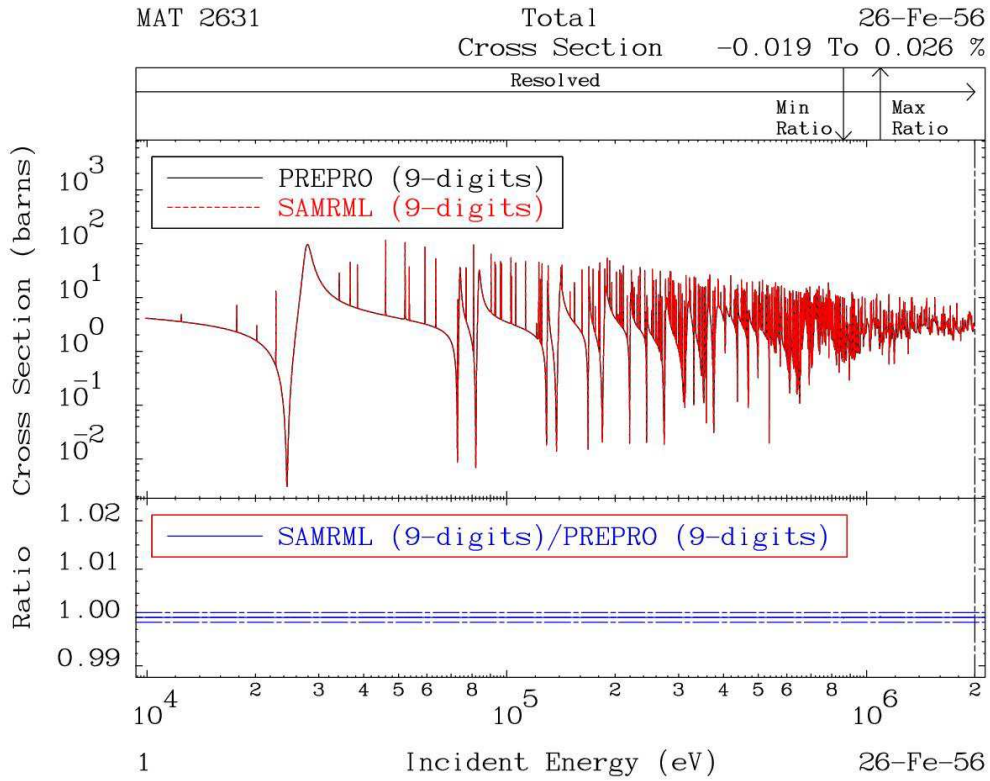


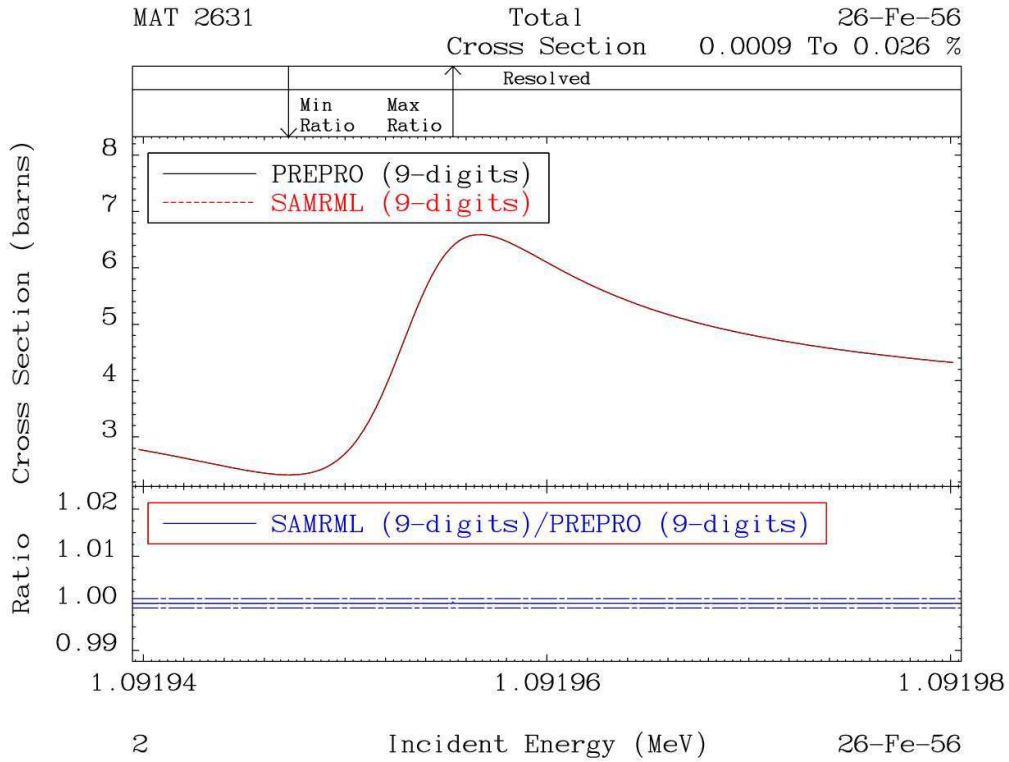


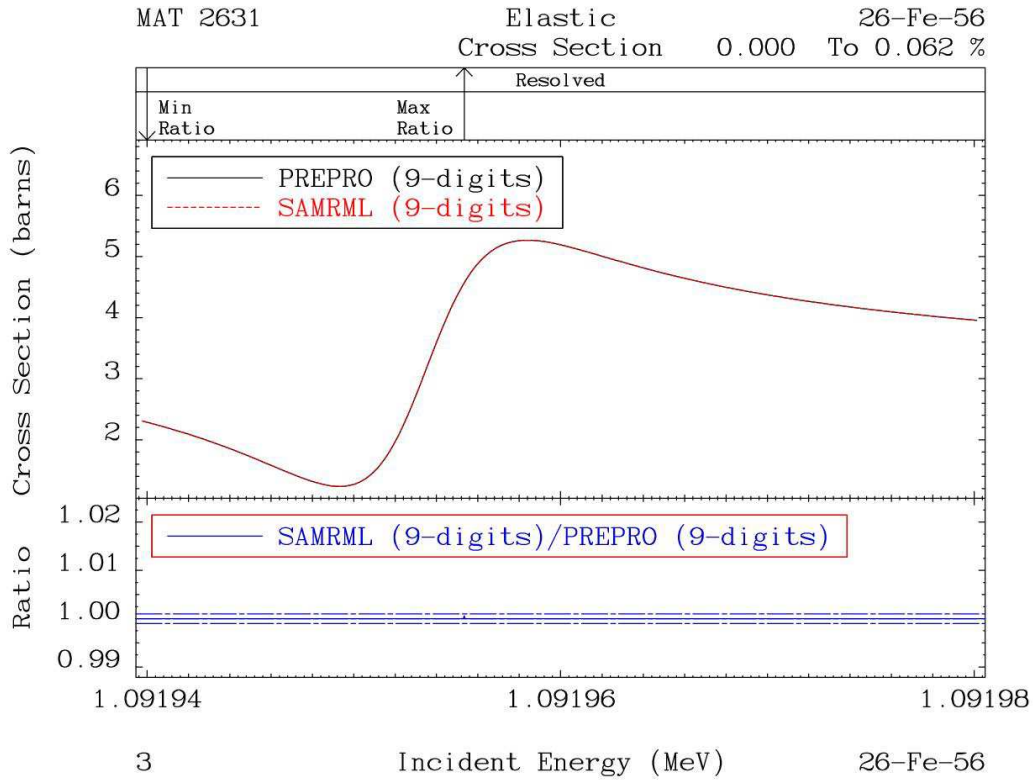

MAT 2631
Elastic
Cross Section
26-Fe-56
-14.14 To 17.68 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-digits)
SAMRML (7-digits)
SAMRML (7-digits)/PREPRO (9-digits)
Cross Section (barns)
Ratio
1.09194
1.09196
1.09198
3
Incident Energy (MeV)
26-Fe-56

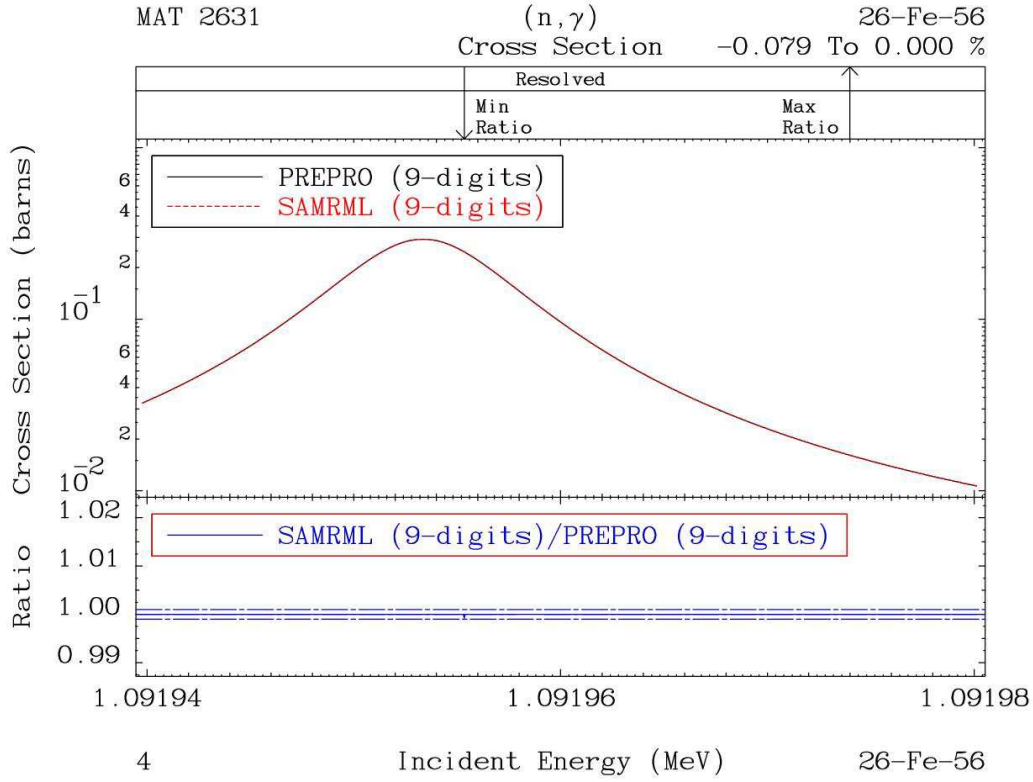

MAT 2631
(n,γ)
Cross Section
26-Fe-56
-9.945 To 10.47 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-digits)
SAMRML (7-digits)
SAMRML (7-digits)/PREPRO (9-digits)
Cross Section (barns)
Ratio
1.09194
1.09196
1.09198
4
Incident Energy (MeV)
26-Fe-56

