Checking the resolved resonance region in EXFOR database

Gottfried Berton
Société de Calcul Mathématique (SCM)

Oscar Cabellos
OECD/NEA Data Bank

JEFF Meetings - Session JEFF Experiments
November 20 - 24, 2017
Boulogne-Billancourt, France

1. Presentation of the SCM activities

- Mathematical modelling company, established in 1995;
- Creates mathematical tools for decision help;
- Specialized in robust modelling;
- Main branches of activities: energy, environment, health, transportation, scientific assistance to large projects…
- Our work in nuclear sector:
  - Malfunctions in sensor networks;
  - Outlier detection, reconstructing missing information;
  - Looking for zones with highest risk;
  - Evaluating the performance of a network of sensors (e.g TELERAY);
  - Taking into account the uncertainties in computational codes.

2. Objectives

- ❑ Cross-checking the experimental data (EXFOR) with the evaluated ones
- ❑ Providing a list of suspicious data
- ❑ Ranking the entries to see which data are potentially erroneous and which are reliable
- ❑ Applying the work on most nuclear data:
  - – Isotopes and natural elements
  - – Threshold reactions, isomeric transitions, angular distributions, etc.
  - – Neutron reactions.
- ❑ Taking the uncertainties of both EXFOR and ENDF into account

3. Methodology in 2016

- Compute the distance between a curve (PENDF) and a set of points (EXFOR)
- The distance is the interval between two 95% vertical confidence intervals for EXFOR and ENDF
- Compute the min distance over the discretized horizontal confidence interval

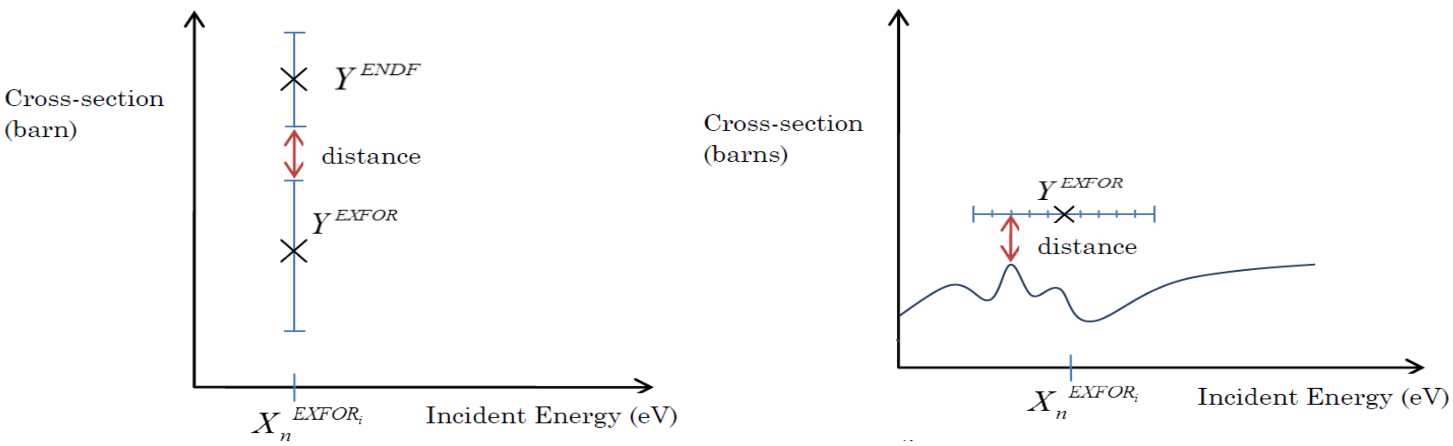


Fig. 1. General principle of the method

- Definition of a “Ranking value” to identify the potential problems in EXFOR or ENDF:

$$\text{ratio} = \frac{\text{distance}}{\max(\sigma_{EXFOR}, \sigma_{ENDF})}$$

4. Implementation

1) Finding the right scale for abscissa and discretizing it in 50 intervals

2) Constructing the resonance indicator as the “relative variance”

3) Computing the distance ratios for each intervals:

   - In a no-resonance interval: average of the pointwise distances

   - In a resonance interval: difference between integral of EXFOR and ENDF

4. Implementation

4) Averaging the ratios of the 50 intervals and computing the final ranking in “A”, “B”,…, ”E”

5) Compute the rank of the worst single point to detect single outliers (Fig. 2)

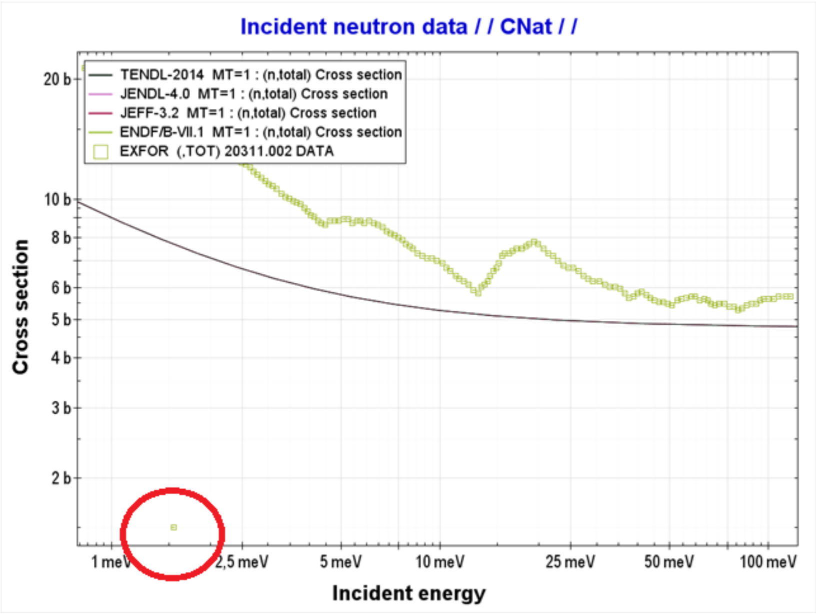
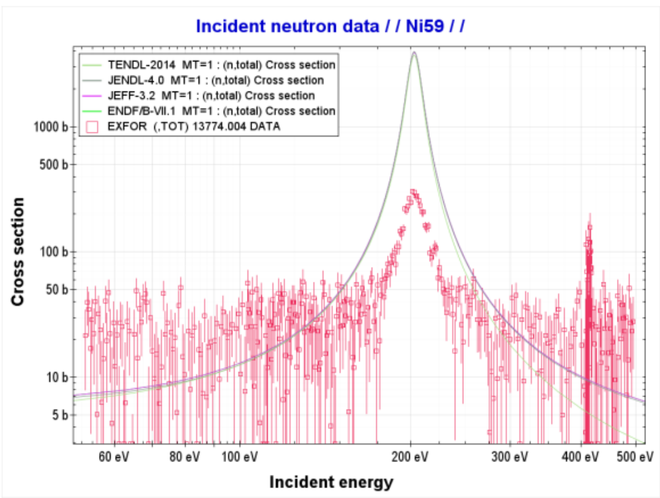


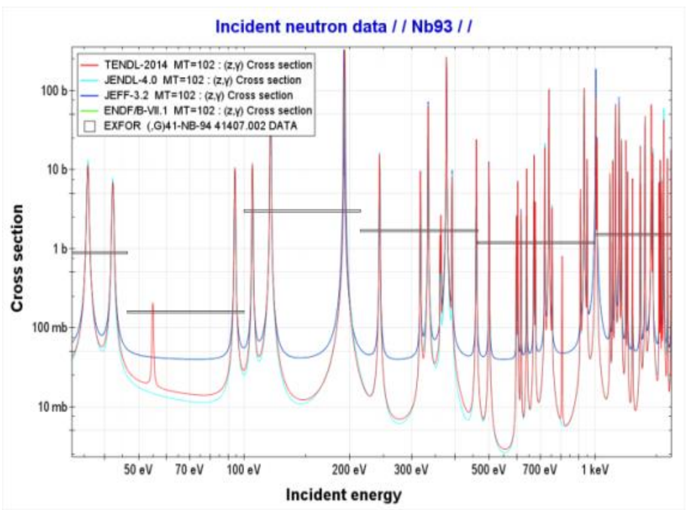
Fig. 2. Single point aberrant in Carbon natural element

4. Implementation

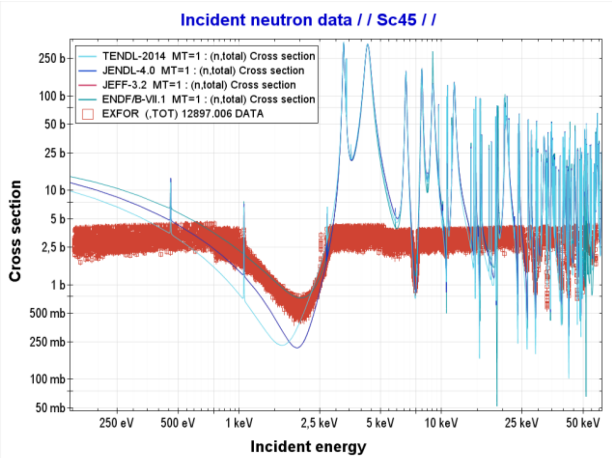
- ❑ This method has limitations in the resonance intervals

