# Unresolved Resonance Range format, formalism and interpretation

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# ENDF-102 URR formalism

- Only the SLBW LRF=1 formalism for ur parameters is allowed

- Single level Breit-Wigner;
  no resonance-resonance interference
  one single-channel inelastic competitive reaction allowed

- LSSF flag
  LSSF=0, MF-3 contains partial background to be added
  LSSF=1, MF-3 contains infd xs, MF-2 is used solely for the calculation of self-shielding factor ssf

- Inconsistency

$\Gamma_x$ can be given if LRF=2, in U238 accounted for by CALENDF but not by NJOY, PREPRO, PURM or AUROX that read in the infd xs in MF-3 disregarding the competition widths in MF-2.

# Direct cross section contributions

- LSSF=1

- One need to be sure that the direct inelastic (that is not accounted for in MF-2 assembly) has been added to the compound one

- Direct and compound angular distribution are very different, direct is forward peaked while compound is more symmetrical

- With LSSF=1 the “direct” component can be added as “background”, but the MF-4 (angular distribution) is the same !!

- For Pu239 : direct component 18.1% at 3.00E+05

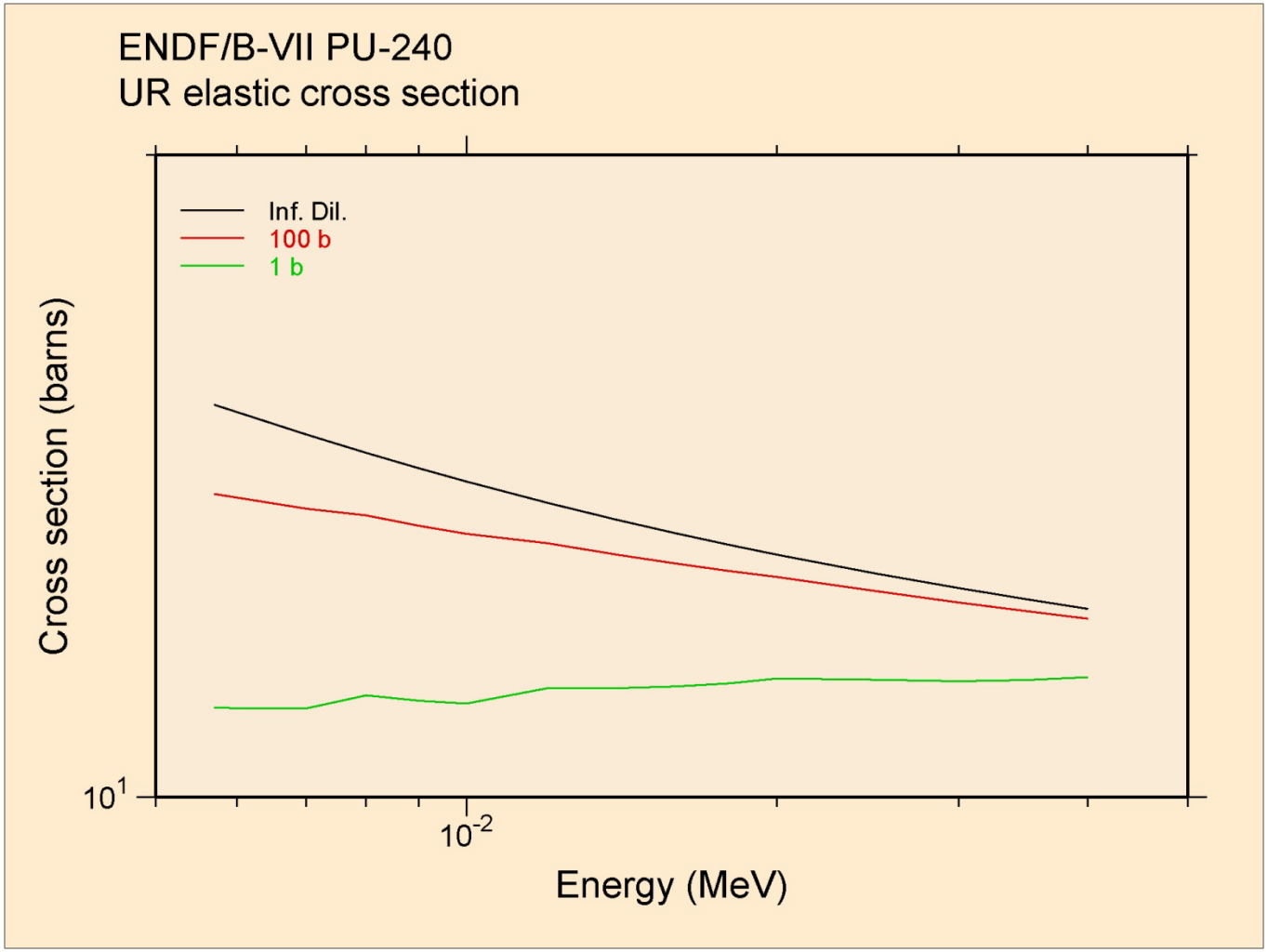
**TALYS U-238**

Discrete Inelastic cross section - Level 1, Spin= 2.0 Parity= +, Direct component contributions to the total level

| Energy | Direct |
|---|---|
| 5.00E+04 | 0.80% |
| 5.50E+04 | 0.97% |
| 6.00E+04 | 1.15% |
| 8.00E+04 | 1.87% |
| 1.00E+05 | 2.55% |
| 1.20E+05 | 3.19% |
| 1.40E+05 | 3.74% |
| 1.60E+05 | 4.24% |
| 1.80E+05 | 4.69% |
| 2.00E+05 | 5.08% |
| 2.04E+05 | 5.15% |
| 2.06E+05 | 5.19% |
| 2.08E+05 | 5.22% |
| 2.10E+05 | 5.26% |
| 2.16E+05 | 5.36% |
| 2.20E+05 | 5.42% |
| 2.22E+05 | 5.46% |
| 2.24E+05 | 5.49% |
| 2.26E+05 | 5.52% |
| 2.30E+05 | 5.58% |
| 2.50E+05 | 5.87% |
| 2.60E+05 | 6.01% |
| 2.70E+05 | 6.14% |
| 2.80E+05 | 6.27% |
| 2.90E+05 | 6.39% |
| 3.00E+05 | 6.51% |

# Pu-240 ur, PT derived ssf impact, new graphs

SSF's are channels dependent MT=1,2,102 18 and 4 (4 only for CALENDF PT's)

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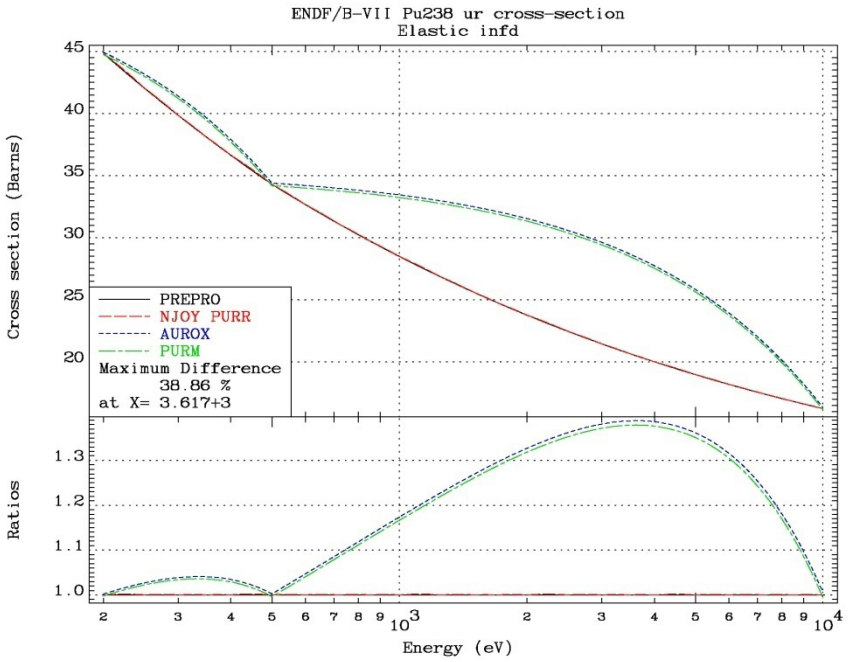
# Unresolved resonance range computation

New in NJOY-296 (not -259)
PREPRO since many years

- Parameter against cross section interpolation impact
- INT = 5 not accounted for AUROX or PURM




| Evaluation | UR range (eV) | Points/decade | INT | LSSF | Shape |
|---|---|---|---|---|---|
| W-184 | 2.65E+03- 1.00E+05 | 3 / 2.5 | 5 | | lin-lin |
| U-233 | 6.00E+02- 4.00E+04 | 17 | 2 | 1 | rough |
| U-238 | 2.00E+04- 1.49E+05 | 18 | 5 | 1 | lin-lin, Gx |
| Pu-238 | 2.00E+02- 1.00E+04 | constant | | | |
| Pu-239 | 2.50E+03- 3.00E+04 | 48 | 2 | | rough |
| Pu-240 | 5.70E+03- 4.00E+04 | constant | | | |

