# Monte Carlo Adjustment:

*an application to $^{239}$Pu from ENDF/B-VII.0*

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① Methodology: TALYS + Monte Carlo + benchmarking

② Goal:

⟹ *Can we use Monte Carlo to create/adjust data libraries ?*

③ Example with $^{239}$Pu

⟹ *500 (and more) random nuclear data libraries*

④ Results 1:

⟹ *Search for the optimum entire file/evaluation*

⑤ Results 2:

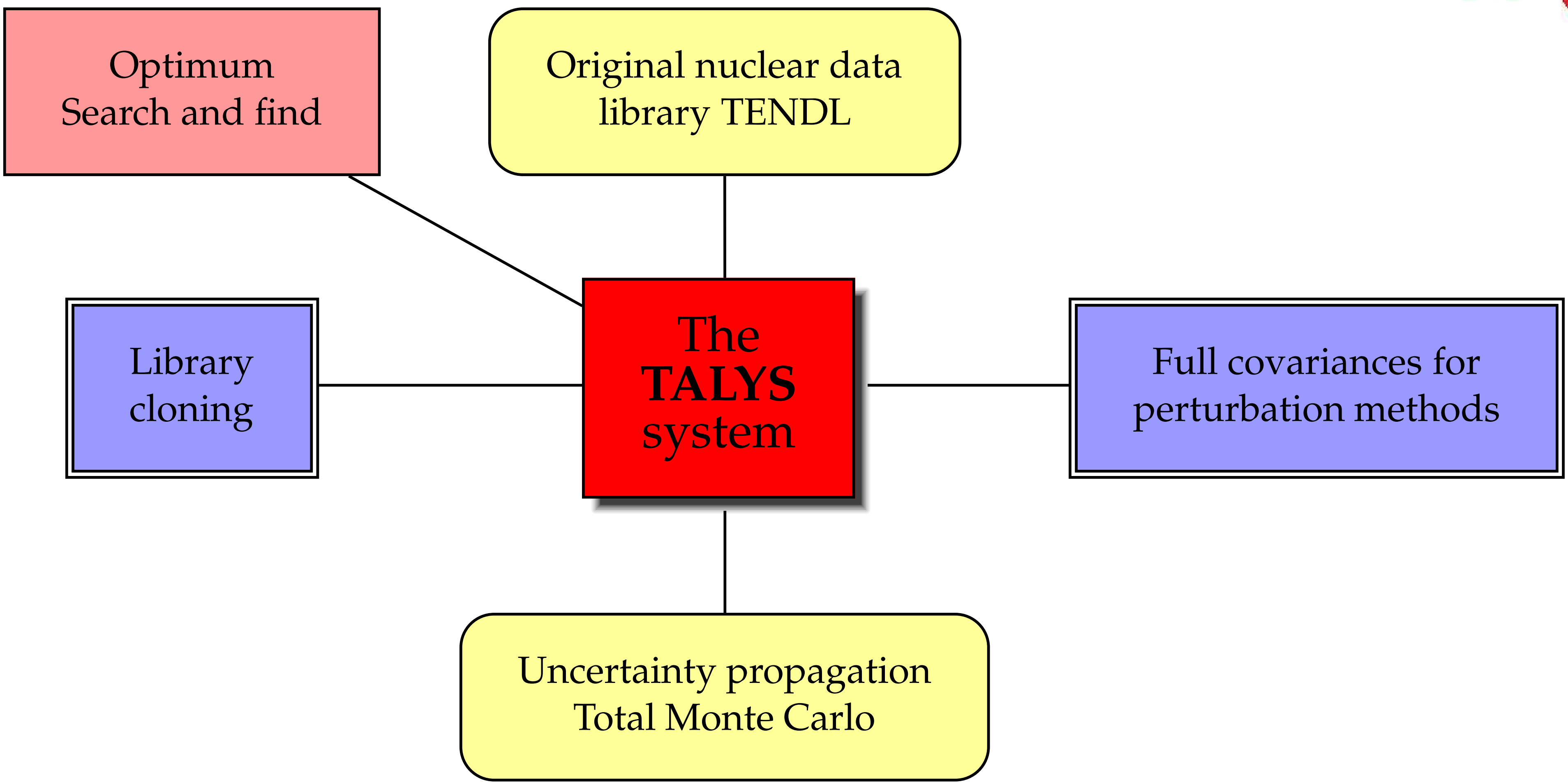
⟹ *Search for the optimum fission neutron spectra*

⑥ Secret plan:

⟹ *to be achieved by 2013*

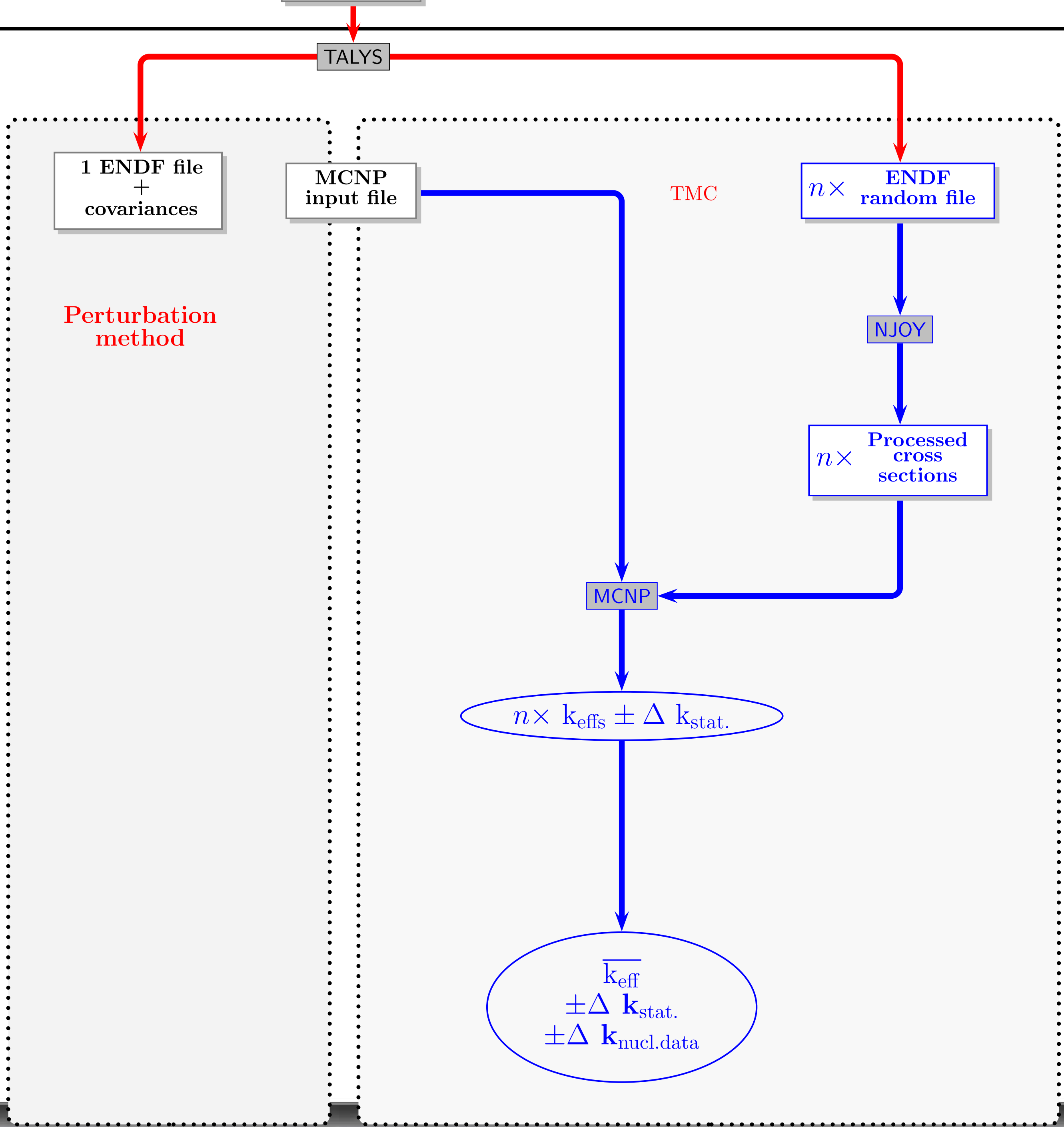
⑦ Conclusions

## The TALYS system and outcomes




Our work is based on the "TALYS system". Completely different applications are possible, all unprecedented.