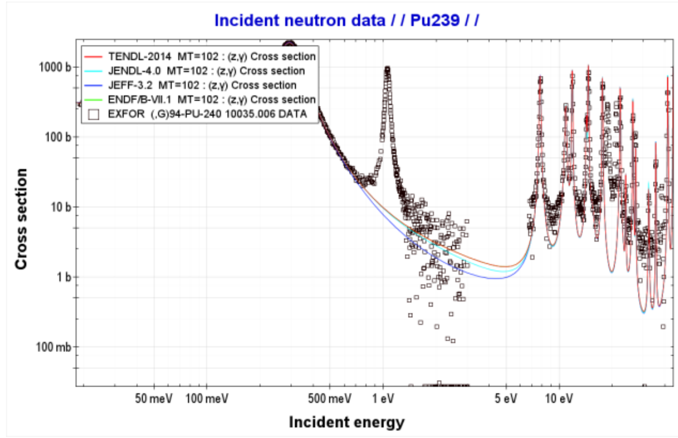
- ❑ Effect of resolution broadening in region of high variability: the cross-section measured is an averaging of the theoretical cross-sections at different energies

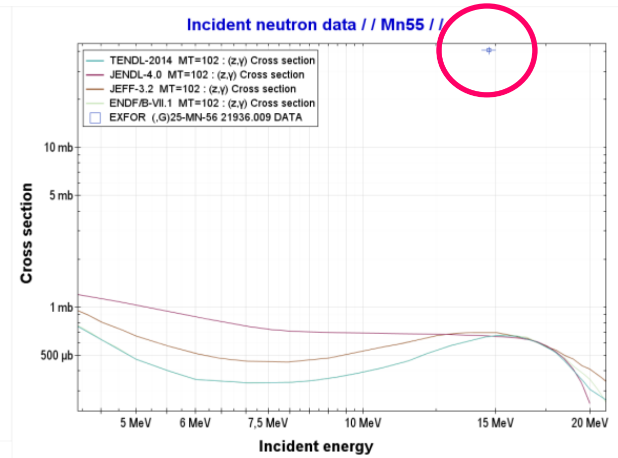


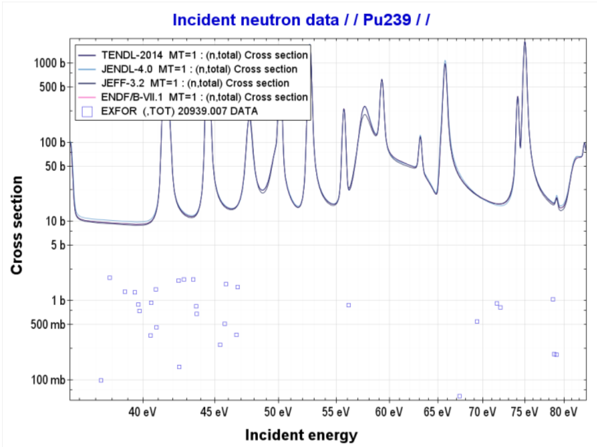


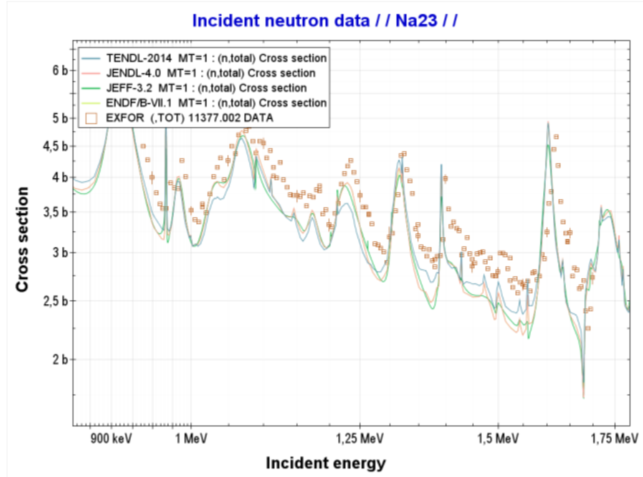
5. Results (2016)

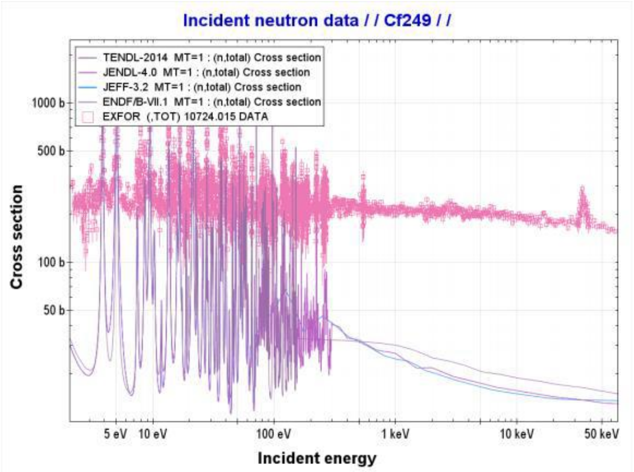












6. SCM´s Methodology applied in RRR (2017)

- Recover the resolution function in order to:
  - Compare PENDF and EXFOR in resonance region
  - Assess the shape of the resolution function (for n_TOF and GELINA entries)
  - Verify if the resolution changes with energy
  - Detect isolated sets of points and outliers: impossibility to find a resolution function, abnormally high resolution, etc.
  - Find missing peak in ENDF (or contamination in EXFOR)
  - Check normalization

6. SCM´s Methodology applied in RRR (2017)

- Discretize the energy domain so that there are 50 resonance peaks in each energy bin

- For each energy bin:

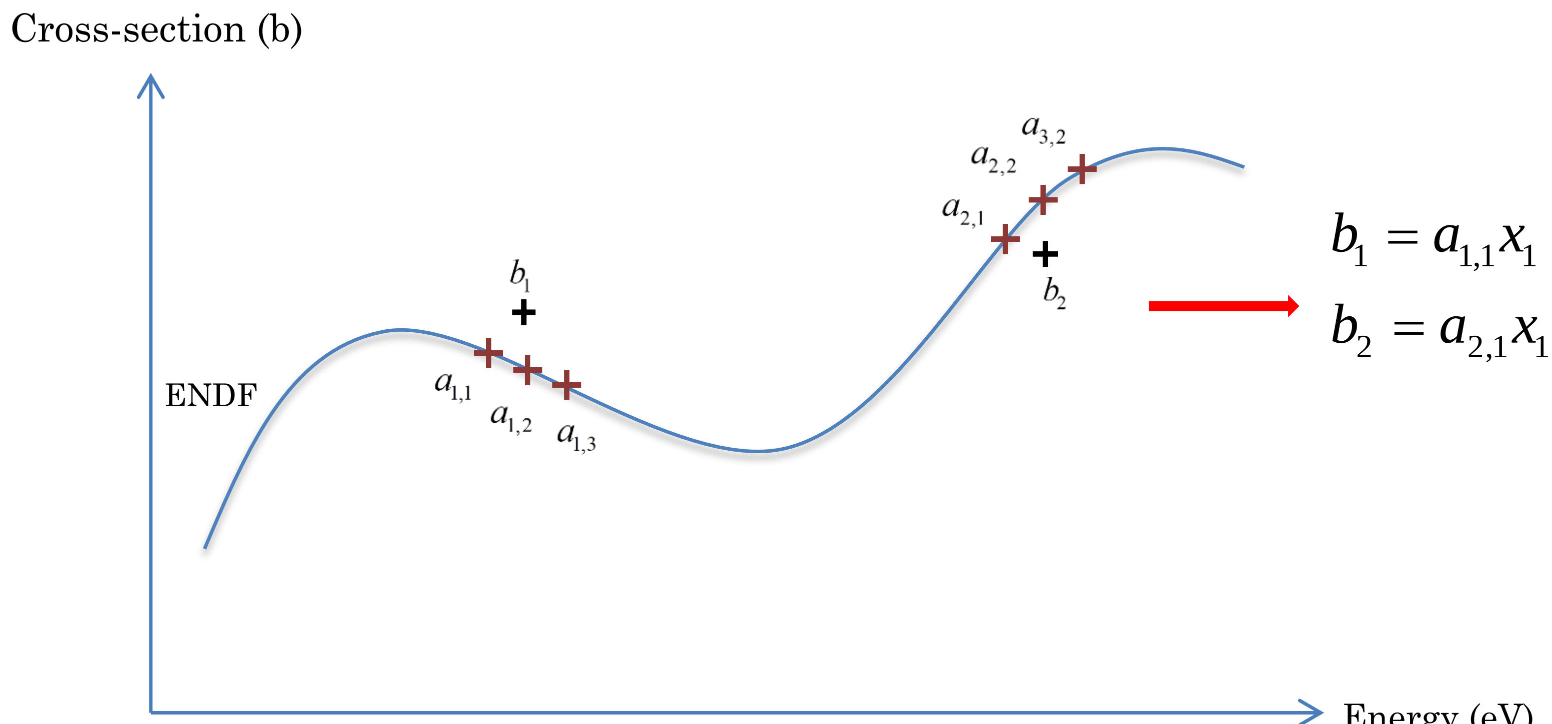
  - "Checking Normalization" by computing the ratio between integral of EXFOR and PENDF

  - Calculate the resolution function: the EXFOR "curve" is a moving average of the ENDF curve: find the coefficients x_j of this averaging

6. SCM´s Methodology applied in RRR (2017)

- Discretize the energy domain so that there are 50 resonance peaks in each energy bin

- For each energy bin:



$$b_1 = a_{1,1}x_1 + a_{1,2}x_2 + a_{1,3}x_3$$
$$b_2 = a_{2,1}x_1 + a_{2,2}x_2 + a_{2,3}x_3$$

$x_1 = ?$

$x_2 = ?$

$x_3 = ?$

6. SCM´s Methodology applied in RRR (2017)

- Discretize the energy domain so that there are 50 resonance peaks in each energy bin

- For each energy bin:

  - Calculate the resolution ΔE: how spread is the resolution function is

  - Check this value against resonance energy $\Delta E/E$

    - Is it an abnormally high value?

    - Does this ratio change for the different energy bins?