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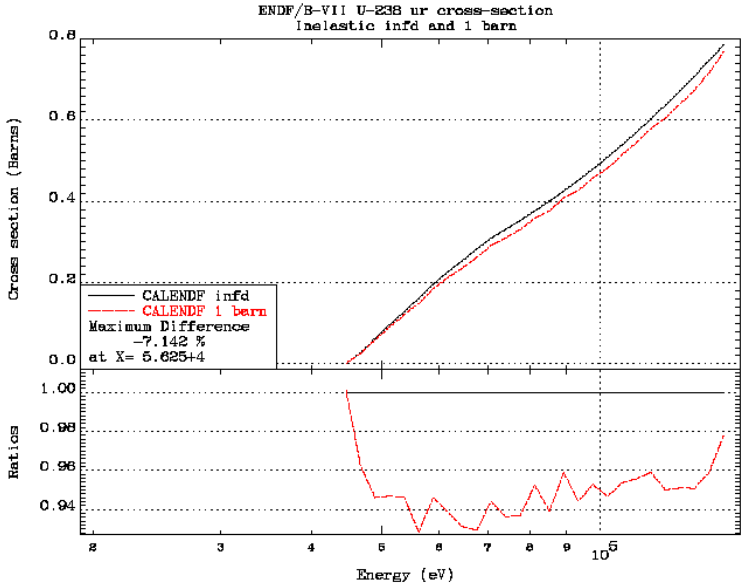
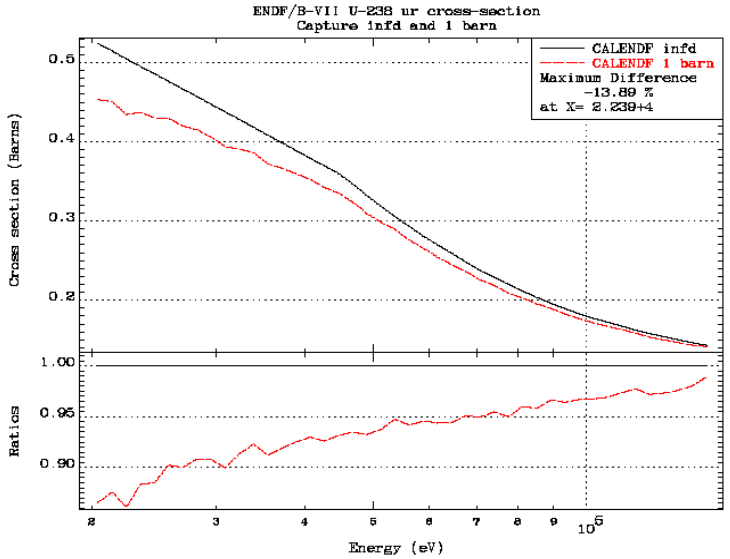
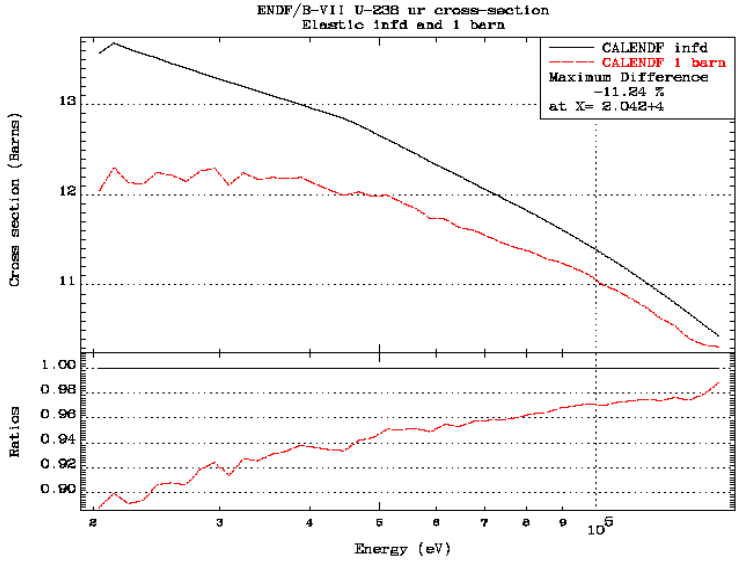
# CALENDF PT's U-238 self-shielded cross-section




Inelastic 7% (unique..)
Capture 14%
Elastic 11%

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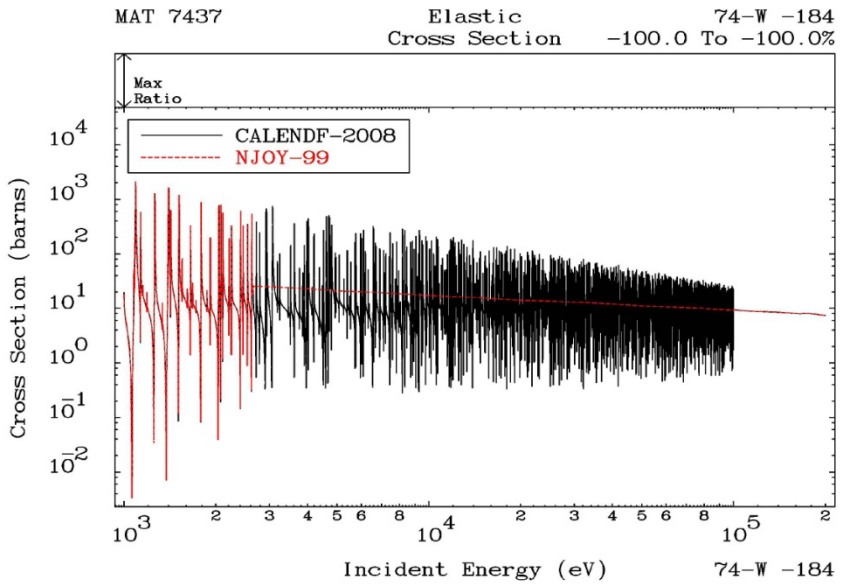
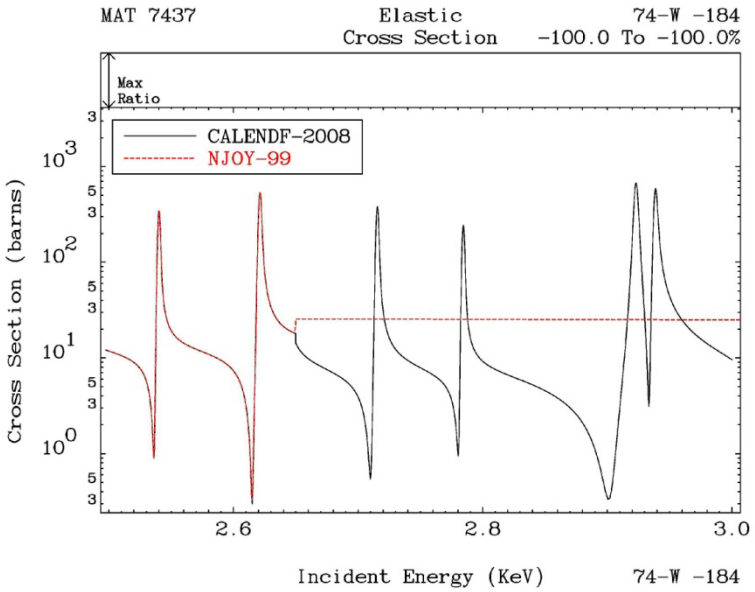
# CALENDF pointwise data – W-184




Statistically generated resonances

Peak and depress

Different SSF

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# Effective cross sections comparisons

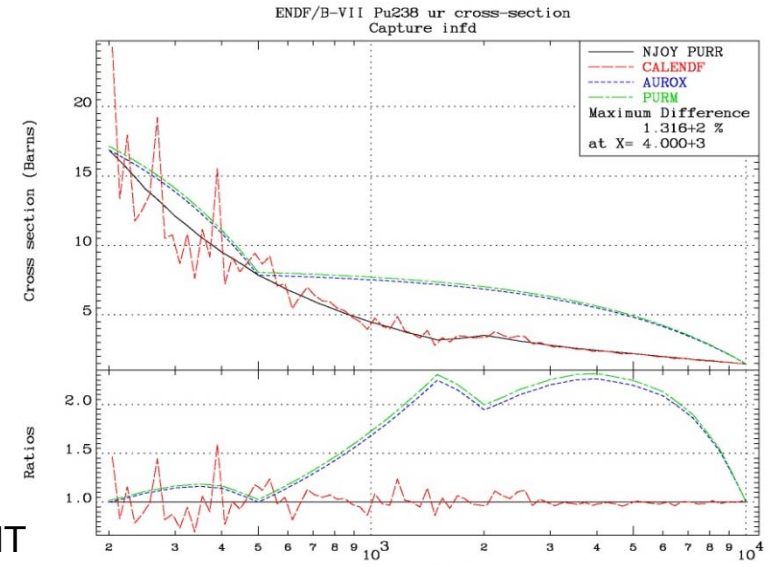
- Four different processing codes; NJOY-PURR, CALENDF, AUROX and PURM on the six evaluations

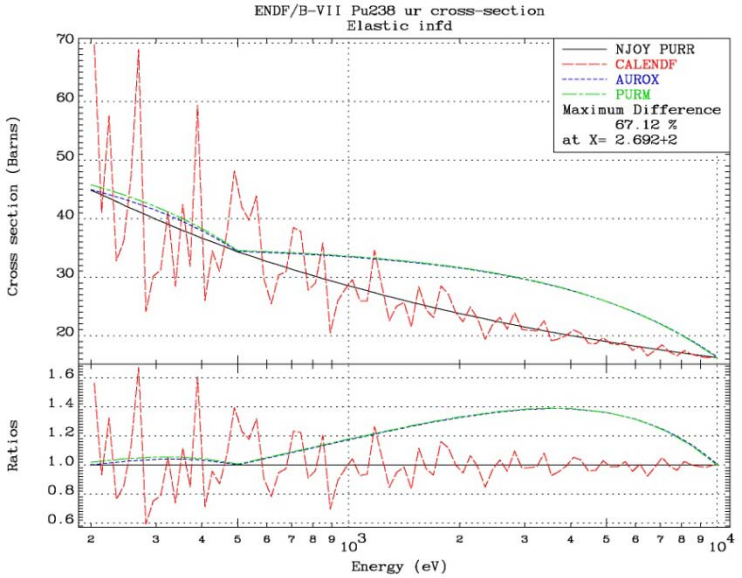
- Those isotopes have been chosen to encompass most cases encountered in the unresolved energy range of any ENDF/B-VII or JEFF-3.1.1 evaluations.