# Idea: TALYS +( $n$ TALYS input files ) Monte Carlo = Total Monte Carlo

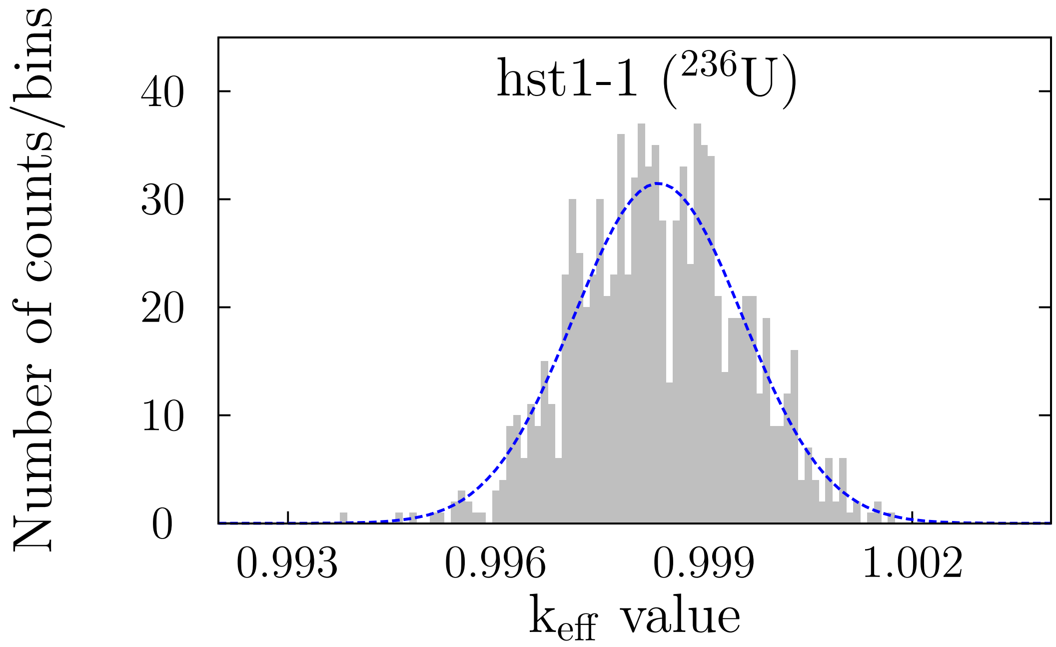


# (1) Total Monte Carlo: examples

*n* ENDF file + *n* MCNP calculations $\Longrightarrow$ *n* different $k_{eff}$

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

$$\sigma^2_{total} = \sigma^2_{statistics} + \sigma^2_{nuclear\ data}$$




Basic and original ideas developed and presented by D. Smith in 1991, 2004 and 2007. Test on a unique benchmark by T. Kawano in 2006 (Jezebel $^{239}$Pu fission cross section).

# Example 1 of innovative approach on $^{239}$Pu

Total Monte Carlo + selection
$\Longrightarrow$ adjustment

① Use TALYS 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 500 random $^{239}$Pu evaluations

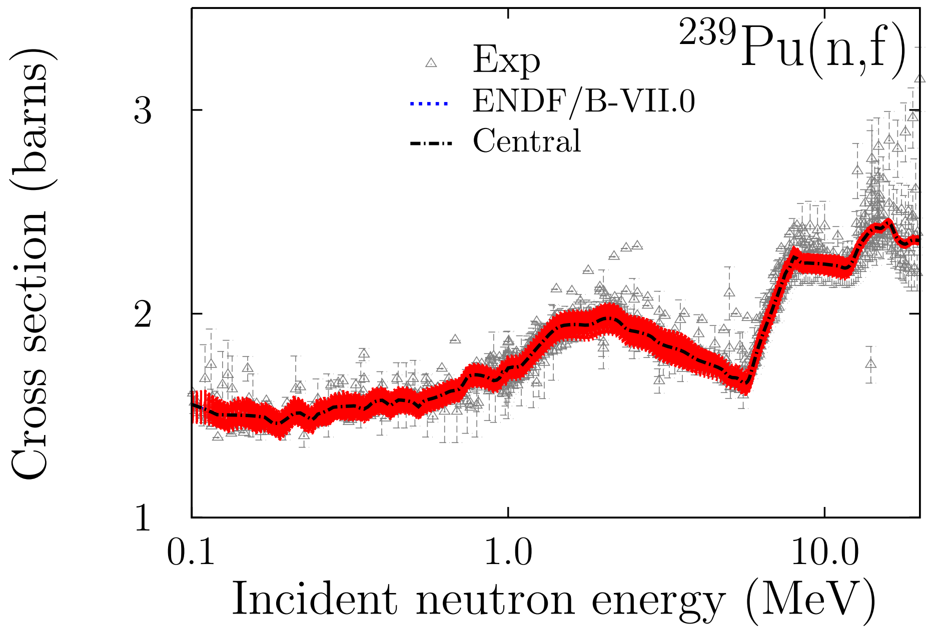
③ Benchmarks the $n \geq 500$ files with the same set of criticality benchmarks

