New ^{239}Pu adjustment method for ANDES WP2/3:

covariances, uncertainty propagation and evaluation

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Contents

Goals

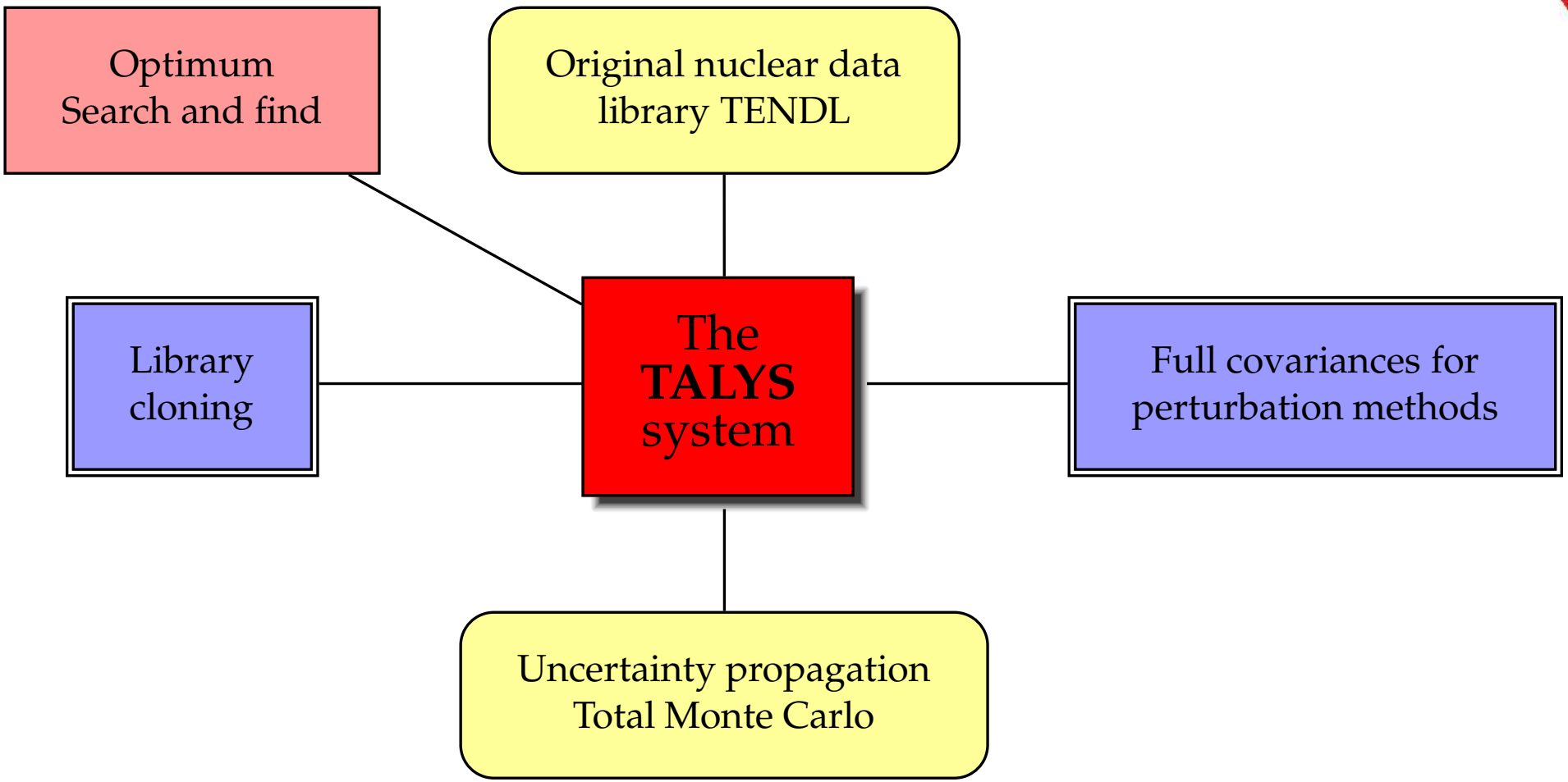
In ANDES, we can perform the evaluation and adjustment of ^{239}Pu with the latest and most advanced methods used in the nuclear data community:

1. The general nuclear reaction code TALYS,
2. the TALYS system (used at NRG to produce evaluations),
3. Total Monte Carlo,
4. Evaluation/adjustment.

Outcome: integration of the complete evaluation chain at one place

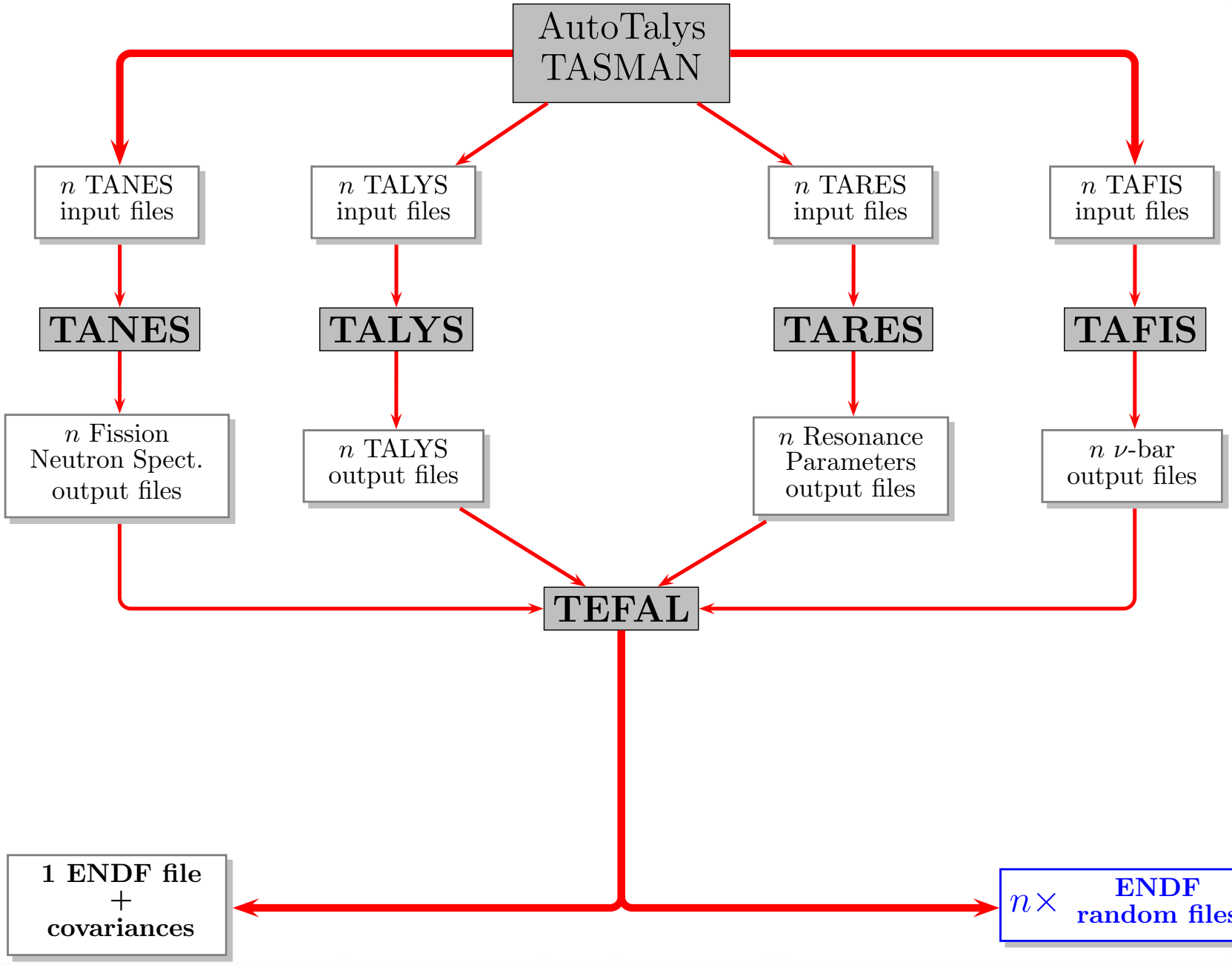
$\Longrightarrow$ consistent and simultaneous evaluation & adjustment (WP2/3), covariance production WP2 and uncertainty propagation for ^{239}Pu WP3.

The TALYS system and outcomes



Our work is based on the ”TALYS system”. Different outcomes are possible.

The TALYS system

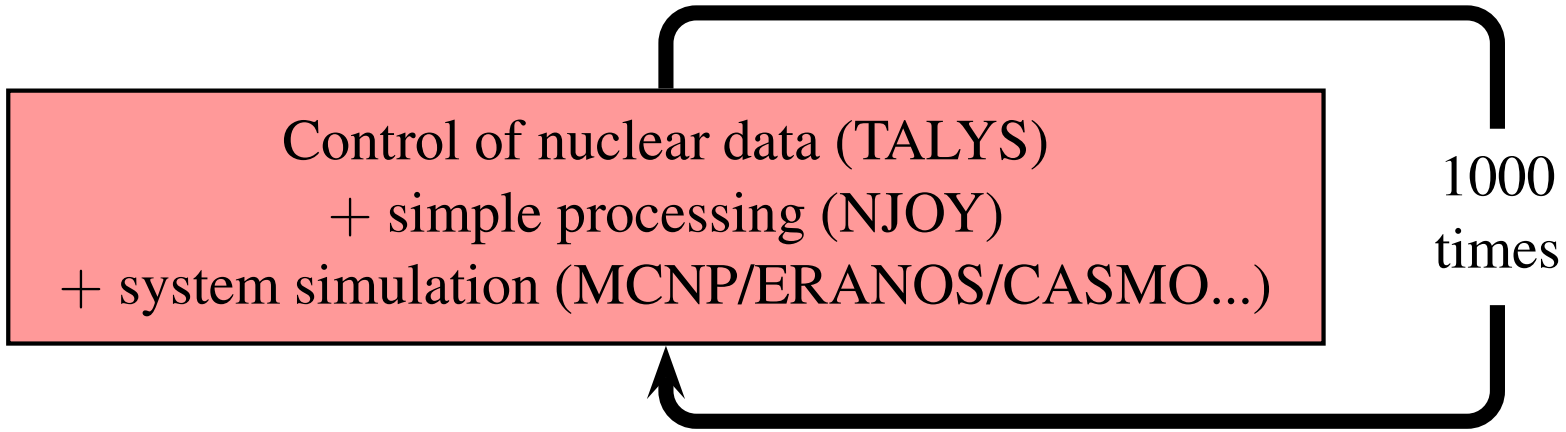


(1) Possibilities at NRG: uncertainty propagation

① Obtain uncertainties for ANDES due to nuclear data uncertainties

② Systematic approach, reliable and reproducible

Solution (1): Total Monte Carlo (or TMC)