- The minimum energy encountered for an unresolved range is 1 eV and the maximum is 1 MeV.

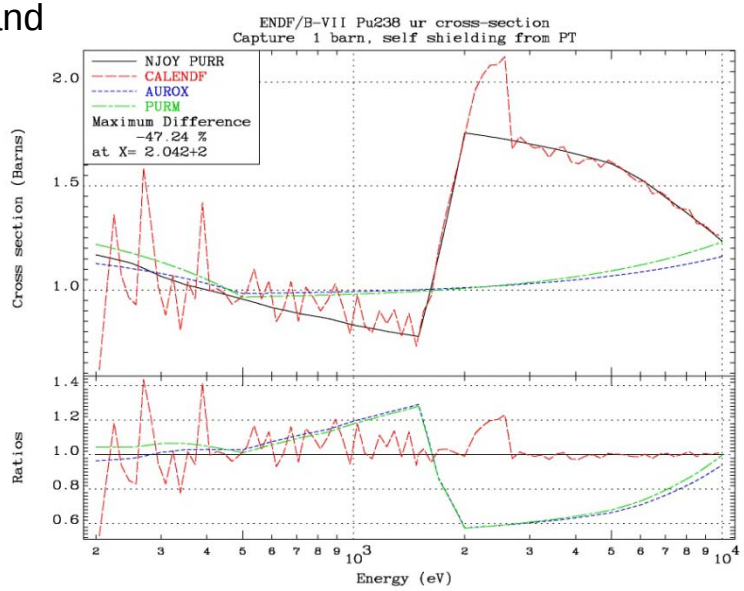
- What was asked of the participants were all unresolved range cross-sections in the unresolved range of those six ENDF/B-VII evaluations, at 293.6 Kelvin, both infinitely dilute, and 1 barns, in simple 2E11.4 column format. However simple this may seem, it took quite a few iterations to finalize the series of graphs in this section

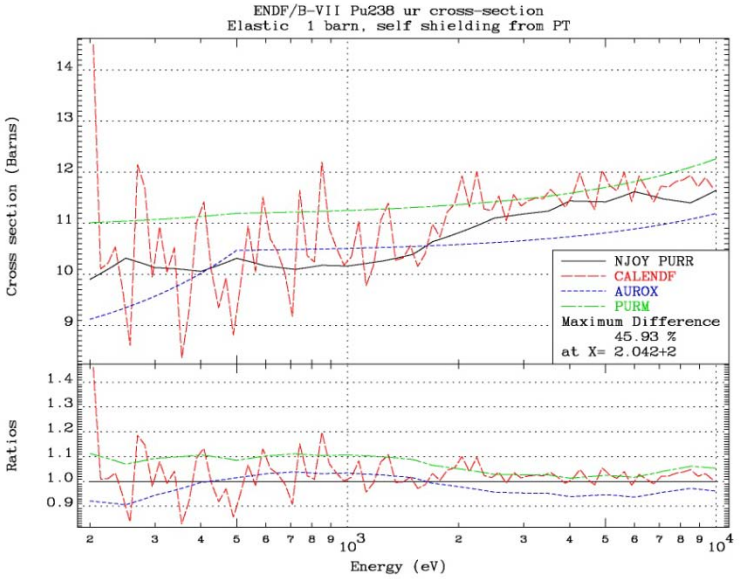
# Pu238 UR cross sections, INT = 5




Missing INT for AUROX and PURM

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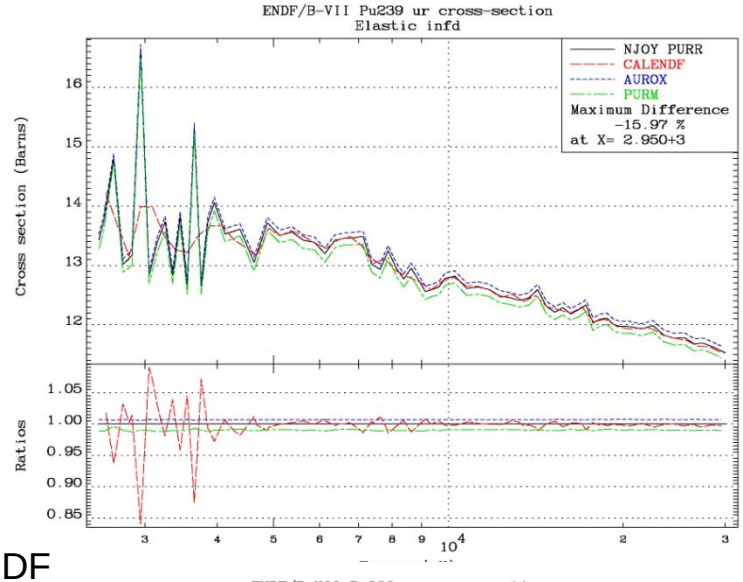
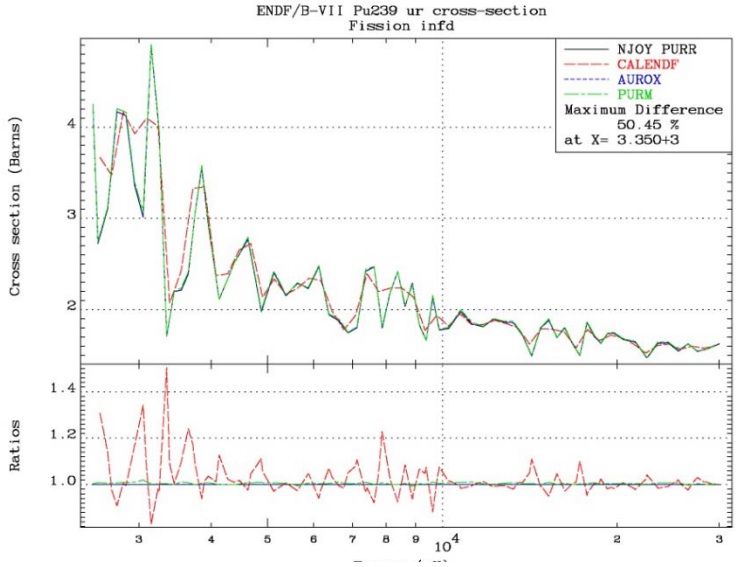
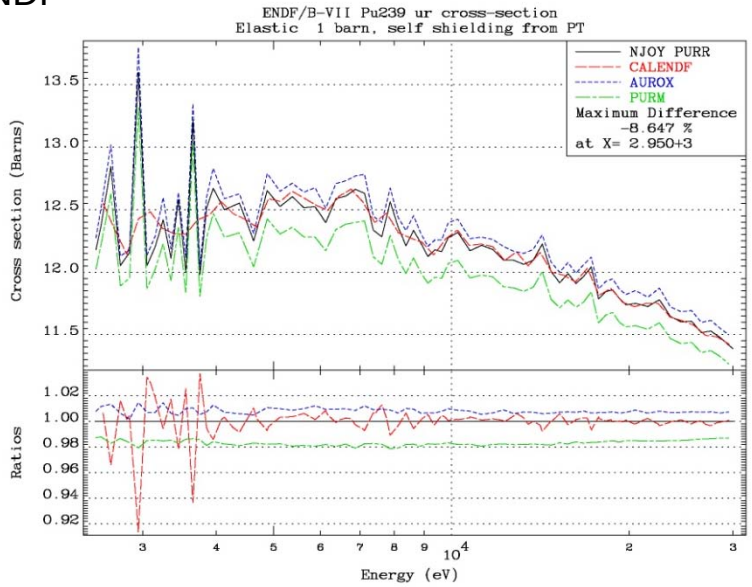
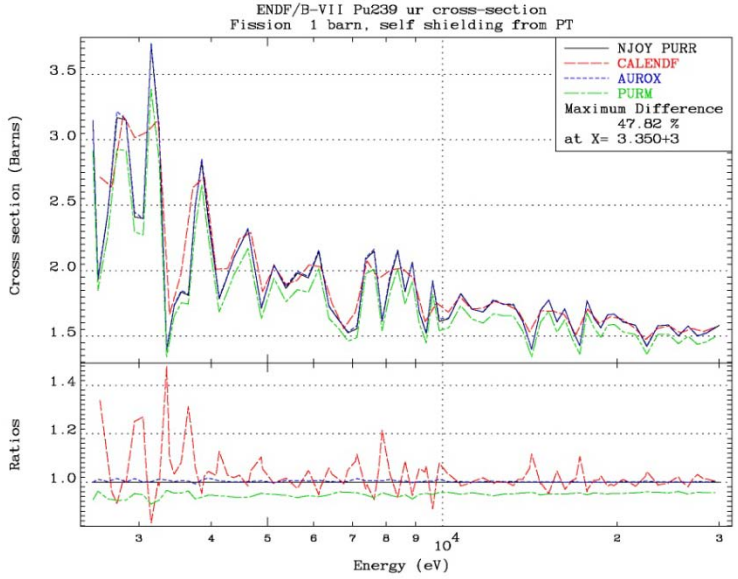
# Pu239 UR cross sections, AUROX corrected