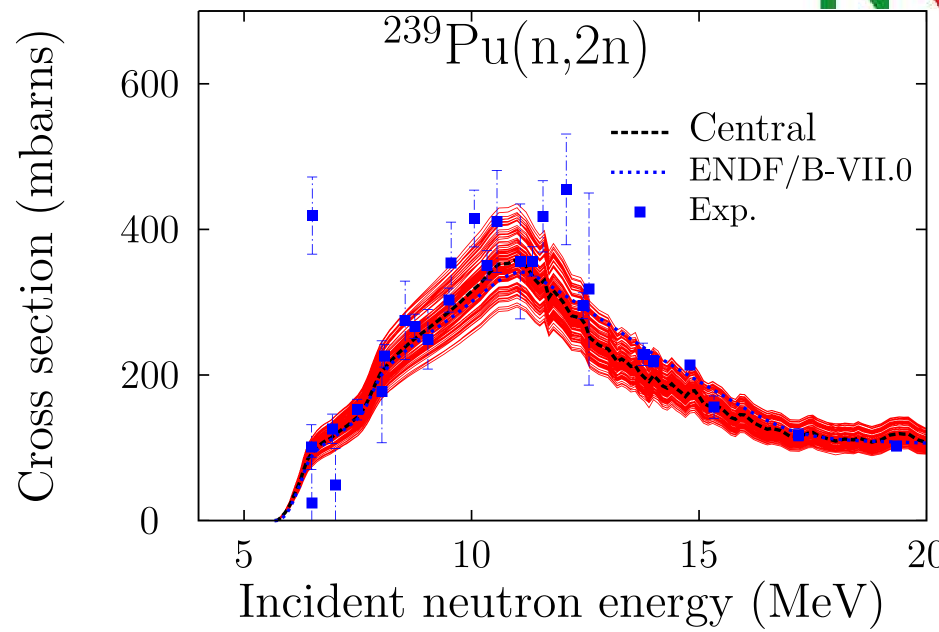
④ Select the best random file

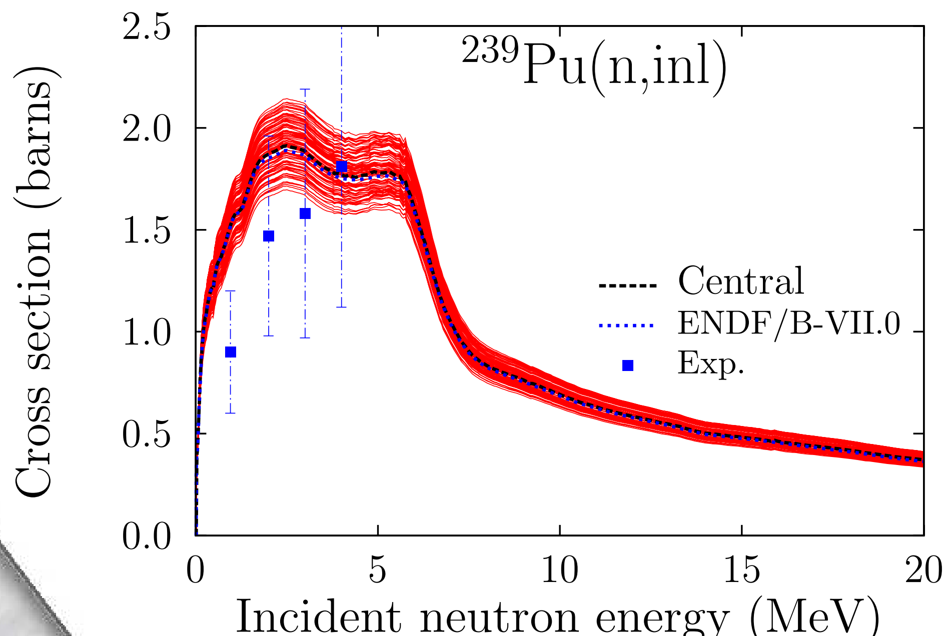
⑤ Create JEFF-3.2β = JEFF-3.1.1 + new $^{239}$Pu

Example: 100 benchmarks, 500 random files $\Longrightarrow$ 500 TALYS + NJOY and $100 \times 500 = 5 \cdot 10^4$ MCNP loops, 1.4 years on a single processor, or 5 days on 100 processors (3 GHz)

