LLNL-TR-461199

A Short History of ENDF/B Unresolved Resonance Parameters

by
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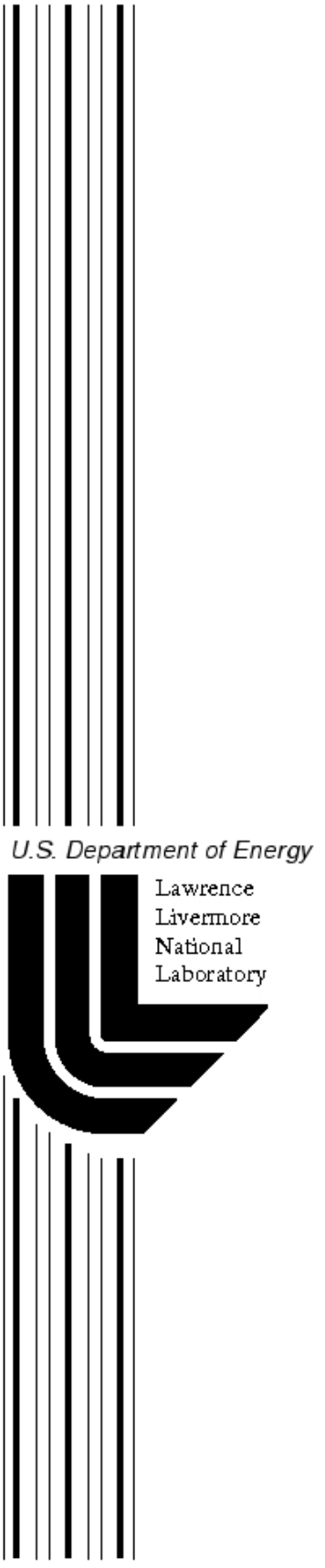
October 31, 2010



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Overview

This paper is designed to address two topics relating to ENDF/B data in the unresolved resonance region [1],

1) **Part 1: For years code users have pointed out and complained that various ENDF data processing codes, in particular PREPRO [2] and NJOY [3], produce different answers from one another for the cross sections in unresolved resonance region. First I assure code users that NJOY has now been updated to agree with PREPRO, so that this problem has now been solved.**

2) **Part 2: Next, this paper documents why we saw these differences; the emphasis here is on explaining what my own codes do [2], but I will also try to briefly outline what other codes do, so the reader can understand why we were producing different answers.**

The first topic should be of general interest to all readers, particularly users of our codes, whereas the second topic will be of more limited interest only to those readers who are interested in the details of our calculations in the unresolved resonance region. Now that our PREPRO and NJOY results agree we consider this problem solved and no further action is necessary.

Part 1: Our Codes now Agree

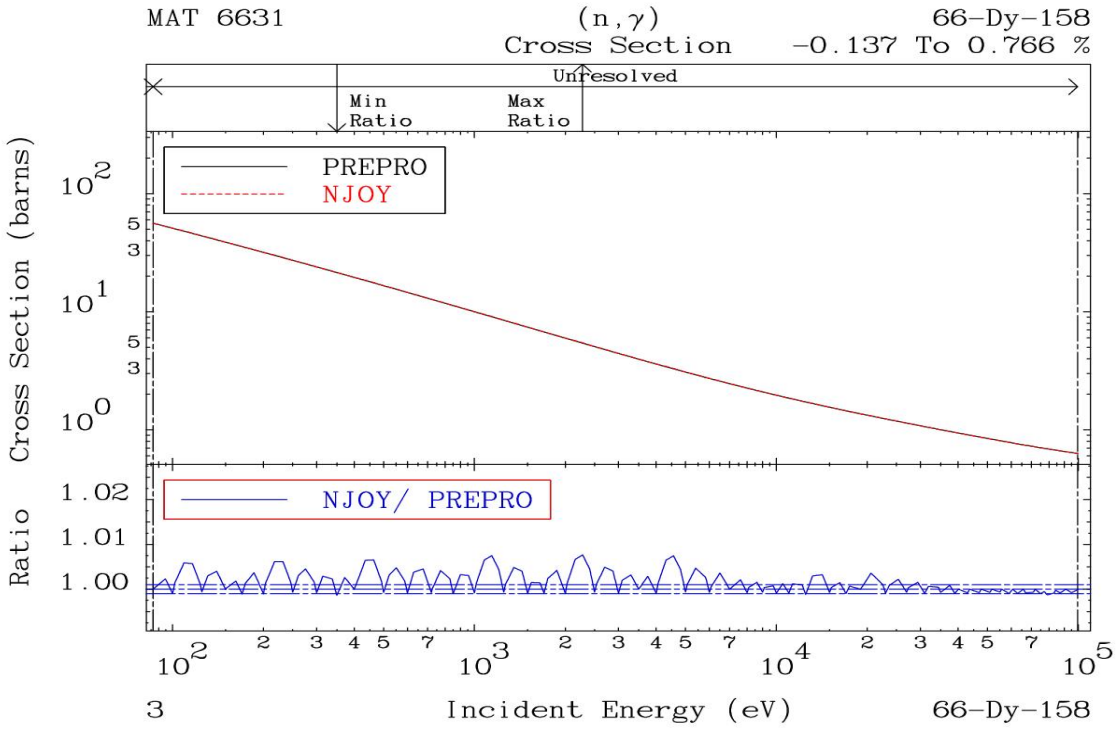
PREPRO [2] and NJOY [3] unresolved resonance region results differed for one reason: how they interpolated in energy. In the unresolved resonance region parameters are defined in tabular form at a series of fixed energies. At the energies where parameters are

tabulated PREPRO and NJOY results agree, i.e., given a unique set of parameters at any given energy both codes use the same model to calculate cross sections at that energy.

Where they differed is in interpolating between the energies are which parameters are tabulated. NJOY interpolates cross sections, whereas PREPRO interpolates parameters. A quick read of the ENDF-102 formats and procedures manual [1] seems to indicate that we should interpolate cross sections; however this procedure leads to non-physical results, whereas interpolating parameters lead to physically acceptable results with the expected energy dependent shape similar to 1/v variation. After reviewing the details of ENDF-102 [1], and the results shown in the appendix of the paper, where we see differences of over a factor of two (over 100% difference), it was decided to update NJOY to interpolate parameters.

It is important to understand that today the PREPRO and NJOY results in the unresolved resonance region closely agree. Code users should be aware that they should be using the most recent version of NJOY in order to obtain these more accurate results. It is also important for code users to understand that while NJOY was updated in order to obtain this agreement, PREPRO was not changed at all, so that earlier results from PREPRO for the unresolved resonance region are still valid.

In the appendix you will see a comparison of PREPRO and NJOY results before NJOY was updated. In particular in the appendix note 66-Dy-158 capture which shows a different of up to over 112% (over a factor of two). For comparison see the below results after NJOY was updated. The 112% differences have been reduced to a fraction of 1%.



Part 2: A Brief History

Throughout the first 20 years of the ENDF/B system [1] there was no confusion or ambiguity as to how to define cross sections in the unresolved resonance region. Evaluations included tabulated unresolved resonance parameters and an interpolation law to allow these parameters to be defined at ALL energies, not just the energies at which they are tabulated. In addition once we knew the parameters at any energy, we had only one model (single-level Breit-Wigner) to uniquely define cross sections at that energy. The only reason this convention was changed was to accommodate the limitations of data processing codes and computers over 20 years ago. Obviously our codes and computers today are so much better and faster than they were 20 years ago, that these considerations do not apply today, and yet we are still stuck with this approximation. **Today this is not very controversial since PREPRO [2], NOY [3], AMPX [4] and CALENDF [5] all agree that at least some form of parameter interpolation is what should be used.**

Mine is not the first paper on this subject. An excellent review and comparison of code results is "**Unresolved Resonance Range Cross Section, Probability Tables and Self Shielding Factors**" [7]; ref [7] is more general than paper that you are now reading, in that it covers in detail a variety of codes and the unresolved region data that these codes produce, both unshielded and shielded. I highly recommend that anyone who wants more detail on this subject read this paper. The paper [7] generally reaches the same conclusions that I present here, which is basically that: **Cross section interpolation does not work; it produces results that R.J. MacFarlane recently described as "absurd" [8]; at least some form of parameter interpolation is required to obtain physically acceptable results.**

Details

There is what I consider to be a very poor approximation in the ENDF/B system [1], to interpolate cross sections, rather than parameters in the unresolved resonance region. To my knowledge this is the only time that the objective of having ENDF/B only include the very best physics and data was compromised. The only justification claimed at the time for this approximation was solely to accommodate the limitations of the data processing codes and computers that existed 20 years ago. Today with the advances in codes and computers that we have seen over the last 20 years there is absolutely no justification at all for this approximation. As we will see later in this report this approximation leads to results that differ by factors of three or four; let me repeat that – we are not talking about differences of a few per-cent – we see factors of 300% to 400% or even more. More to the point: Why were the limitations of somebody's computer codes allowed to be incorporated into the ENDF system? In doing this the basic data that everyone in the World uses was compromised. Generally if you have a code problem you deal with it yourself; you shouldn't ask everybody else to be limited by your problem.

Here I briefly outline the history of ENDF/B unresolved resonances parameters, in the hope that this explains how we got into the current situation.

What we Expect

When we calculate average cross sections in the unresolved resonance region starting from unresolved parameters, physically we expect cross sections that are what I will call "1/v-like". By this I mean that the energy dependent cross section will decrease with increasing energy roughly as 1/v, that is, inversely as the square root of energy. The complete energy dependence will be defined by,

1) Usually slowly varying parameters
2) Penetration, shift factor, etc., that are also slowing varying functions of energy
3) The 1/v term, which compared to the other terms is rapidly varying

Even for parameters that are constant over an extended energy interval, it is important to understand that the cross section will still be energy dependent. For example, in many actual cases evaluations will define parameters that are constant over an entire energy decade or more. In this case we expect the cross sections to be close to 1/v, with only a few per-cent difference, due to the small change in penetration, shift, etc. So that over a decade of energy with 1/v-like variation we expect the cross section to vary by more than a factor of three. Naturally when the parameters are energy dependent the situation is more complicated, but even then a good rule of thumb is that the cross sections should be "1/v-like". Indeed when we see parameters with strong and rapid changes we start to question what "unresolved" means.

In the Beginning

The ENDF/B system originated about 1965, some 45 years ago, at Brookhaven National Laboratory. From the beginning of ENDF/B through the fourth version of this library, ENDF/B-IV, the definition and conventions for unresolved resonance parameters was clear and resulted in unique answers. Unresolved parameters were treated just like any other table of ENDF/B data. In ENDF/B **tables of data are uniquely defined at all energies**, not just the energies where they are tabulated. This is accomplished by defining data at discrete energies PLUS an interpolation law that can be used to uniquely define the data at ANY ENERGY between those energies at which it is tabulated. Let me repeat this, because it is important: **The interpolation law with each table defined how to interpolate ONLY the data that is actually tabulated in the table; this was true throughout ENDF.**

There was never any complaint or uncertainty about how to define parameters at any energy; once parameters were interpolated to define them at any energy we could in turn uniquely define the corresponding cross sections at that energy. Unfortunately, in the 1980's in the transition from ENDF/B-IV to ENDF/B-V the Cross Section Evaluation Working Group (CSEWG) was told that it was expensive to process unresolved resonance data and it was suggested that the convention be changed to instead of interpolating parameters, users could instead use the parameters at the energies at which they were tabulated to calculate cross sections at those energies, and to then interpolate CROSS SECTIONS, rather than PARAMETERS to define cross sections at all other

energies. **At the time CSEWG was assured that this change in convention would have no significant impact on results; in fact this turned out not to true at all.**

I should mention that the original intent of ENDF/B was to present the best possible physical data for use in our applications. This change in the convention for unresolved parameters is the only case that I can think of in which the original intent of ENDF/B was compromised solely to meet the needs of some data processing code. In changing convention there was no attempt to physically justify this change; indeed it has always been obvious that the original convention was physically better. The only justification for this approximation was that many years ago due to the limitation of the then current computers, processing codes could use this approximation to process unresolved data faster. Many times in using data we may run into limitations in our codes and/or computer power, and we are forced to make approximations. **That is nothing new; we personally make the best approximations we can and then we personally deal with the consequences. But this is the only case that I know of where someone's limitations were allowed to propagate into the actual ENDF system where they would affect everyone.**

In my opinion ENDF/B should focus on always providing the BEST physical data. Any approximation that a data user wishes to subsequently make in interpreting this data should be strictly up to the user, and NEVER be a part of the ENDF/B system. The only case that I can think of where this approach was violated was in the case of unresolved resonance parameters. **In my humble opinion this compromise should never have been accepted as part of ENDF/B, and we have been paying for this compromise ever since; long after our computers have become so powerful that the original justification is simply no longer relevant.**

Once ENDF/B-V was released by the National Nuclear Data Center (NNDC), I updated my PREPRO code [2] to use the new unresolved resonance convention, processed all of ENDF/B-V using my codes, and I returned my results to NNDC. They compared my ENDF/B-V results to my earlier ENDF/B-IV results and my phone immediately began to ring, telling me that my codes must have errors in them. **The differences between many evaluations in the ENDF/B-IV library that were carried forward to ENDF/B-V without any changes in the data, showed enormous differences in the unresolved resonance region**; at that time we saw differences of 300% to 400%; even today we see over 100% differences, see examples later in this report. It didn't take too long to track the source of the difference not to errors in my code, but directly to the change in convention to interpolate cross sections rather than parameters.