Only CALENDF differs

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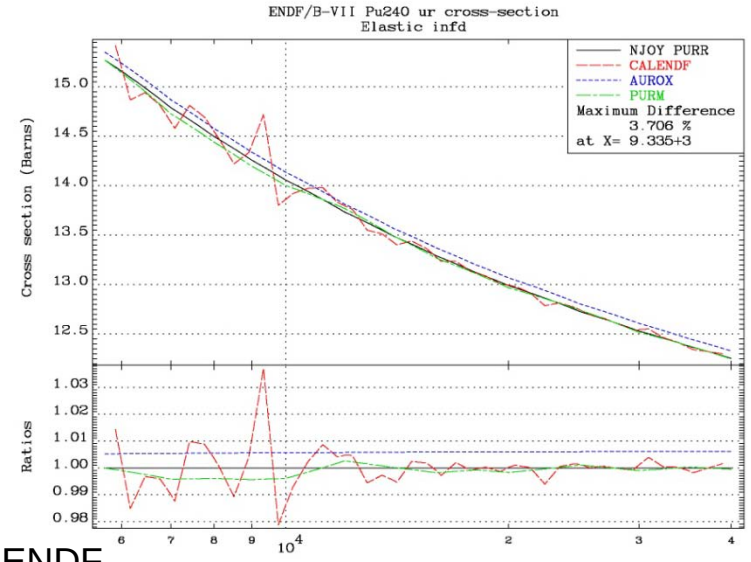
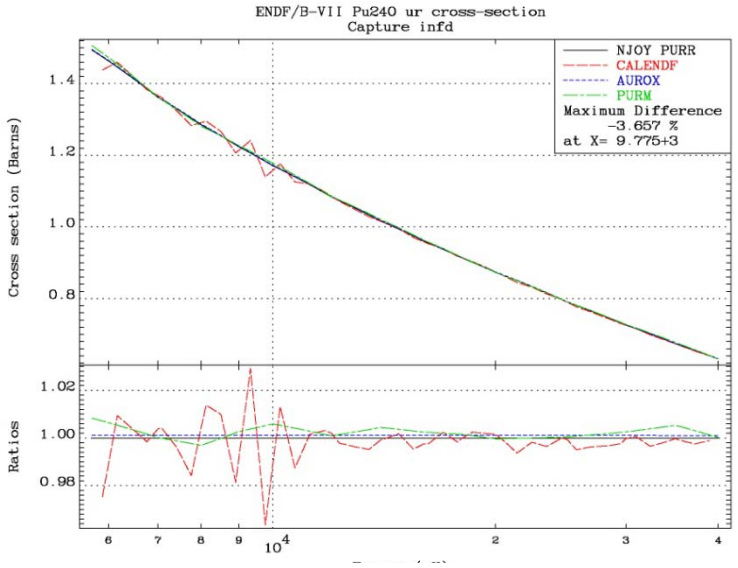
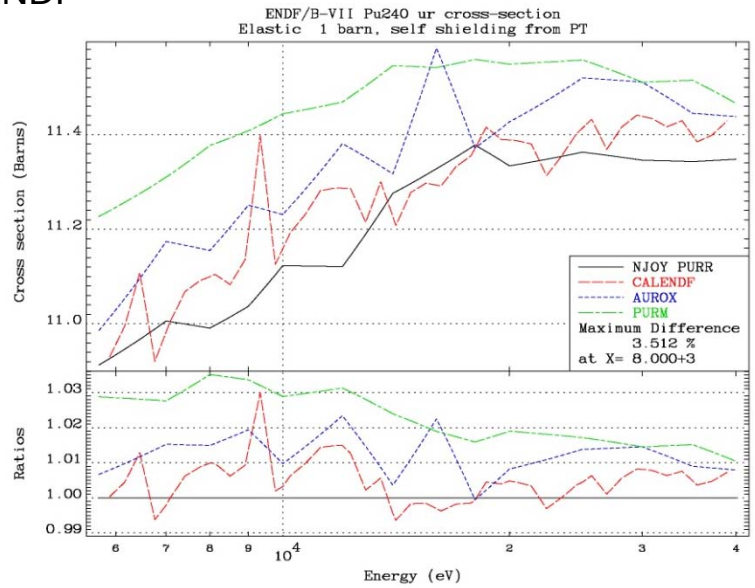
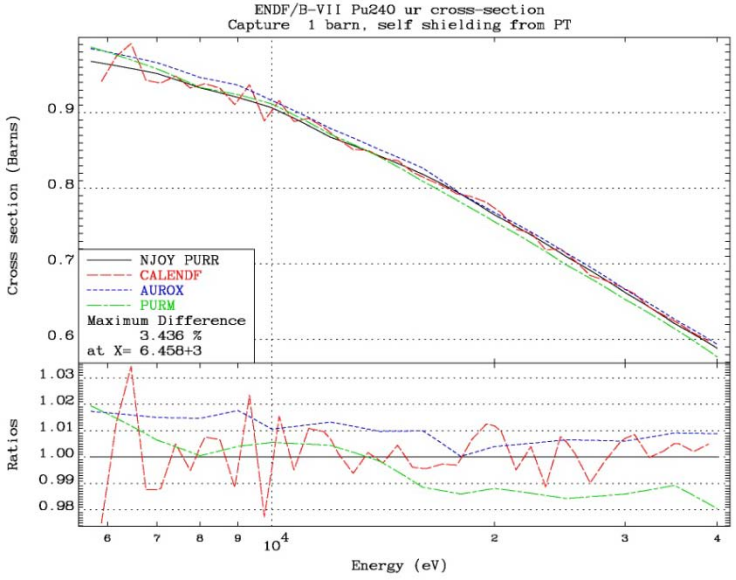
# Pu240 UR cross sections, PURM corrected




Only CALENDF differs

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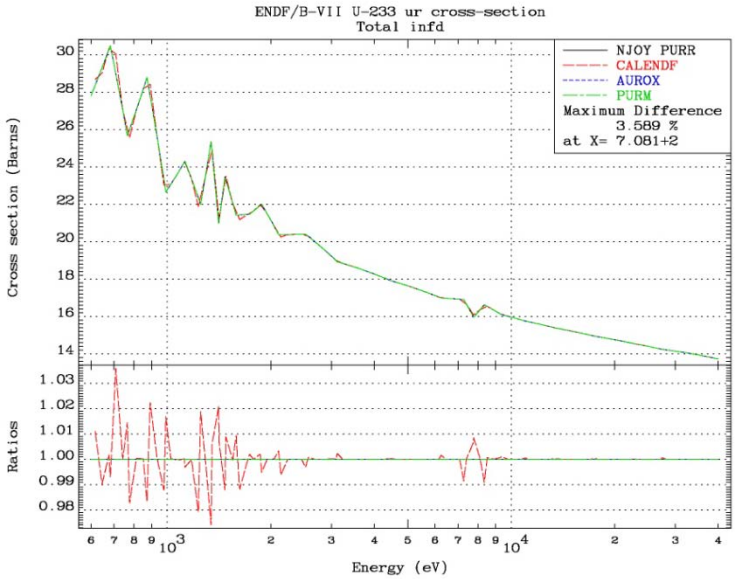
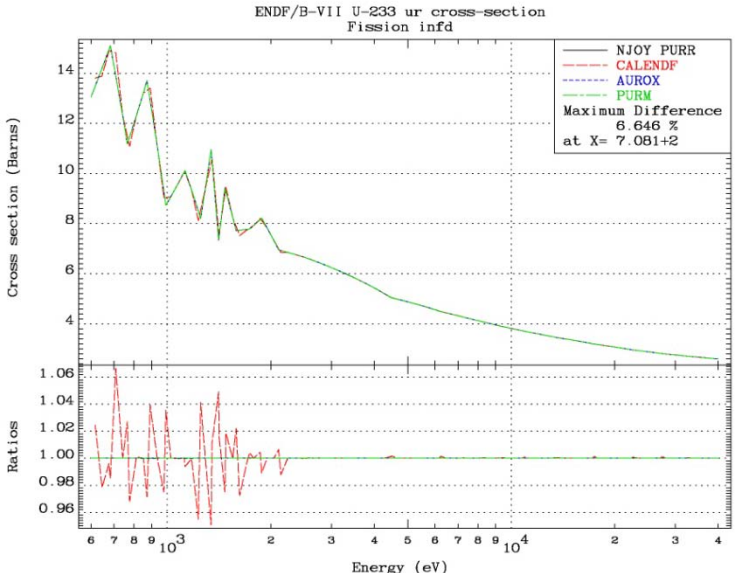
# U233 UR cross sections, 20% at 1 barn, LSSF=1