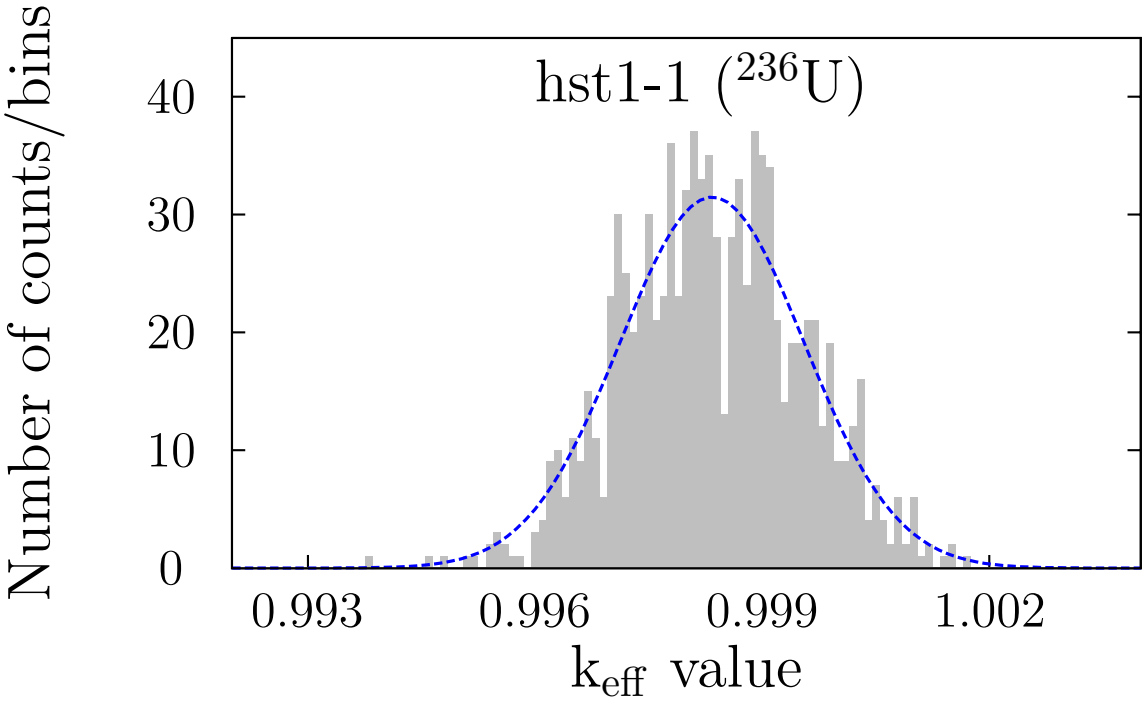


TMC has been successfully applied to different system (fusion benchmarks, criticality benchmarks, GEN-III and GEN-IV reactors) for k_{eff}, void coefficient, Doppler effect, inventory, radiotoxicity. Results are presented in many papers.

(1) Total Monte Carlo: examples

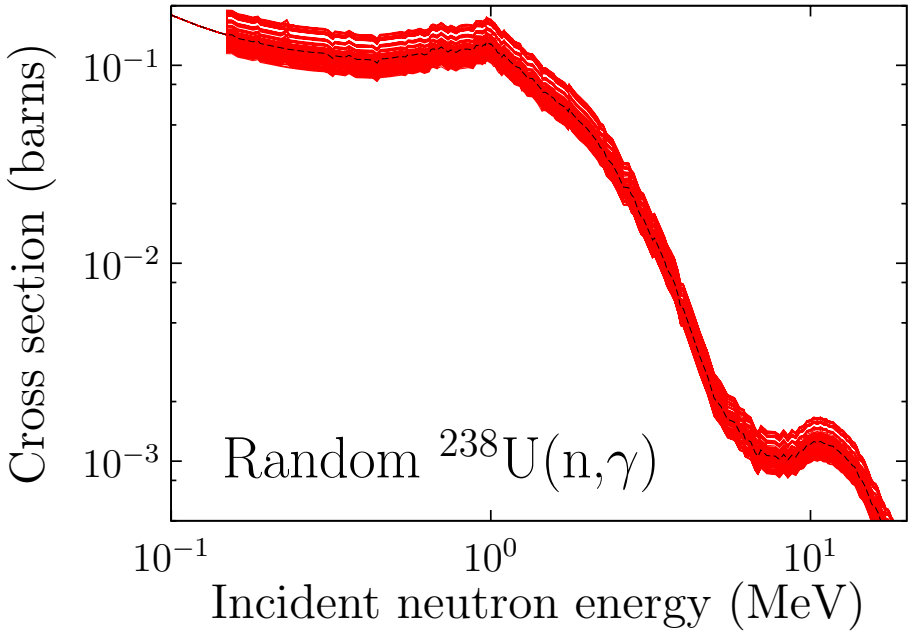
For each random ENDF file, the benchmark calculation is performed with MCNP. At the end of the *n* calculations, *n* different k_{eff} values are obtained. In the obtained probability distribution of k_{eff}, the standard deviation σ_{total} reflects two different effects:

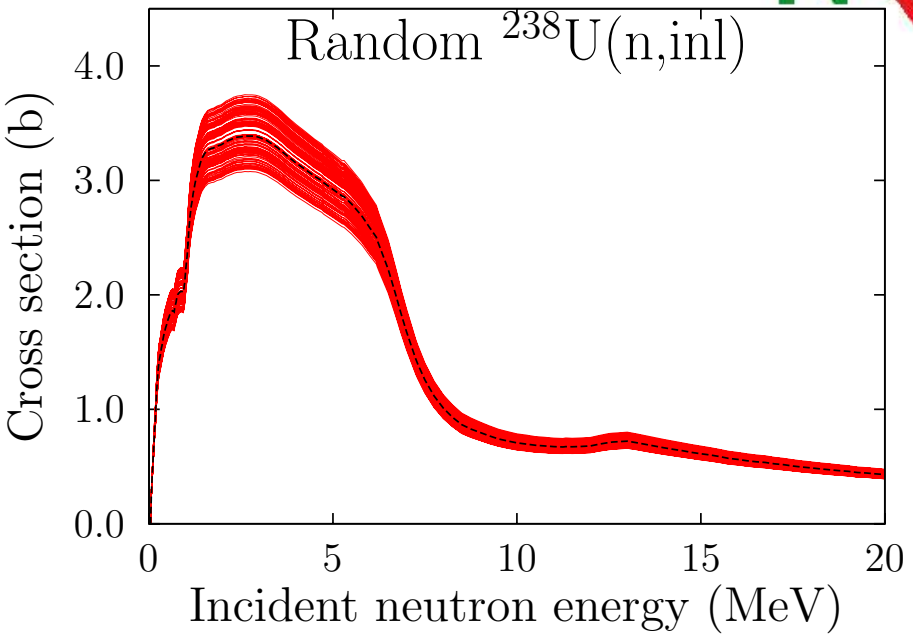
$$\sigma^2_{total} = \sigma^2_{statistics} + \sigma^2_{nuclear\ data}. \quad (1)$$

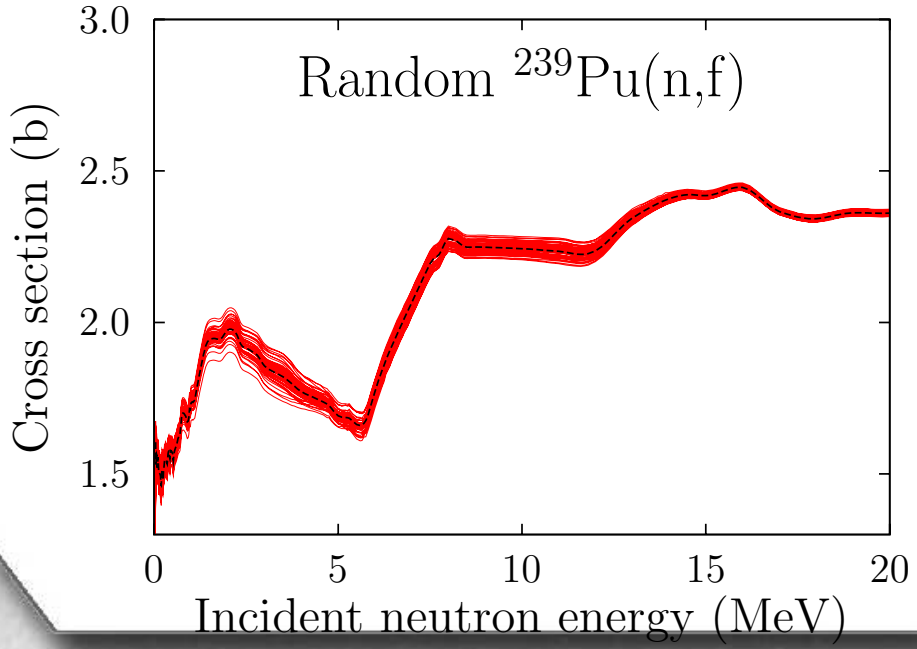


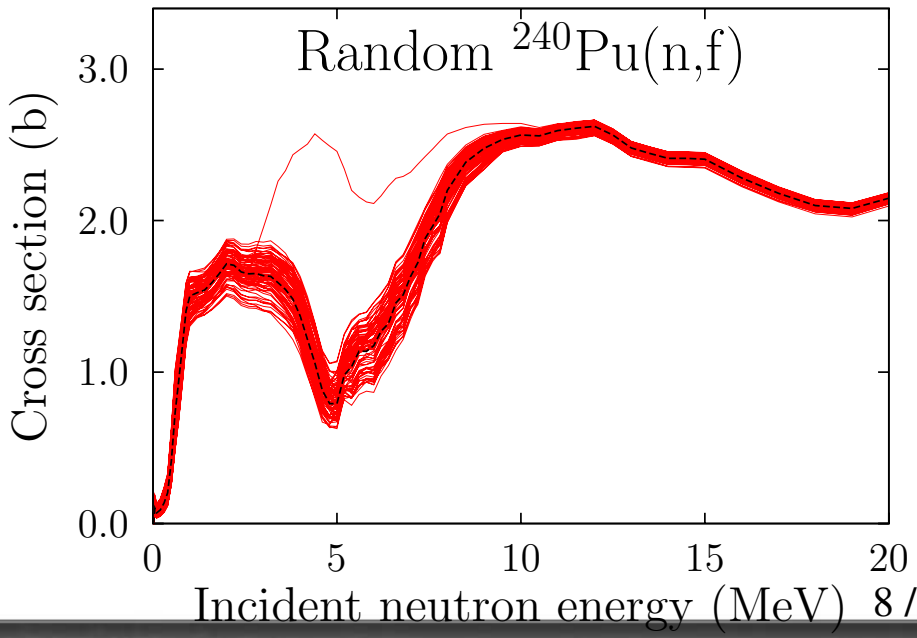
Each random file is completely different than another one: nu-bar, resonance parameters, cross sections...