This convention that CSEWG was assured would not have any impact on results, was actually resulting in differences in cross sections of up to factors of three or four (300% to 400%), with the cross sections based on cross section interpolation resulting in totally non-physical "bumps" in the cross section, so it was obvious they were WRONG; again, see the figures later in this report.

What to do?

Once we saw the difference between the ENDF/B-IV and ENDF/B-V results we realized that CSEWG had been mislead; rather than having no significant effect this convention had a major effect and produced physically unacceptable cross sections. The National Nuclear Data Center (NNDC), located at Brookhaven National Laboratory, was obviously reluctant to admit such a fault in the newly released ENDF/B-V data library. Yet we obviously could not accept such enormous differences in cross sections, so it was decided to effectively cancel the change in convention by further clarifying what it says in the ENDF-102 formats and convention manual.

ENDF-102 had recently been modified for the new convention to state (these are all quotes from ENDF-102[1])

For energy-dependent formats (LRF=2, or LRF=1 with LFW=1), the recommended procedure is to interpolate on the *cross sections* derived from the unresolved resonance parameters (URP). This is a change from the ENDF/B-III and IV procedure, which was to interpolate on the parameters.

We added to this the additional constraint,

It is recommended that evaluators provide the URP's on a mesh dense enough that the difference in results of interpolating on either the parameters or the cross sections be small. A 1% maximum difference would be ideal, but 5% is probably quite acceptable.

What this statement does not state is what we should do when evaluators do not supply parameters on "a dense enough energy grid", Because evaluators are ignoring this recommendation, more recently we added to ENDF-102 the further clarification,

When evaluators do not supply parameters on a dense enough grid processing codes should interpolate parameters to a finer energy grid until this criteria is met.

At the time of the release of ENDF/B-V I checked to insure that not one single evaluation provided parameters on a dense enough energy grid. Recently I checked a number of current data libraries: ENDF/B-VII, JEFF, JENDL, CENDL,…, this is thousands of evaluations, and I found that even **today not one single evaluation provides parameters on a dense enough energy grid**.

As such it seemed clear 20 years ago and is still clear today, that processing codes MUST **interpolate unresolved parameters** to a dense energy grid that the difference between interpolation of either parameters or cross sections is small **– that is EXACTLY what ENDF-102 says, and that is exactly what my PREPRO codes do [2].**

Problem Solved?

At the time 20 years ago I assumed that we had effectively short circuited the poor approximation to interpolate cross sections and the problem was solved. Except for the brief period after the release of ENDF/B-V that it took us to realize how poor this approximation was, my codes have always used the more physically acceptable procedure to interpolate parameters. Let me repeat this to be sure it is clear: **My PREPRO [2] codes have always used the original ENDF/B convention to interpolated parameters and continue to do so today.**

Unfortunately the problem was not solved. It turns out that unbeknown to me over the last 20 years some processing codes have continued to use the approximation to interpolate cross sections. The non-physical results are shown later in this report. In the appendix I show comparisons of PREPRO [2] versus NJOY [3] of results produced at the beginning of 2009. **Be assured that since then NJOY has been updated to interpolate parameters, so that today (summer 2010), PREPRO and NJOY results are in close agreement, e.g., see the figure in Part 1 of this report. Again, let me stress that a primary purpose of this paper is to explain this to PREPRO code users.**

ENDF/B Unresolved Resonance Parameter Formats

In the unresolved resonance region ENDF/B allows evaluations to use any of three different tabulated representations of parameters,

1) All parameters energy independent.
2) Fission parameters energy dependent.
3) All parameters energy dependent.

Since we are discussing interpolation it is of interest to see how interpolation is defined for each of these cases,

1) No interpolation law (INT) is defined
2) No interpolation law (INT) is defined, but the text says use lin-lin
3) Interpolation law (INT) is defined in the format

This format has not changed since the beginning of ENDF, and in particular it was not modified when the rule to interpolation cross sections rather than parameters was adopted. The interpolation laws defined for these three different representations made sense when interpolating parameters, but make no sense when interpolating cross sections. I don't care what it says in ENDF-102 when evaluators give us parameters tabulated on a sparse energy grid with energy intervals of a decade or more we simply cannot calculate cross sections at these energy points and assume linear variations over a decade or more in energy. **Physically that is nonsense and it the one and only source of the ENORMOUS differences we see in the figures in the appendix.**

It is important to understand that in many cases unresolved parameters are defined as 1) constant, so **there is no interpolate law associated with them**; in cases 2) only fission parameters are energy dependent the text says to **always use lin-lin (there is no choice)**, and only in case 3) is any interpolation law explicitly defined in the format. So you might ask: what does it mean to interpolate cross sections rather than parameters, since even in the cases where parameters are constant, independent of energy, **the cross sections are still energy independent, so they MUST be interpolated**. Also the energy dependent variation of cross sections based on the combination of unresolved parameters and model relating parameters and cross sections is different for elastic, capture and fission, and therefore different for the total. This means that there is no one single interpolation law that is best for interpolating ALL of the cross sections. In contrast parameters are usually constant or slowly varying with energy and interpolating all parameters does not present any serious problems. **See the appendix for many examples of differences, and note that the difference in the energy dependent variation of cross sections usually results in bigger differences for capture than for elastic, because their energy variations are different and not easily defined by a single interpolation law, which is all that is available with the unresolved parameters.**

These various representations never presented any problem or non-uniqueness with the older convention to interpolate parameters; then in each case the energy dependent shape of cross sections was based on the combination of the variation of the unresolved resonance parameters and the model relating parameters and cross sections. But with the new convention to interpolate cross sections there were immediately obvious problems. For example, in the simplest case where parameters were physically independent of energy the evaluator was free to represent these parameters in the ENDF/B format in any of three allowed forms. With the older convention to interpolate parameters this did not present any difficulty and all three representations led to exactly the same cross sections. **In contrast, using the newer convention to interpolate cross sections was leading to codes calculating three different answers, for exactly the same resonance parameters, differing only in how they were coded in the ENDF/B format; this makes no physical sense at all.**

Suddenly with this new convention we were faced with unresolved resonance parameters that were tabulated at say two energies a decade apart where the old convention to interpolate parameters would calculate physically acceptable energy dependent cross sections (close to 1/v variation), whereas the new convention to interpolate cross section resulted in cross sections that were claimed to be linearly interpolable over a decade of energy. **The differences were enormous, with the older convention to interpolate parameters resulting in physically accepted cross sections, and the newer convention to interpolate cross sections resulting in, how can I diplomatically say this: RUBBISH!!! See the appendix for many examples of these differences.**

It is also worth noting that often unresolved resonance parameters are used to generate **ladders of resonances**, that are then used either directly in Monte Carlo calculations or to derive averaged unresolved region cross sections. This ladder approach involves using the unresolved region level spacings and widths to randomly sample the position and

widths of a series of resonances, at successive energy intervals in the resonance ladder. Essentially to create a ladder we start at some base energy and we sample an energy interval to the position of the next resonance and at this energy we use the average widths at that energy to sample widths for the next resonance in the ladder. We continue advancing in energy, resonance by resonance to the end of our ladder. What the current ENDF-102 rules do not address is: In order to define a ladder we have to define the average widths to samples at the energy of each resonance in the latter. **How can we do this using cross section interpolation? Don't we have to interpolate parameters? I searched ALL of the most recent version of ENDF-102 [1] and found that the word "ladder" is only mentioned three times, and never in the context of how to interpret unresolved resonance region data to construct a ladder.**

Interpolate What and How?

In our applications we are interested in integral results; quantities such as reactions, energy deposited, dose, etc, that depend on defining results at all energies, not just the energies at which cross sections are tabulated. The ENDF format allows us to do this by defining tabulated data and an interpolation law to define data at ALL energies between where they are tabulated. Integrals can be VERY sensitive to how we interpolate [6]. For example, see the differences shown in the appendix; in each case the integral is merely the "area under the curve**". In ALL of these cases this integral differs SOLELY because of what and how we interpolate between tabulated parameter values.** So that for our use the question of what and how to interpolate is crucial.

To be fair the ENDF/B "bible" ENDF-102 [1] is at best confusing as far as its "recommendation" of how to define energy dependent cross sections in the unresolved resonance region. Above I quoted statement from ENDF-102 that first clearly say to interpolate cross sections, and then follows with a contradictory statements that say, but first interpolate parameters to a dense enough energy grid. ENDF-102 also defines the interpolation law (INT); here is another quote from ENDF-102,

INT Interpolation scheme to be used for interpolating between the cross sections obtained from average resonance parameters. Parameter interpolation is discussed in the Procedures Section 2.4.2.

There is only one interpolation law with the unresolved resonance parameters (INT), and based on the above statement from ENDF-102, it seems to clearly state that this is to be used to interpolate cross sections. Yet ENDF-102 says to interpolate parameters to a dense enough energy grid, but nowhere does it say how to interpolate parameters.

When the recommendation to interpolate cross sections, rather than unresolved parameters, was introduced, initially PREPRO [2] and NJOY [3] assumed that the interpolation law defined with the unresolved parameters is what should be used to interpolate cross sections. Unresolved resonance parameters are fairly slowly varying with energy, so in almost all cases linear interpolation is defined to use with the parameters. After initial testing showed that cross section interpolation caused problems

PREPRO returned to interpolating parameters, whereas NJOY continued to interpolate cross sections. **This is the SOLE source of the large differences that we see in the appendix.**

Although parameters vary slowly, the average infinitely dilute cross section do not. Even in the case of energy independent parameters, the cross sections are 1/v-like, so that over a decade of energy they can vary by over a factor of three, and a 1/v-like shape is not at all close to linear. In contrast AMPX [4] was **designed to assume** that the interpolation law with the unresolved parameters applied only to the parameters, and it was assumed that to interpolate cross sections they should use log-log interpolation. The AMPX assumption of log-log variation is physically better in the sense that this assumption better approximates the expected 1/v-like variation of the cross sections when parameters are energy independent; if used this assumption would eliminate the enormous differences between NJOY and PREPRO results shown in the appendix, but still results in 5% to 10% differences when parameters are energy dependent. This is true in principle, however a recent code comparison showed that **although AMPX was designed to assume log-log interpolation, it is actually using lin-lin interpolation and is producing the same results as shown in the appendix; the results produced by NJOY before NJOY was updated**. This result clearly demonstrates the importance of code comparisons, i.e., in designing codes good intentions are not sufficient.

At least to me the recommendations in ENDF-102 are at best confusing and contradictory, but let's look at reality: our codes have interpreted this to mean a variety of things,

1) PREPRO - Interpolate parameters
2) NJOY - Interpolate cross sections, use parameter interpolation law
3) AMPX - Interpolate cross sections, assuming log-log interpolation.
4) CALENDF – Interpolate parameters

Apparently ENDF-102 is confusing enough that NJOY and AMPX can claim to be abiding by the letter of the law, to interpolate cross sections. Similarly, PREPRO can claim that it is abiding by the letter of the law because ENDF-102 also says to first interpolate parameters to a fine energy grid such that there is no significant differences between parameter and cross section interpolation. And CALENDF in generating ladders of resonances has no choice but to interpolate parameters to the energy of each resonance of the ladder.

The bottom line is that the ENDF-102 recommendations are vague enough to allow everybody to claim they are "right", leaving us with a variety of different interpretations and answers. Most important for you to understand is that the above lists how our codes used to interpret unresolved resonance region data. **Today this is not very controversial since PREPRO [2], NOY [3], AMPX [4] and CALENDF [5] all agree that at least some form of parameter interpolation is what should be used.**

The Earth is the Center of the Universe

For decades there have been no changes in how our codes treated unresolved data, and we have lived with whatever results our codes generated. Recently there has been a great deal of discussion about what sounds like a trivial problem of how to interpolate in the unresolved resonance region. Unfortunately in my humble opinion this discussion has lost contact with reality. The nearest analogy I can think of is the clergy during the middle ages debating about how many angels can dance on the head of a pin; obviously an unresolved problem (no pun intended). They also debated more serious problems, such as trying to prove using the Bible that the Earth is the center of the Universe. They obviously lost contact with reality, because regardless of what it says in the Bible we physically know that the Earth is not the center of the Universe. But back then they were so serious about this that you could get burned at the stake as a heretic if you claimed the Earth was not the center of the Universe.