7. Finding a resolution function

- To find the coefficients x_i , solving the system:

$$\sum_{j=1}^{n} x_j a_{i,j} = b_i, \ i = 1, \ldots, N \qquad x_j \geq 0, \ j = 1, \ldots, n$$

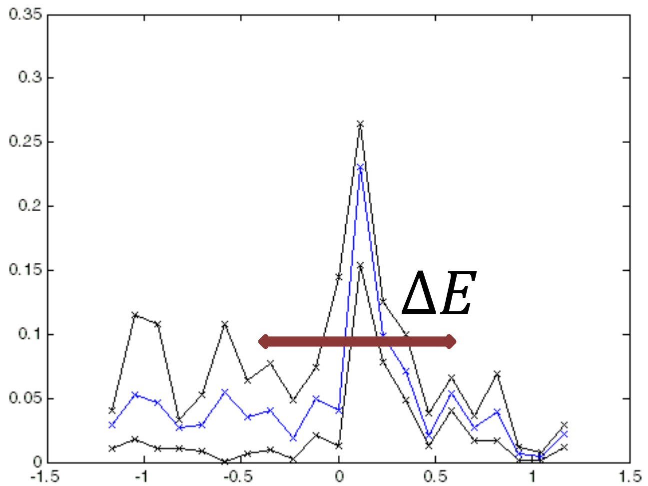
- b_i is the cross-section of EXFOR
- $a_{i,j}$ cross-section of ENDF at energies around EXFOR energy
- n the number of coefficients, N the number of EXFOR measures

7. Finding a resolution function

- Solving using the least squares method

- To take into account uncertainties, use probabilistic method: Archimedes method

  - Allows to calculate for each coefficient the expectation (blue), and lower/upper bounds (black)



  - Calculate the uncertainty upon the resolution to obtain $\Delta E \pm \delta$

7. Finding a resolution function

Archimedes method:

1. Generating a candidate resolution function, i.e a set of coefficients x_j
2. At each EXFOR energy i
   - Applying the broadening on the PENDF curve using the resolution function x_j
   - Comparing this PENDF value to the EXFOR cross-section b_i: define probability p_i to be around b_i using the uncertainty on each measure
3. Calculating the weight of the candidate solution as $\Phi = p_1 p_2 \dots p_N$
4. Normalizing by the sum of the weights when generating all the solutions

7. Finding a resolution function

- Each candidate solution has a probability associated

- For each candidate we can calculate the resolution ΔE

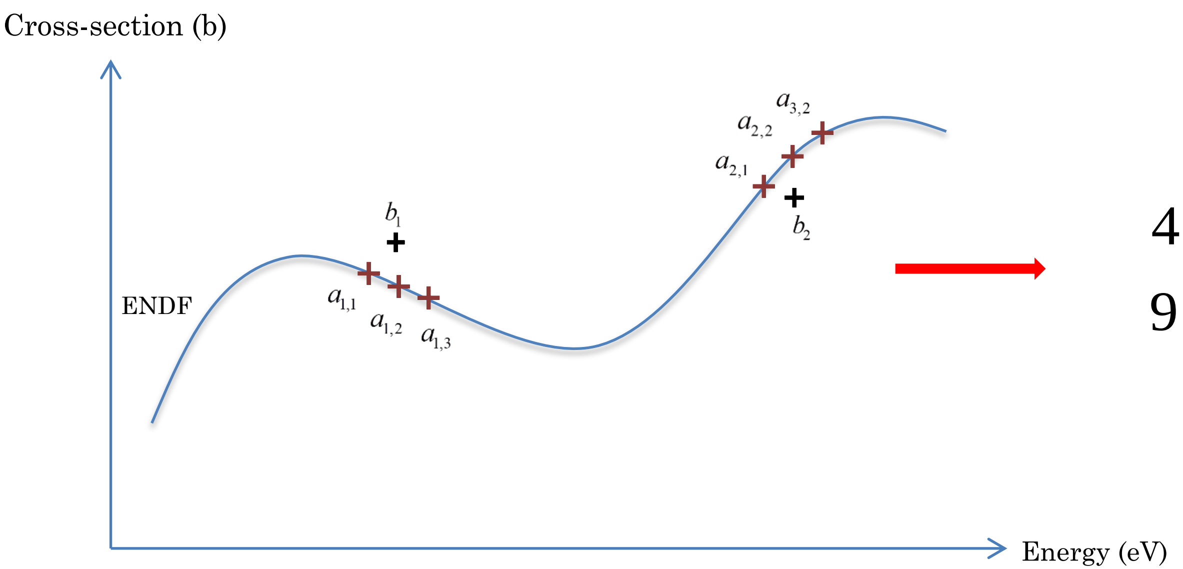
- Eventually, we obtain a probability law upon the resolution, and each coefficient x_j

- It works also for non-linear systems and any kind of uncertainty (not only Gaussian)

7. Finding a resolution function

How to generate the candidates solutions?

- Numerical example:
  - $b_1 = 10b$ with standard deviation $2b$, 95% probability to be in $[4; 16]$
  - $b_2 = 12b$ with standard deviation $1b$ 95% probability to be in $[9; 15]$
  - We obtain a system of inequalities:



$$4 \le 9.1x_1 + 9.5x_2 + 10.2x_3 \le 16$$
$$9 \le 10.1x_1 + 9.4x_2 + 11.3x_3 \le 15$$

7. Finding a resolution function

- These inequalities are the intersection of half-spaces, and form a convex space

$$4 \leq 9.1x_1 + 9.5x_2 + 10.2x_3 \leq 16$$
$$9 \leq 10.1x_1 + 9.4x_2 + 11.3x_3 \leq 15$$

- We generate only candidate solutions in this convex subspace by performing a random walk in it

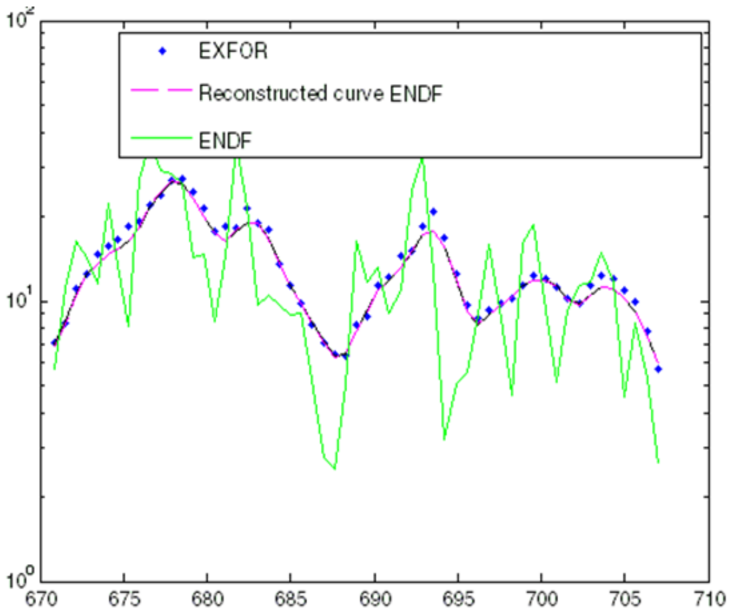
- Checking existence of a solution to this system above using simplex algorithm.

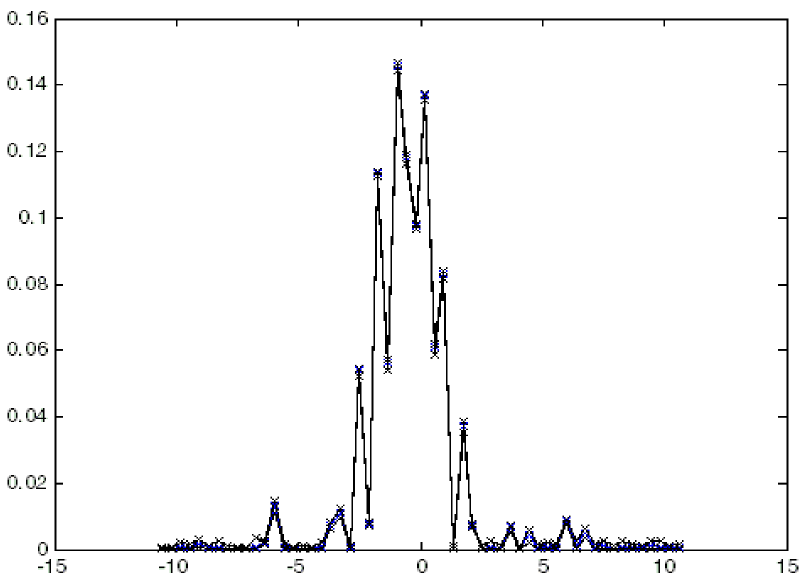
- No solution could mean:

  - too small EXFOR uncertainties with respect to the distance with ENDF
  - isolated set of points

8. Results

- ❑ Example of resolution function obtained for n_TOF data (figure at right)