SAMRML: 9 digit energies

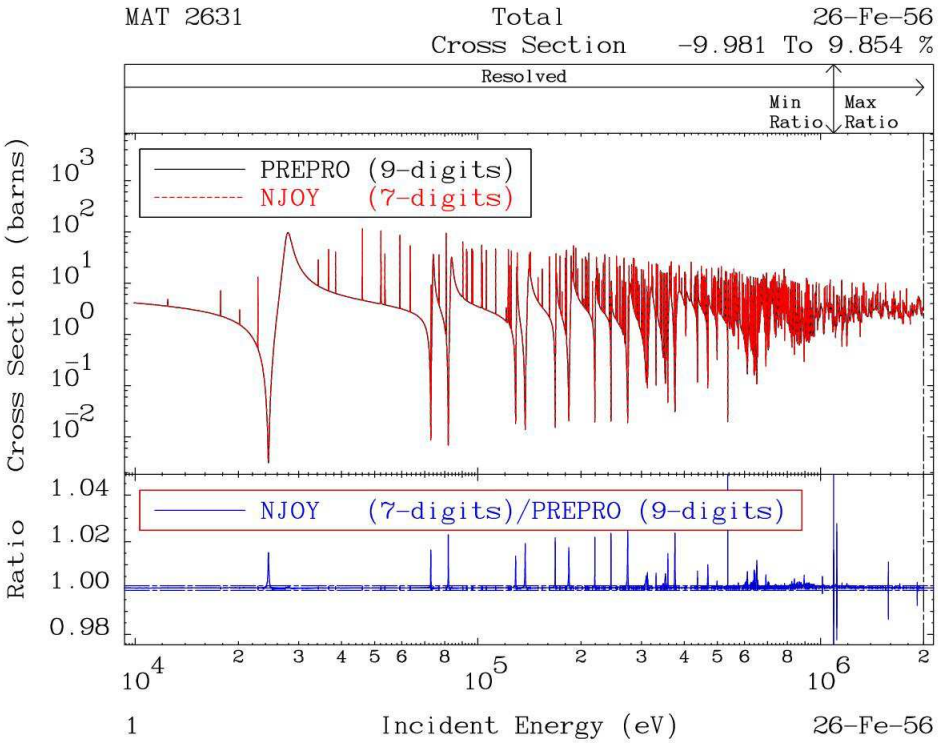


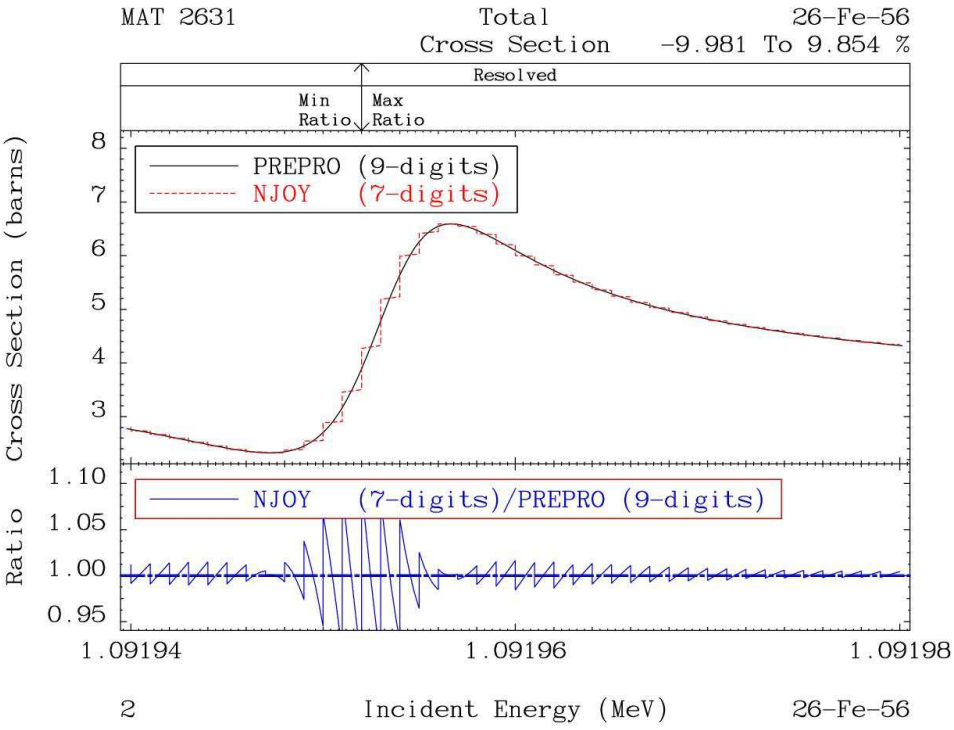


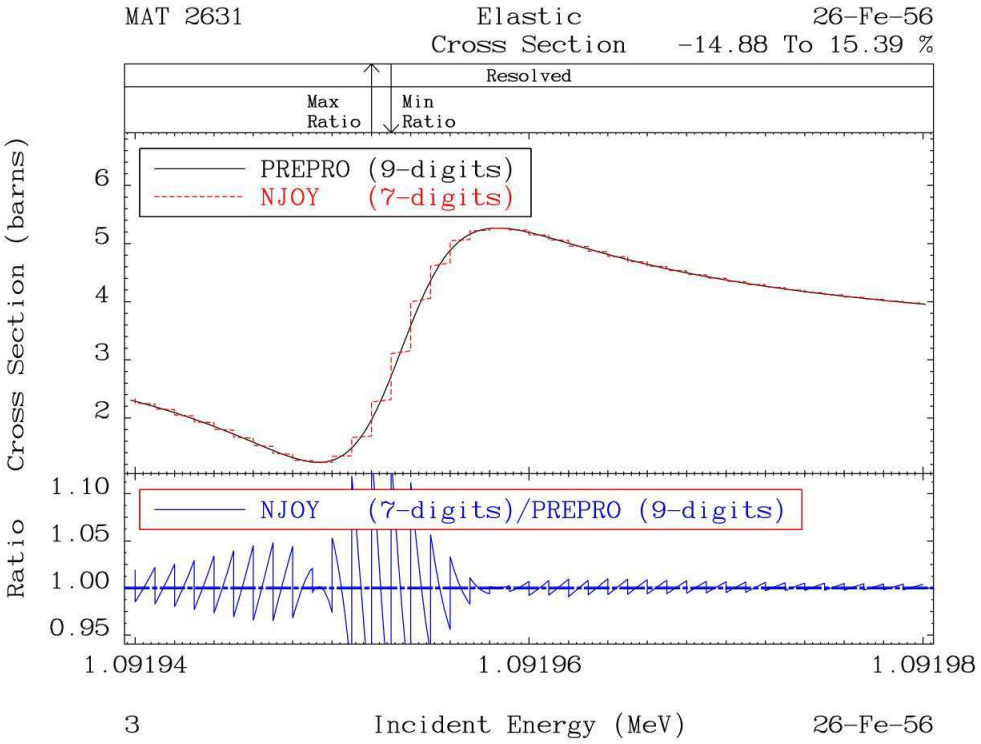

MAT 2631
Elastic
Cross Section
26-Fe-56
0.000 To 0.062 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-digits)
SAMRML (9-digits)
SAMRML (9-digits)/PREPRO (9-digits)
Ratio Cross Section (barns)
1.09194
1.09196
1.09198
3
Incident Energy (MeV)
26-Fe-56

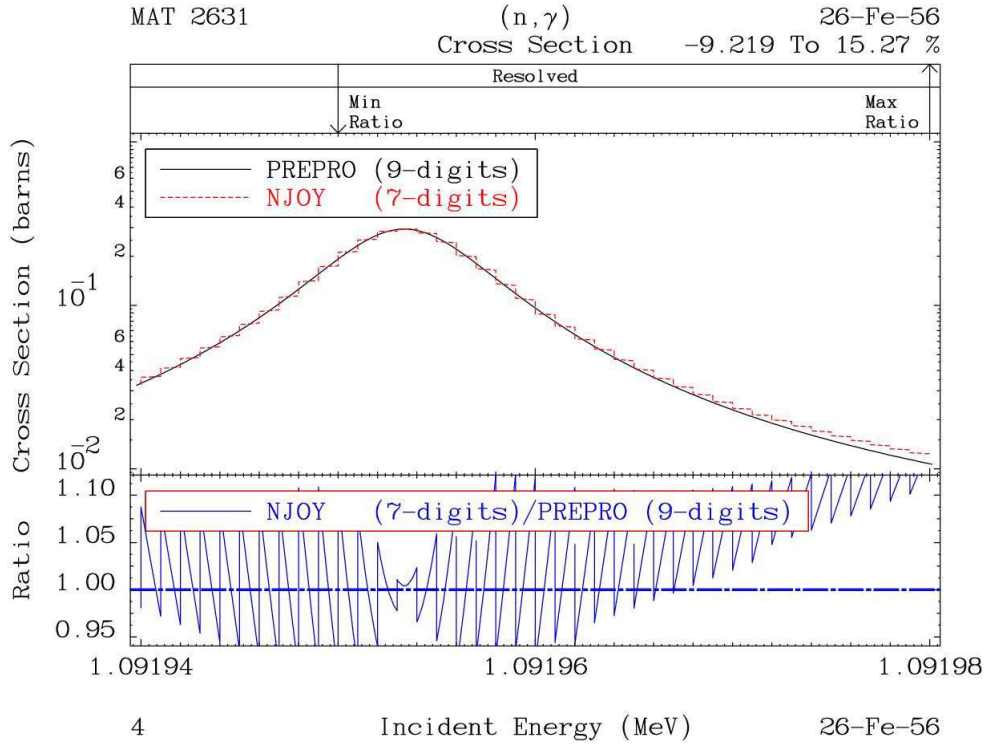

MAT 2631
(n,γ)
Cross Section
26-Fe-56
-0.079 To 0.000 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-digits)
SAMRML (9-digits)
SAMRML (9-digits)/PREPRO (9-digits)
Ratio Cross Section (barns)
1.09194
1.09196
1.09198
4
Incident Energy (MeV)
26-Fe-56