Today there is a great deal of discussion back and forth debating what it says in the "ENDF/B Bible", ENDF-102: does it say interpolate cross sections between the energies at which parameters are tabulated, or does it say first interpolate parameters to a dense grid, or does it say something else. These discussions are losing contact with reality in the same way that the clergy was losing contact with reality trying to interpret the Bible. Back then it did not matter what the Bible said, because physically the Earth is not the center of the Universe, and today it does not matter what ENF-102 says, because physically we cannot calculate cross sections at the sparse energy grid supplied by evaluators and use cross section interpolation between these energies. **Sorry, but physically cross section in the unresolved resonance region are simply not linear over large energy intervals, and if you assume they are you get the "absurd" [8] results shown in the appendix.** I always try to have my codes produce what I consider to be the most physically accepted results. So that in this case I must ignore all the debate and confusion as to what it says in ENDF-102, and I produce results based strictly on the best physics, which is older ENDF convention to interpolate parameters. **Therefore I am an admitted ENDF heretic and probably a candidate for burning at the stake.**

Is This Important?

In recent years there has been a flurry of activity concerning ENDF unresolved resonance region data. There was so much interest that an International sub-committee was formed to determine whether ENDF should be extended to allow other resonance formalisms in the unresolved resonance region; today only the single-level Breit-Wigner formalism is allowed. It was **hypothesized** that using other formalisms could lead to changes in the unresolved cross sections of a few per-cent.

Therefore I was amused at the reaction when the differences shown in the appendix where seen by people. First came shock, then embarrassment, but finally denial in the claim that these differences are not important. I found this amusing because the same people who were promoting an International sub-committee to look for a few per-cent

differences due to methods, are now claiming that 100% or more differences are unimportant.

People also claim that it is even today it is too expensive to use parameter interpolation; I find this claim laughable. Today when we have process a material like U-238 we may have over 100,000 tabulated energy points for the cross sections. Of these someplace between 30 to 100 energy points may be in the unresolved resonance region energy range. I say 30 to 100 because it depends on how one interprets the unresolved parameters. Today processing these 30 to 100 energy points is trivial compared to the overall time to process all of the over 100,000 energy points for a material like U-238. Yet there are still some who continue to cling to the claim that assuming cross section interpolation is more efficient because it will produce the 30 points while parameter interpolation produces the 100 points. Guys: 30 points or 100 points out of 100,000, it is still overall trivial to process the unresolved resonance region data. Everyone is certainly free to believe whatever they want, but my experience is that processing and using the unresolved data is a trivial part of the overall time consumed, and the results shown in the appendix, indicate that those people who want to save a trivial amount of time are ignoring what we call **Howerton's first law [9]: "We are in no rush for the wrong answer."**

What can I say; I suppose I should have expected this. As they say "Beauty is in the eye of the beholder", and human nature makes us view things to best meet our own personal needs. **So is this important? In my personal view, yes, it is important. Indeed if we can change ENDF cross sections by factors of three or four and not see important effects, we would not need ENDF at all.**

Using LSSF=1 Option

To me this relatively new ENDF option sounded like a GREAT IDEA. Since people were noting differences in the infinitely dilute cross sections calculated in the unresolved resonance region, this option (LSSF=1) was designed to allow evaluators to include in their evaluators tabulated infinitely dilute cross sections, in MF=3. The convention would then be to use the evaluator supplied tabulated cross sections (MF=3) as a normalization to define infinitely dilute cross sections, and the unresolved resonance region parameters (MF=2) to only define self-shielding factors.

Evaluators could then use the BEST experimentally measured and theoretical models to define tabulated infinitely dilute cross sections in MF=3. They could then derive unresolved resonance region parameters using the only ENDF-102 approved model, namely single level formalism, to agree with their tabulated MF=3 cross sections.

Alternatively, evaluators could just rely on the tabulated parameters, and it was hoped that with this option evaluators would use a verified code, such PREPRO [2], to start from their unresolved parameters on a sparse energy grid, to calculate cross sections on a dense energy grid that could then be used directly in their evaluations. If done this way this would solve the problem created because ALL evaluators define parameters on a

very sparse energy grid (again, often with energy points a decade or more apart), and still supplying cross sections on a dense enough energy grid (for example, as calculated by PREPRO).

Again, let me stress that this sounded like a GREAT to me.

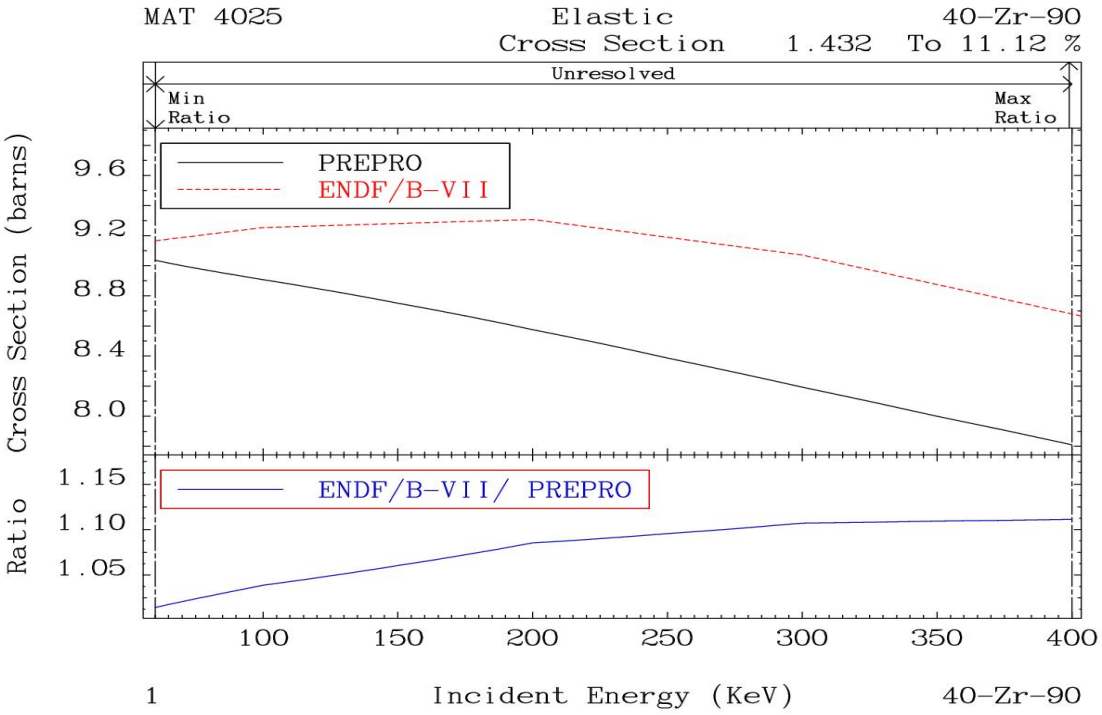
In contrast our worst fear was that rather than supplying tabulated MF=3 cross sections on a dense energy grid, evaluators would merely calculate and tabulate cross sections on the sparse energy grid on which the parameters are given. This only makes the situation worse, because their tabulated cross sections on a sparse energy grid merely reproduces the BIG differences shown in the appendix to this report. **Unfortunately, based on looking at current evaluations this is what evaluators are doing, which only makes things worse. Earlier our codes at least had a chance to interpret their parameters given on a sparse energy grid to produce correct energy dependent cross sections. But once evaluators supply cross sections and say that is what they recommend, we are stuck with it.** A major part of the problem seems to be that evaluators do not appreciate the importance of interpolation; again, let me stress that what is important to us are integrals, not simply values at the discrete energies where evaluators tabulate data.

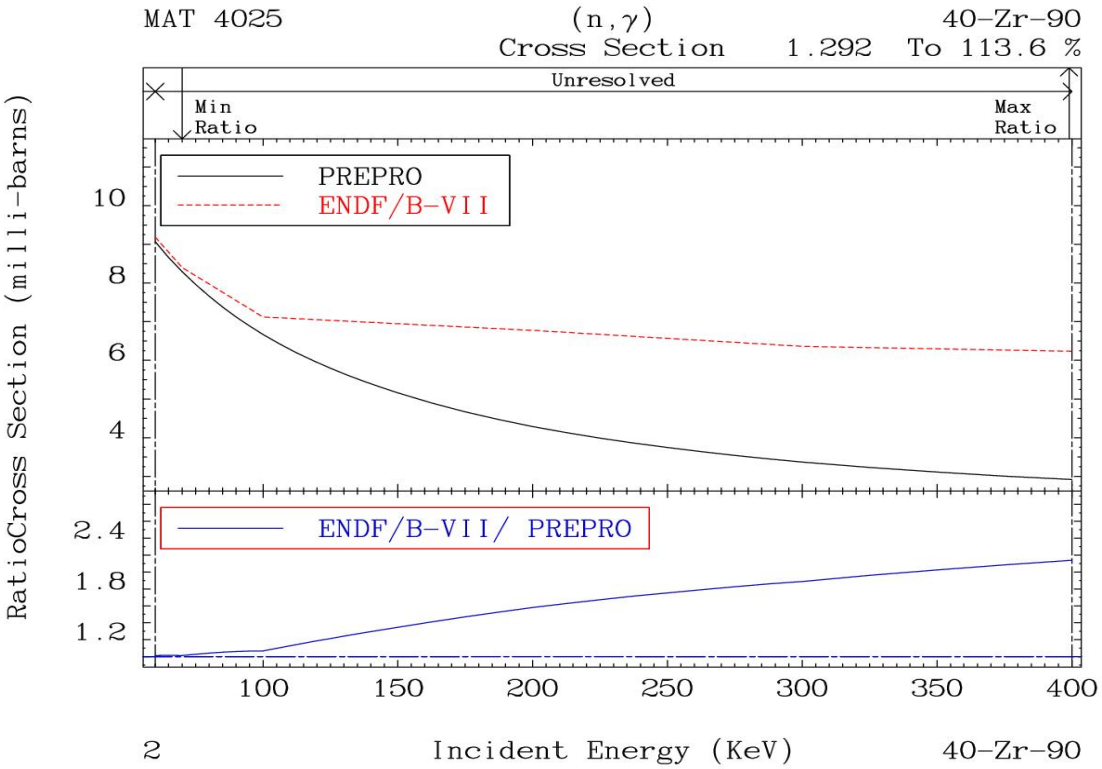
We have always had excellent agreement for the infinitely dilute cross sections calculated at energies where parameters are tabulated [2, 3]. It never occurred to us that not only would evaluators calculate cross sections only at the sparse energies where parameters were tabulated, but that they would use methods other than the verified methods that we have used for many years [2, 3]. Unfortunately, this is what we find in current evaluations.

The overall result is that we started with a fairly simple to understand interpolation problem in the unresolved resonance region, and now we have an even worse situation, where even the normalization of the infinitely dilute tabulated cross section is now in question.

Below is but one example, comparing results tabulated by the evaluator using LSSF=1 (identified as ENDF/B-VII) and what I calculate based on the unresolved parameters also tabulated by the evaluator (identified as PREPRO). Here we see differences for the elastic by over 12% and capture by over 113%. Note, that unresolved parameters are tabulated at the upper energy limit of the unresolved resonance region at 400 keV, and yet this is the energy where we see the latest difference, i.e., obviously the evaluator is not using a verified method from one of our codes [2, 3] to define their tabulated infinitely dilute cross sections.

Currently I still think the LSSF=1 option is a GREAT idea. Hopefully we are merely going through growing pains while evaluators learn how to correctly use this option. For now the best I can suggest is CAVEAT EMPTOR.