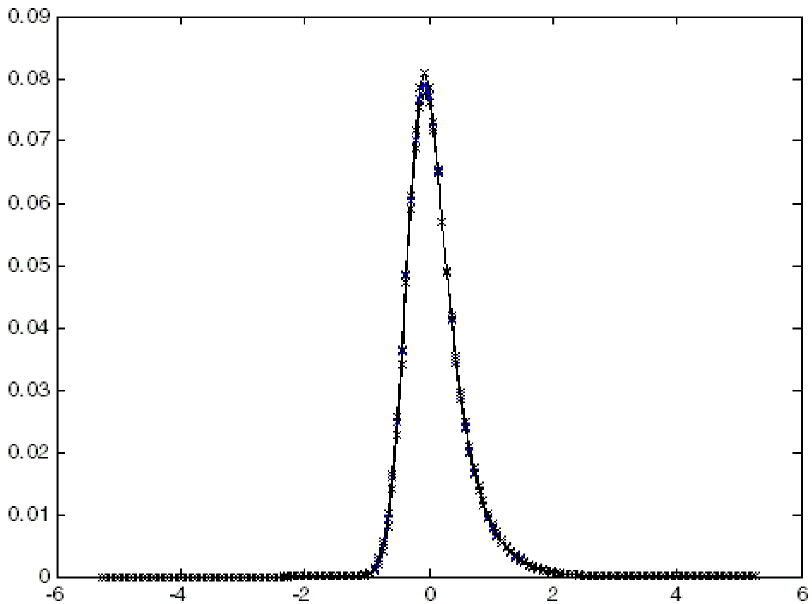


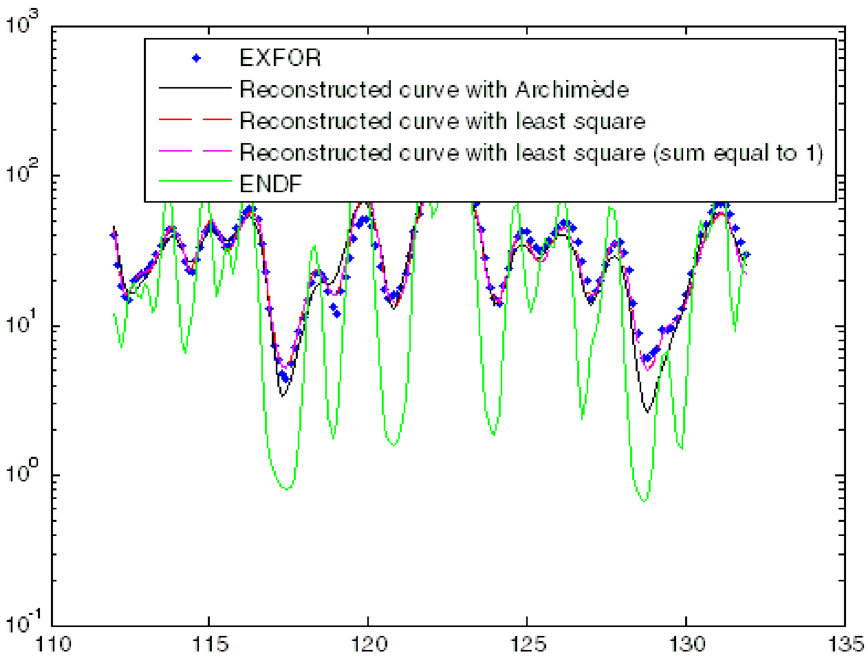
  - Green line: ENDF
  - Pink line: Broadened ENDF using coefficients on figure at right
  - Blue: EXFOR

- ❑ Usually small resolution (0.8% approximately in the example above)

8. Results

- ❑ Added constraint on the shape (convolution of exponential and multiple gaussians as used in SAMMY code)

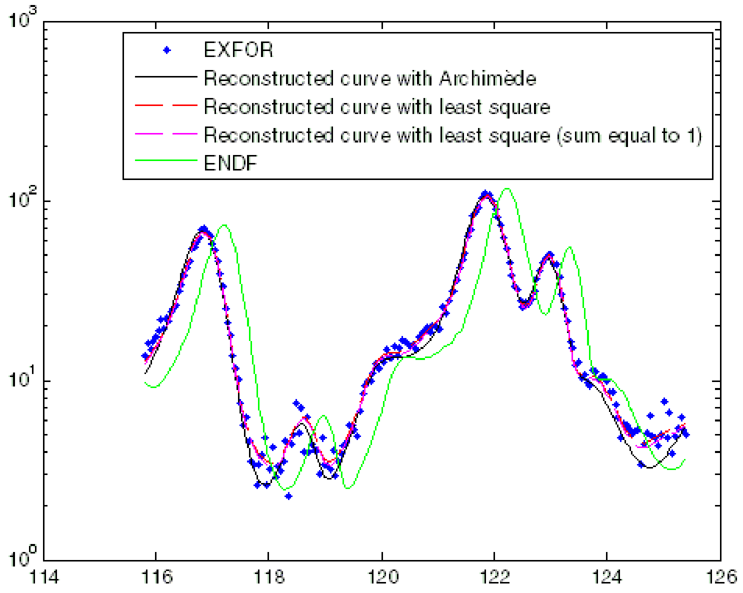


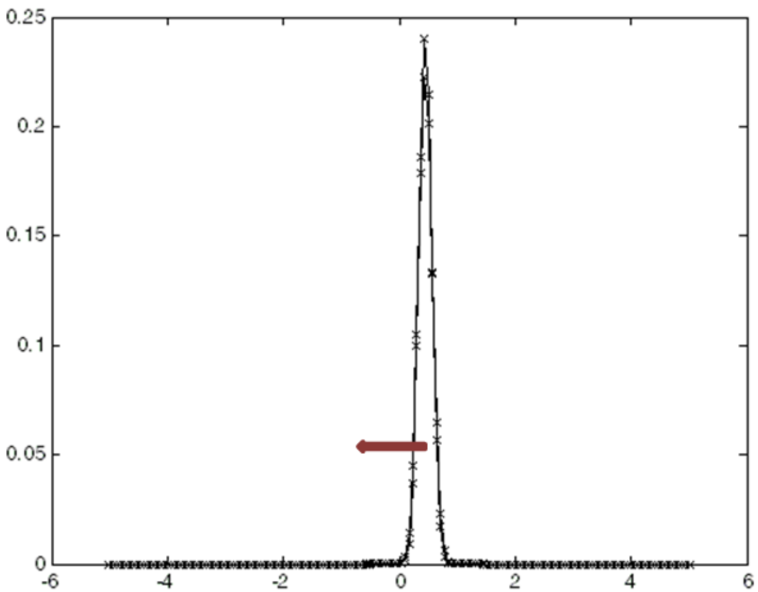


- ❑ Adding such constraint often leads to poor match between “broadened ENDF” and EXFOR

9. Data

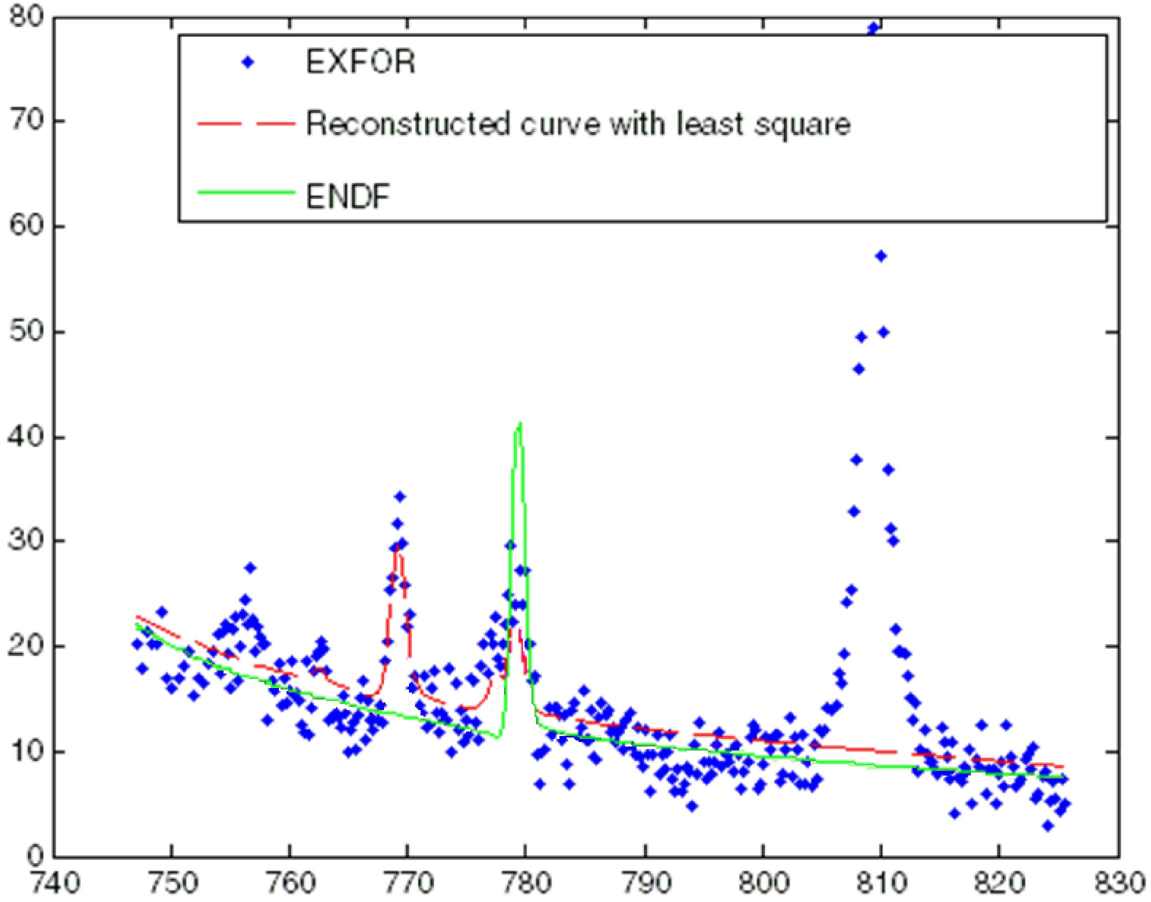
- Data processed at room temperature (Doppler broadening)
- Applied to large entries (TOF measurements from GELINA and CERN)
- Resolution function defined on an interval energy of 50% around the resonance energy
- Horizontal shift between ENDF and EXFOR: recenter afterwards the resolution function obtained to align ENDF to EXFOR.