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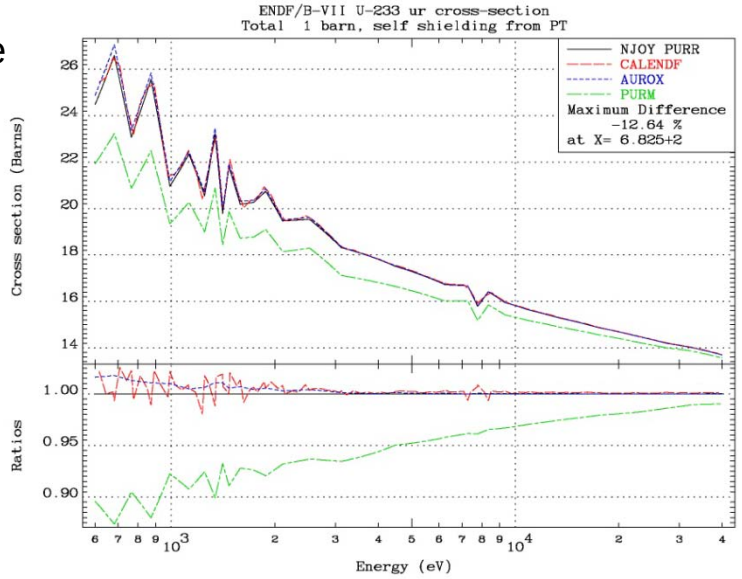
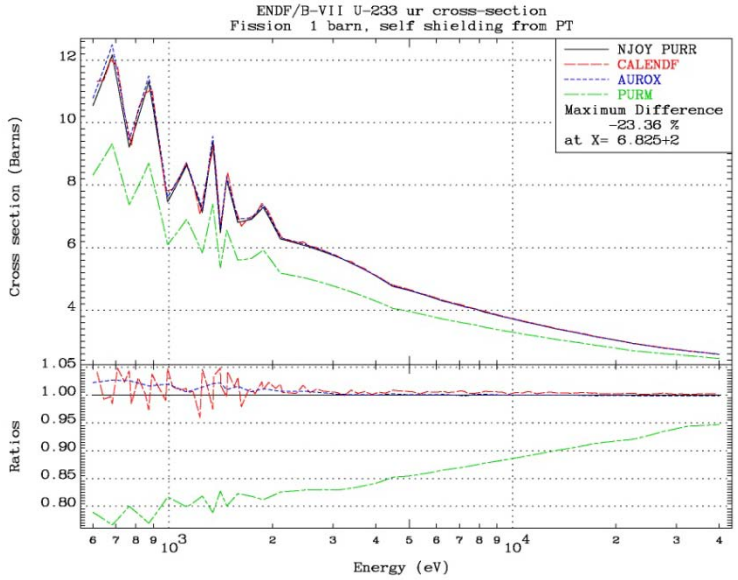
1 barn not acceptable

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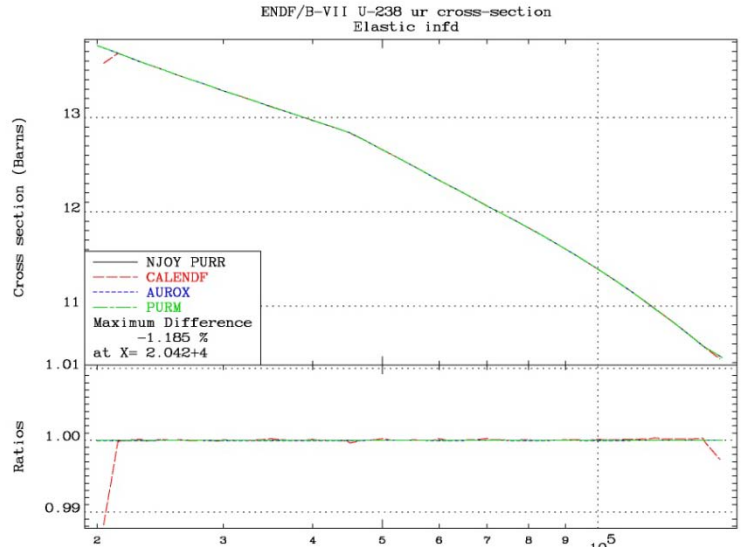
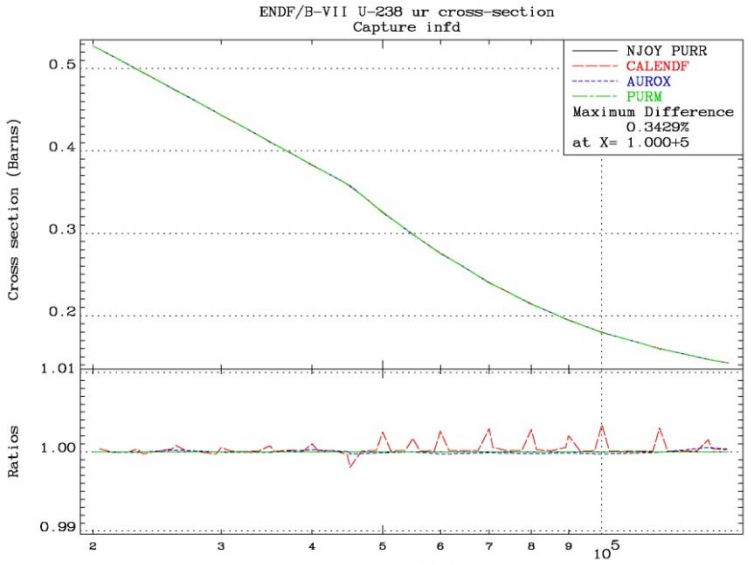
# U-238 UR cross sections, 1 to 2% at 1 barn, LSSF=1

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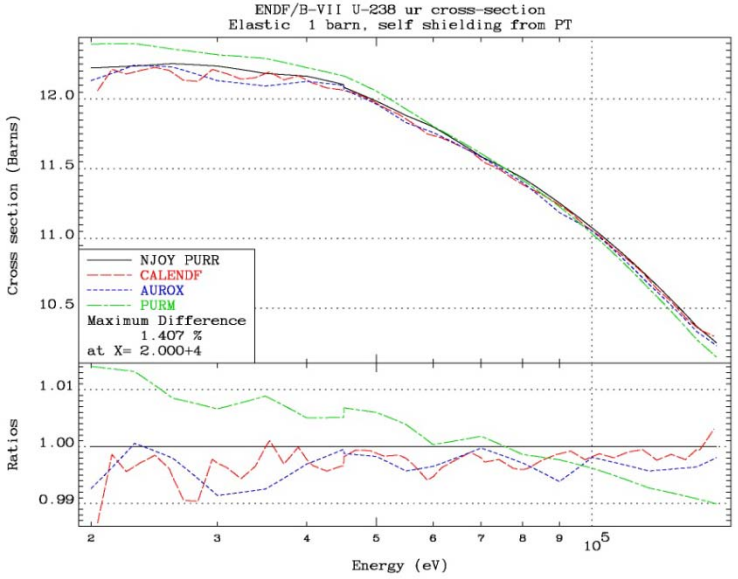


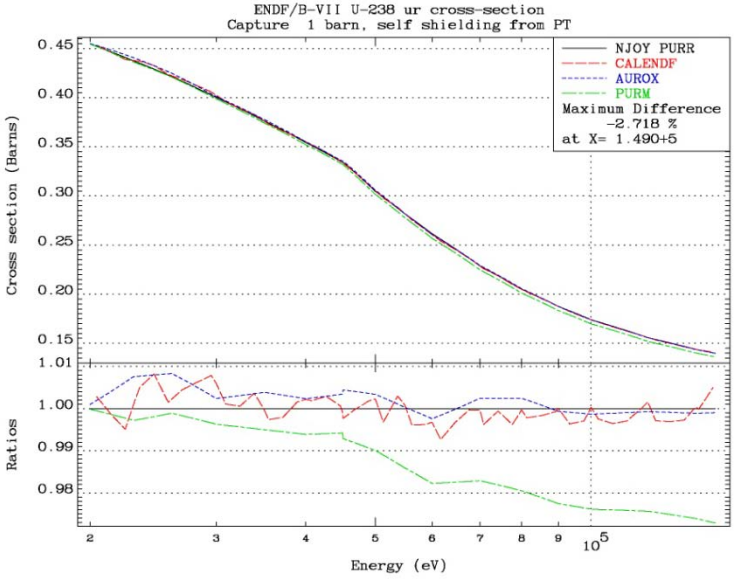


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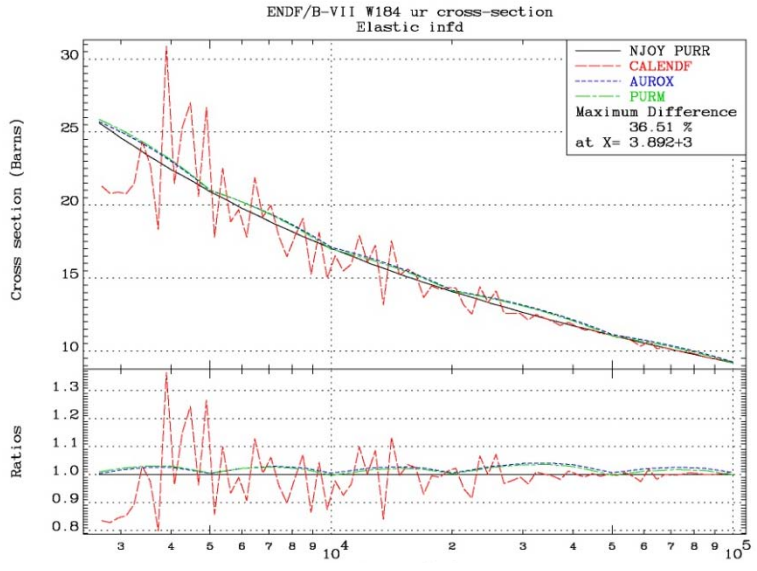
# W-184 UR cross sections, 20% at 1 barn