(1) Nuclear data: examples of random cross sections

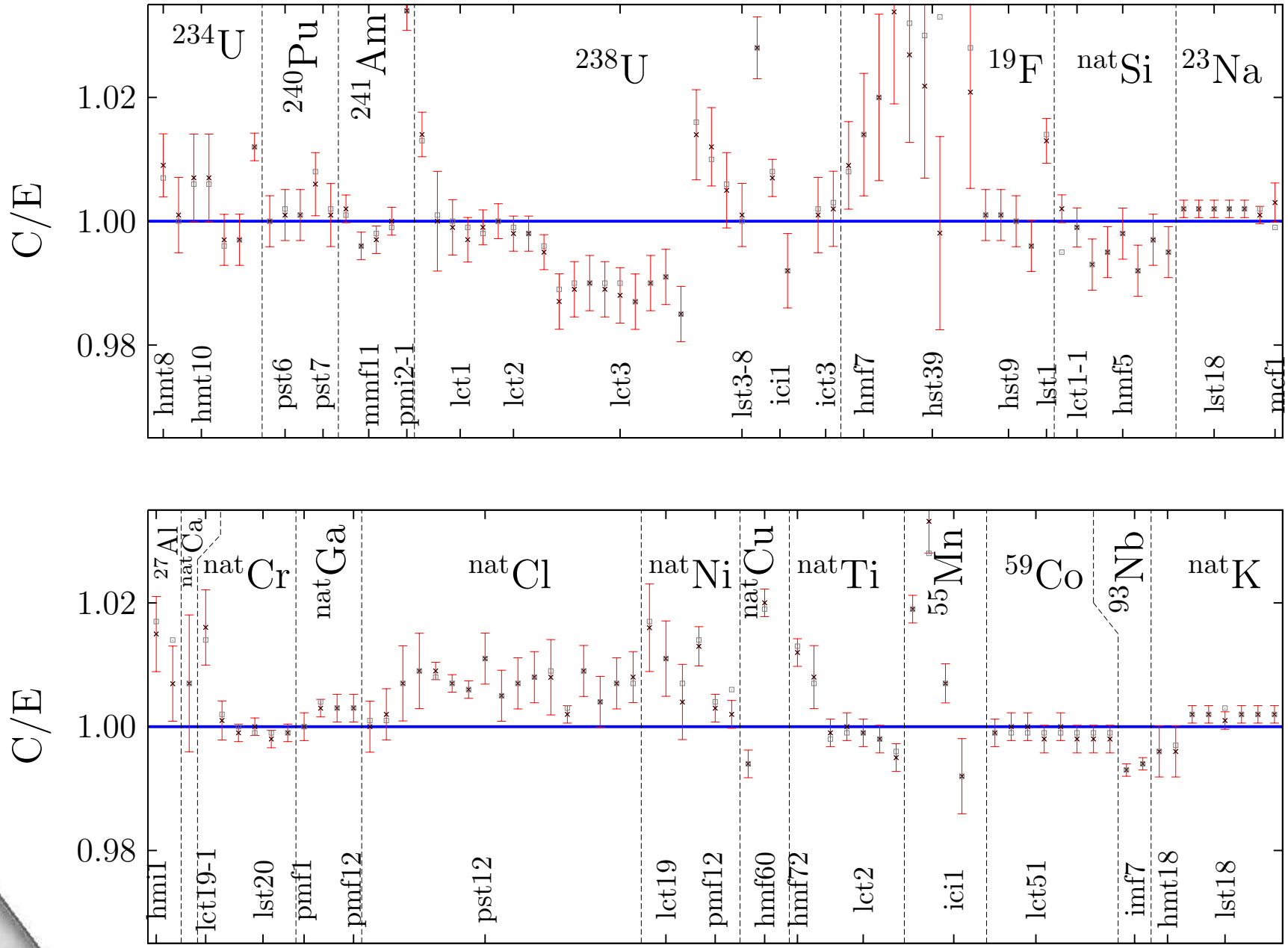








(1) Examples of results for a few criticality benchmarks



(2) Example of the *Random search* on ^{239}Pu

① Use the ”TALYS system” to create a single ^{239}Pu evaluation close or equal to ENDF/B-VII.0 or JEFF-3.1.1

② Randomize all model parameters (resonances, nubar, fission neutron spectrum, TALYS parameters) to create $n > 500$ random ^{239}Pu evaluations

③ Benchmarks the n files with the same set of criticality benchmarks

④ Select the best random file

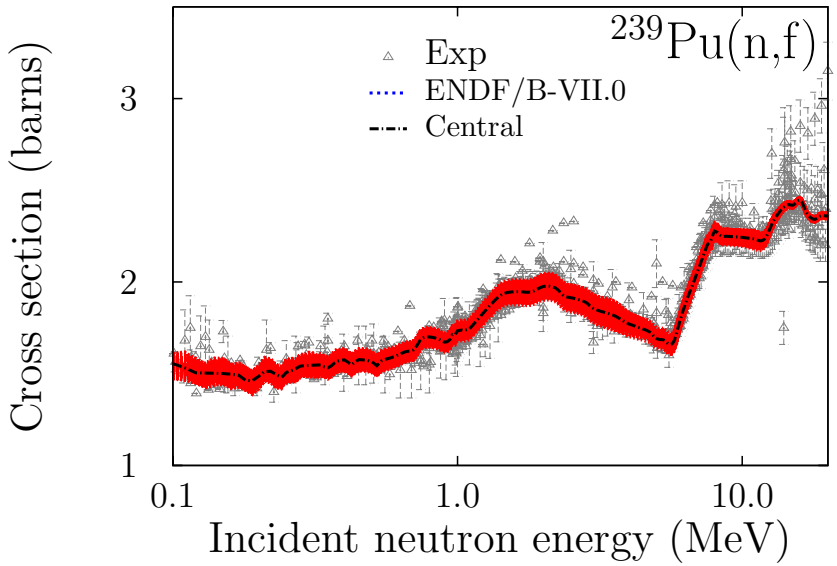
⑤ *Collaboration with LANL to analyze the fission neutron spectrum with TMC*

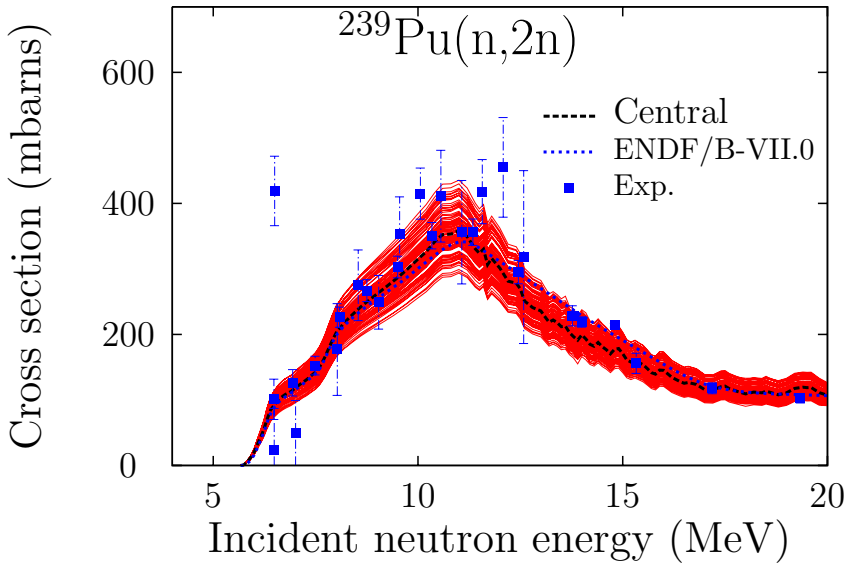
This method is presented in

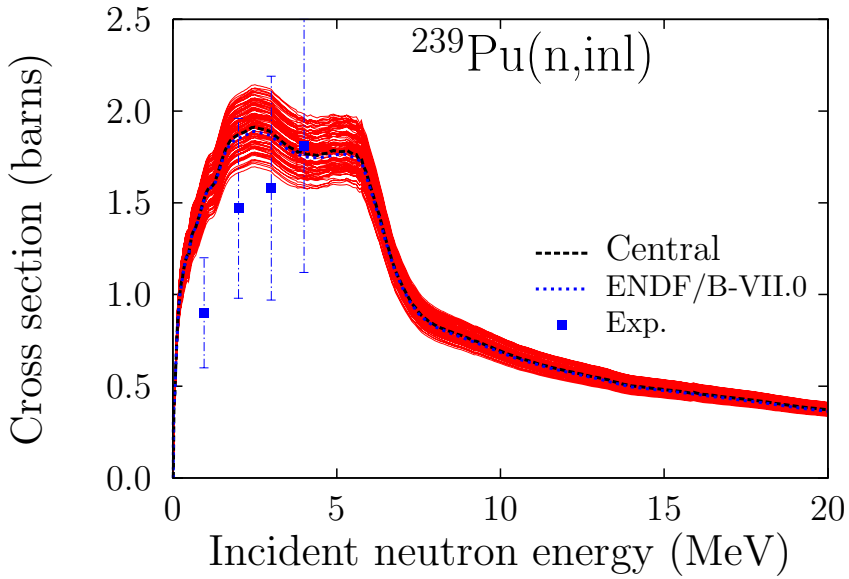
1) ”*How to randomly evaluate nuclear data: a new data adjustment method applied to* ^{239}*Pu*”, D. Rochman and A.J. Koning, accepted in Nucl. Sci. and Eng., Sept. 2011.

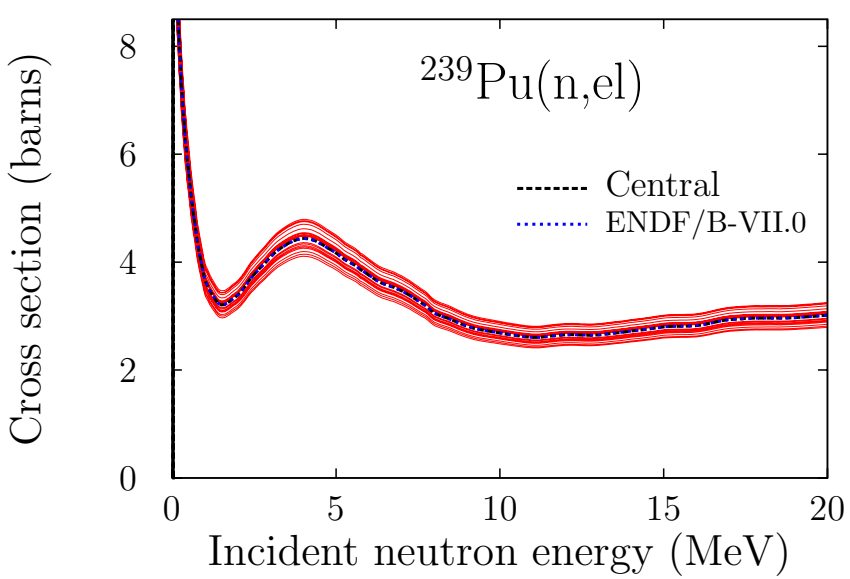
2) ”*Evaluation and adjustment of neuron-induced reactions of* ^{63,65}*Cu*”, D. Rochman and A.J. Koning, submitted to Nucl. Sci. and Eng., 2011.