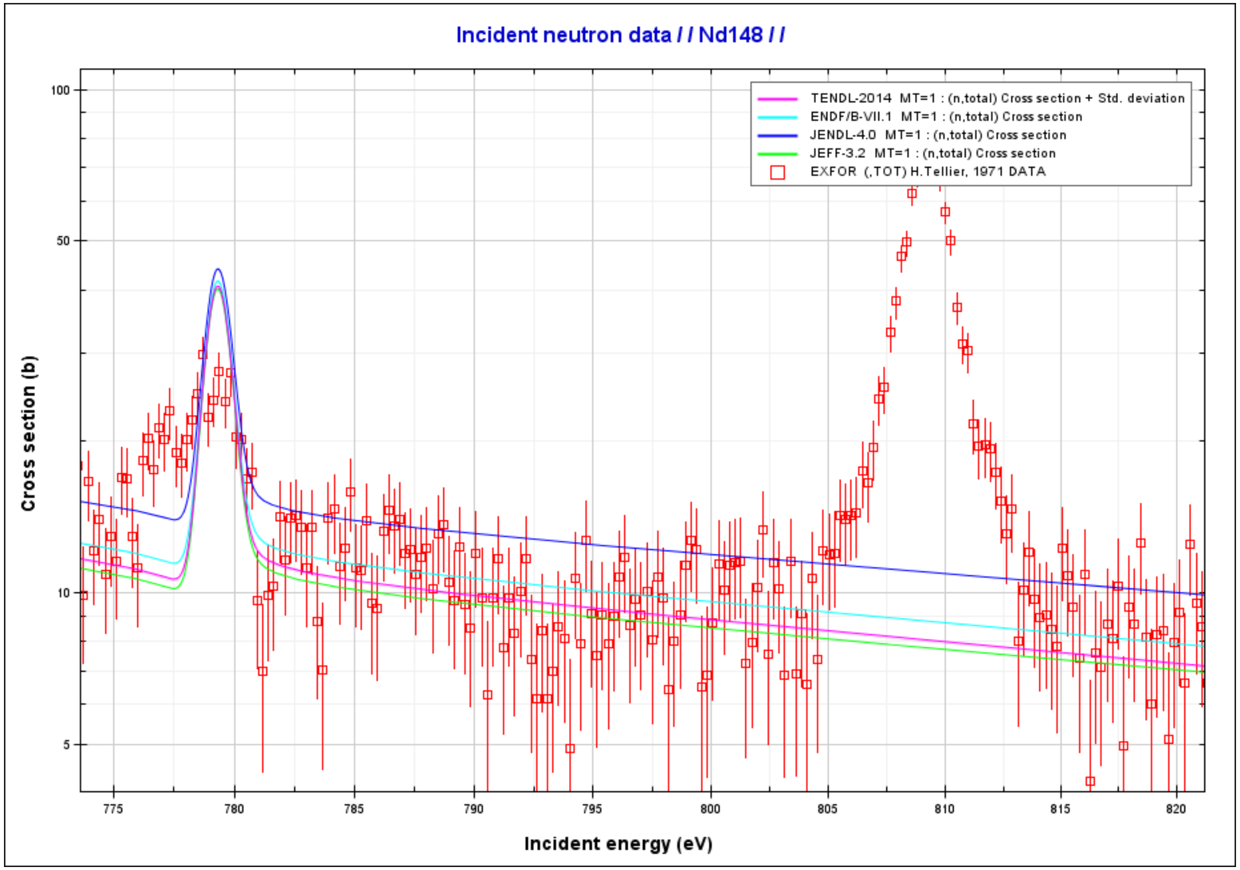
10. Find missing peak

- Case 1: contamination from another isotope in EXFOR



10. Find missing peak

- Case 1: contamination from another isotope in EXFOR

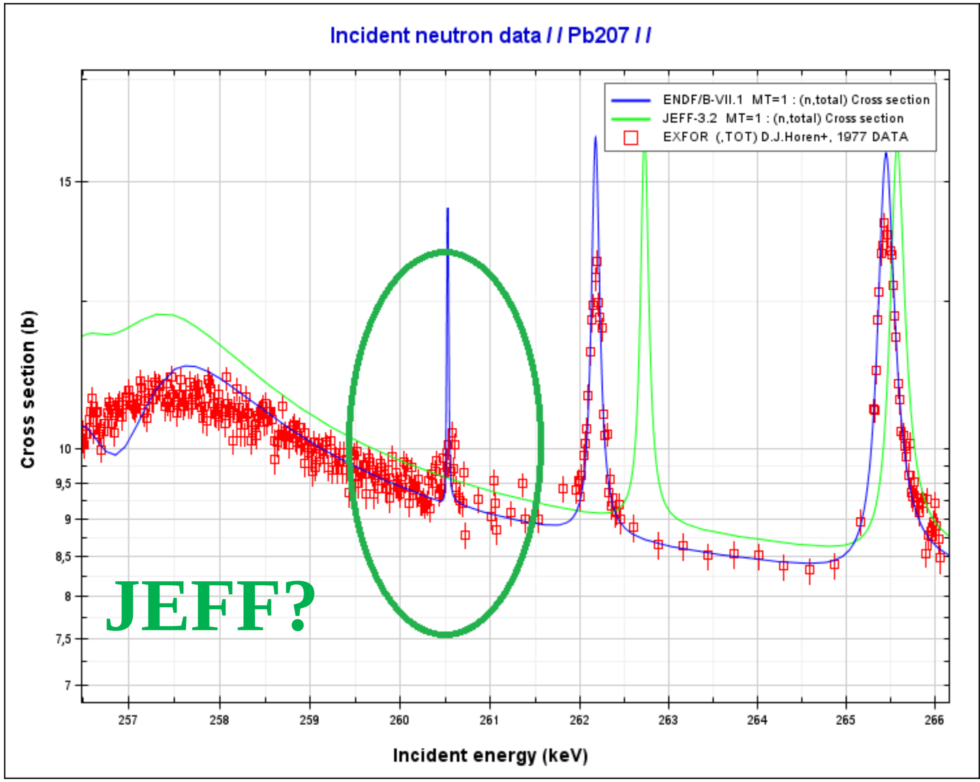


10. Find missing peak

- **Case 2: missing resonance in ENDF**

Method to detect it:

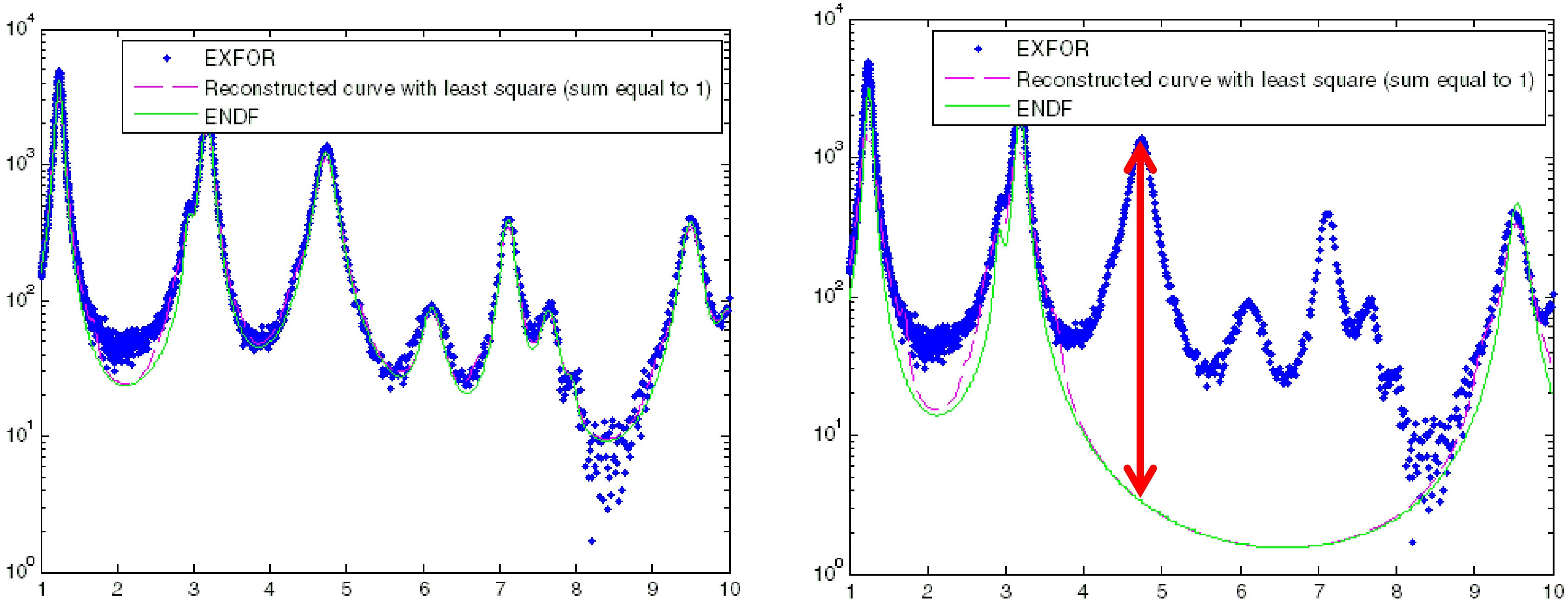
- "Broadening" of each ENDF using the RF
- For each local maximum in EXFOR, calculate the distance EXFOR/ENDF
- If large distance, count the number of resonance peaks around this peak for each evaluator
- If there is disagreement between the evaluators on the number of peaks: report



Peak for ENDF but not for JEFF

10. Find missing peak

- **Case 2: missing resonance in ENDF**
  - One more example



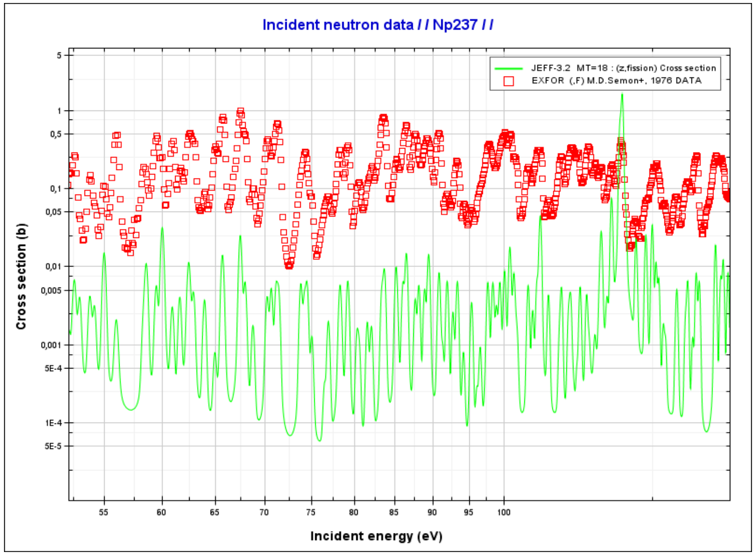
ENDF (OK) TENDL (??)