NJOY: 7 digit energies

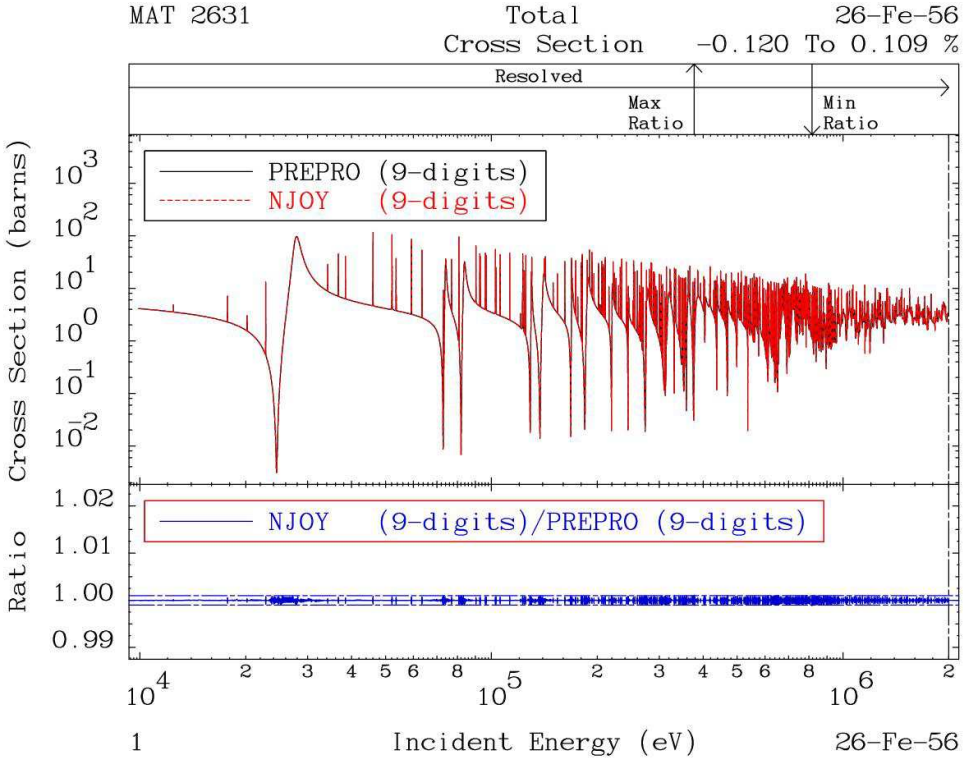


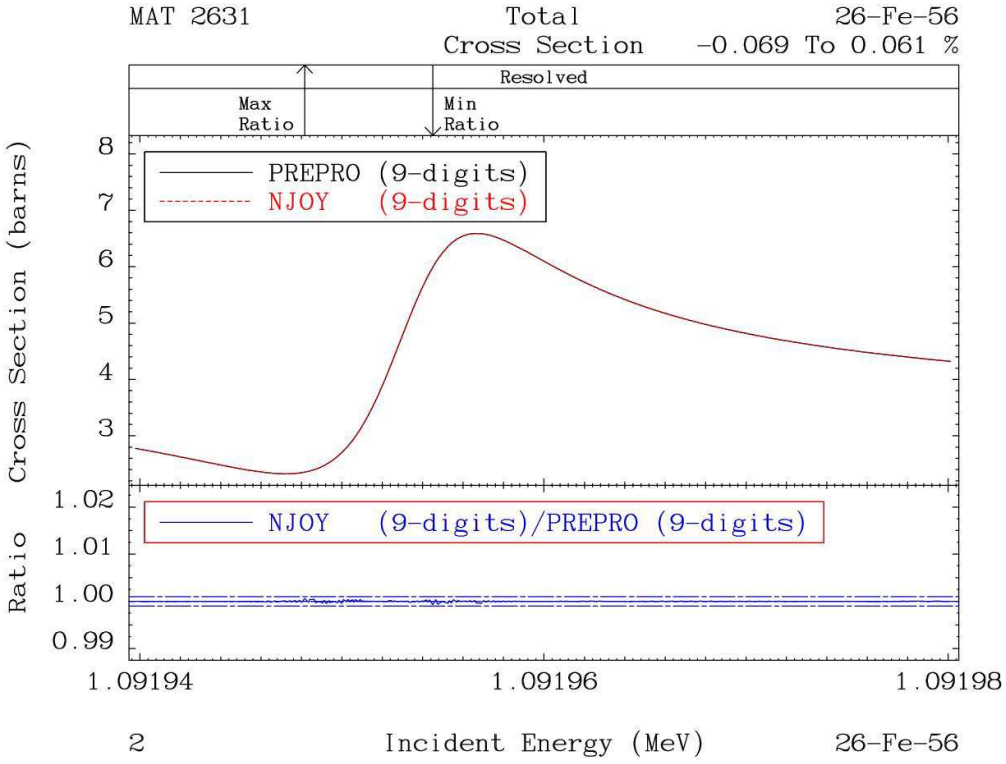


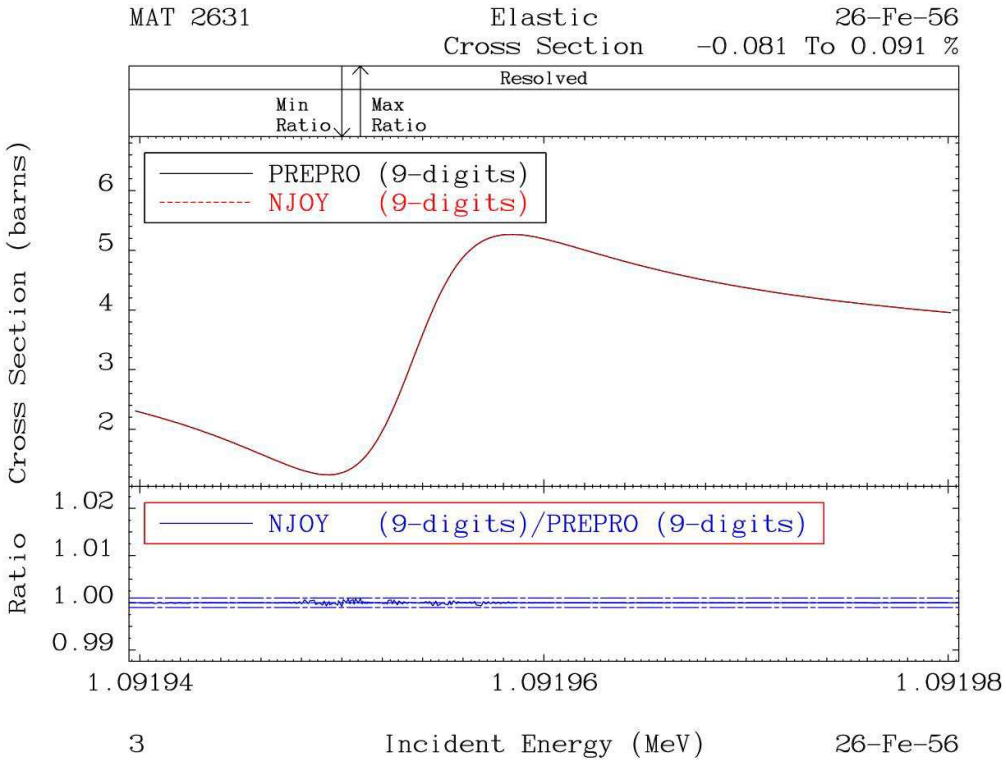

MAT 2631
Elastic
Cross Section
26-Fe-56
-14.88 To 15.39 %
Resolved
Max Ratio
Min Ratio
PREPRO (9-digits)
NJOY (7-digits)
Cross Section (barns)
6
5
4
3
2
NJOY (7-digits)/PREPRO (9-digits)
Ratio
1.10
1.05
1.00
0.95
1.09194
1.09196
1.09198
3
Incident Energy (MeV)
26-Fe-56