(2) Possibilities at NRG: Random search of the *best* ^{239}Pu

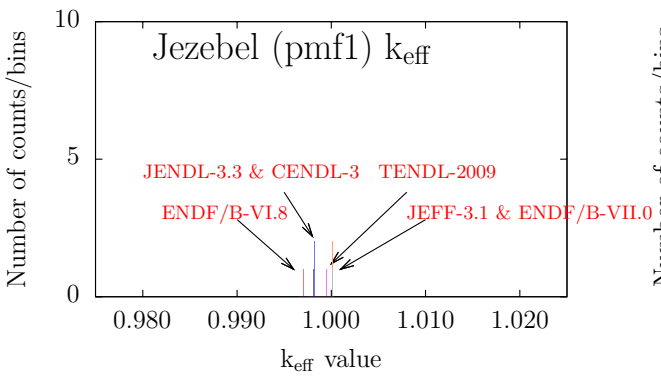


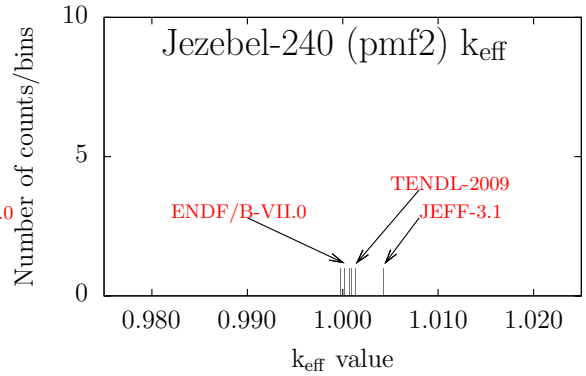


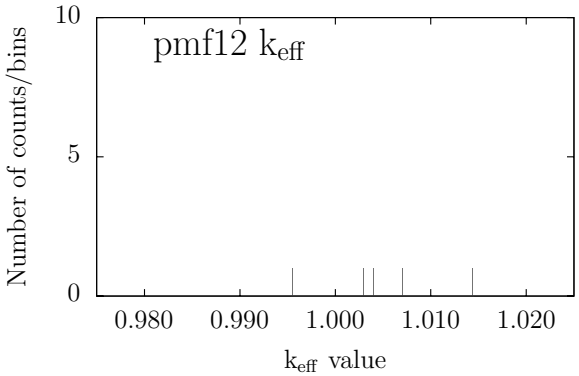


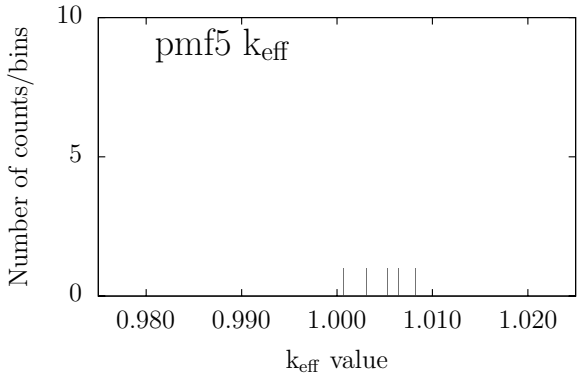


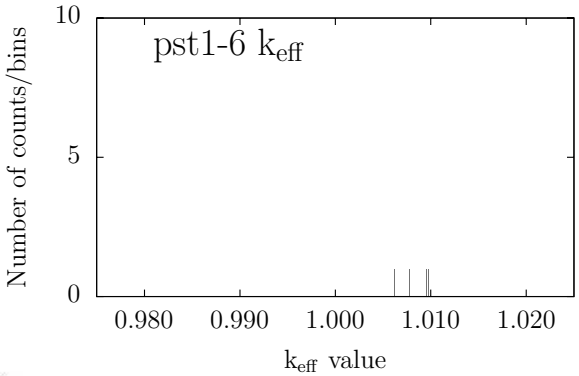
(2) Benchmarking: simple example with 6 k_{eff} benchmarks

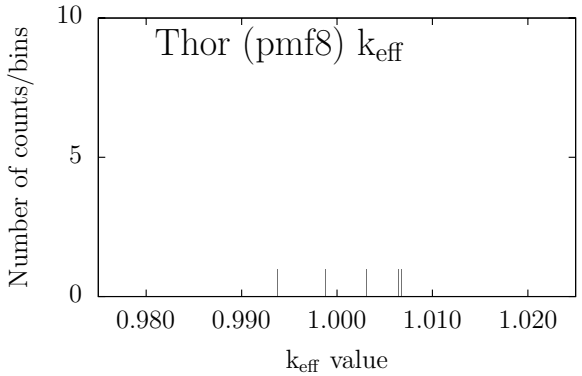












χ^2

JEFF-3.1.1:	$1.14e^{-4}$
JENDL-3.3:	$1.71e^{-4}$
TENDL-2009:	$3.66e^{-4}$
ENDF/B-VI.8:	$1.72e^{-4}$
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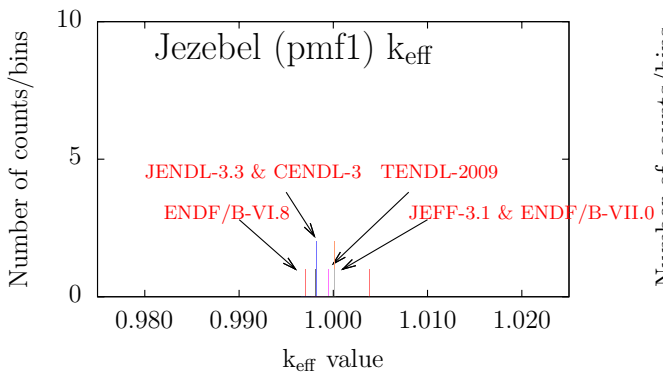

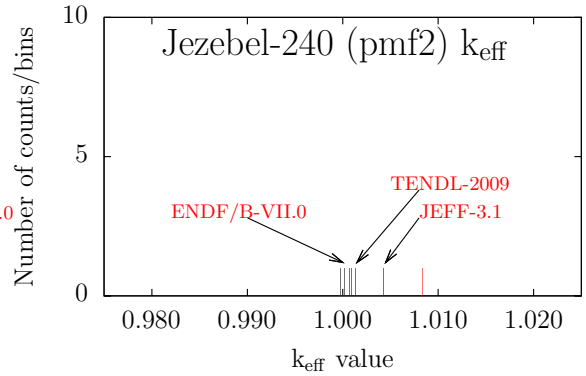

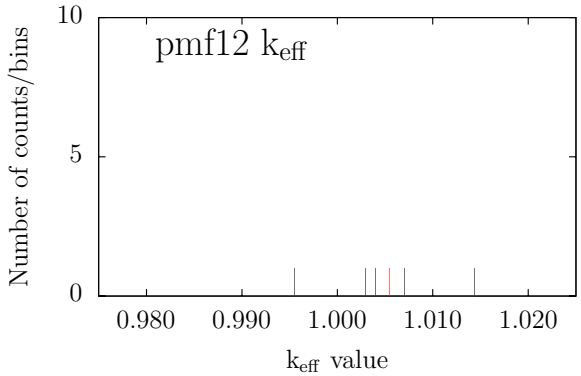

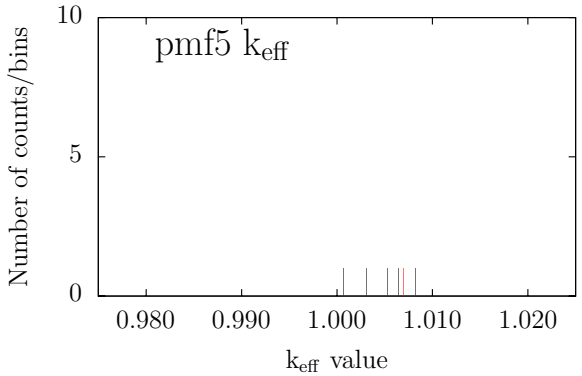

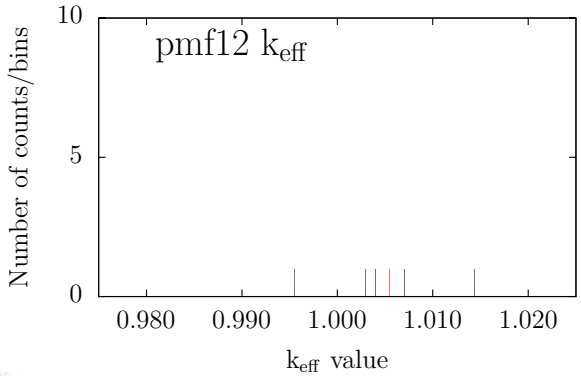

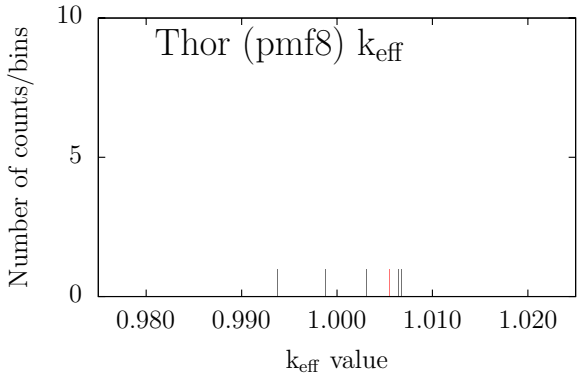

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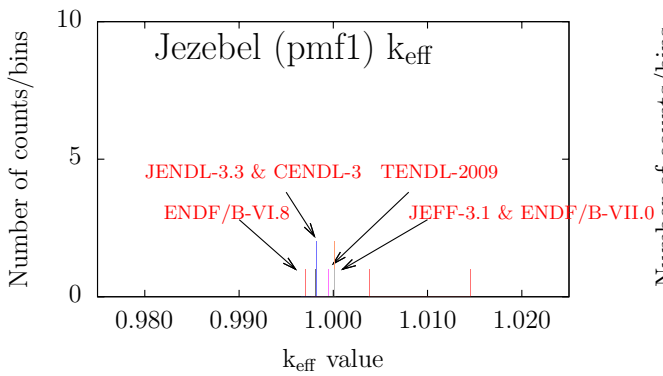