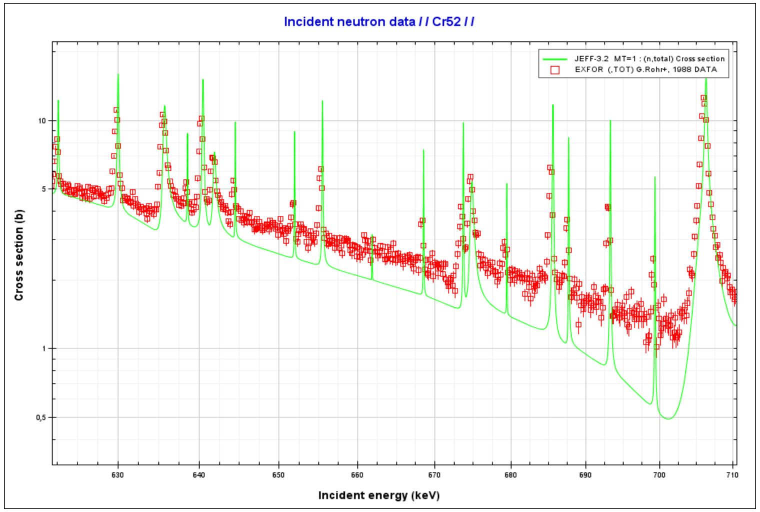
11. Find problem in normalization

- ❑ First case: integrals don't match, no ambiguity
Something wrong independently of resolution

- ❑ Second case: is the vertical shift due to normalization problem or resolution broadening?

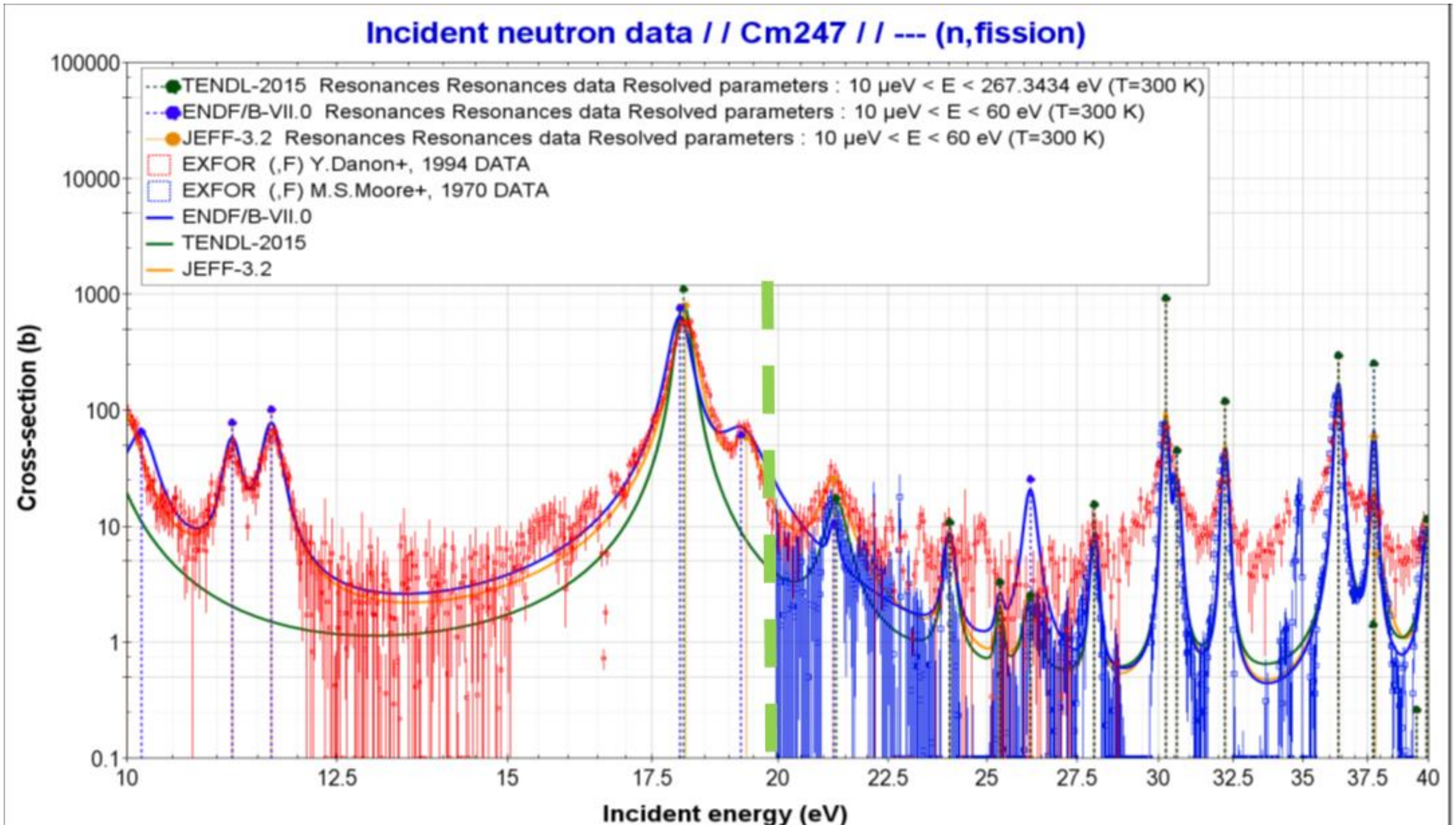
  - ○ Can we say it visually? No, to verify:
  - ○ check the existence of a resolution function having sum equal to one?
  - ○ yes: the shift is due to resolution effect
  - ○ no: the shift is due to a normalization problem



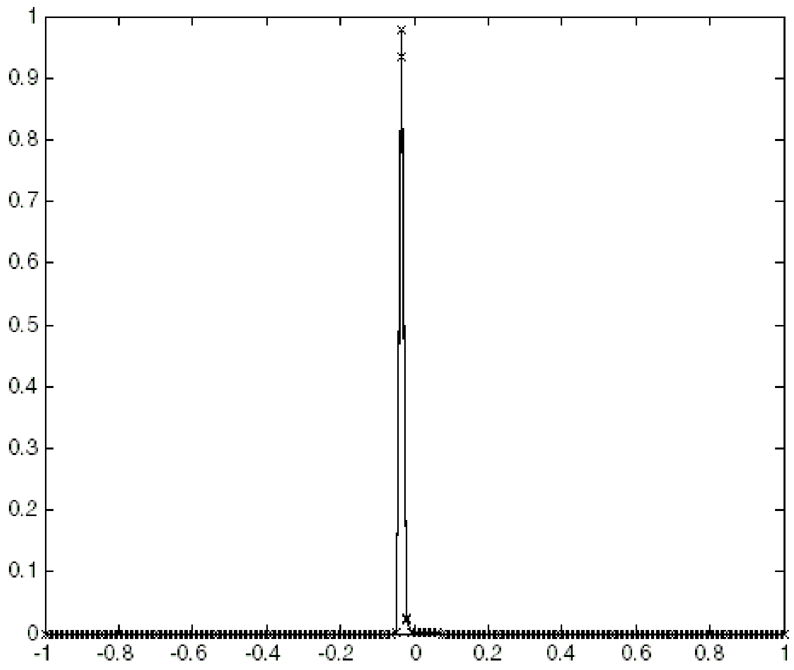


12. Change in resolution

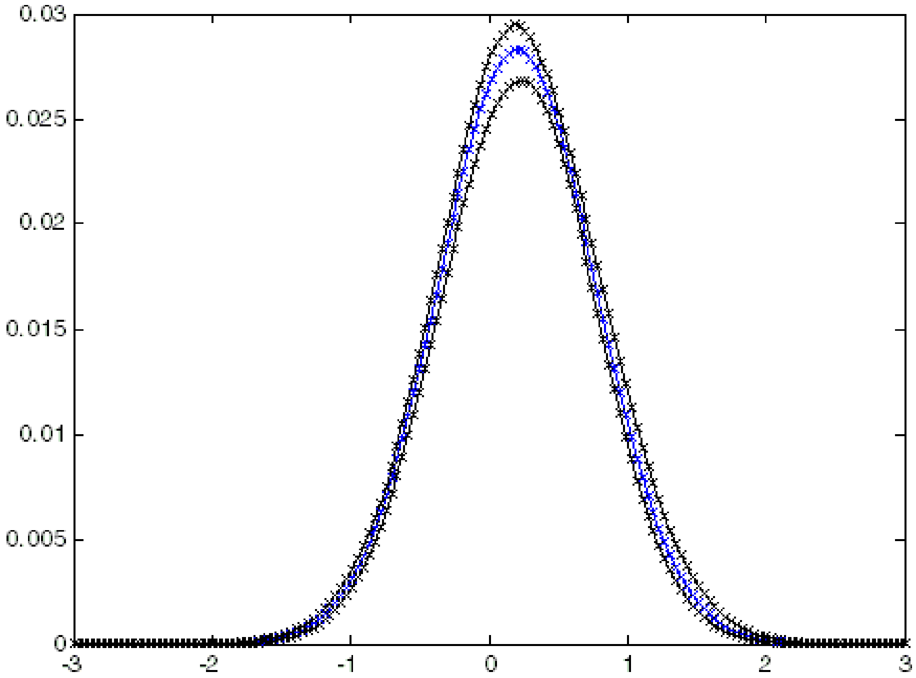
- Is there a change in resolution ΔE at a certain energy?