MAT 4025
Elastic
Cross Section
1.432 To 11.12 %
40-Zr-90
Unresolved
Min Ratio
Max Ratio
PREPRO
ENDF/B-VII
ENDF/B-VII/ PREPRO
Cross Section (barns)
Ratio
9.6
9.2
8.8
8.4
8.0
1.15
1.10
1.05
100
150
200
250
300
350
400
1
Incident Energy (KeV)
40-Zr-90


MAT 4025
(n,γ)
Cross Section
1.292 To 113.6 %
40-Zr-90
Unresolved
Min Ratio
Max Ratio
PREPRO
ENDF/B-VII
ENDF/B-VII/ PREPRO
RatioCross Section (milli-barns)
10
8
6
4
2.4
1.8
1.2
100
150
200
250
300
350
400
2
Incident Energy (KeV)
40-Zr-90

Conclusions

This paper is designed to address two topics relating to ENDF/B data in the unresolved resonance region [1],

1) **Part 1: For years code users have pointed out and complained that various ENDF data processing codes, in particular PREPRO [2] and NJOY [3], produce different answers from one another for the cross sections in unresolved resonance region. First I assure code users that NJOY has now been updated to agree with PREPRO, so that this problem has now been solved.**

2) **Part 2: Next, this paper documents why we saw these differences; the emphasis here is on explaining what my own codes do [2], but I will also try to briefly outline what other codes do, so the reader can understand why we were producing different answers.**

The first topic should be of general interest to all readers, particularly users of our codes, whereas the second topic will be of more limited interest only to those readers who are interested in the details of our calculations in the unresolved resonance region. Now that our PREPRO and NJOY results agree we consider this problem solved and no further action is necessary.

Acknowledgements

I thank **Mary Chin** (CERN), for reminding me of this problem, and providing her NJOY vs. PREPRO comparisons, some of which are included in the appendix. I thank **Bob MacFarlane** for providing the NJOY output I used to create the other comparisons in the appendix.

I also thank my friends who reviewed a preliminary version of this paper; their comments and suggestions have been incorporated into this paper and I feel they have significantly contributed to improving this paper. The reviewers in alphabetical order include: **S. Ganesan** (BARC), **Maurice Greene** (ORNL, retired), **Dave Heinrichs** (LLNL), **Mike Herman** (NNDC, BNL), **Bob MacFarlane** (LANL), **Jean Christophe Sublet** (CEA), and **Andrej Trkov** (IJS).

References

[1] **ENDF format:** "ENDF-6 Formats Manual: Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VII", CSEWG Document ENDF-102, edited by Michael Herman and Andrej Trkov, (July 2010). Note, that the ENDF formats and conventions have had a number of updates, latest being the ENDF-6 formats, available on-line at http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf

[2] "**PREPRO 2007**: 2007 ENDF/B pre-processing Codes", IAEA-NDS-39, Rev. 13, March 17, 2007, by Dermott E. Cullen, Nuclear Data Section, International Atomic Energy Agency, Vienna, Austria. These codes are available FREE on-line at http://www-nds.iaea.or.at/ndspub/endf/prepro/

[3] **NJOY:** "The NJOY Nuclear Data Processing System, Version 91," Los Alamos National Laboratory report LA-12740-M, by R. E. MacFarlane and D. W. Muir, (October 1994) is still the latest official manual.

[4] "**AMPX:** A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B", by N.M. Greene, et al., ORNL-TM-3706, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1976.

[5] **CALENDF**-2005: User manual", ISSN 0429-3460, Report CEA-R-6131, France (2006)**,** by J-Ch. Sublet, P. Ribon, M. Coste-Delclaux.

[6] **ENDF Cross Sections are not Uniquely Defined**, LLNL-TR-446331 June 2010, by Dermott E. Cullen, Lawrence Livermore National Laboratory, available on-line at, http://home.comcast.net/~redcullen1/Papers/nonunique/nonunique.pdf

[7] **Unresolved Resonance Range Cross Section, Probability Tables and Self Shielding Factors**, Report ISSN 0429 – 3460, June 2009, by J-C Sublet, et al.

[8] **Private Communication**, R.J. MacFarlane [2009]

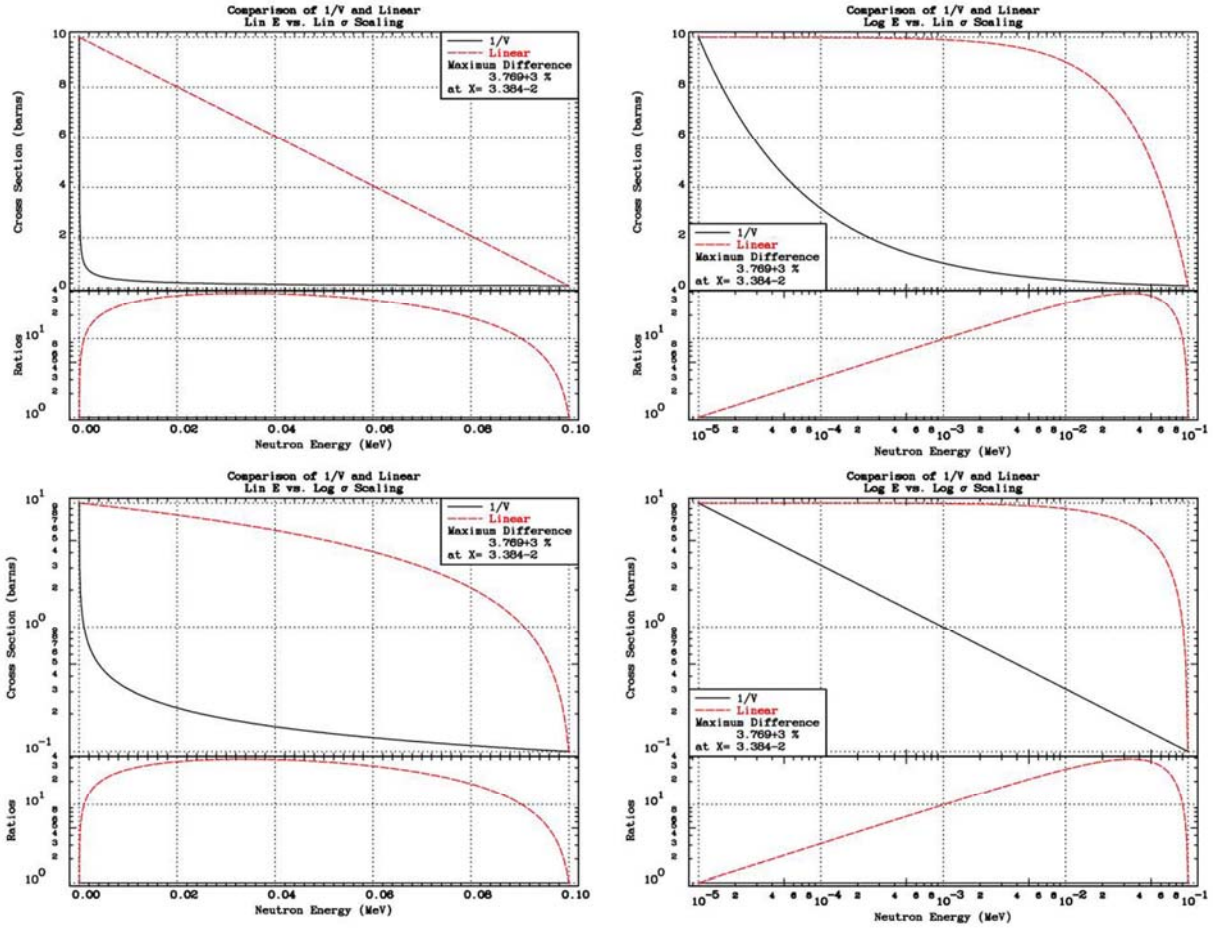
[9] **Private Communication**, R.J. Howerton [1975]

Appendix A: The Effect of Scaling on What you see

When comparing data using non-linear scaling for a figure, you may be confused by what you see. Here we show exactly the same data: 1/v compared to Linear, using four different scales for the figures: all combination of linear and log scaling for energy and cross section (four results).

In the first figure (upper, left), with lin-lin scaling **we see the Linear data as a straight line**, compared to the 1/v that rapidly decreases; the result being a difference of over 3700% (over a factor of 37). This may be the most familiar view to you.

Now look at the other figures using exactly the same 1/v and Linear data, with the only difference being the x and y scaling of the figure (linear or log). By the last figure (lower, right), with log-log scaling, **we now see that it is the 1/v that appears as a straight lin**e, and the Linear appears as a curve, well above the 1/v. Regardless of how we display the data the ratio remains the same. **Be assured that this is not a mistake or an optical illusion; this is the effect of how the figures are scaled. PLEASE be aware of this when viewing the following figures.**



Appendix B: 66-Dy-158 unresolved resonance parameters at 86.2 eV and 1000 eV

- Parameters are tabulated at 86.2 eV and 1000 eV, but no energies between these two
- There are 5 (L, J) states
- For all 5 the capture width is exactly the same at both energies
- The level spacing and elastic width are almost the same, within ~ 1%

In this case there is no question about what the widths and spacing are at any energy between 86.2 eV and 1000 eV; obviously the parameters are constant over this entire energy range, regardless of what interpolation law is used. The following plots illustrate the results based on cross section interpolation (NJOY) and parameter interpolation (PREPRO). **Let me stress the differences shown below are from the beginning of 2009. Since then NJOY has converted to parameter interpolation, and NJOY and PREPRO now closely agree.**

All Unresolved Parameters Energy Dependent

L Value---------- 0
Number of J Values---------- 1

Energy (eV)	Level Spacing (eV)	Competition Width (eV)	Neutron Width (eV)	Capture Width (eV)	Fission Width (eV)	Total Width (eV)
86.2000000	14.2979500	0.0	.002859589	.106000000	0.0	.108859589
1000.00000	14.2759200	0.0	.002855184	.106000000	0.0	.108855184

L Value---------- 1
Number of J Values---------- 2

Energy (eV)	Level Spacing (eV)	Competition Width (eV)	Neutron Width (eV)	Capture Width (eV)	Fission Width (eV)	Total Width (eV)
86.2000000	14.2979400	0.0	.002144691	.050000000	0.0	.052144691
1000.00000	14.2759200	0.0	.002141388	.050000000	0.0	.052141388
86.2000000	7.62373500	0.0	.001143560	.050000000	0.0	.051143560
1000.00000	7.61199200	0.0	.001141799	.050000000	0.0	.051141799

L Value---------- 2
Number of J Values---------- 2

Energy (eV)	Level Spacing (eV)	Competition Width (eV)	Neutron Width (eV)	Capture Width (eV)	Fission Width (eV)	Total Width (eV)
86.2000000	7.62373600	0.0	.001143560	.106000000	0.0	.107143560
1000.00000	7.61199200	0.0	.001141799	.106000000	0.0	.107141799
86.2000000	5.65740100	0.0	8.48610E-4	.106000000	0.0	.106848610
1000.00000	5.64868600	0.0	8.47303E-4	.106000000	0.0	.106847303

Appendix C: Examples of the Problem when Interpolating Cross Sections

All of the following examples compare NJOY [3] and PREPRO [2] results as of the beginning of 2009. At that time PREPRO interpolated parameters and NJOY interpolated cross sections**; this was the ONLY difference between their treatments, and as such is the only source of the differences that we see in the below figures.**

In these figures we see "bubbles" in the NJOY cross sections because of the difference between the 1/v-like results that we expect, and non-physical linear variation between the energies at which parameters are tabulated. For example, in the below first two plots of 66-Dy-158, parameters were tabulated first at 86.2 eV followed by 1 keV (an energy step of over a factor of 10). As a result we see differences of over 18% for elastic and 112% for capture; i.e., the capture is over twice as big as it should be because of this interpolation error. **Note that the differences in almost all cases overestimate the cross sections, so that not only does this introduce an ERROR, but also a BIAS.**

Since then based on the differences that we found, NJOY has converted from cross section to parameter interpolation. As a result, today both NJOY and PREPRO produce very similar results, corresponding to the PREPRO results shown below.

The bottom line is that today both NJOY and PREPRO are using some form of the original ENDF-102 convention to interpolate unresolved parameters between the energies at which they are tabulated, rather than the newer approximate convention to interpolate cross sections. This is being done because results based on cross section interpolation are a poor approximation, resulting in non-physical cross sections, that even a casual reader can see in the below examples.

This might seem to contradict the current ENDF-102 recommendation to interpolate cross sections, except that the ENDF-102 recommendation also says,

It is recommended that evaluators provide the URP's on a mesh dense enough that the difference in results of interpolating on either the parameters or the cross sections be small. A 1% maximum difference would be ideal, but 5% is probably quite acceptable.