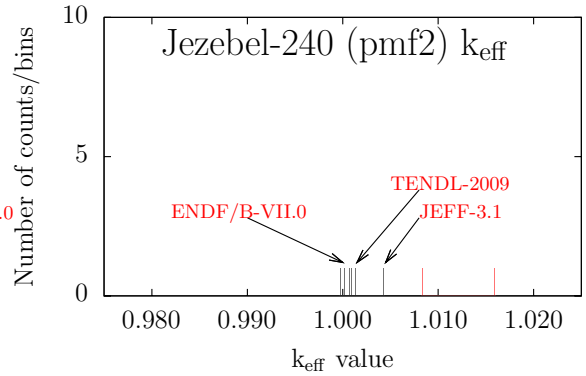

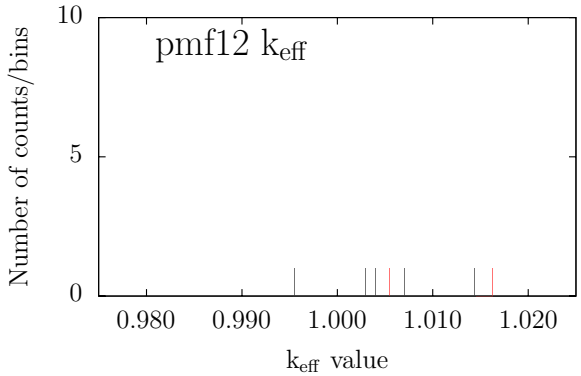

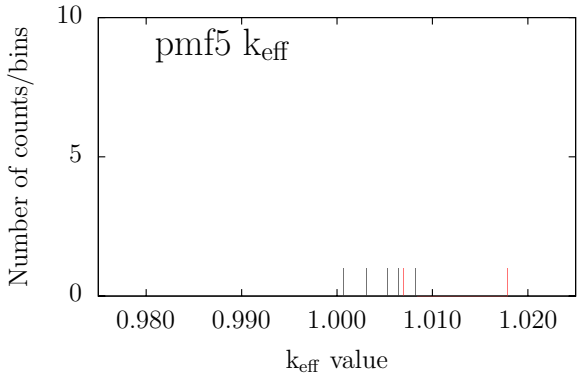

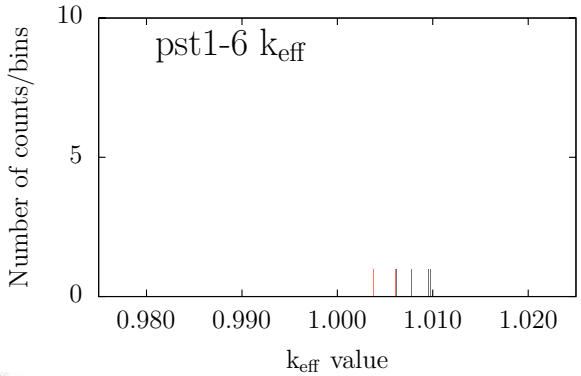

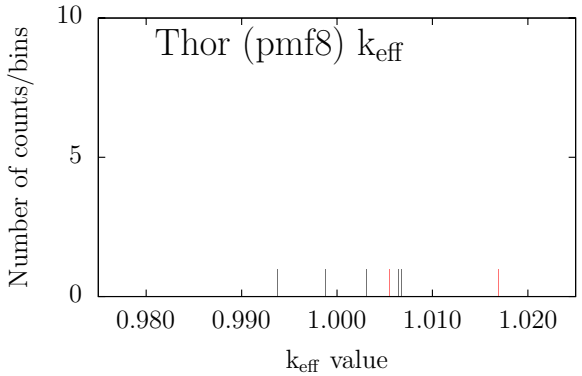

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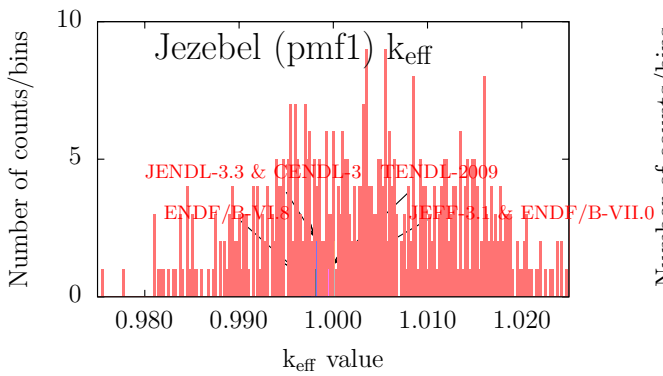
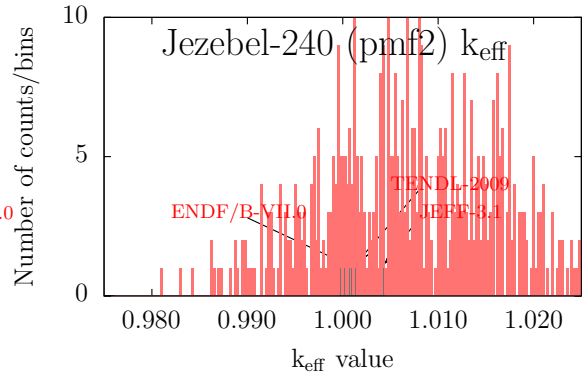
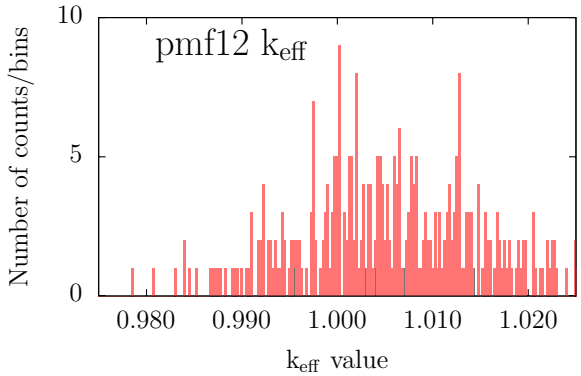
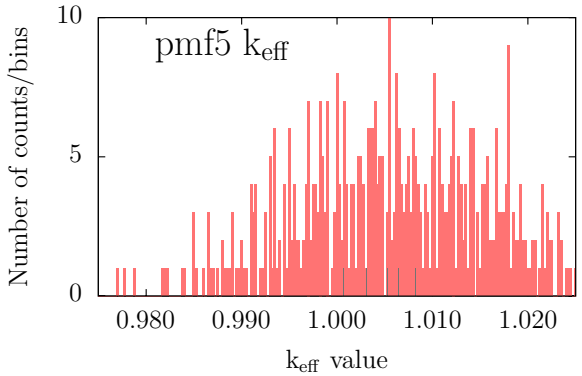
random 0:	$2.29e^{-4}$
random 1:	$13.4e^{-4}$

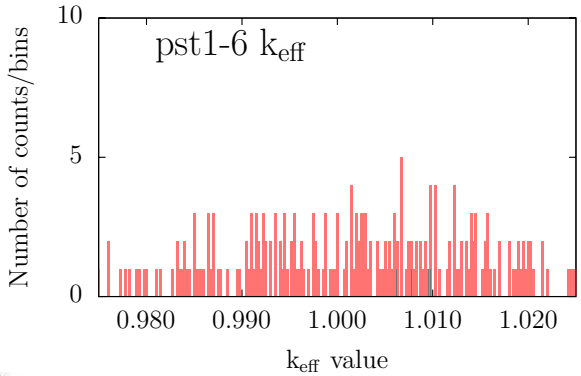
(2) Benchmarking: 6 k_{eff} benchmarks with random ^{239}Pu

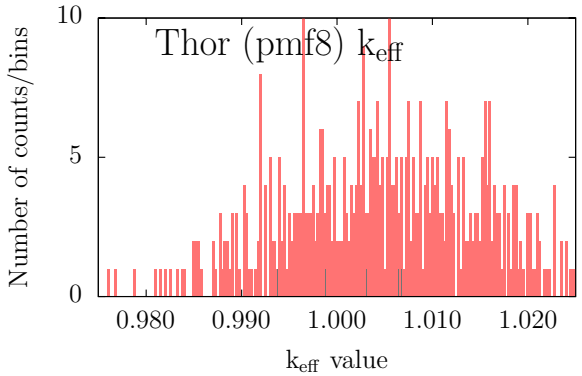












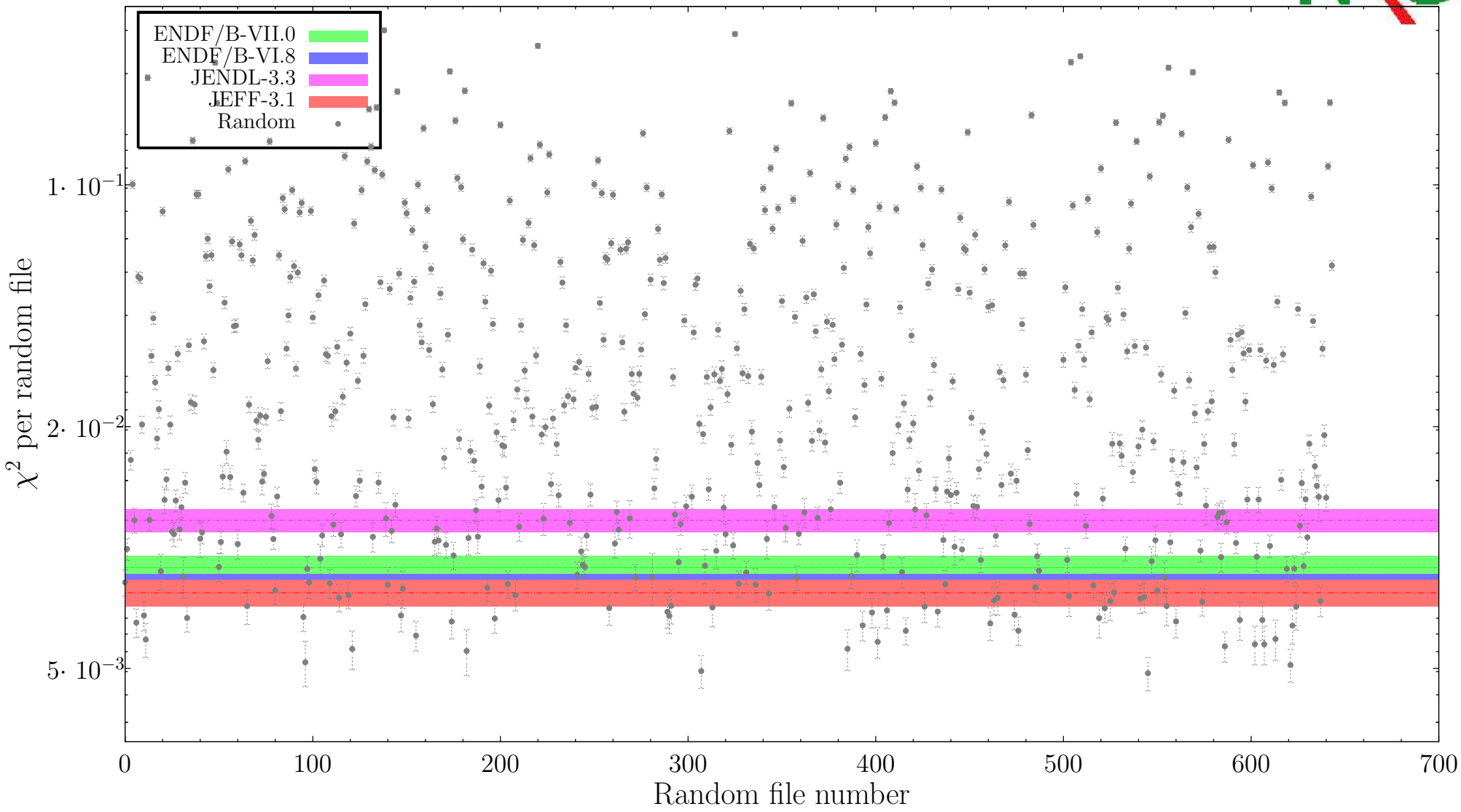
(2) Real case: 120 ^{239}Pu benchmarks

Table 1: List of plutonium benchmarks selected for the random search.