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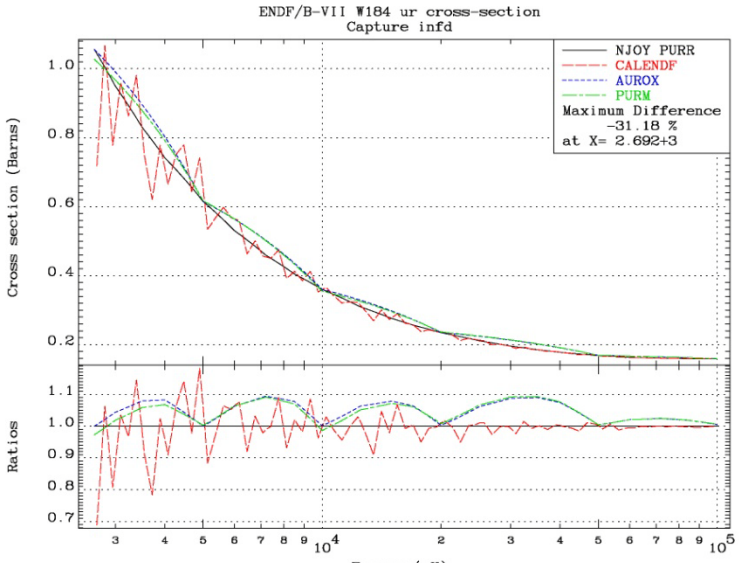
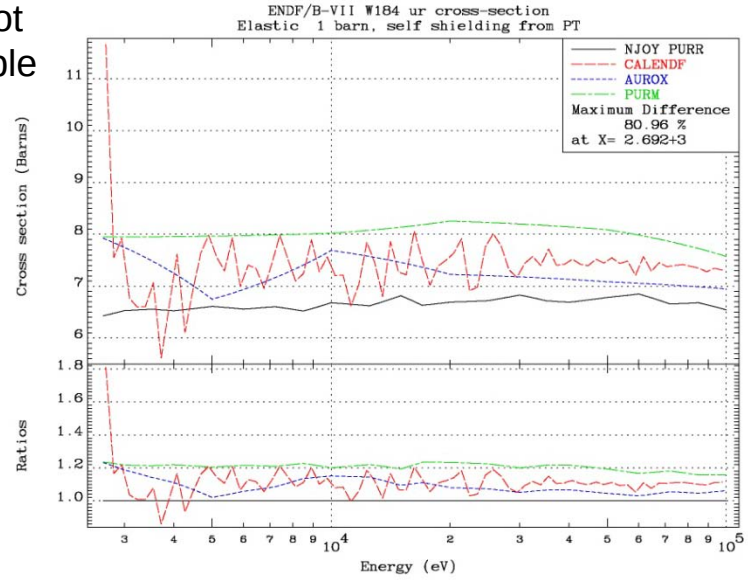
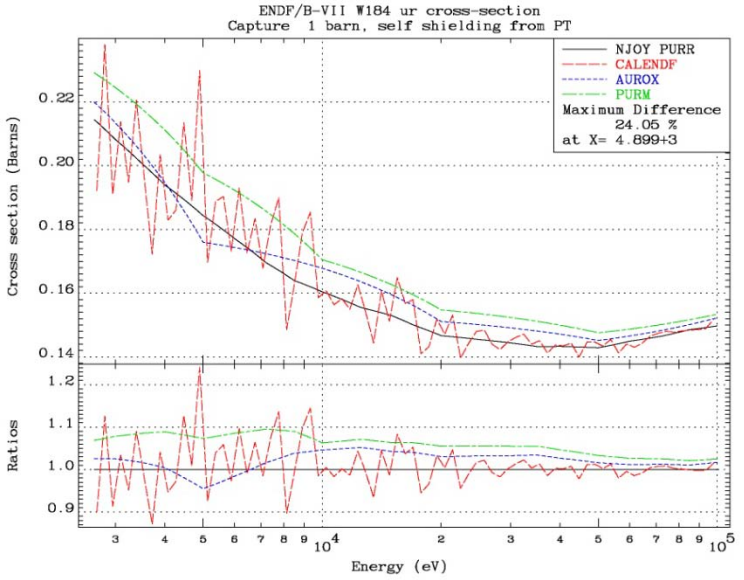



1 barn not acceptable

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# Conclusions

- The primary conclusion is that these four processing codes usually agree within a target accuracy of 1% for both infinitely dilute and 1-barn self-shielded effective cross sections (with the exception of PURM) **when the parameters files data and ENDF-102 rules have been properly and consistently** interpreted by both the evaluators and those who processed the data. In our comparison, **this only occurred on one fourth (1/4)** of the evaluations.

- A secondary conclusion derives from the fact that processing codes have to palliate the data format deficiencies, either because the format rules have not been well defined, have been interpreted differently, or are inconsistent or unphysical.

- Check what your transport code is using, do not assume, what you have seen is NOT what you have got, infinitely dilute versus shielded.

- ENDF cross sections are not uniquely defined and definitely not uniquely processed

# Facts

- Evaluator exploits: SAMMY, REFIT, FITACS and a lot of experiences, know how's, but so few of them now a days…fortunately there is also McGNASH, TALYS, CCONE, …

  What they show is not what you are using !

- Processor uses: NJOY, PREPRO, AMPX, CALENDF, ….where are you my friends ???

  Do not assume all is the same ! It gives what you are using

- Reactor physicist handles: SCALE, PARTISN, WIMS, APOLLO, MONK, MCNP, TRIPOLI, ERANOS…..

  Are you sure that all but the cross section is perfect ?

  Are reactor physics codes programs stay idle during the past 20 years ?

Reactor physicist DO NOT use the evaluator's product, but their strict interpretation through the philter of processing code and their own … the last few years have unearthed discrepancies….and unturned stones

Fission, absorption, reaction rates in general and eigenvalue in particular are customary quantities, although produced, used and misused by too few that only have in mind "their" cherished and uniquely important application ….

# Conclusions

- The ENDF-102 rules should be revised, as evolutions not major modifications, along the following lines:

- CALENDF's way: a format need to be defined (ENDF-102) but different specifications may also be applied
- Allow for other formalisms in the URR : MLBW, RML
- Account for the effect of multiple fission channels.
- Allow all competition channels to be open in this range, e.g., inelastic levels, direct components, charge particle emissions. This would make the sum-up and energy interpolation rules clear, but would not require that everybody could or should use them all.
- Privileges, enforces LSSF=1 formalism (self-shielding from file 2, cross section in file 3) if you can be sure that the SSF's can be correctly predicted and applied, else LSSF=0.
- Make the formats and specifications unambiguous.

# LSSF dilemma

- LSSF =0

Prerequisite: exact average parameters to properly interpret them but it assure a proper SSF's implementation

- LSSF=1

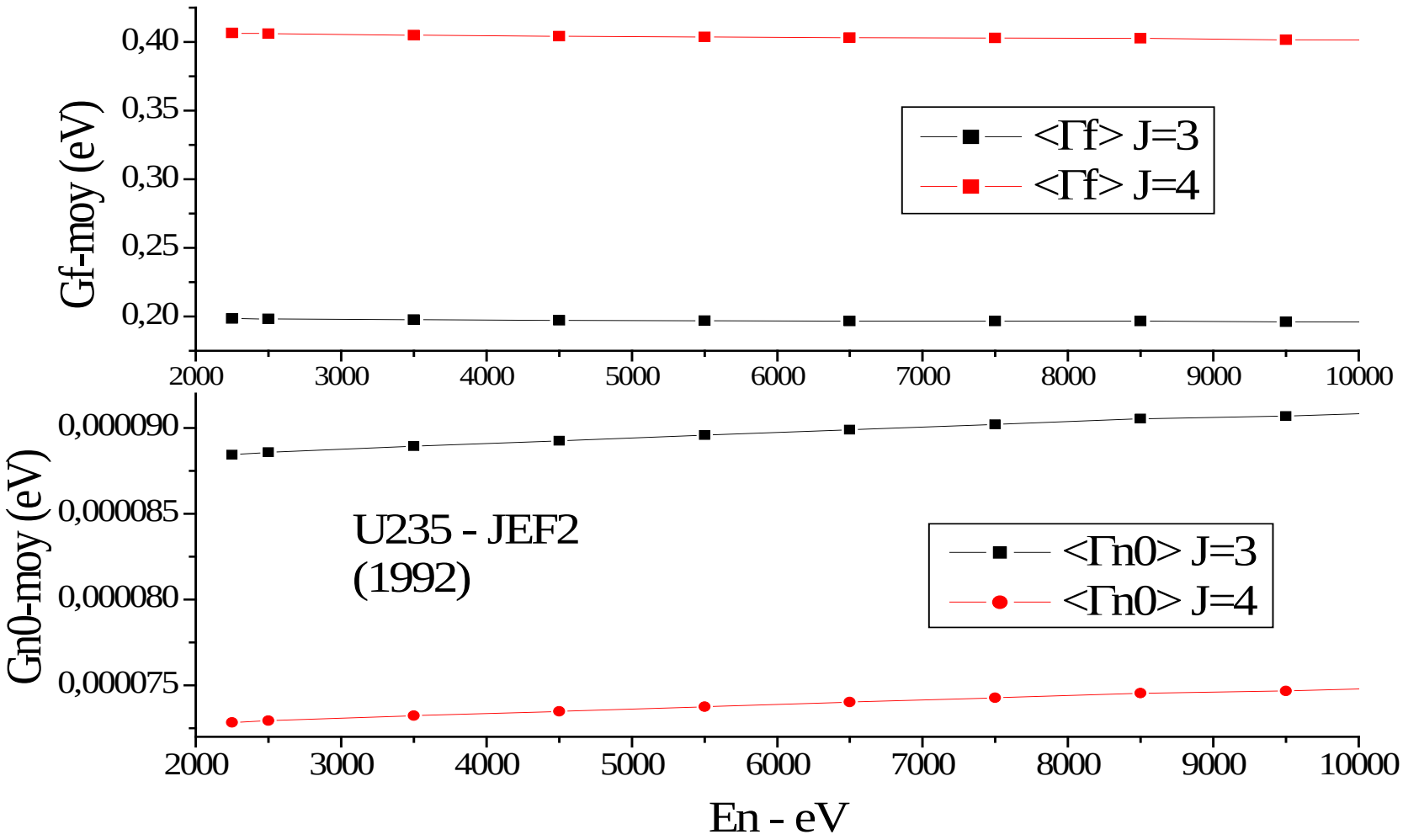
Ensure good cross sections mean value but the SSF are also applied to the residual !!! when it exists ; and what about the angular distribution ?? Is ensuring an average enough ??