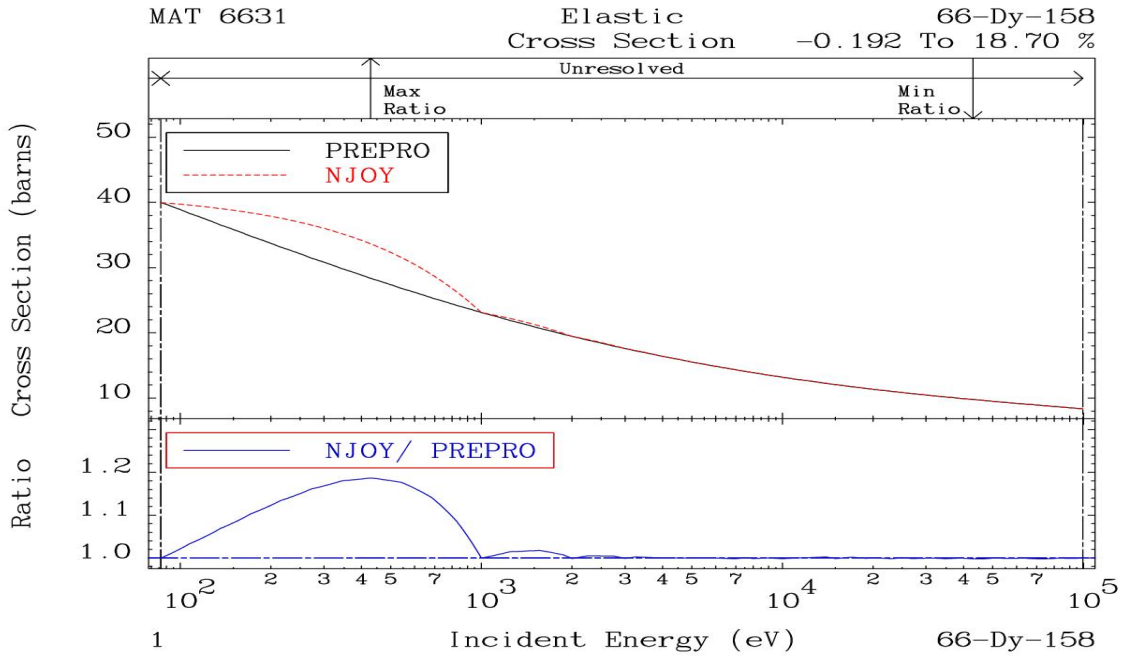
Recently this was further clarified in ENDF-102 to state,

When evaluators do not supply parameters on a dense enough grid processing codes should interpolate parameters to a finer energy grid until this criteria is met.

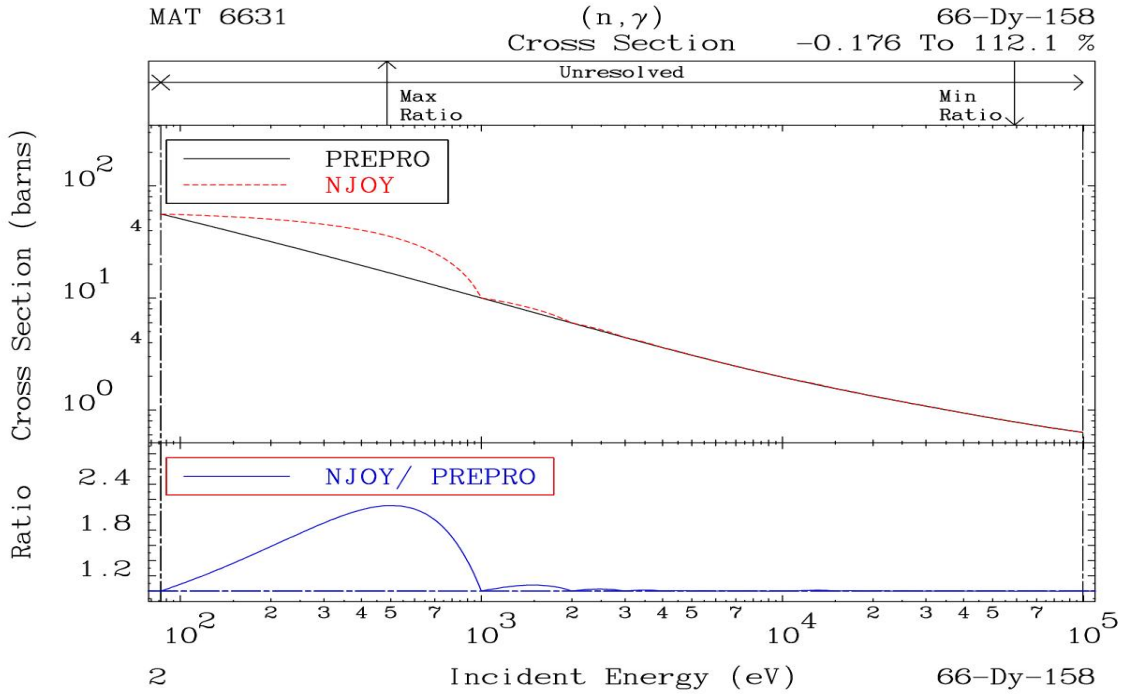
It is important to understand that currently NO evaluation (ENDF/B-VII, JEFF, JENDL, CENDL,…) includes parameters tabulated on a mesh dense enough to avoid large differences. **As a result the current ENDF-102 rules tell us that processing codes, such as NJOY and PREPRO, MUST interpolate parameters to a finer energy grid, which is what they are doing TODAY.**

Comparisons of NJOY and PREPRO infinitely dilute unresolved resonance region

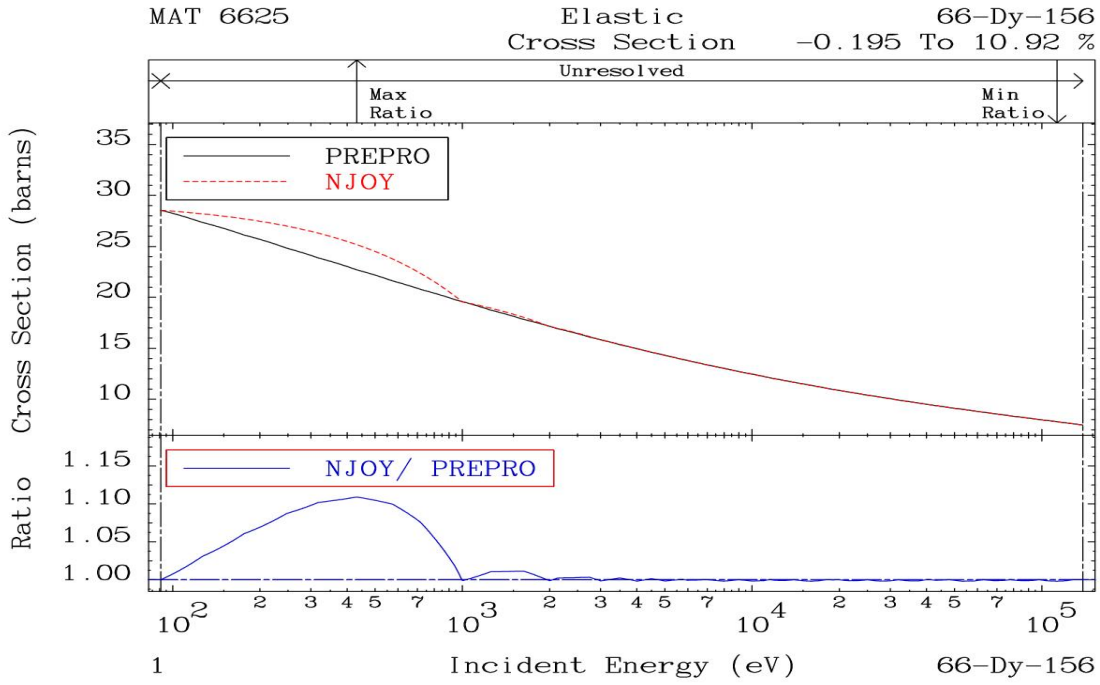
66-Dy-158 elastic (MT=2): 18% difference



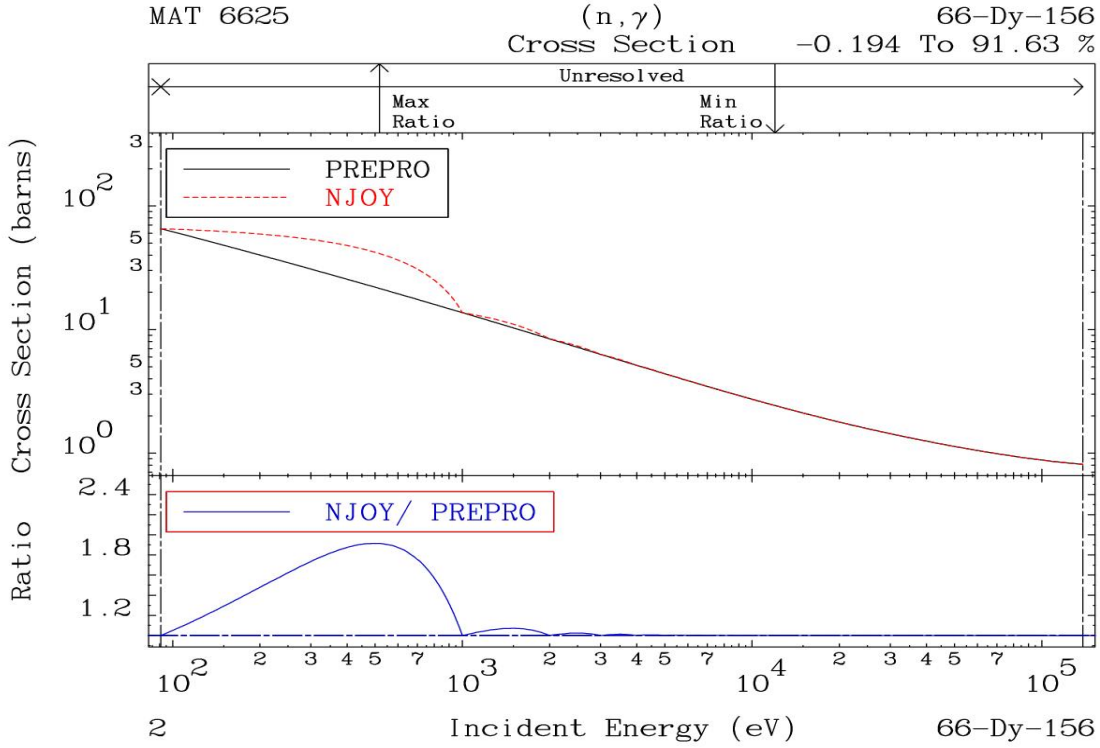
66-Dy-158 capture (MT=102): 112% difference



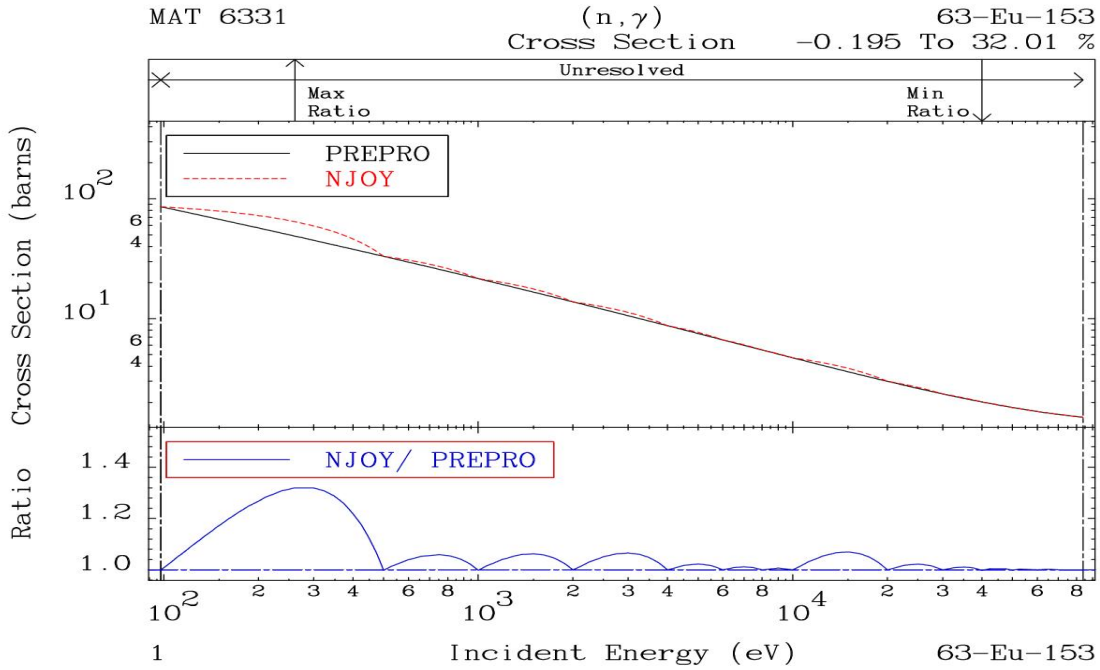
66-Dy-156 elastic (MT=102): 11% difference