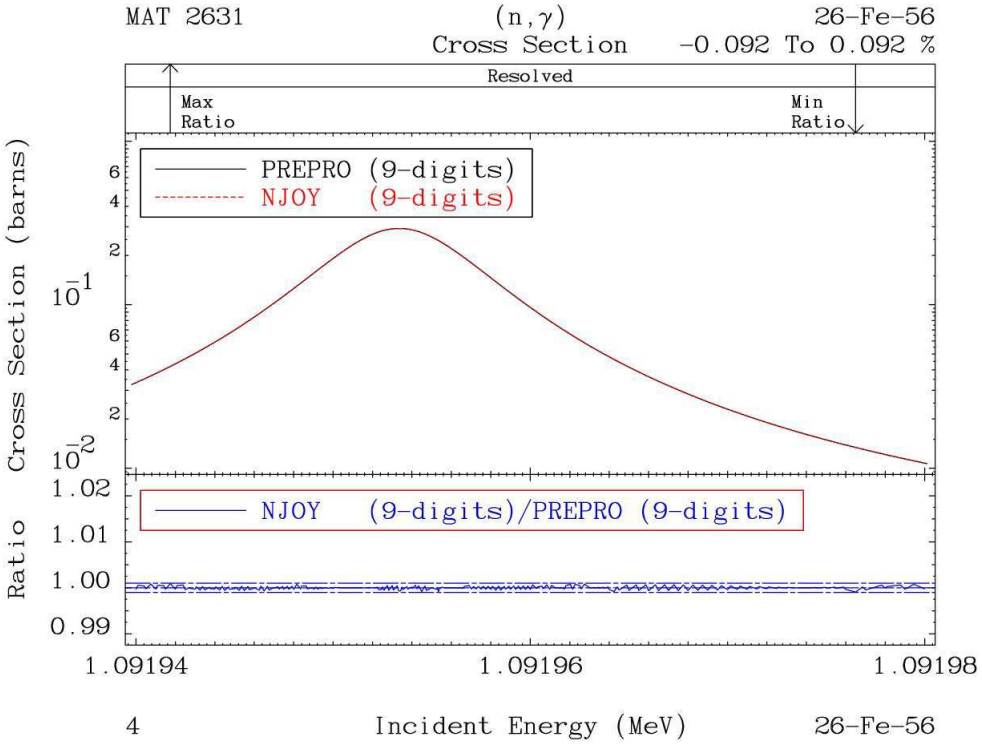

MAT 2631
(n,γ)
Cross Section
26-Fe-56
-9.219 To 15.27 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-digits)
NJOY (7-digits)
Cross Section (barns)
6
4
2
10^-1
6
4
2
10^-2
NJOY (7-digits)/PREPRO (9-digits)
Ratio
1.10
1.05
1.00
0.95
1.09194
1.09196
1.09198
4
Incident Energy (MeV)
26-Fe-56

NJOY: 9 digit energies






MAT 2631
Elastic
Cross Section
26-Fe-56
-0.081 To 0.091 %
Resolved
Min Ratio
Max Ratio
PREPRO (9-digits)
NJOY (9-digits)
NJOY (9-digits)/PREPRO (9-digits)
Cross Section (barns)
Ratio
1.09194
1.09196
1.09198
Incident Energy (MeV)
3
26-Fe-56


MAT 2631
(n,γ)
Cross Section
26-Fe-56
-0.092 To 0.092 %
Resolved
Max Ratio
Min Ratio
PREPRO (9-digits)
NJOY (9-digits)
NJOY (9-digits)/PREPRO (9-digits)
Cross Section (barns)
Ratio
1.09194
1.09196
1.09198
Incident Energy (MeV)
4
26-Fe-56

Cross Sections: 9 digits versus 7 digits

Since our objective is to reproduce the cross sections to within 0.1%, one might assume we only need to know any cross sections to an accuracy of 3 or 4 digits. However, this does not allow for the fact that cross sections are often defined by sums or differences. For example, we may define our total as the sum of its parts; in the simplest case without fission and below the inelastic threshold we have:

Total = Elastic + Capture

You might then assume that obviously this means: Capture = Total - Elastic

But use caution. The General Reich-Moore (LRF=7) ENDF treatment does not directly define the capture cross section; it is defined by subtracting. Similarly in Monte Carlo calculations codes often select a reaction by subtracting cross sections, e.g., is it elastic? If not, subtract the elastic and try the next reaction.

As a result in a perfect world we could assume: Capture = Total - Elastic

But in the real world where cross sections can vary over many orders of magnitude and we must deal with the finite accuracy of computers, this seemingly simple relationship is difficult to actually achieve within our target accuracy of 0.1%.

At 521082.982 eV

	9-digits	7-digits
Total	2.53264165	2.532642
Elastic	2.53259305	2.532593
Capture	0.0000485970	0.0000485970
Capture = Total - Capture	0.00004860	0.000049
Difference	-0.0000000030	-0.0000004030
Per-Cent	-0.006%	-0.829%

To illustrate the problem we need only consider one energy point in Fe-56 where the Total and Elastic agree to almost 5 digits (see, the above table). This means if we try to define the Capture as the difference, with cross sections truncated to 9 digits we only have about 4 digits remaining to define the Capture. And with 7 digit accuracy we only have about 2 digits remaining. In this situation we can easily see (see the above table) that we can still achieve our 0.1% target with 9 digit cross sections, but **not** with 7 digit cross sections. In the above table we can see that 9 digit cross section truncation results in 0.006% error (well within our 0.1% target), whereas 7 digits result in 0.829%, or roughly 100 times larger than the 9 digit results, which is exactly what we would expect when we lose 2 digits (9 versus 7). The following pages show results using cross sections truncated to 7 and 9 digits; these results include:

1) PREPRO 7 digit – there are no such results, because PREPRO has been using 9 digit output for energy and cross section for many years, since circa 2000.

2) PREPRO 9 digit results that show first a comparison of the total and elastic, to illustrate that the two are equal over almost the entire energy range, except near some resonances where capture makes a significant contribution. Next, I compare the capture cross section tabulated in the evaluation to that defined as Total-Elastic. Here we see a maximum difference of about 0.01%, an order of magnitude below our target 0.1%.

3) AMPX 9 digit – since AMPX is using binary files its cross sections are not subject to output precision truncation, so we need not show them here. **This is an excellent example of why I consider AMPX to be the Gold Standard as far as precision.** "We need not", but for completeness I include AMPX 9 digit results, that show excellent agreement when AMPX results are output in the ENDF character format.

4) SAMRML 7 digit results showing differences up to about 1.4%, over the entire energy range. The second detailed figure shows the differences are where we would expect them to be; they are largest between resonances, but also affect the shape of the capture resonances. The resulting 1.4% difference is 14 times our target 0.1% accuracy.

5) SAMRML 9 digit results show results similar to the PREPRO 9 digit results, with maximum differences of about 0.01%, an order of magnitude below our target 0.1%.

6) NJOY 7 digit results are similar to the SAMRML 7 digit results, with differences up to about 1%, over the entire energy range. Again, the detail figure shows where these differences occur. The resulting 1% difference is 10 times our target 0.1% accuracy.

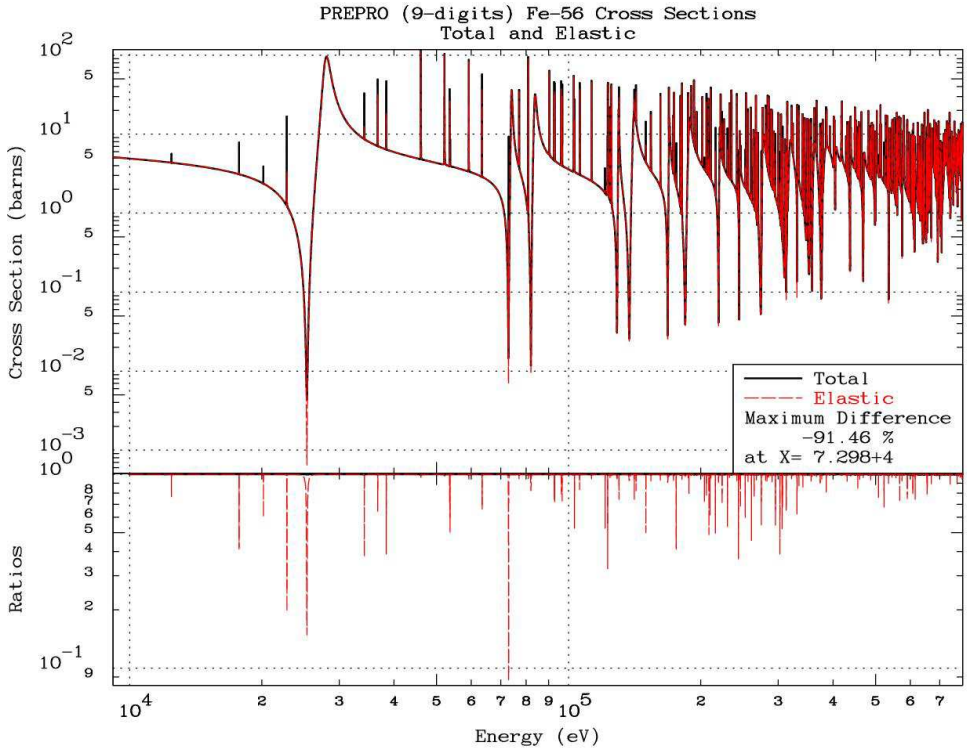
7) NJOY 9 digit results show results similar to the PREPRO 9 digit results, with maximum differences of less about 0.01%, an order of magnitude below our target 0.1%.