Name	Cases	Name	Cases	Name	Cases	Name	Cases
pmf1	1	pmf2	1	pmf5	1	pmf6	1
pmf8	1	pmf12	1	pmf13	1	pci1	1
pmi2	1	pst1	6	pst2	6	pst3	8
pst4	13	pst5	9	pst6	3	pst7	9
pst8	29	pst12	22	pmm1	6		

$$\chi^2 = \sum_{i=0}^{n} \frac{(C_i - E_i)^2}{C_i}, \tag{2}$$

(2) χ^2 values for random ^{239}Pu evaluations



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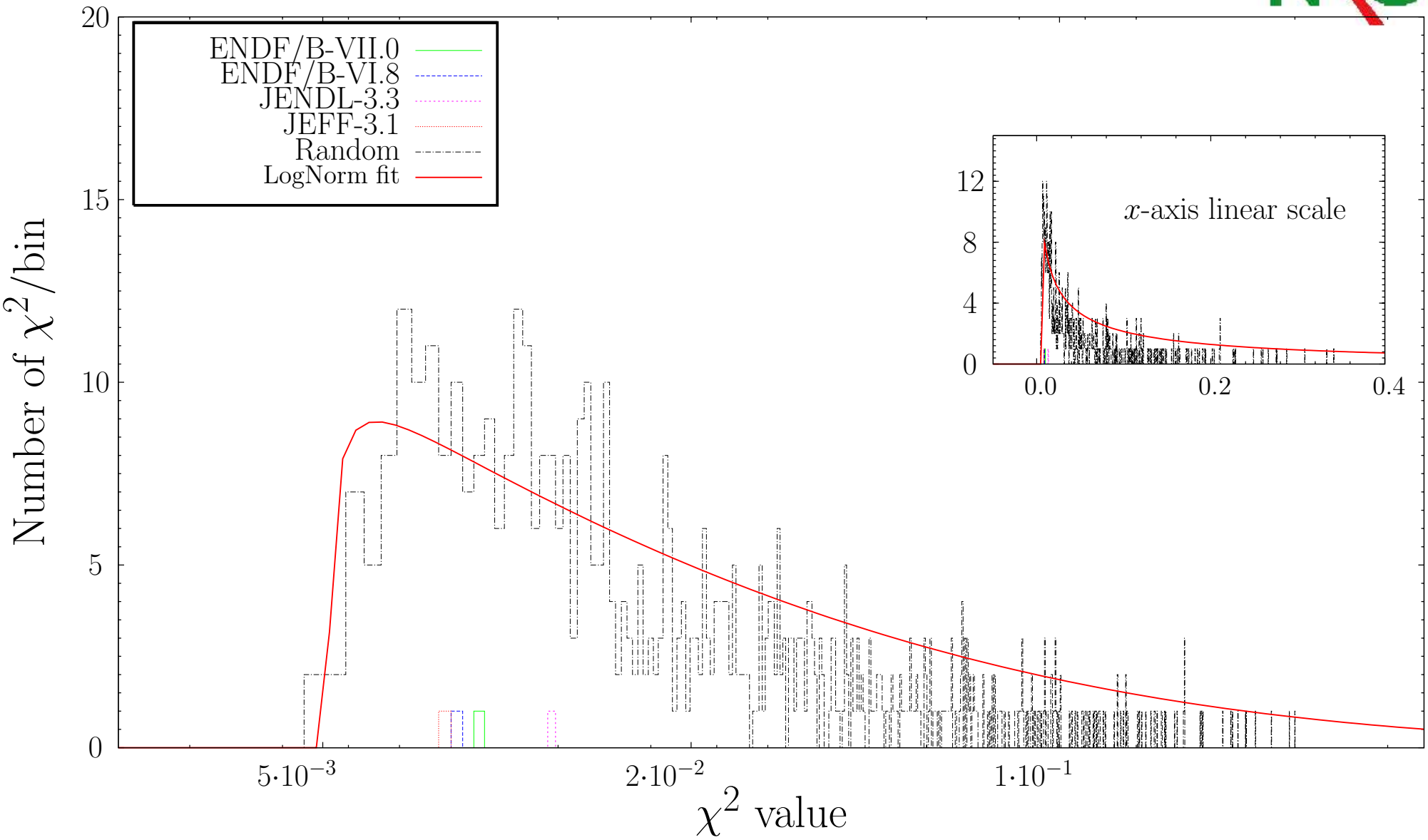

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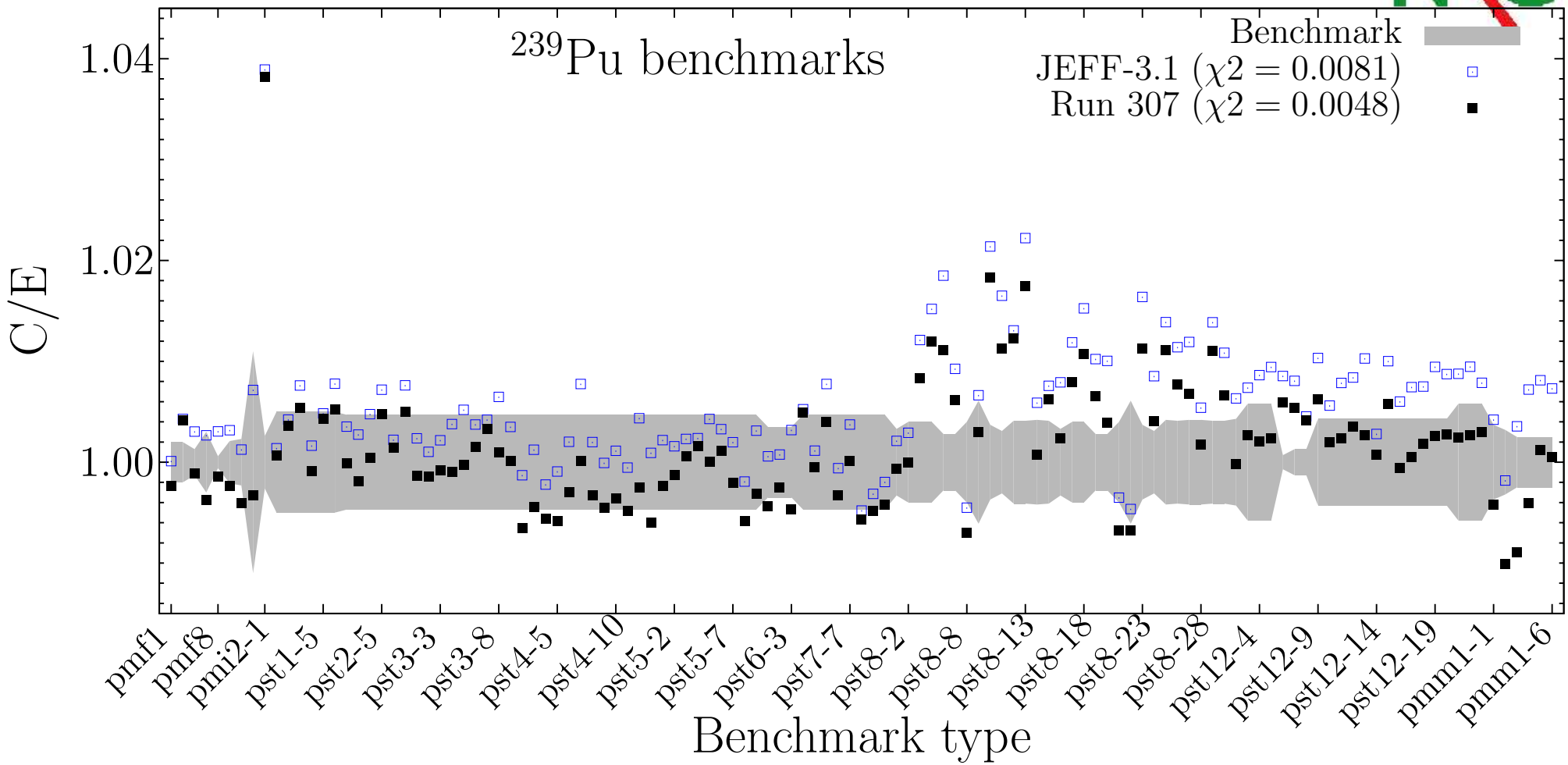
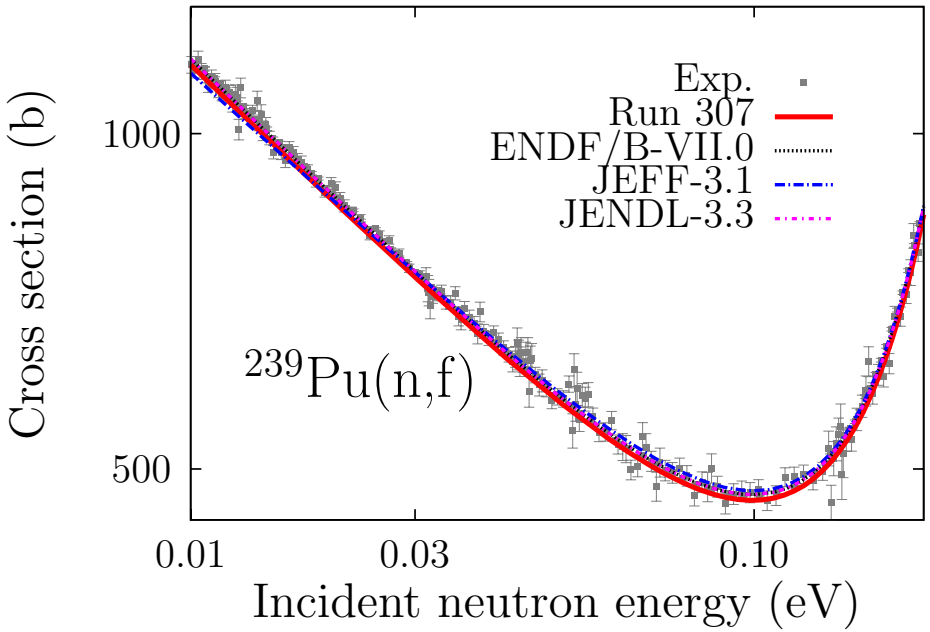
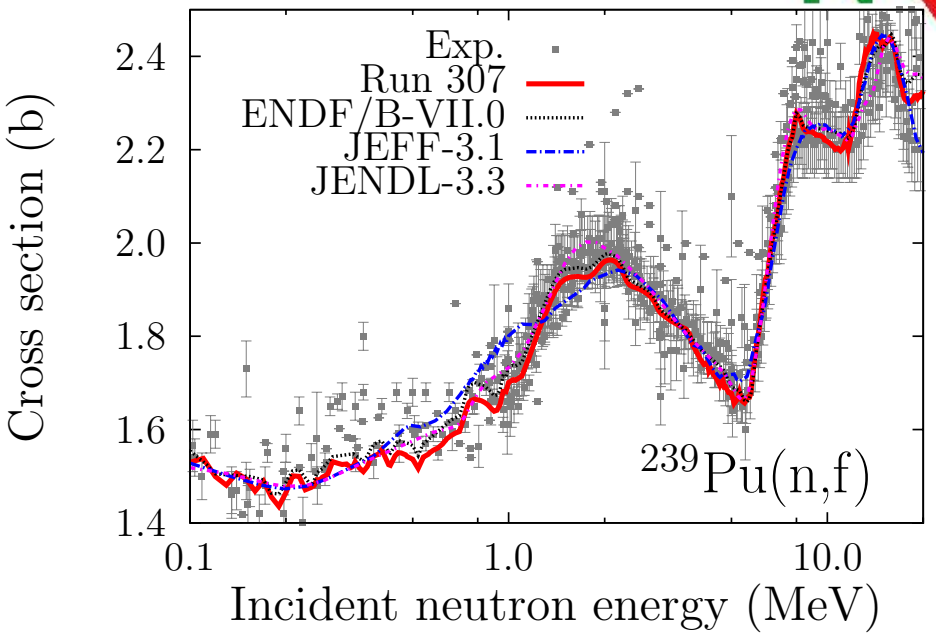
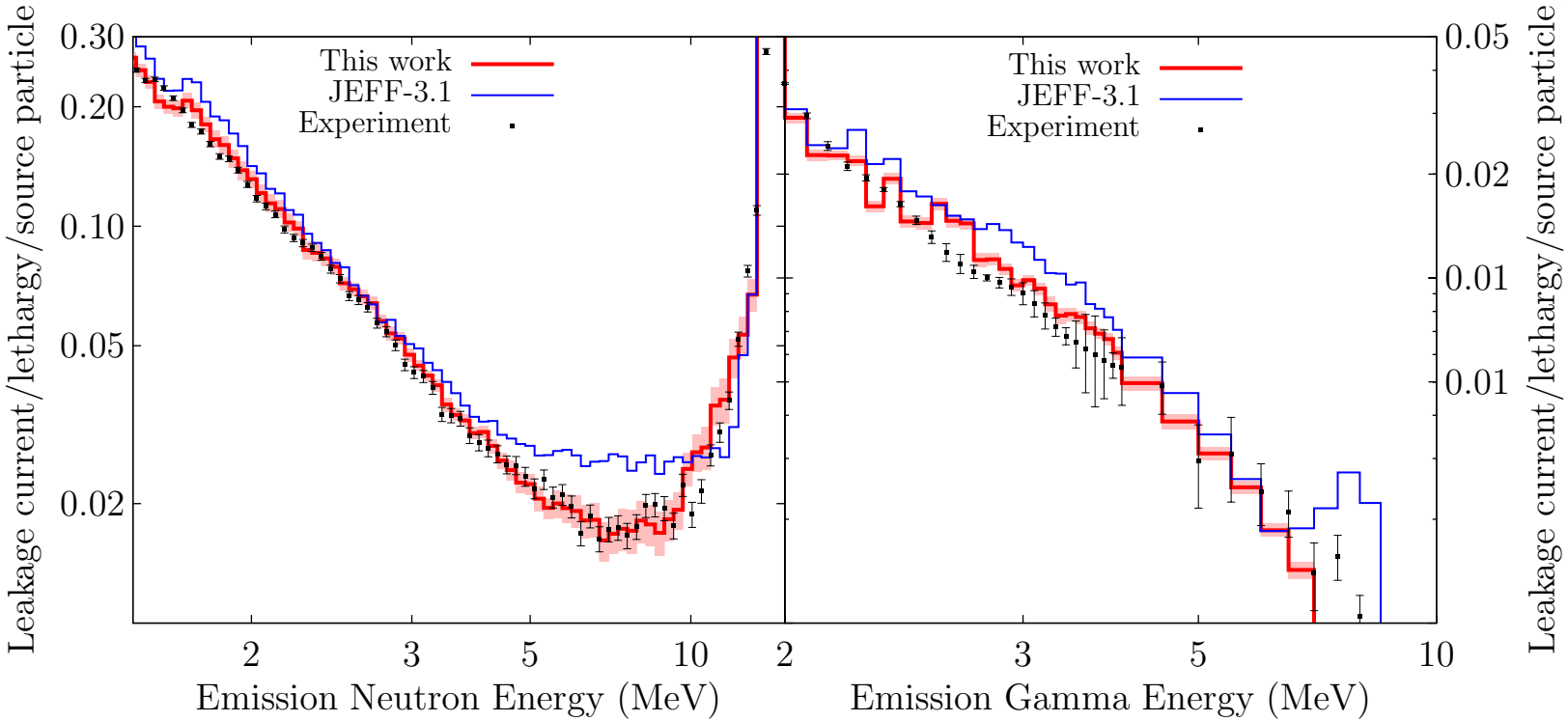