12. Change in resolution



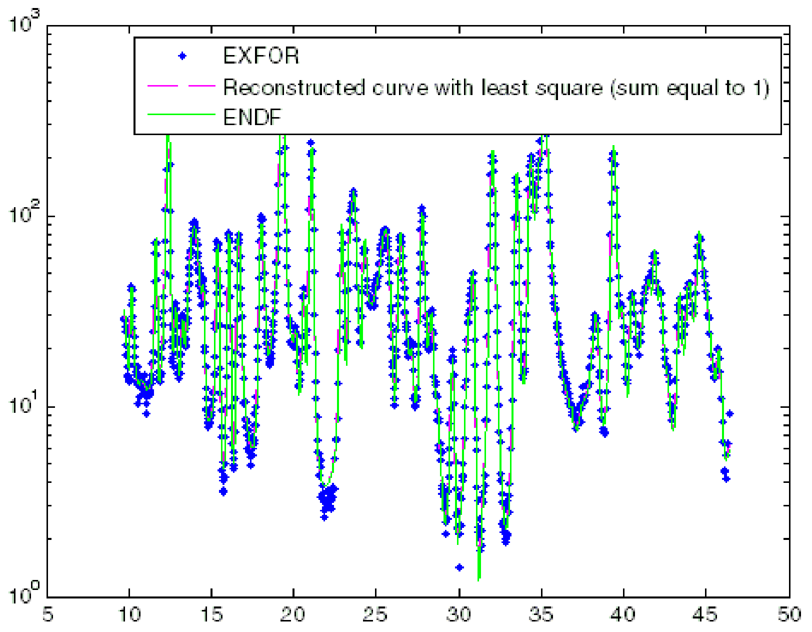
Energy <20eV (green line)



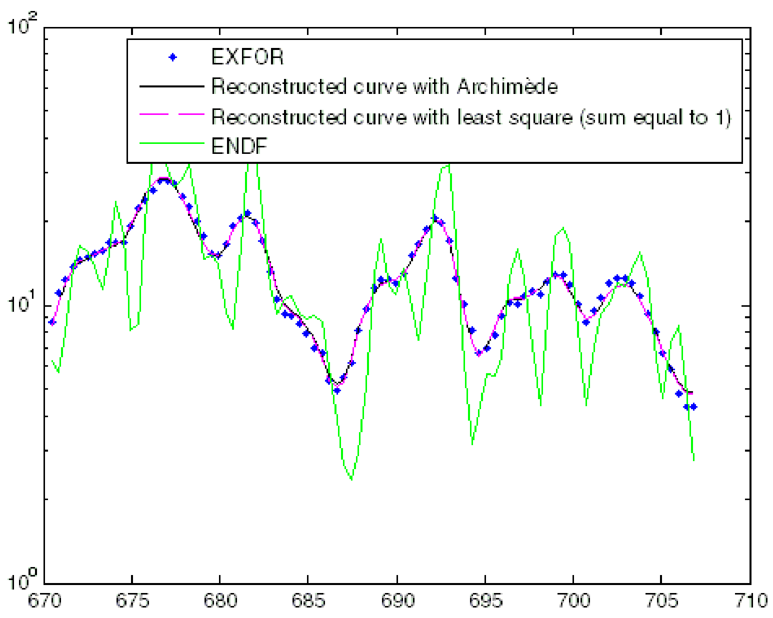
Energy >20eV

12. Change in resolution

- Take into account relative resolution $\Delta E/E$
- The ratio $\Delta E/E$ remains the same at left and right



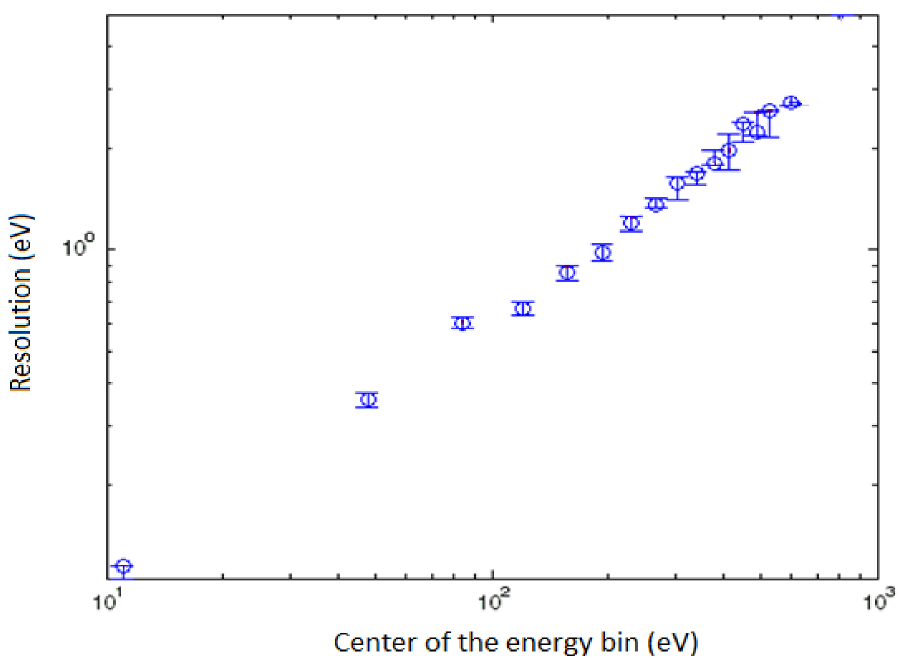
Energy 5 – 50 eV



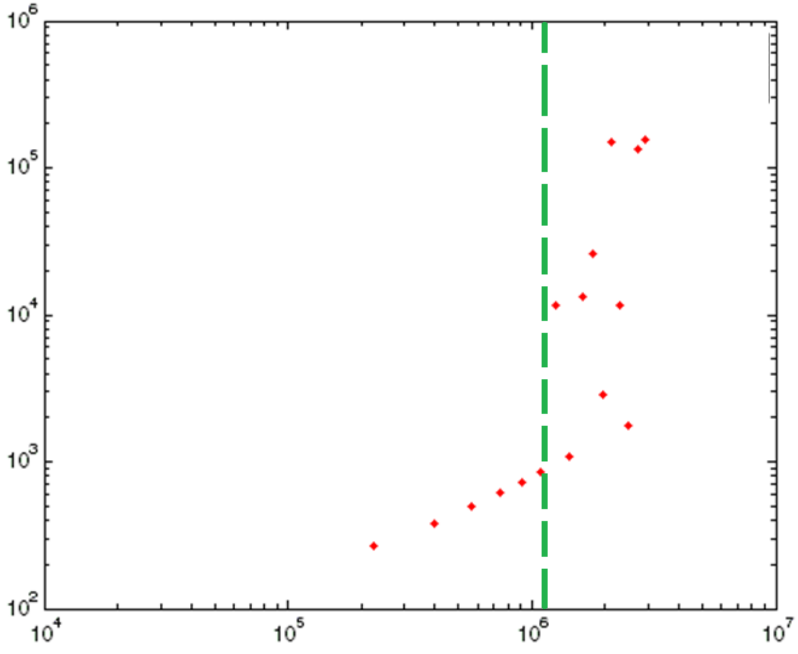
Energy 670 – 710 eV

12. Change in resolution

Plot for each energy bin, the resolution obtained. For two different entries:



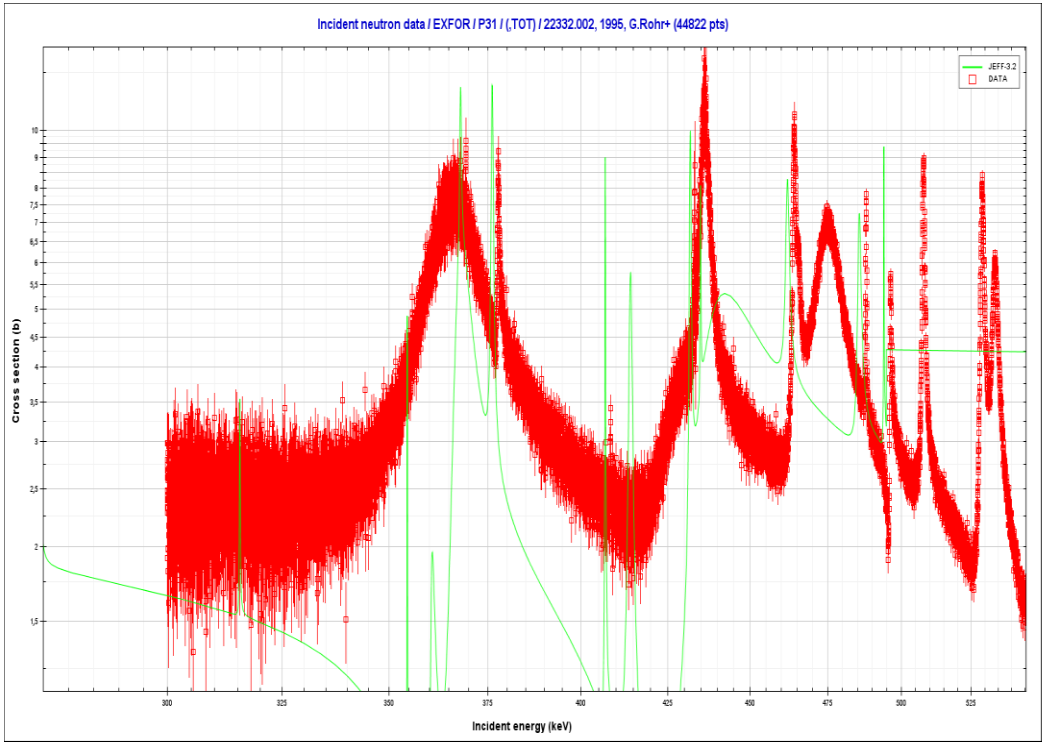
Entry #1: No change in resolution



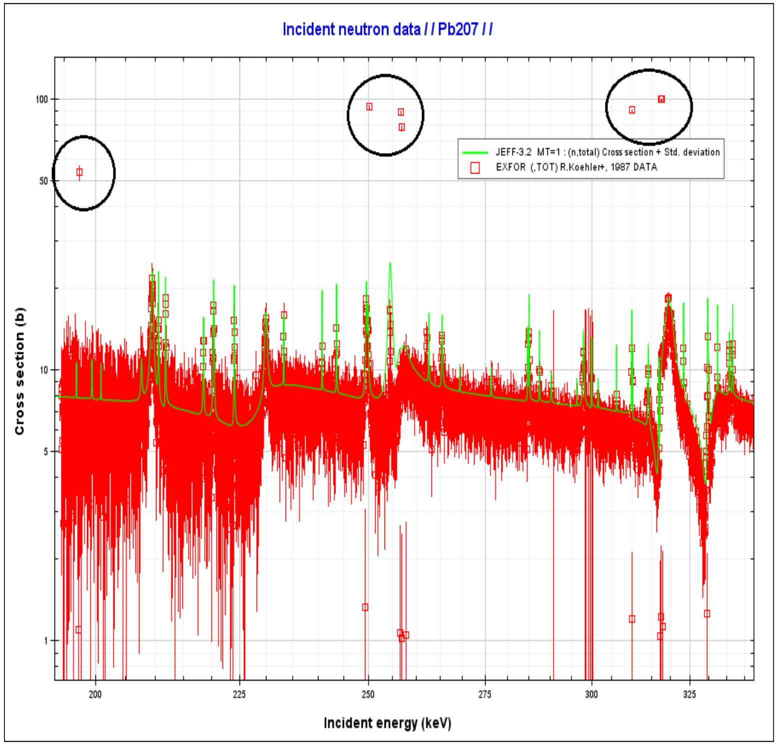
Entry #2: Change in resolution at 1 MeV

13. Find outliers

- After "correction" for resolution broadening, pointwise comparison allows to detect outliers in resonance region (n_TOF data):

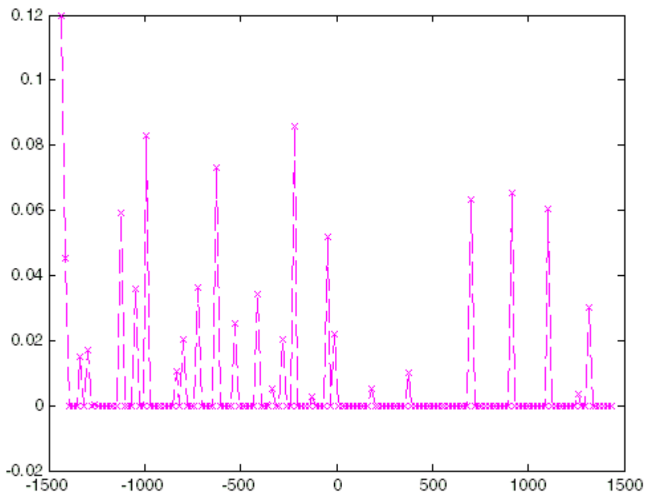


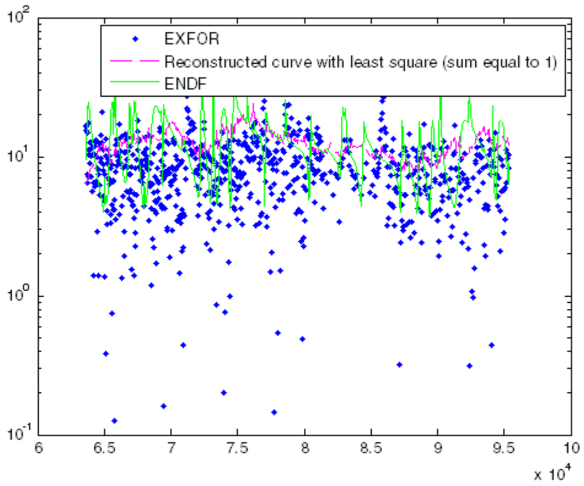
subentry 22332.2



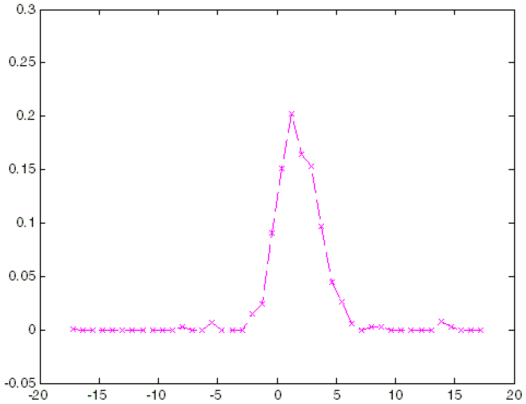
13. Find outliers

- Check also situations of strange resolution function or impossible to calculate:



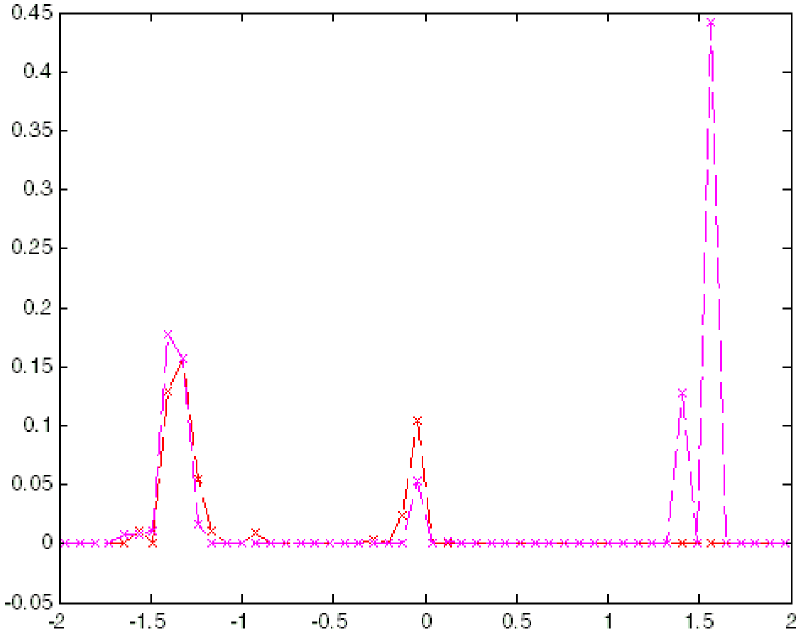


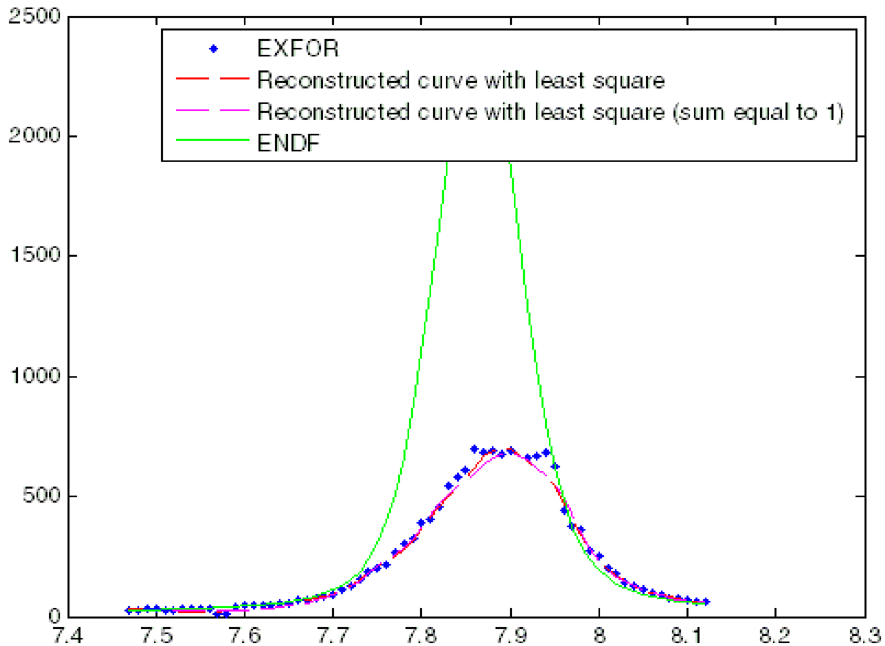
- Generally, decreasing when away from the center of the distribution



14. Other remark

- Is there a physical constraint on the resolution function that should be added?
- Why should be Gaussian?
- Different resolution functions can lead to the same result (pink and red)





15. Conclusion

- This work allowed to compare the ENDF and EXFOR in the resolved resonance zone
- Checking missing peak in ENDF
- Detecting isolated sets of points and potential outliers
- Assessing the resolution function for n_TOF and GELINA data per energy bin and how the resolution changes with energy