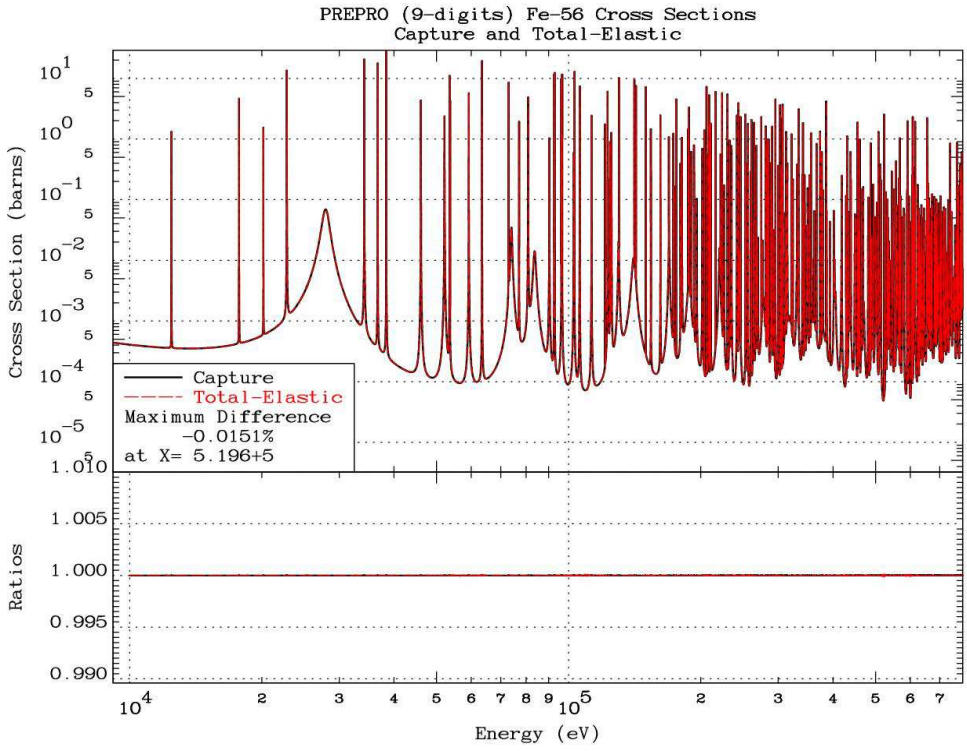
Let me stress that these differences are not due to any changes WITHIN these codes, but rather solely due to changes in their output to the ENDF format. **Indeed, the agreement between 9 digit results from ALL of the codes shows that INTERNALLY INSIDE COMPUTERS they are ALL producing very similar, accurate results**. But those that use 7 digit output have a design flaw, that once recognized can be easily corrected.

In summary, consider that Fe-56 was merely the first evaluation that I checked and discovered this problem with 7 digit truncation. There are 423 evaluations in ENDF/B-VII.1, and of these I doubt that Fe-56 is the worst example of the problem with not representing cross sections to as high a precision as possible. When using 7 digit cross sections the roughly 1% error that we found here should be considered merely 'the tip of the iceberg'; there are bound to be many more cases where the error is much worse.

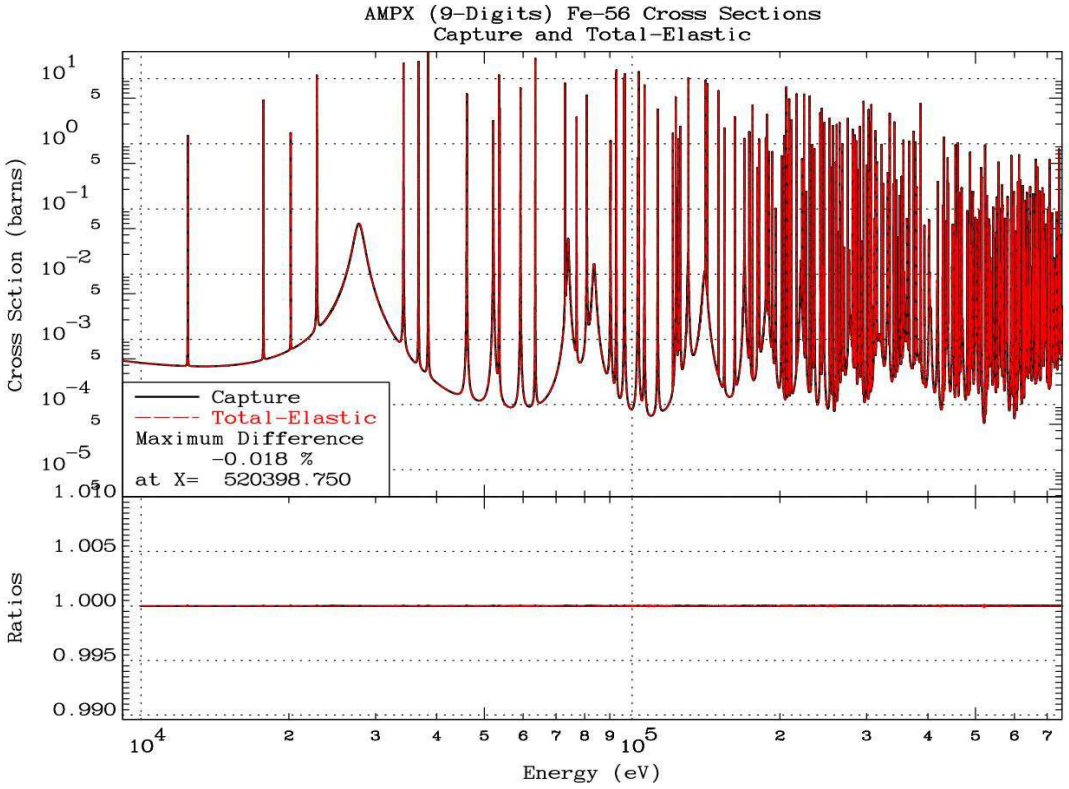
These results clearly show the importance of outputting results to the ENDF format as precisely as possible. What is most important to understand is that this uncertainty is not necessary; there is no disadvantage to not defining cross sections using 9 digit cross section output, but there ARE OBVIOUSLY DISADVANTAGES TO NOT USING 9 digit cross section output. The bottom line is: as far as 7 digit truncation CAVEAT EMPTOR: Let the user BEWARE.