Rigor, strictness would encourage LSSF=0

Now an example Pu-239 URR

**yesterday, today and… tomorrow**

# Yesterday : smooth variation of the average parameters

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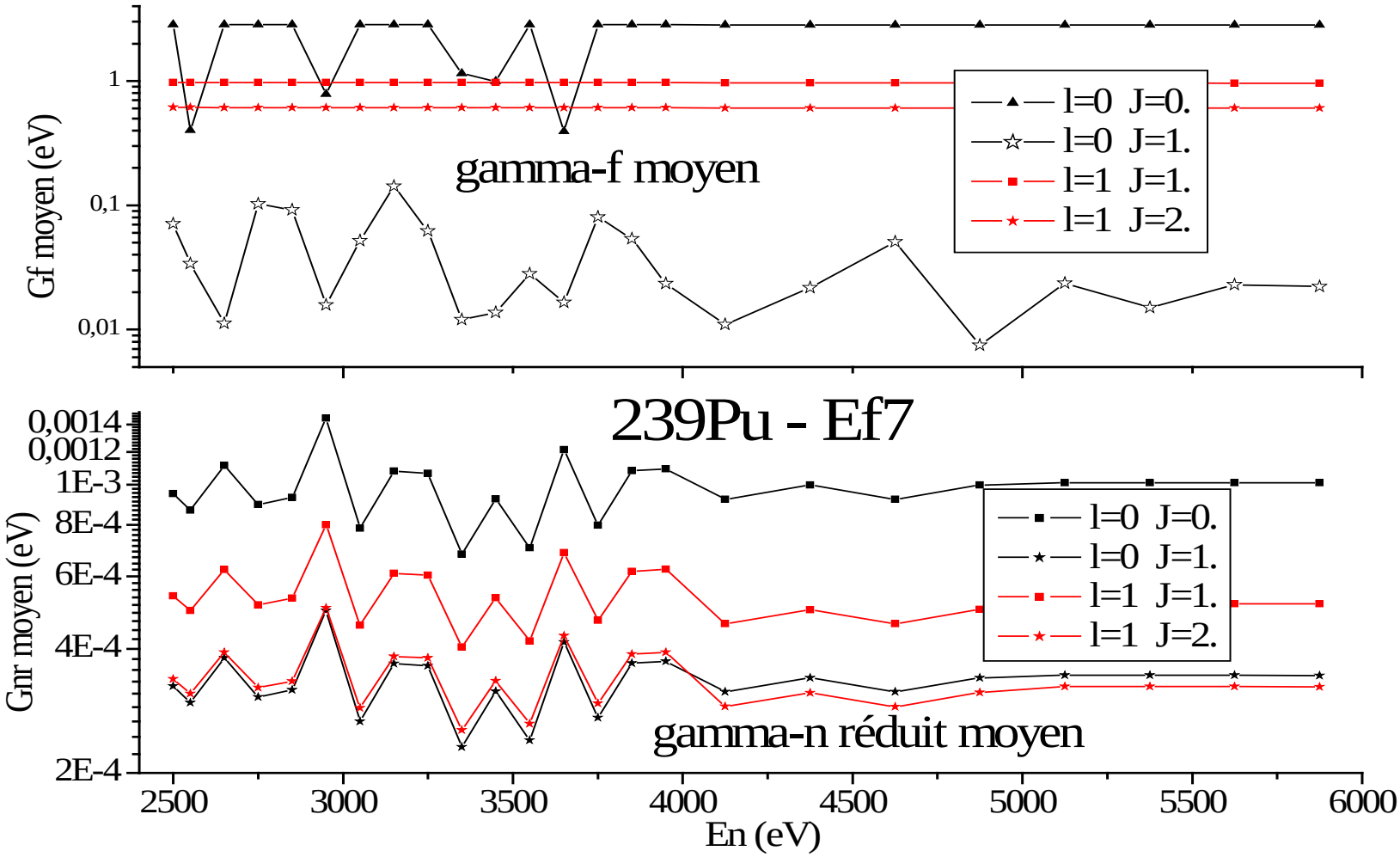
# Today: ENDF-B-VII = JEFF-3.1.1 Pu-239

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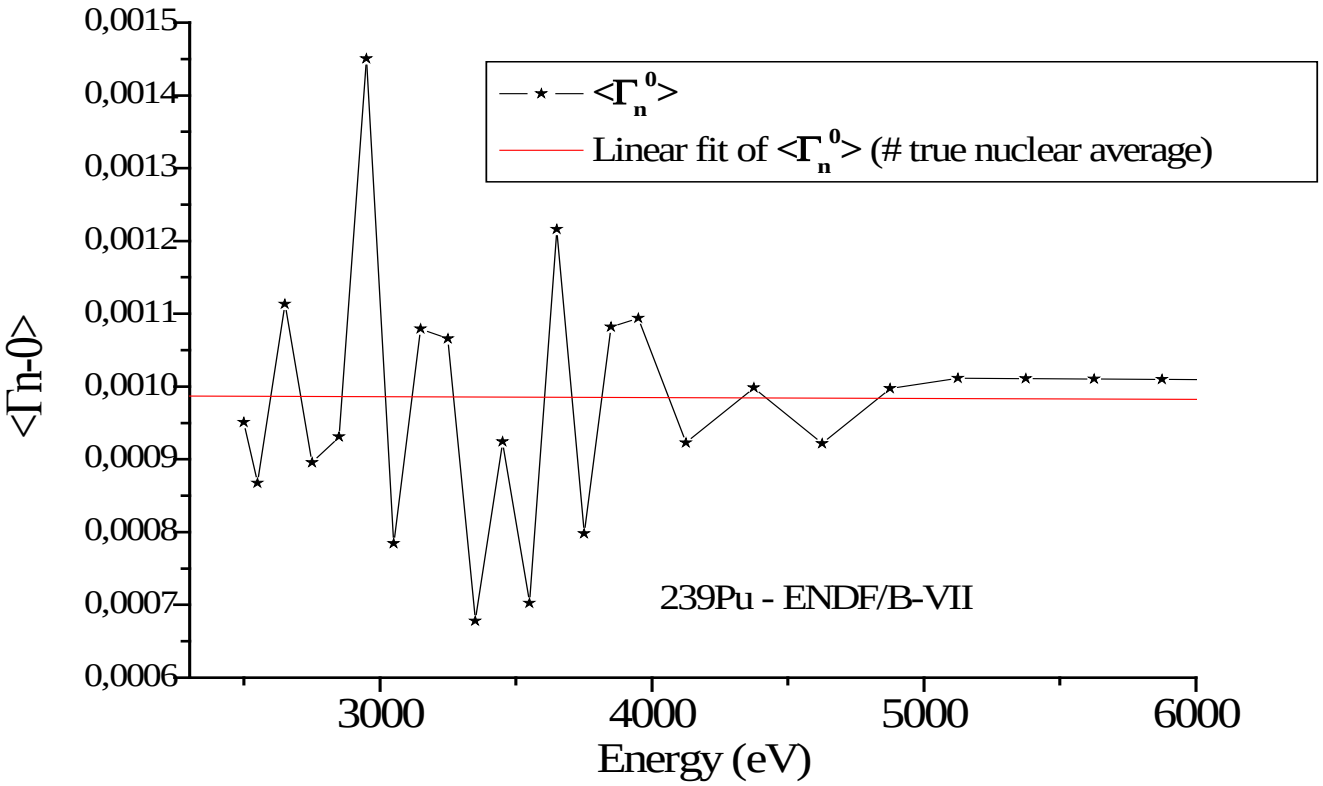
# Caution !