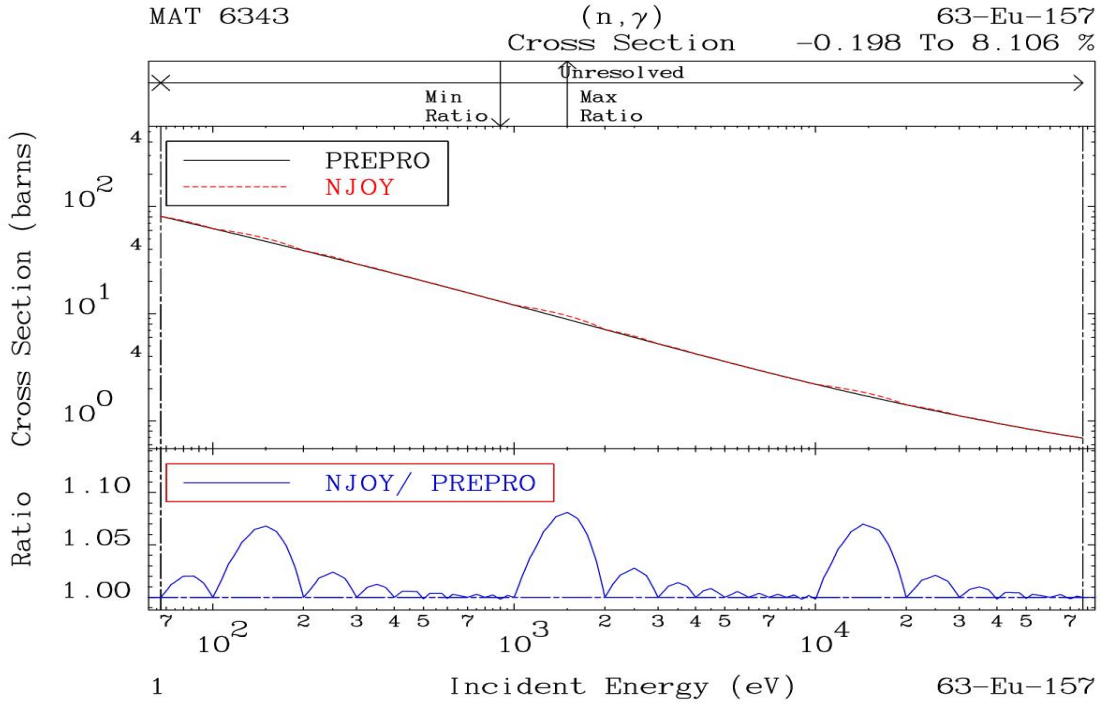
66-Dy-156 capture (MT=102): 91% difference



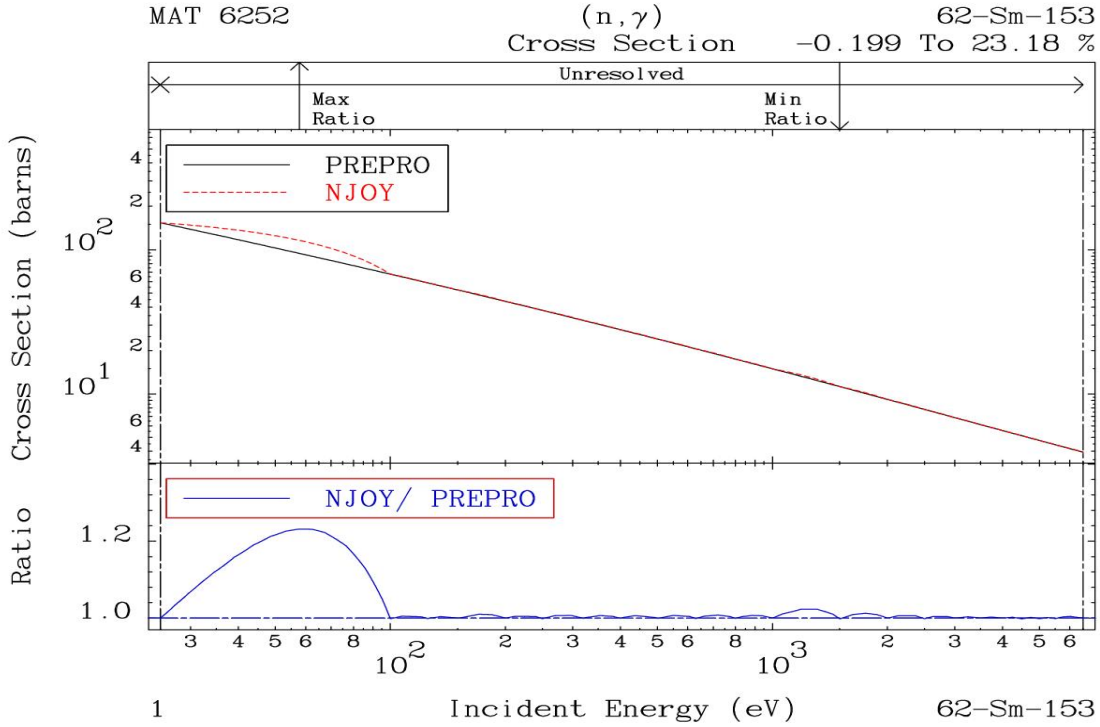
63-Eu-153 capture (MT=102): 32% difference



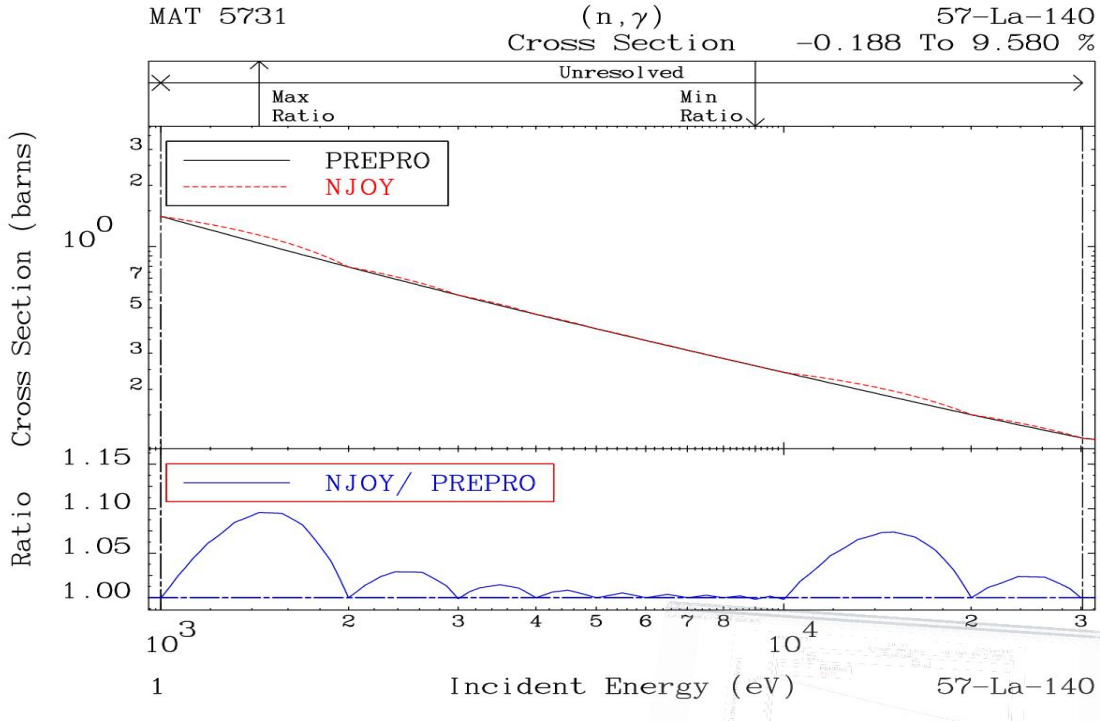
63-Eu-157 capture (MT=102): 8% difference



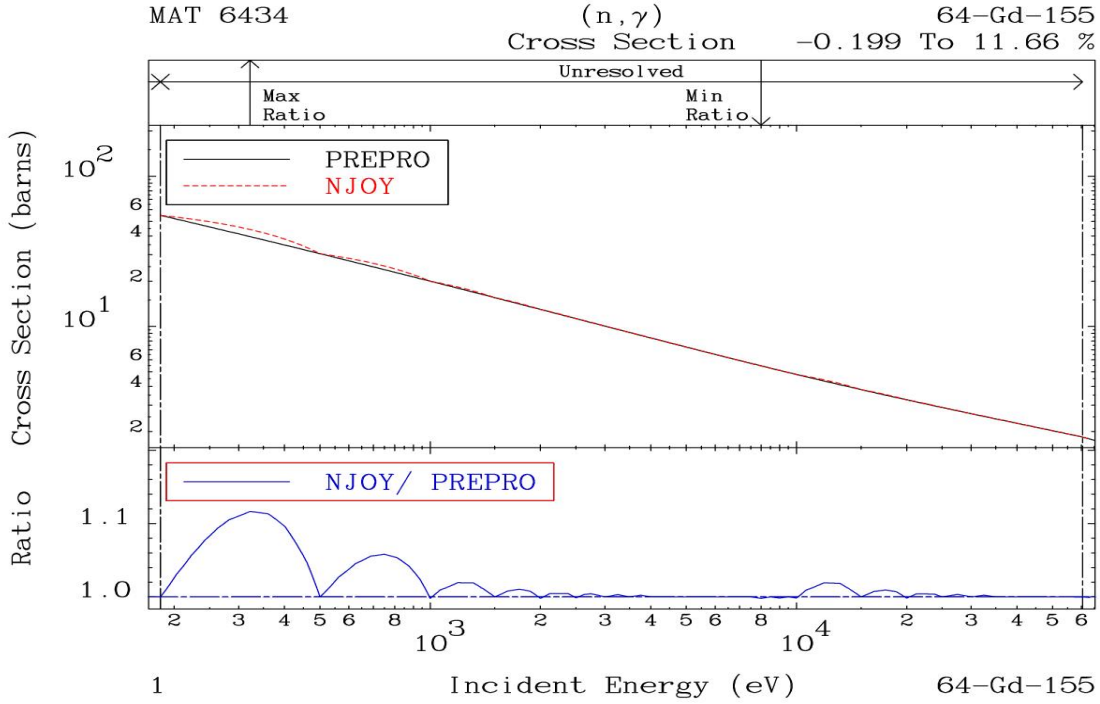
62-Sm-153 capture (MT=102): 23% difference



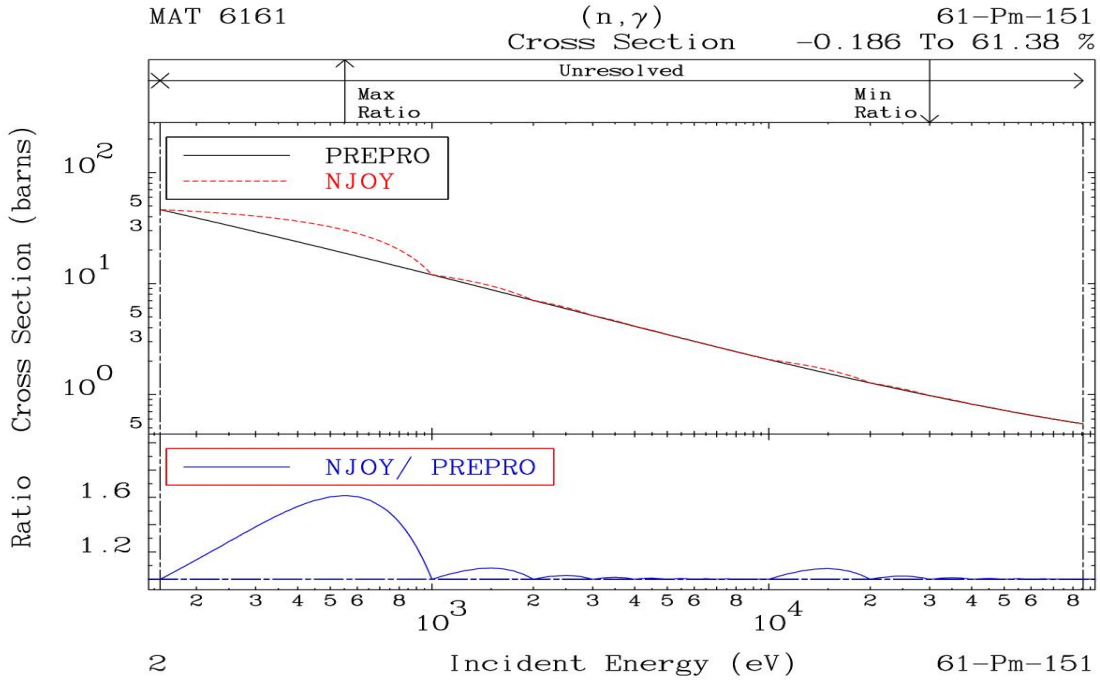
57-La-140 capture (MT=102): 9% difference