(2) Best ^{239}Pu for this set of benchmarks



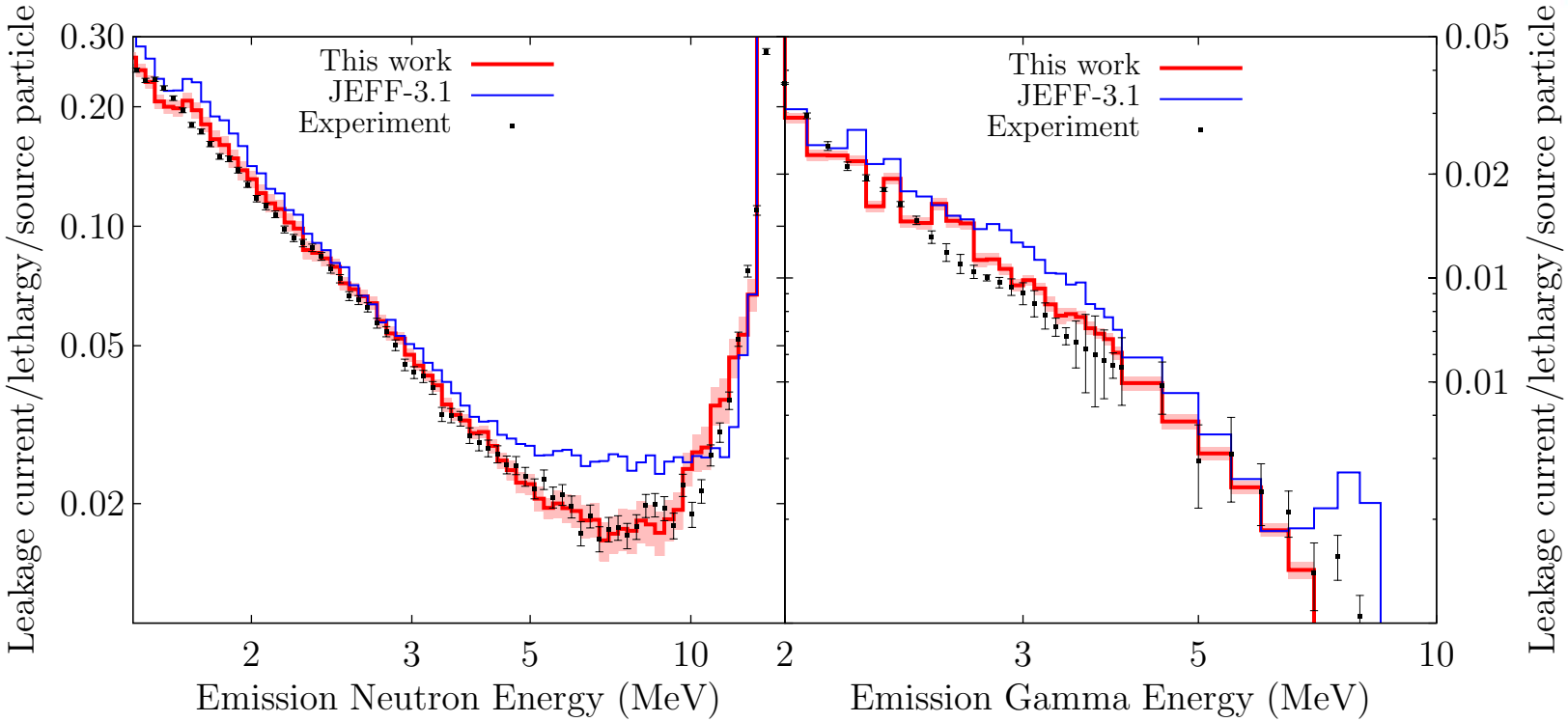


(2) Monte Carlo Sensitivity (Cu case)



Example for random ^{63}Cu and ^{65}Cu applied to the 14 MeV neutron leakage Oktavian benchmark. Which reaction helped to improve the calculation ?

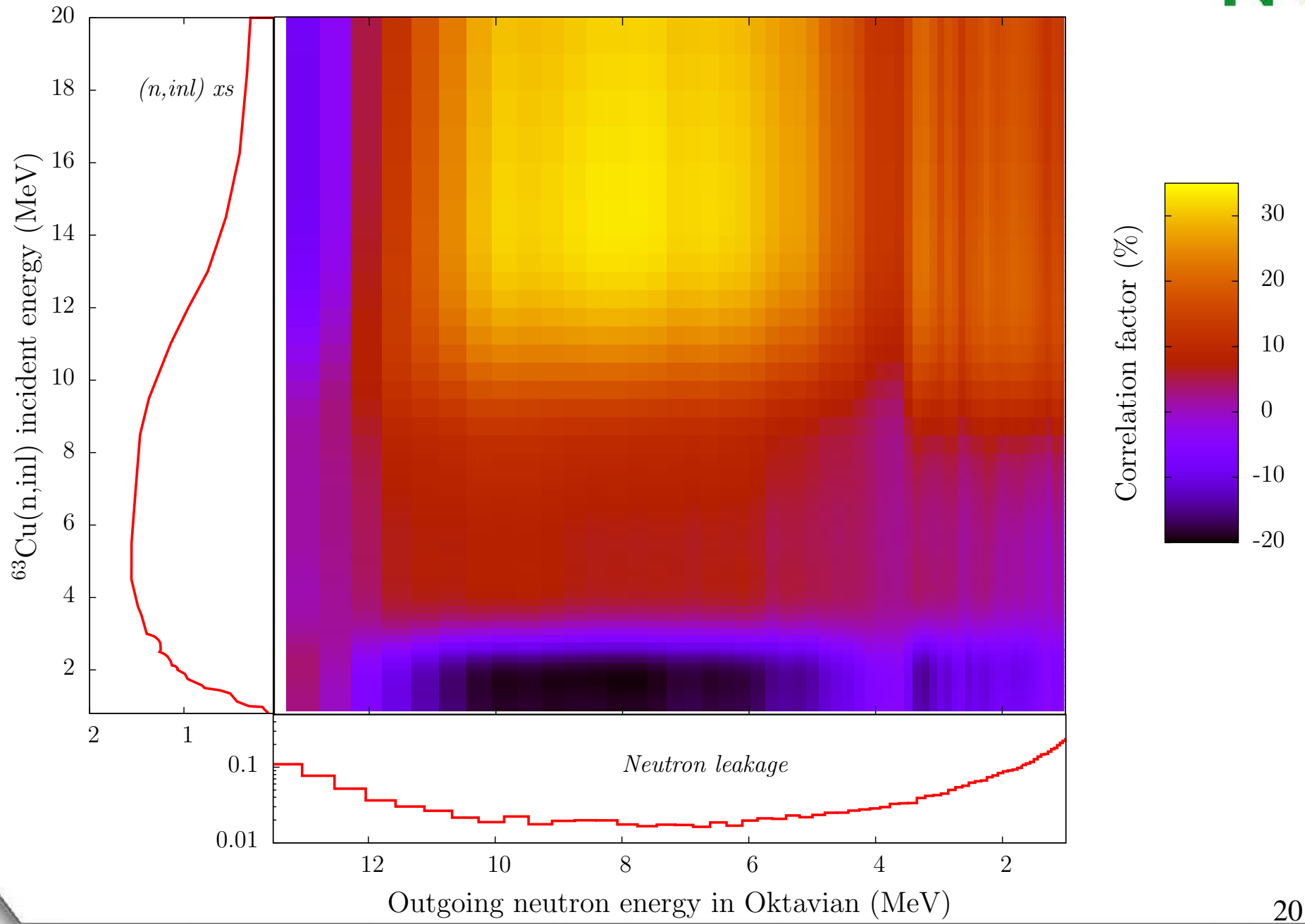
(2) Monte Carlo Sensitivity (Cu case)