- These fluctuations are Porter and Thomas fluctuations
- The parameter distributions should not be based on these local averages but on the real nuclear average

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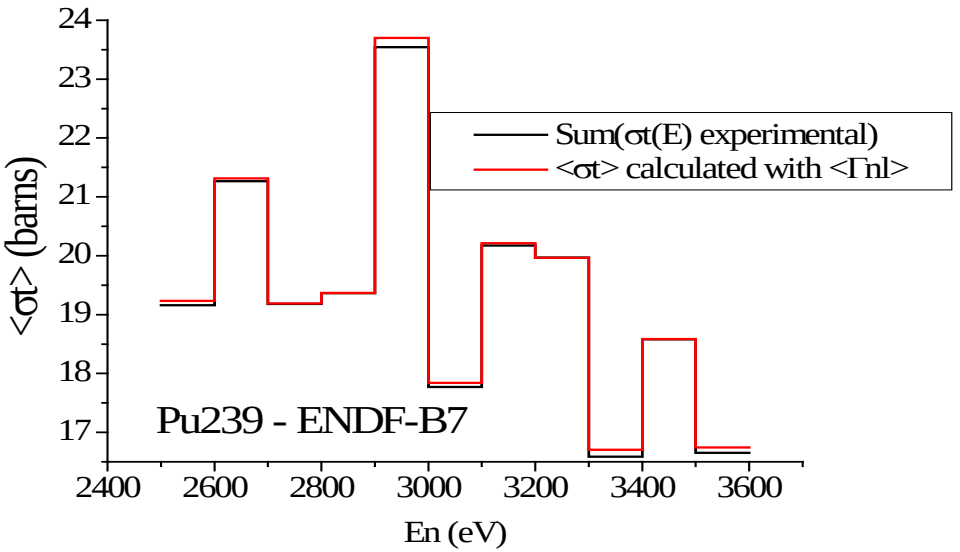
# How ? what are these local averages ?

- Generate several random sets of resonance parameters
- Select the set for which the average is equal to the local average
- But how these values are been predicted ?
- An assumption:  they described a specific energy range around every energy point.
- We tested the following hypothesis: every point $E_n$ described the range ($E_n$-50:$E_n$+50) eV ➔ perfect agreement.

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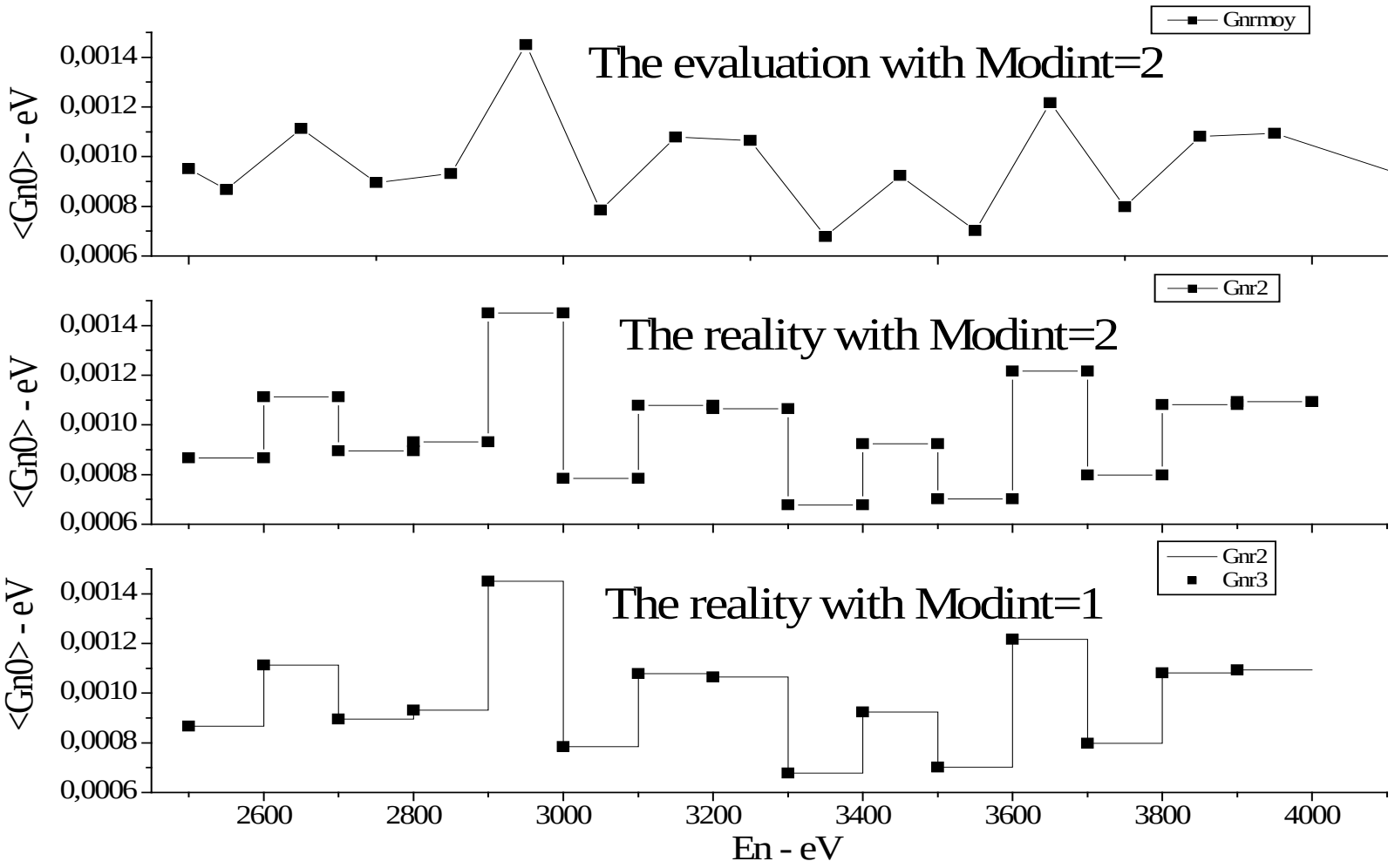
# Then, what should be in the evaluation ?

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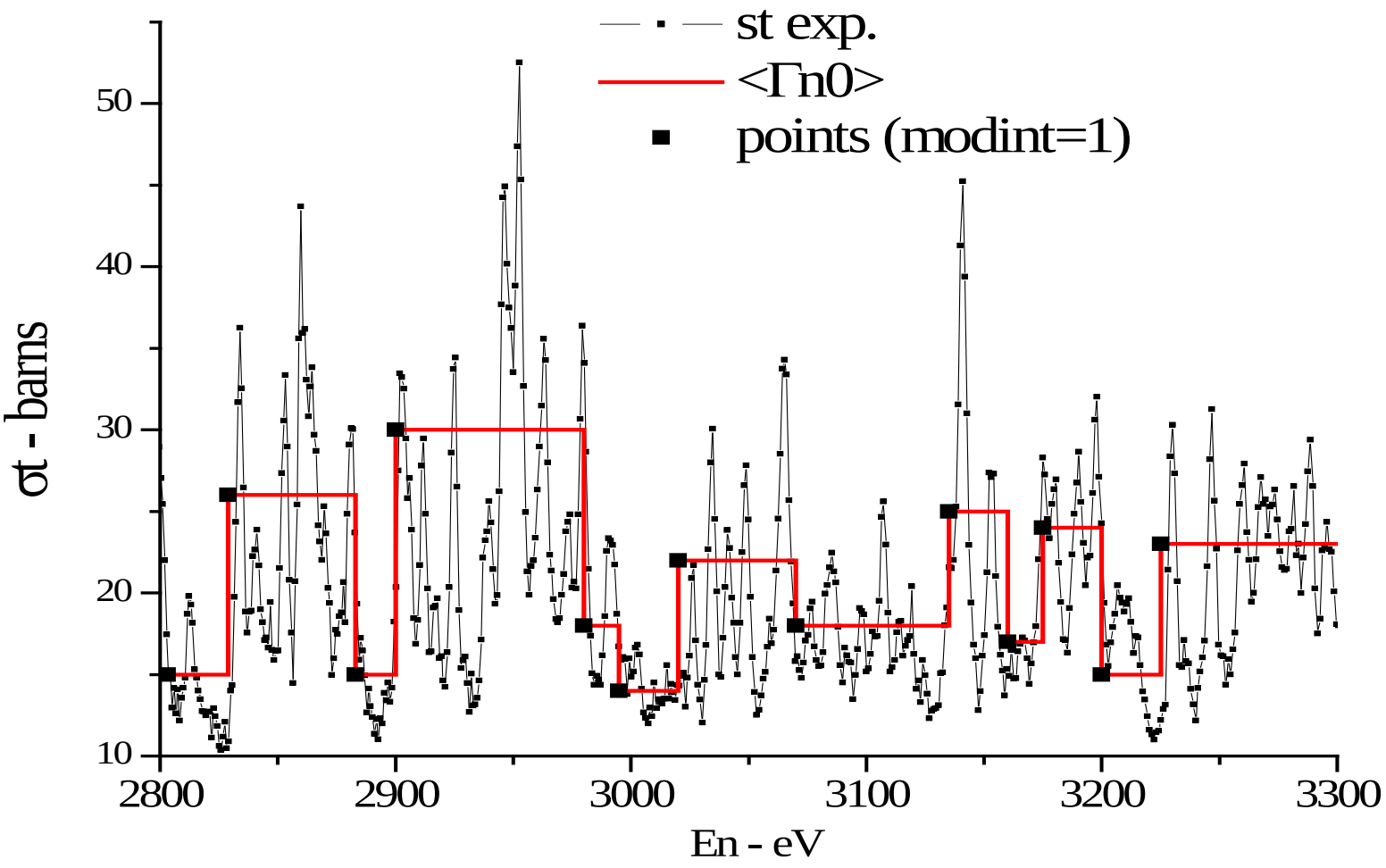
# New evaluation with variable energy band




Crude example of a more accurate xs description

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# Recommendations

- A possible improvement would be the insertion of some large resolved resonances in the URR.
- Add locals description of the averages with INT=1, from selected random sampling.

- These small modifications would improve the description of the URR and are actually possible respecting the present ENDF format.

- Format improvement, evolution need to be allowed on physic grounds and not only with engineering considerations in mind,…. because if not the outcome of many (already tuned) effects, including many compensation, makes a mockery of using nominal value and uncertainty based V&V processes.