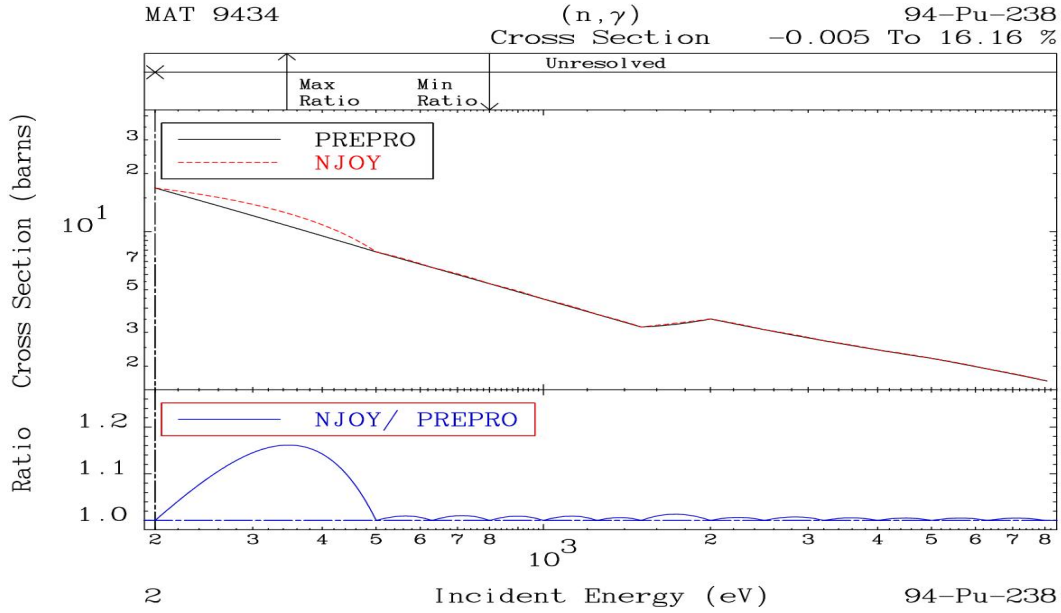
64-Gd-155 capture (MT=102): 11% difference



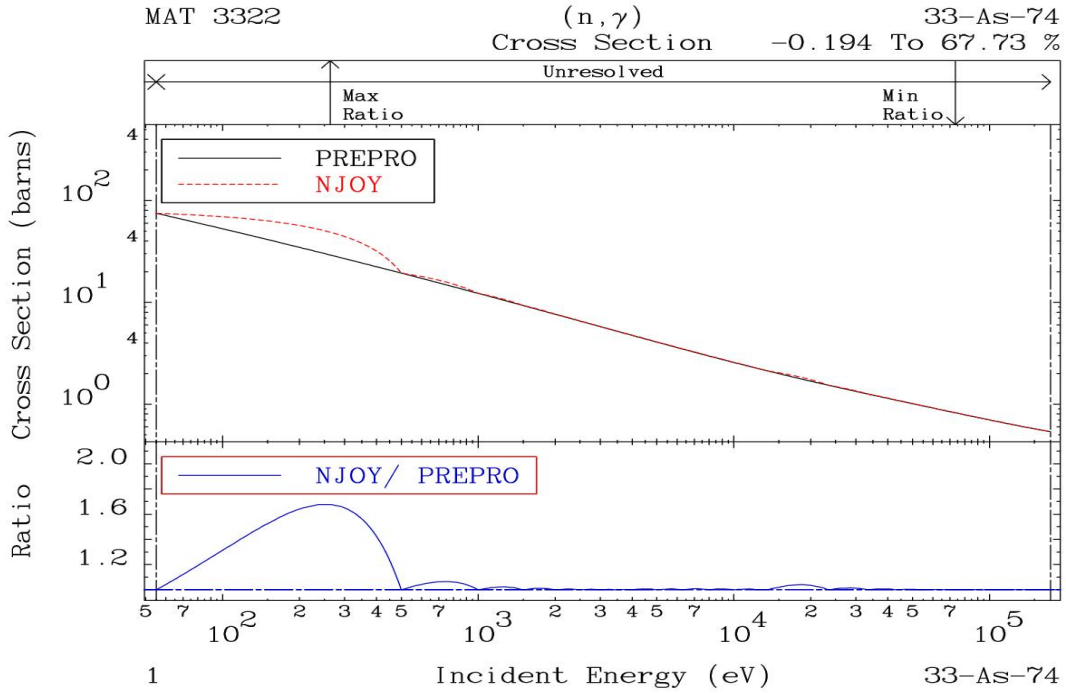
61-Pm-151 capture (MT=102): 61% difference



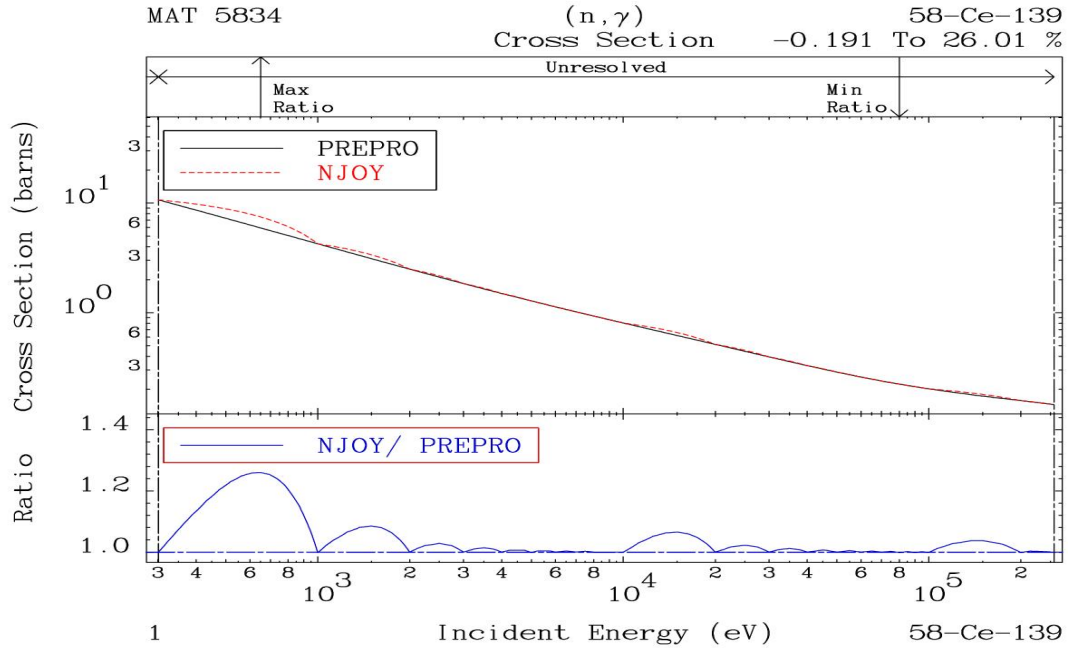
94-Pu-238 capture (MT=102): 16% difference



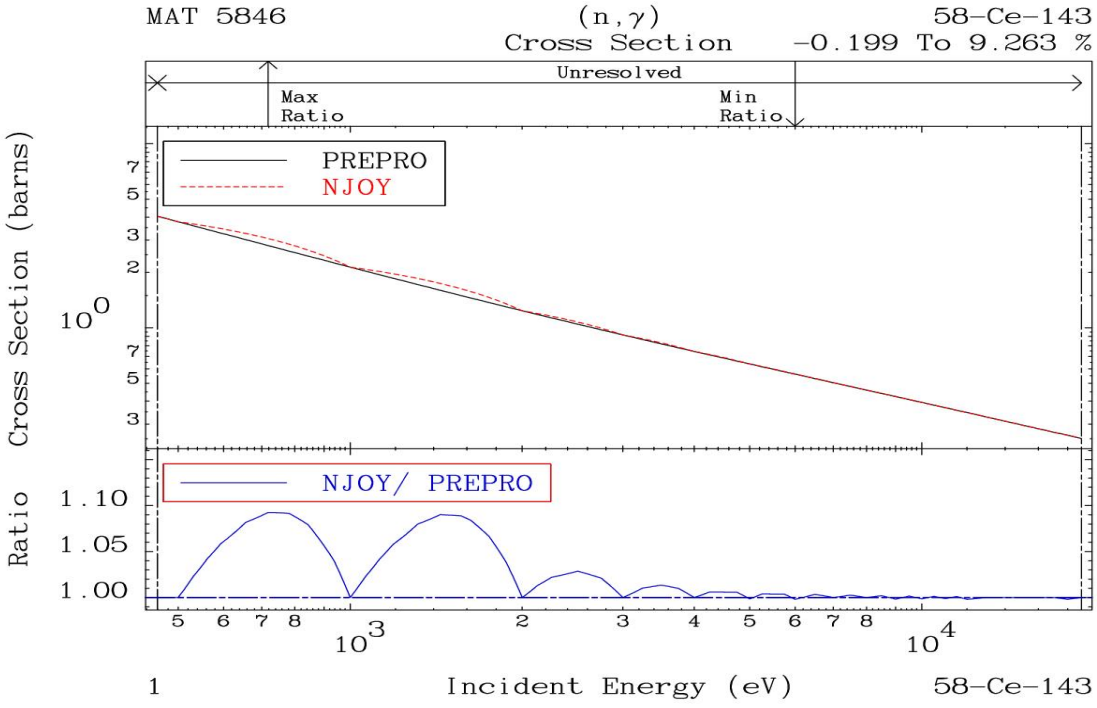
33-As-74 capture (MT=102): 67% difference



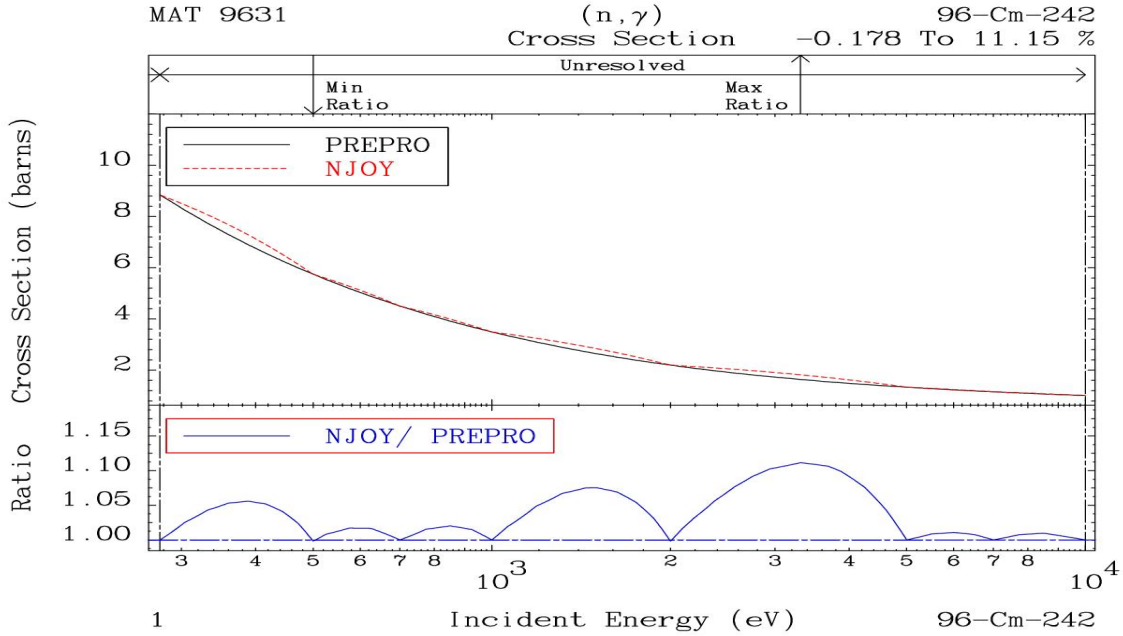
58-Ce-139 capture (MT=102): 26% difference