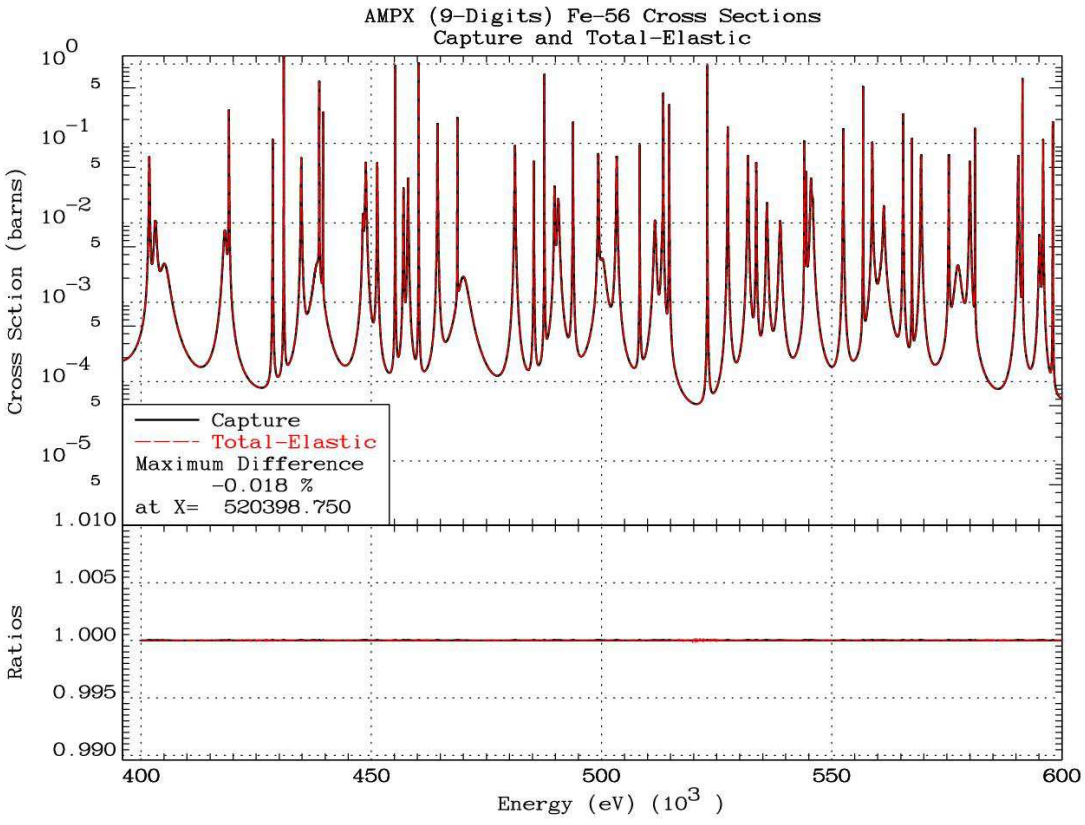
PREPRO 9 digit Cross Section



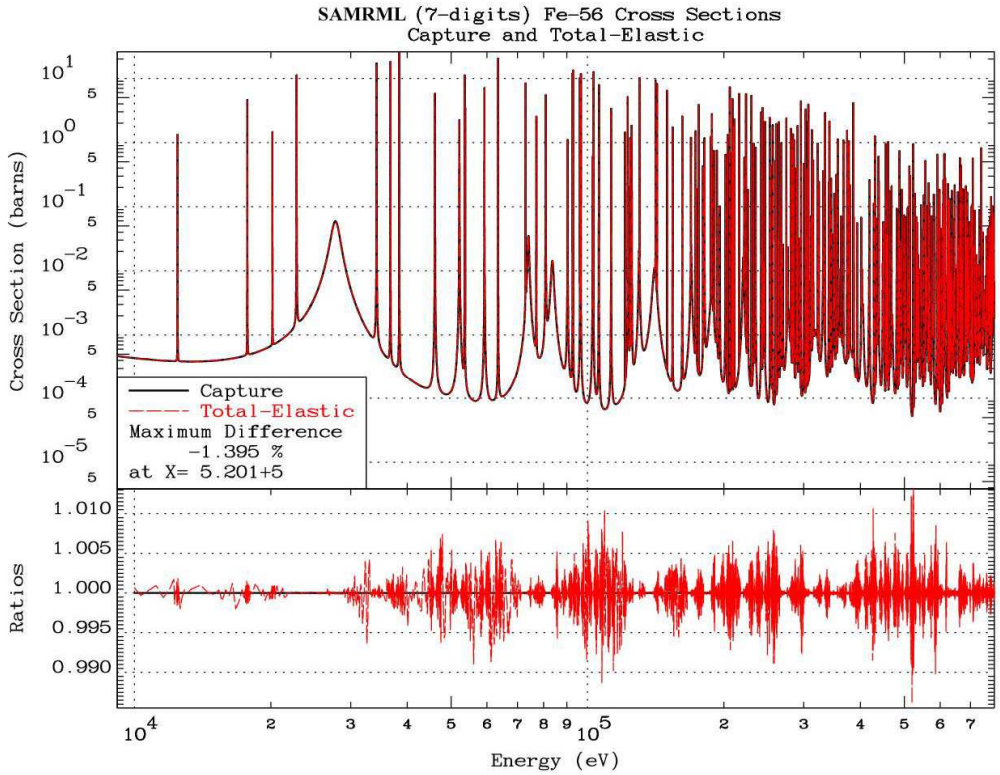


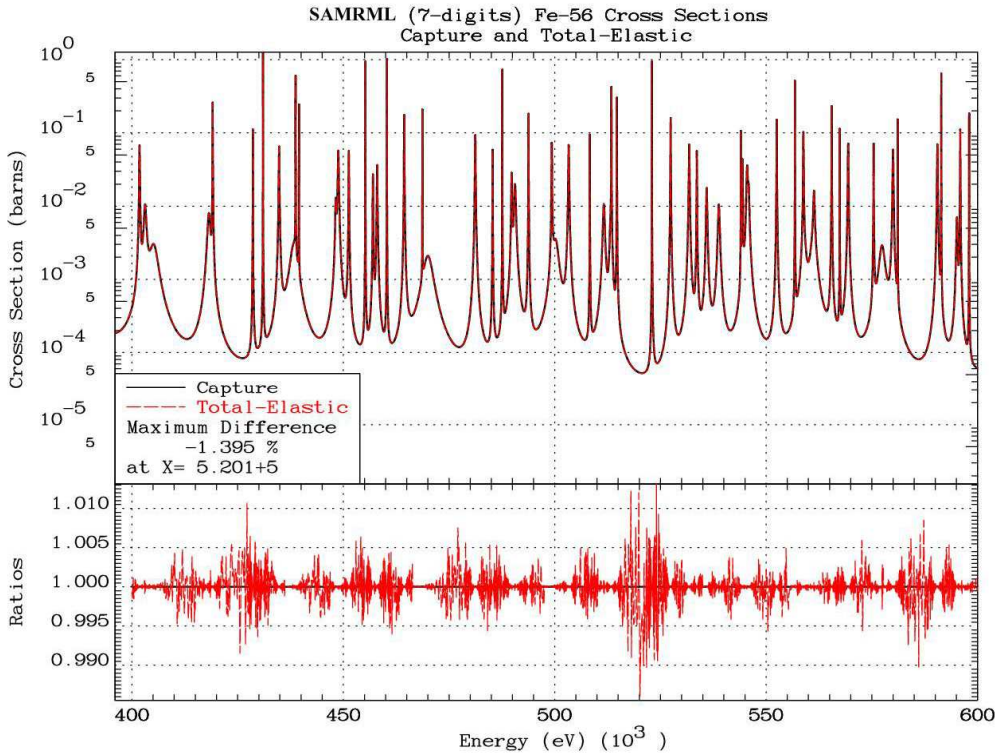
AMPX 9 digit Cross Sections



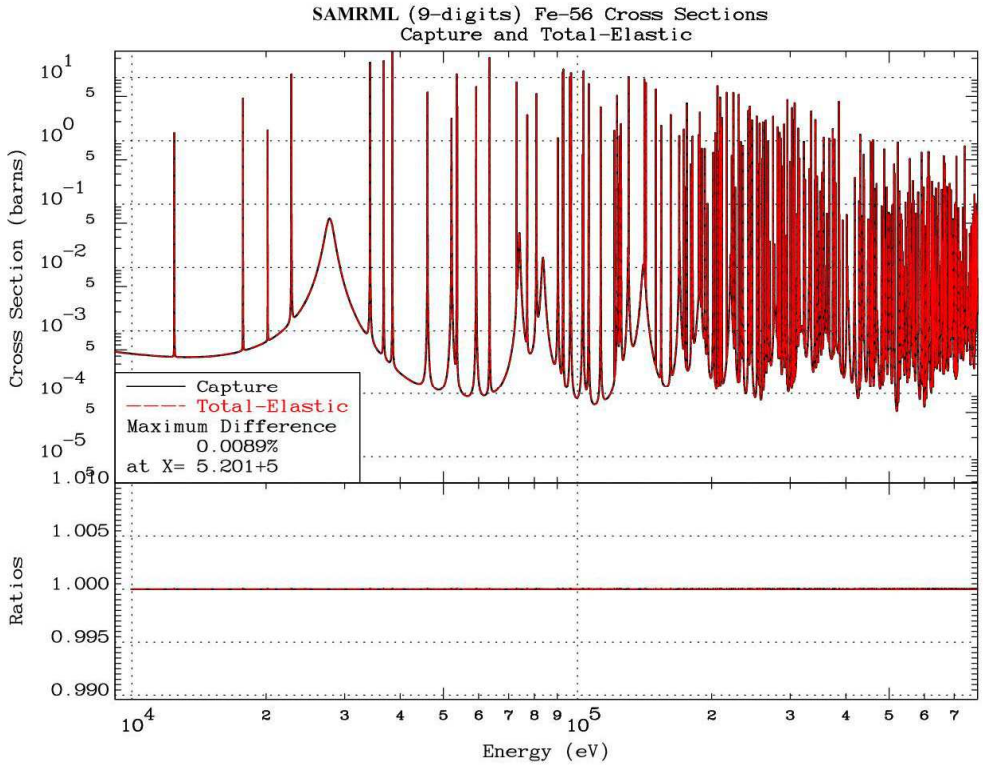


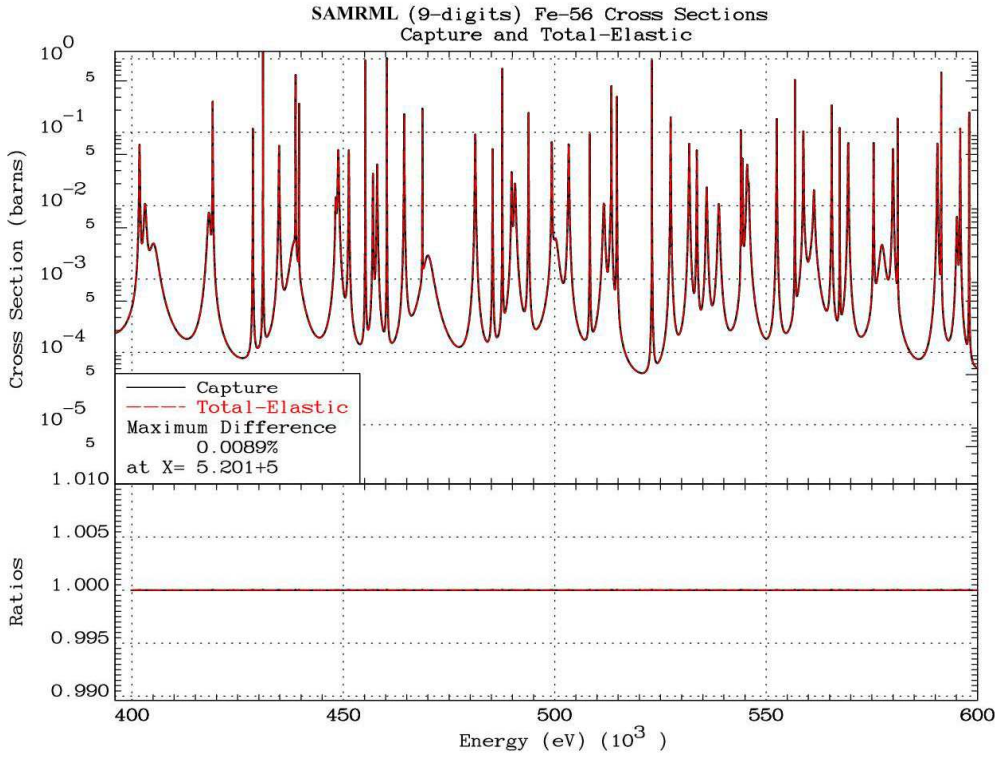
SAMRML 7 digit Cross Sections



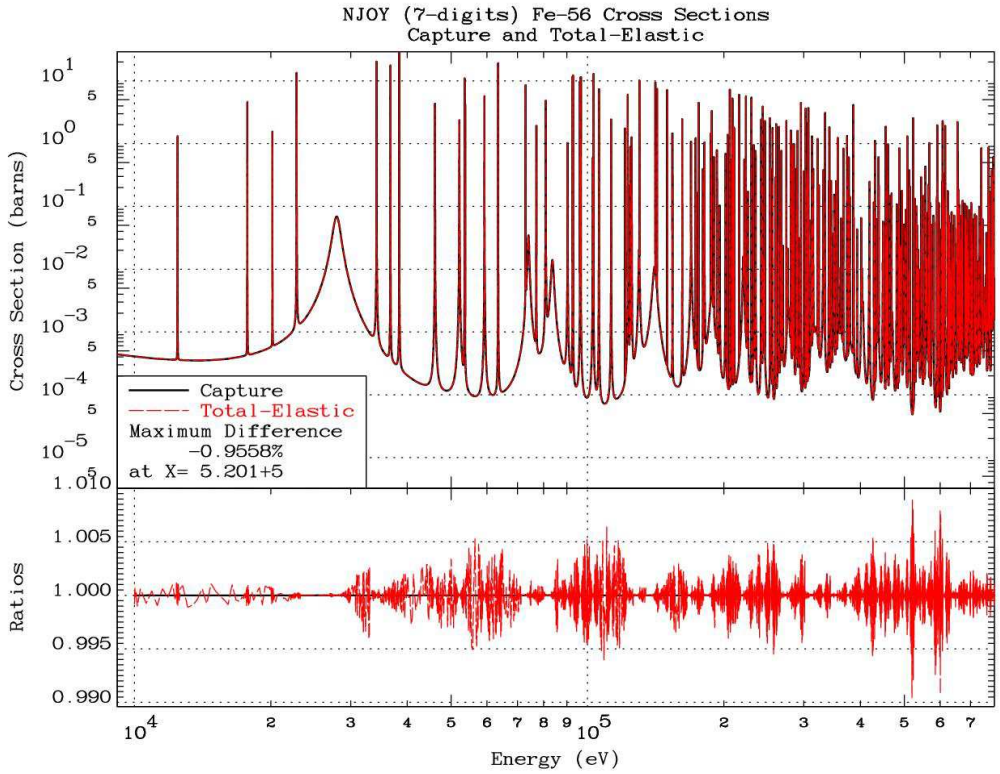


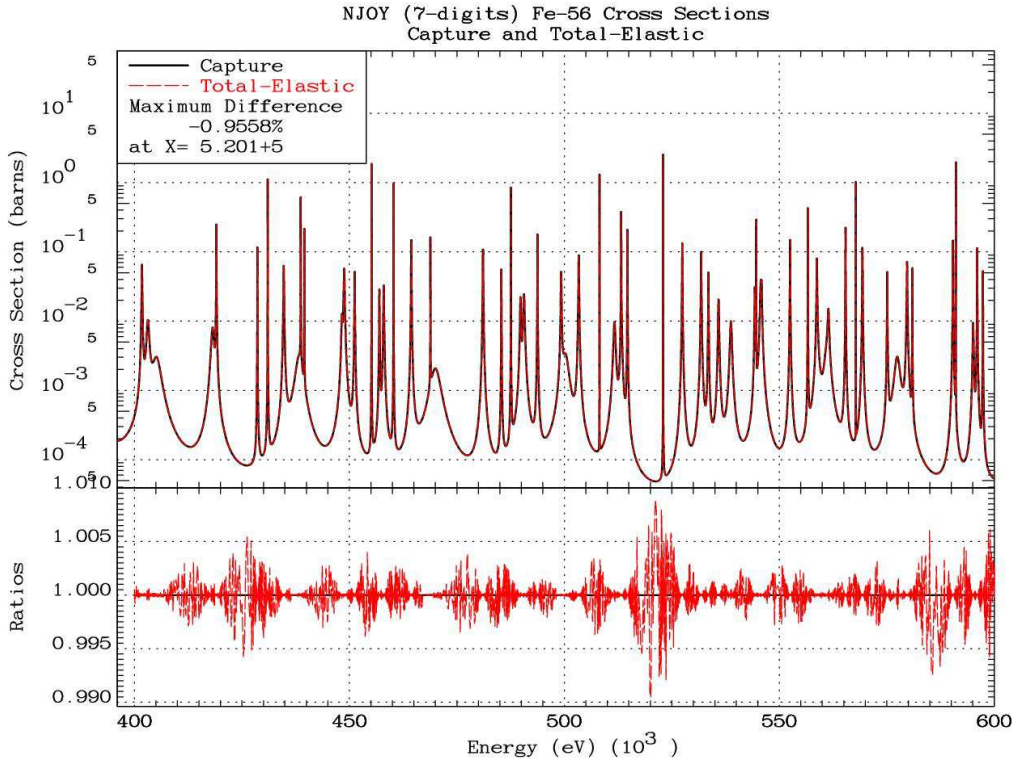
SAMRML 9 digit Cross Sections



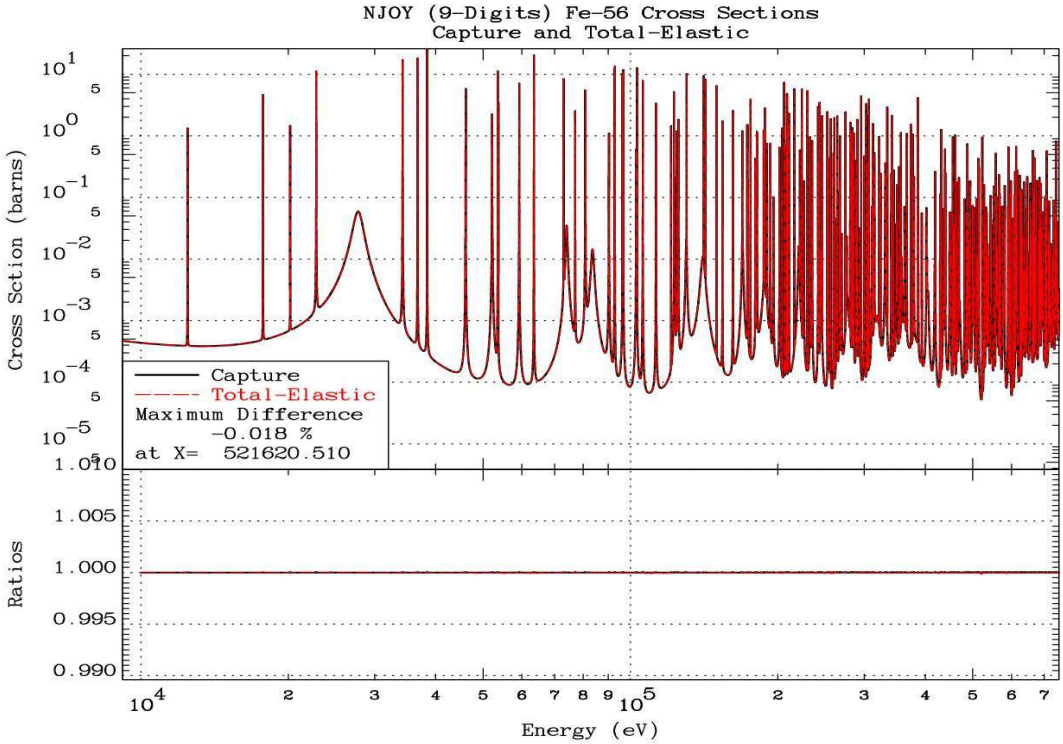


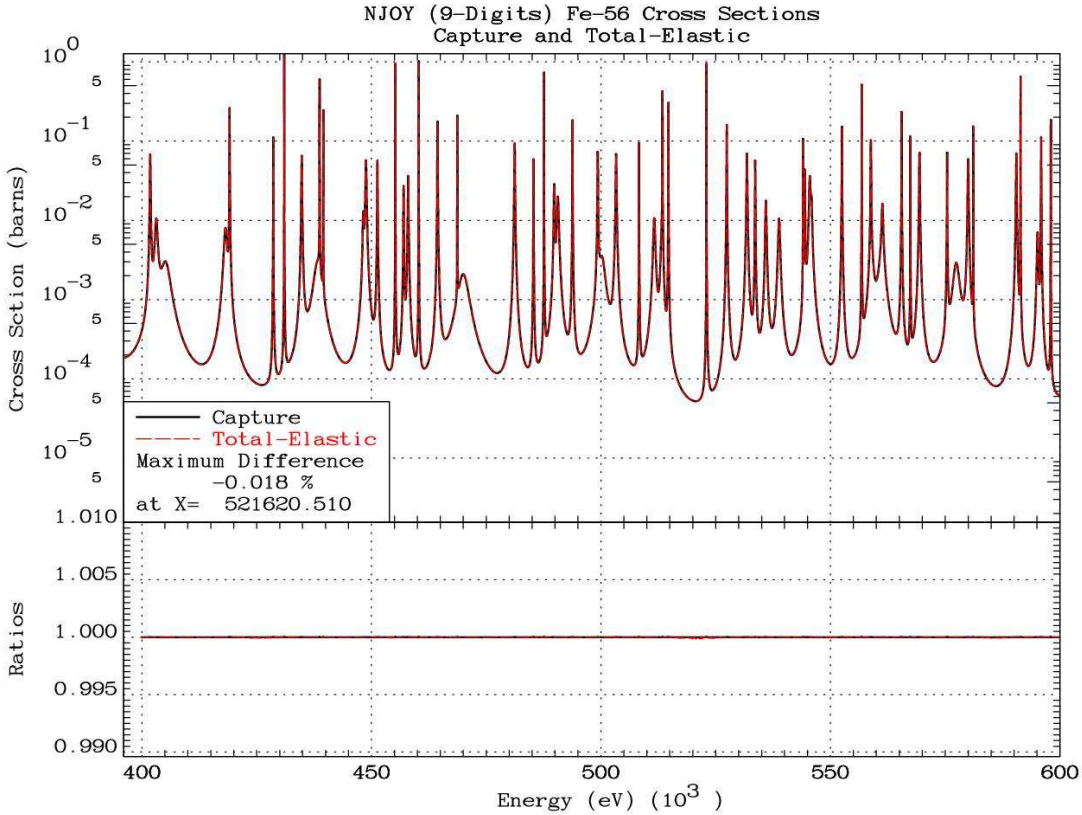
NJOY 7 digit Cross Sections





NJOY 9 digit Cross Sections





Conclusions

C**urrently our nuclear data processing codes are very accurate** in the calculations that they perform **INSIDE COMNPUTERS**. However, at the beginning of this study (2012), most of them dropped the ball in what should be a trivial final step to **output their results into the ENDF format** [1]. This is obviously a very important step, because without accurately outputting their results, we would not be able to confidently use their results in our applications. This is indeed a very important step, but unfortunately it is one that is not given the attention it deserves; hence we come to the purpose of this paper.

Here I documented first the state of a number of nuclear data processing codes as of February 2012, when this comparison began, and then the current state, November 2013, of the same codes; **I have delayed publishing results until now to give participants time to distribute updated codes and data.** The codes compared include, in alphabetical order: AMPX [2], NJOY [3], PREPRO [4], and SAMMY/SAMRML [5]. During this time we have seen considerable improvement in output results, but we still haven't reached the point that I hoped we would be at today, i.e., I hoped that by now not just the codes included in this study, but rather all codes would be using standard, high precision formats for ENDF data.