Example for random ^{63}Cu and ^{65}Cu applied to the 14 MeV neutron leakage Oktavian benchmark. Which reaction helped to improve the calculation ?
Answer: sensitivity S:

$$S_{il} = \frac{\sum_{k=1}^{K}(p_l^{(k)} - p_l^{(0)})(\sigma_i^{(k)} - \sigma_i^{(0)})}{\sum_{k=1}^{K}(p_l^{(k)} - p_l^{(0)})^2} \frac{p_l^{(0)}}{\sigma_i^{(0)}}, \qquad i = 1,N, \quad l = 1,L. \tag{3}$$

(2) Monte Carlo Sensitivity (Cu case)



(2) Monte Carlo Sensitivity (Cu case)

Many types of correlation can be found this way, which were never obtained before:

1. nuclear data vs. neutron or gamma leakage,
2. nuclear data vs. criticality benchmarks,
3. neutron or gamma leakage vs. criticality benchmarks,
4. criticality benchmarks vs. criticality benchmarks,
5. neutron leakage vs. neutron leakage, and
6. neutron leakage vs. gamma leakage.

(3) Covariance generation with TALYS via Monte Carlo

Let $\vec{\mathbf{p}}$ be the vector of the L adjustable nuclear model parameters that are relevant to the problem under consideration, *i.e.*

$$\vec{\mathbf{p}} = \{p_1, \ldots, p_l, \ldots, p_L\} \Longrightarrow p_l^{(k)} = p_l^{(0)} \pm \Delta p_l, \qquad l = 1, L$$

The basis of our method is to let TALYS perform many calculations:

$$\vec{\sigma}^{(k)} = T(\vec{\mathbf{p}}^{(k)})$$

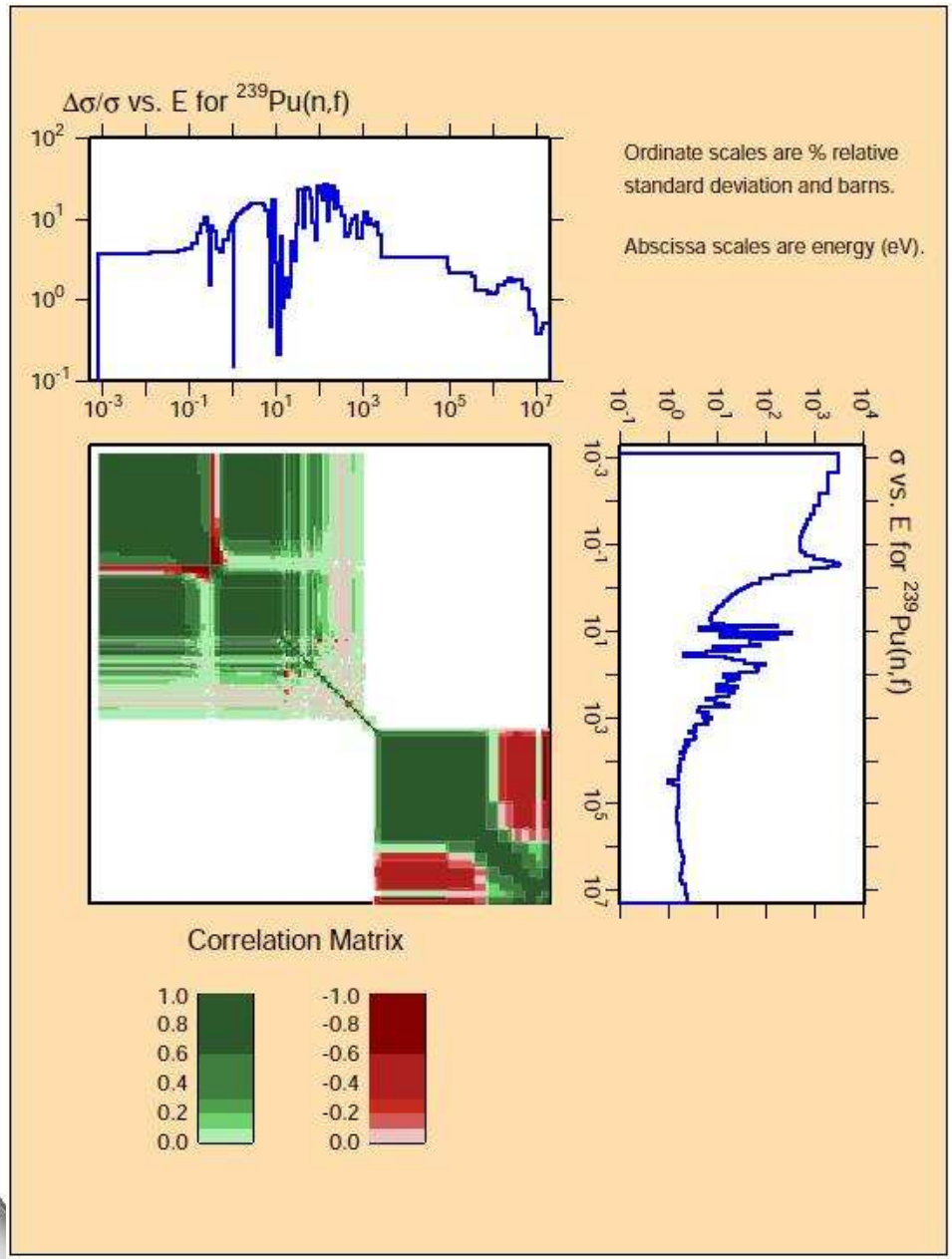
The average covariance matrix for cross sections is given by

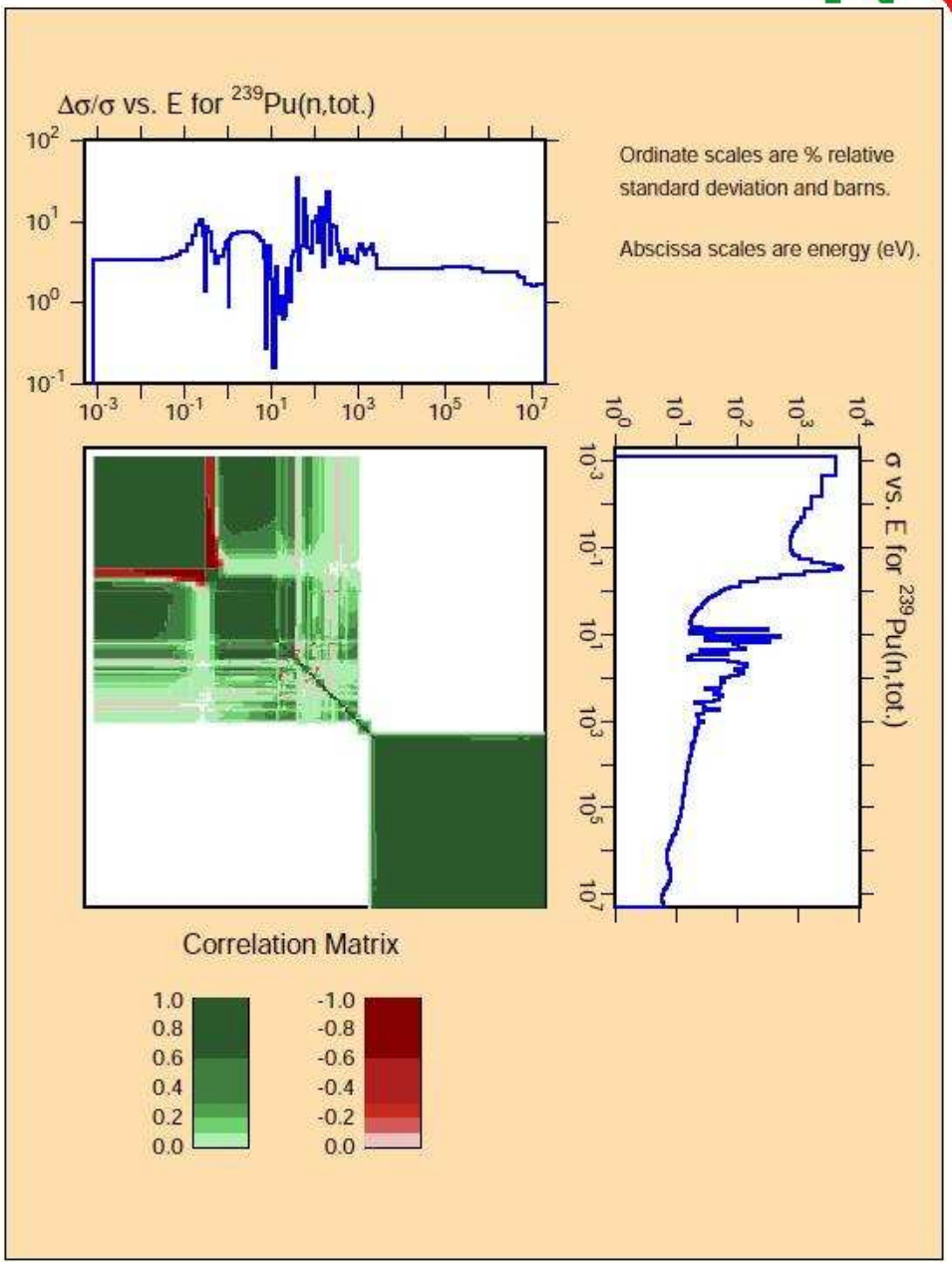
$$V_{ij} = \frac{1}{K} \sum_{k=1}^{K} (\sigma_i^{(k)} - \sigma_i^{(0)})(\sigma_j^{(k)} - \sigma_j^{(0)}), \qquad i, j = 1, N,$$

where K is the total number of TALYS runs needed for statistical convergence. The average calculated cross sections are

$$\bar{\sigma}_i = \frac{1}{K} \sum_{k=1}^{K} \sigma_i^{(k)}, \qquad i = 1, N,$$

(3) Example of ^{239}Pu covariances





Plans for ANDES WP 2/3

- WP2: Random search for the best χ^2 with a given set of benchmarks
  - Benchmarks defined end 2010
  - Perform the search of ^{239}Pu
  - Obtain ^{239}Pu cross sections and covariances (WP2) and use it in WP3
- WP3: Uncertainty for a set of criticality benchmarks
  - Thermal and fast benchmarks
  - Total Monte Carlo method
  - Use libraries from WP2
  - Other benchmarks