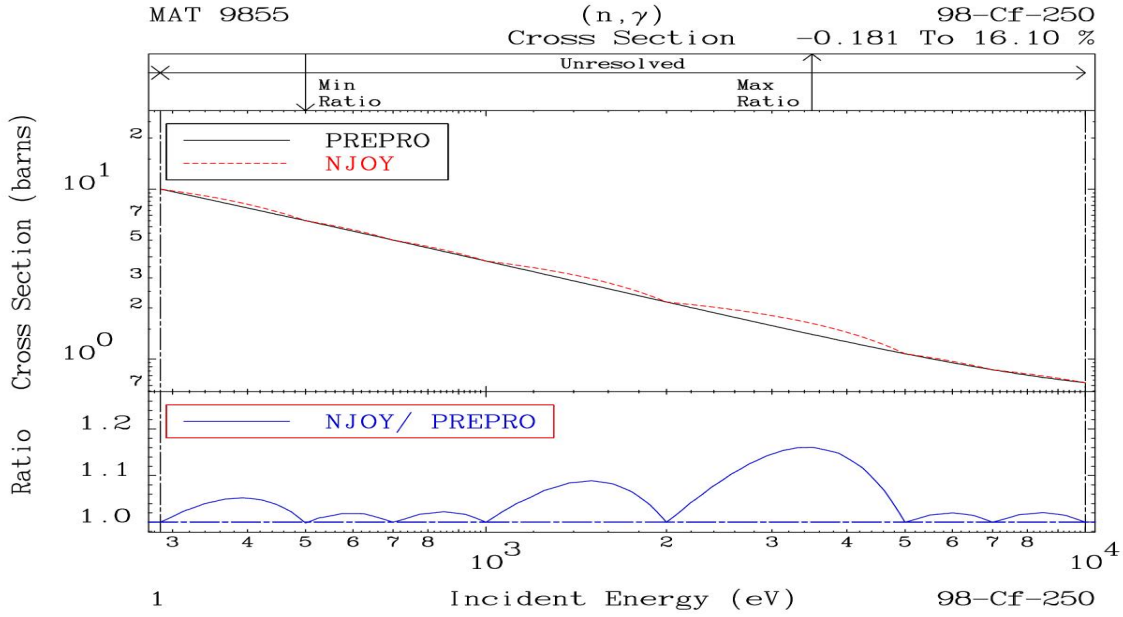
58-Ce-143 capture (MT=102): 9% difference



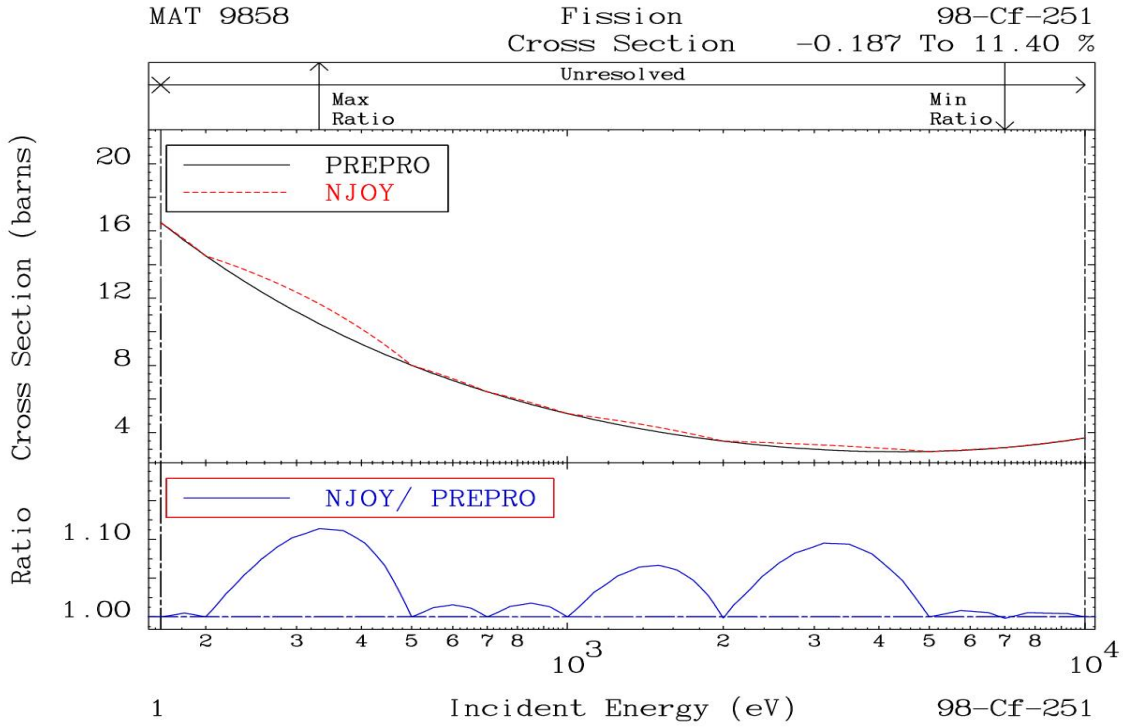
96-Cm-242 capture (MT=102): 11% difference



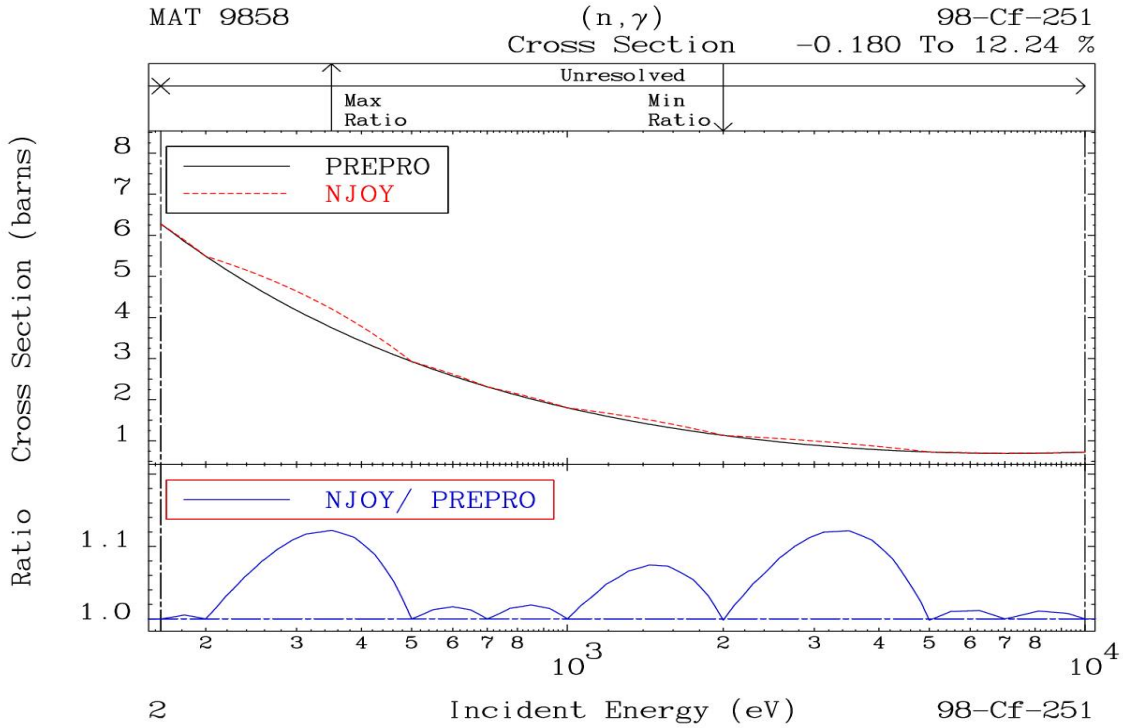
98-Cf-250 capture (MT=102): 16% difference



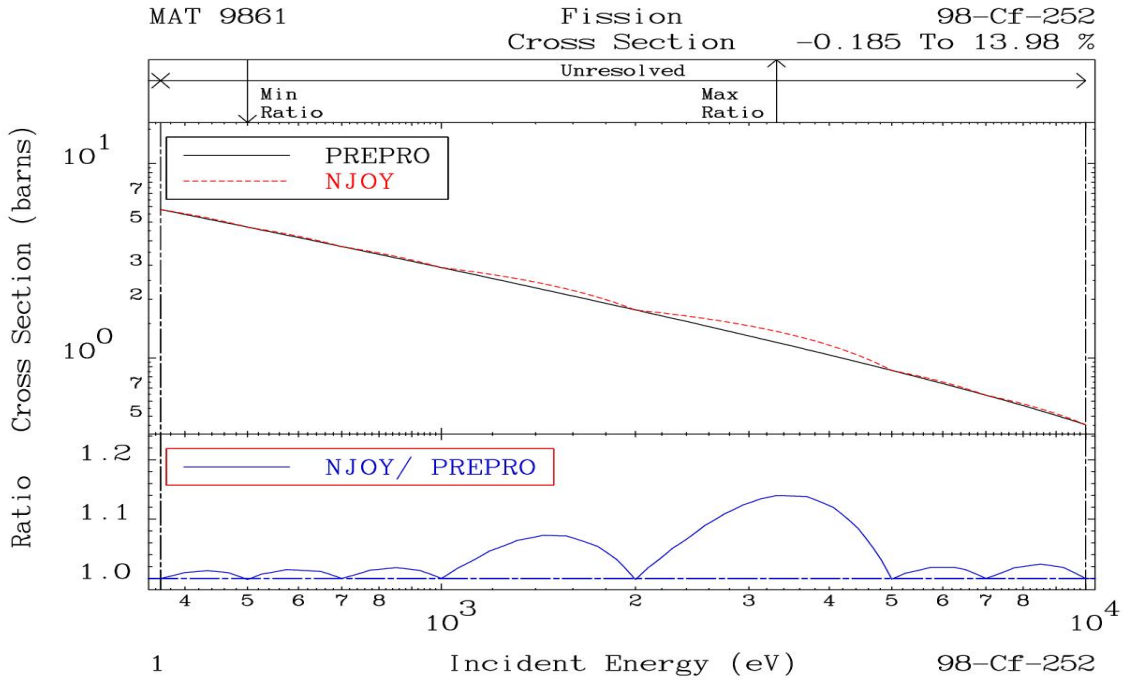
98-Cf-251 fission (MT=18): 11% difference



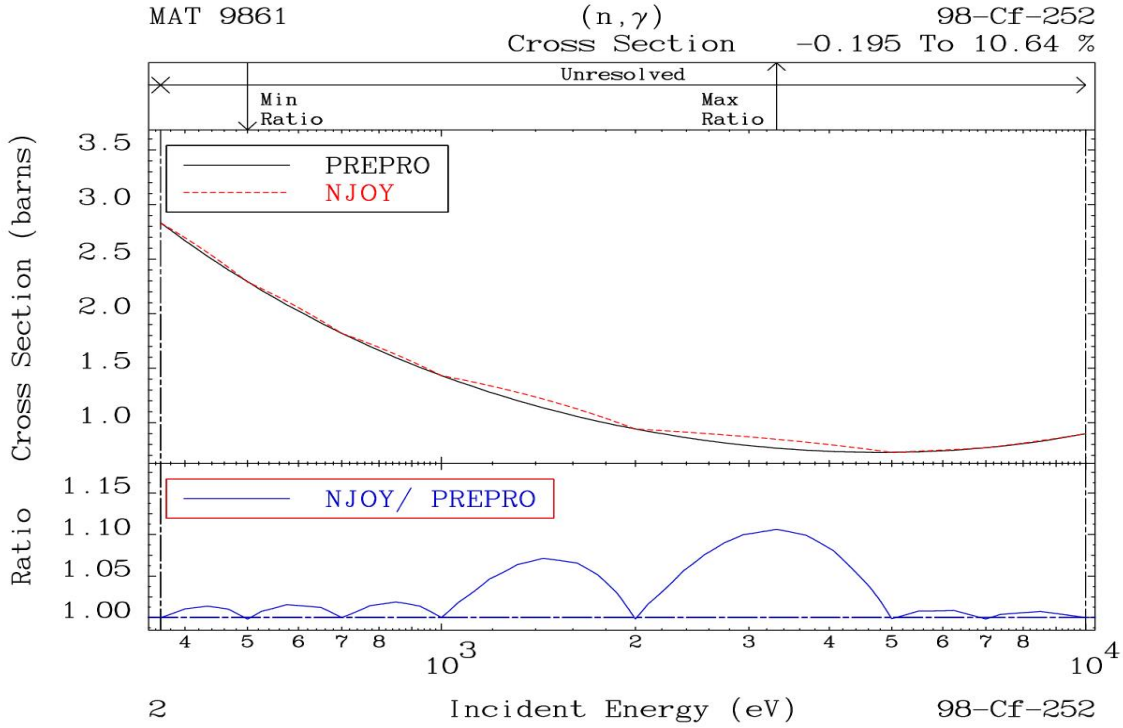
98-Cf-251 capture (MT=102): 12% difference



98-Cf-252 fission (MT=18): 14% difference



98-Cf-252 capture (MT=102): 10% difference



98-Cf-253 fission (MT=18): 9% difference