In the first part of this report I considered the precision of our tabulated energies; here we see obvious flaws when less-precise output is used. In the second part I considered the precision of our cross sections; here we see more subtle flaws. **The important point to stress is that once these flaws are recognized it is relatively easy to eliminate them, and produce high precision energies and cross sections.**

This Isn't Rocket Science

My last remark is to suggest that nuclear data users check the data they intend to use, to be sure it is in a standard, high precision format. This isn't rocket science. Just use any text editor to open the ENDF formatted file you intend to use and look at the data:

Example 7 digit energies and cross sections:

```
1.091943+6 2.537448+0 1.091943+6 2.528038+0 1.091944+6 2.519367+02631 3  186263
1.091944+6 2.509997+0 1.091944+6 2.501377+0 1.091944+6 2.492080+02631 3  186264
1.091944+6 2.483543+0 1.091944+6 2.474358+0 1.091944+6 2.465946+02631 3  186265
1.091944+6 2.456919+0 1.091945+6 2.448676+0 1.091945+6 2.439860+02631 3  186266
```

Example 9 digit energies and cross sections:

```
1091943.39 2.52599003 1091943.72 2.50220364 1091944.05 2.478677582631 3  128619
1091944.37 2.45628467 1091944.70 2.43384158 1091945.03 2.412325452631 3  128620
1091945.36 2.39206433 1091945.68 2.37399130 1091946.01 2.357444652631 3  128621
1091946.34 2.34359345 1091946.67 2.33313163 1091946.99 2.327008242631 3  128622
```

Hopefully, here you can immediately see the difference; **I recommend that you not use the lower precision, non-standard format data, e.g., high precision is expected/required as input into ENDL/TART [11] and ACER/MCNP [12].**

Acknowledgments

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References

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Appendix: The Steps Neutron Data Go Through

To me there are four major steps:

1] Experimental Measurements – Much of nuclear data cannot be accurately predicted by nuclear theory, so we need to experimentally measure data. This is particularly true of data in the resonance region. Currently nobody can accurately predict a resonance energy, shape, etc., for any nucleus. We are so far from being able to do this that anyone who comes up with a good model to accurately do it can pack their bags for Oslo to go and pick up their Nobel Prize.

2] Evaluation – Since we do not know from first principles how to predict nuclear data and we cannot afford to measure everything, evaluation is still an art, trying to patch together what we do know (measurements) and we can guess at (nuclear models) to produce what we need in our applications. It is important to understand that to be useful evaluations MUST be complete – saying: I don't know is not an option. The job of the evaluator is to produce a complete set of data even if it involves just guesses or your best estimate, this is better than nothing, and it absolutely necessary if an evaluation is to be used in the steps I describe below. It is also the job of the evaluator to do this as accurately as possible – in particular if at all possible keep the evaluated data 'pure' and do not introduce any assumptions or approximations unless they are required for evaluation – especially, do not introduce limitations based on the present capabilities — or limitations — of today's processing and application codes (described below). Over the last 50 years our evaluator data has come a long way because improved evaluations force, or at least lead to, improvements in our processing and application codes.

3] Processing – Starting from evaluated data in a well-defined computer format (today ENDF is the universally used format [1]), our processing codes make various approximations and transformations to convert from the evaluated data to the form it will be used in applications. I should point out that there is a world of a difference between the form of the evaluated data and what can, or must, be used in application; the differences are basically because of limitations and approximation used in our application codes. Let me stress, as an evaluator these limitations and approximations are not your problem. It is important that you understand that you can help the most by focusing on producing the BEST POSSIBLE evaluated data, with as few limitations and approximations as possible — you do your job, and let the processing and application people do their jobs — don't try to help them by limiting the accuracy and generality of your evaluated data. Ultimately if you limit your evaluation it will limit its use, and reflect badly on the evaluator = YOU!!!

4] Applications – Next is the "proof of the pudding" where the nuclear data is used in our applications. That may sound like the end of the line, but alas in the real world it isn't, because in many cases our calculated results do not agree with our experimental measurements. When this happens we have a closed loop back to more experiments and/or more evaluation, and we iterate until we have agreement.

In summary, that's my view of nuclear data, where I see these four major steps (measurements, evaluation, processing and application). Here I have tried to give the reader an overview of the entire process.

EXFOR and ENDF

Now we come to the nitty-gritty details of what binds these steps together. These days needless to say, we can't do anything without computers, so we need everything we know

about nuclear data in computer readable form. There are two computer formats that we currently use in our work:

EXFOR – the **EX**perimental data **FOR**mat, or **EX**change **FOR**mat (to store and exchange experimental data between data centers), that we use to store experimentally measured data, in a standard form for subsequent use. If you are involved in evaluation you will most probably be involved with data in this format, if you want to compare say your evaluated energy dependent cross section to what has been measured.

ENDF – the **E**valuated **N**uclear **D**ata **F**ormat, that we use to store and exchange evaluated data. Over the last almost 50 years this format has been instrumental in improving our nuclear data. Before ENDF every laboratory, school and company had their own in-house format for data. In most cases each format was designed specifically to address in-house needs, and generally each was incompatible with all of the other evaluated data formats.

Starting in the mid-1960s Henry Honeck at Brookhaven National Laboratory (BNL) began the **ENDF** project in an attempt to come up with one — and only one — common format for all U.S. nuclear data users to use. I should mention that this was not the first such effort – the English were way ahead of us and already had developed and were using a common UKNDF format for their data.

My first job out of graduate school was in 1967 at Brookhaven National (BNL) at the then newly created National Nuclear Data Center (NNDC) — so by now I have been using the ENDF format for 46 years. While working at NNDC I designed the new **EXFOR** system for the experimental data; I modeled EXFOR on the existing ENDF system — that's why today the two formats look so alike.

What's in ENDF?

The contents of a typical evaluation in ENDF actually vary as we go through the steps I described above. Below I will use the ENDF terminology that I think you are by now familiar with. If any terminology or anything else isn't clear here, see ENDF-102 [1], the ENDF "Bible" that defines all of the ENDF formats and procedures.

MF=2 – Resonance parameters
MF=3 – Tabulated cross sections in LAB system
MF=4 – Angular distributions (exact angle-energy correlated) usually in CM – plus uncorrelated data for some reactions in the LAB.
MF=5 – Energy Spectra (no angle information) always in LAB
MF=6 – Double differential data (both angle and energy distributed)

Evaluation

These days a typical evaluation includes:

MF=2 - resonance parameters for most materials, but none for low-Z isotopes.
MF=3 - does not include the resonance contribution (usually elastic, capture and fission), but it does include tabulated cross sections for all other reactions, e.g., inelastic, (n,2n),….
MF=4 - includes correlated data always for elastic, MT=2, and generally for discrete inelastic, all in CM. Also uncorrelated data for (n,2n), and other reactions in LAB.
MF=5 - includes tabulated spectra for many reactions, e.g., (n,2n), fission, in the LAB
MF= 6 – used for materials where (energy, angle) correlation is important, such as Be9 (n,2n)

In summary the evaluated data produced and distributed **DOES NOT INCLUDE ANY TEMPERATURE DEPENDENT DATA**. Generally it doesn't even include complete tabulated cross sections in MF=3; only resonance parameters in MF=2. MF=4 includes elastic angular data in the CM.

Processed

I like to divide this into two parts: First, what I call pre-processing, which is what I do with my PREPRO codes, where I use the ENDF format both for input and output of data. Next the actual processing done by codes such as NJOY (Los Alamos), AMPX (Oak Ridge), MC2 (Argonne) – each laboratory has its own processing code. Unlike my PREPRO codes that use the ENDF format for both input and output, generally these processing codes start with ENDF input, but produce output designed for use by their own in-house application codes – and each laboratory has its own in-house format — seldom is it ENDF; ACER for MCNP, ENDL for TART, etc.

Way back when I worked at NNDC (1967–72) I could see that one flaw in ENDF was that we were standardizing the evaluated data format, BUT not how it was being interpreted; each laboratory would start with the same evaluated data, but they didn't have the resources to accurately interpret the evaluated data, particularly how to go from resonance parameters (MF=2) to energy dependent cross sections (MF=3). This led me to start work on my PREPRO (ENDF pre-processing) codes, to handle in a standard way, as accurately as we could, some steps that every data processing code could then piggy-back on – this gave them the option to either start their processing from the original evaluation or from my PREPRO output.

The things that I included were, start from MF=2 resonance parameters and reconstruct MF=3 tabulated (0 K) cross sections, Doppler broaden to temperatures of interest (I invented my SIGMA1 method of Doppler broadening to do this), For MF=4, reconstruct angular distributions from Legendre coefficients. For MF=5 replace model parameters by tabulated spectra. By ALWAYS having my PREPRO output in the ENDF format allowed users to bypass these initial processing steps and minimize their work — and approximations — and to concentrate on producing the data they need as input to **their application codes.**

In summary the processed data we produce and distribute **DOES INCLUDE TEMPERATURE DEPENDENT DATA** LAB system cross sections in MF=3; usually we distribute MF=3 cross sections at a number of temperatures. For completeness of every evaluation, with the MF=3 data at each temperature we also include exactly the same MF=4 elastic angular data in the CM, even though this data is **TEMPERATURE INDEPENDENT**. That is to say that this MF=4 data is by definition as CM correlated data **TEMPERATURE INDEPENDENT,** i.e., in the CM system temperature has no meaning.

For an example of what's in the entire current ENDF/B-VII.1 library (423 evaluations), see my latest pre-processed results on-line as POINT2012 at my website http://home.comcast.net/~redcullen1/. This includes both the original evaluations and cross sections at many temperatures. If you want to see and/or compare the data to 'see' the effects of Doppler broaden, I recommend you use my COMPLOT code, also available on-line at my website as part of PREPRO2012.

The POINT2012 data and PREPRO2012 codes are also available for FREE on-line at the National Nuclear Data Center, Brookhaven National Lab, http://www.nndc.bnl.gov/, and at the Nuclear Data Section, IAEA, Vienna, https://www-nds.iaea.org/

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