# Nuclear data: random $^{239}$Pu in the thermal and fast range



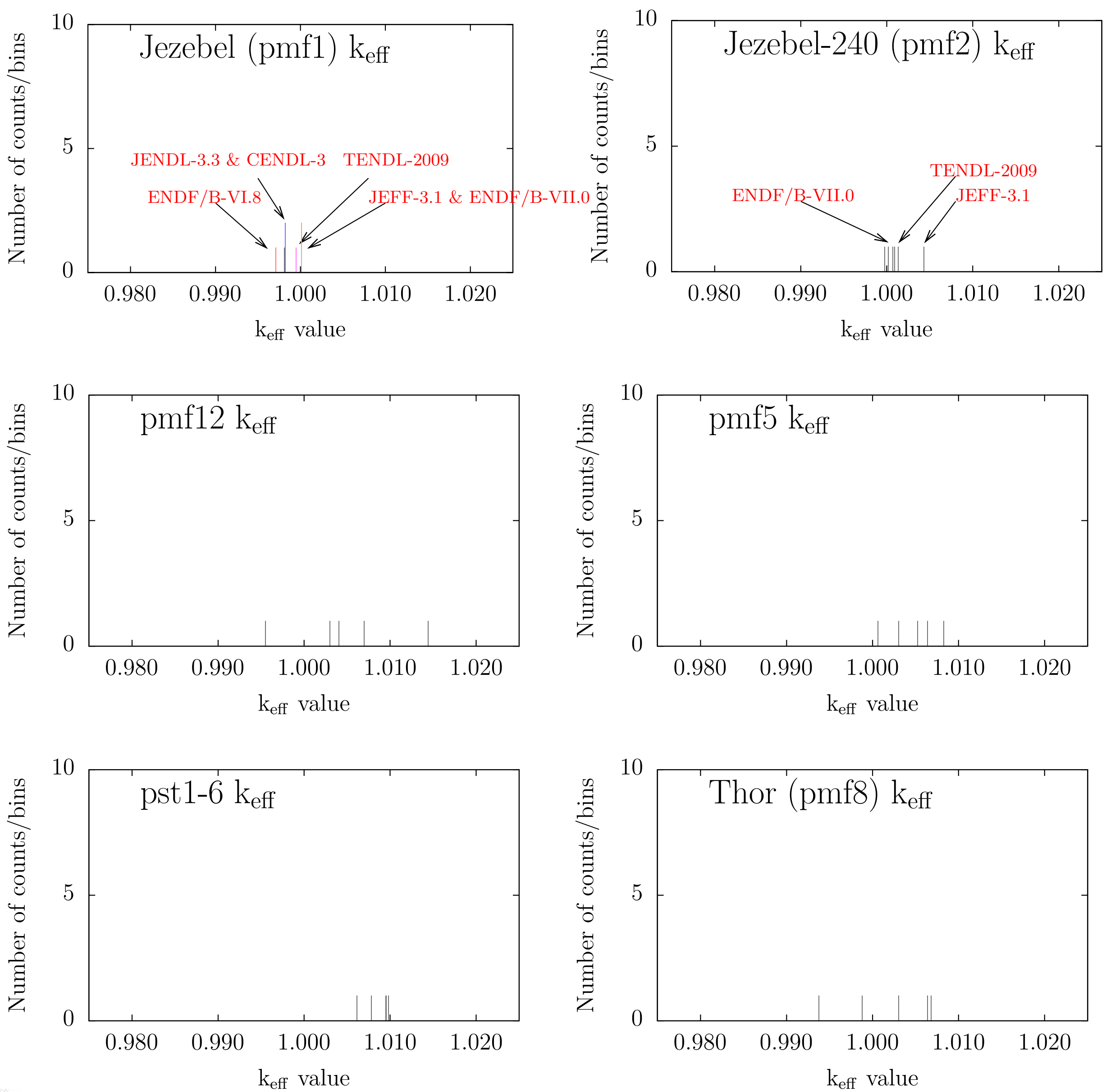




(1) Central cross sections *almost* equal to ENDF/B-VII.0 or JEFF-3.1

(2) Random cross sections obtained from random model parameters

(3) Similar results in MF1, 2, 4, 5 and 6

# Benchmarking: simple example with 6 $k_{eff}$ benchmarks




| | $\alpha$ |
|---|---|
| JEFF-3.1.1: | $1.14e^{-4}$ |
| JENDL-3.3: | $1.71e^{-4}$ |
| TENDL-2009: | $3.66e^{-4}$ |
| ENDF/B-VI.8: | $1.72e^{-4}$ |
| ENDF/B-VII.0: | $1.69e^{-4}$ |

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

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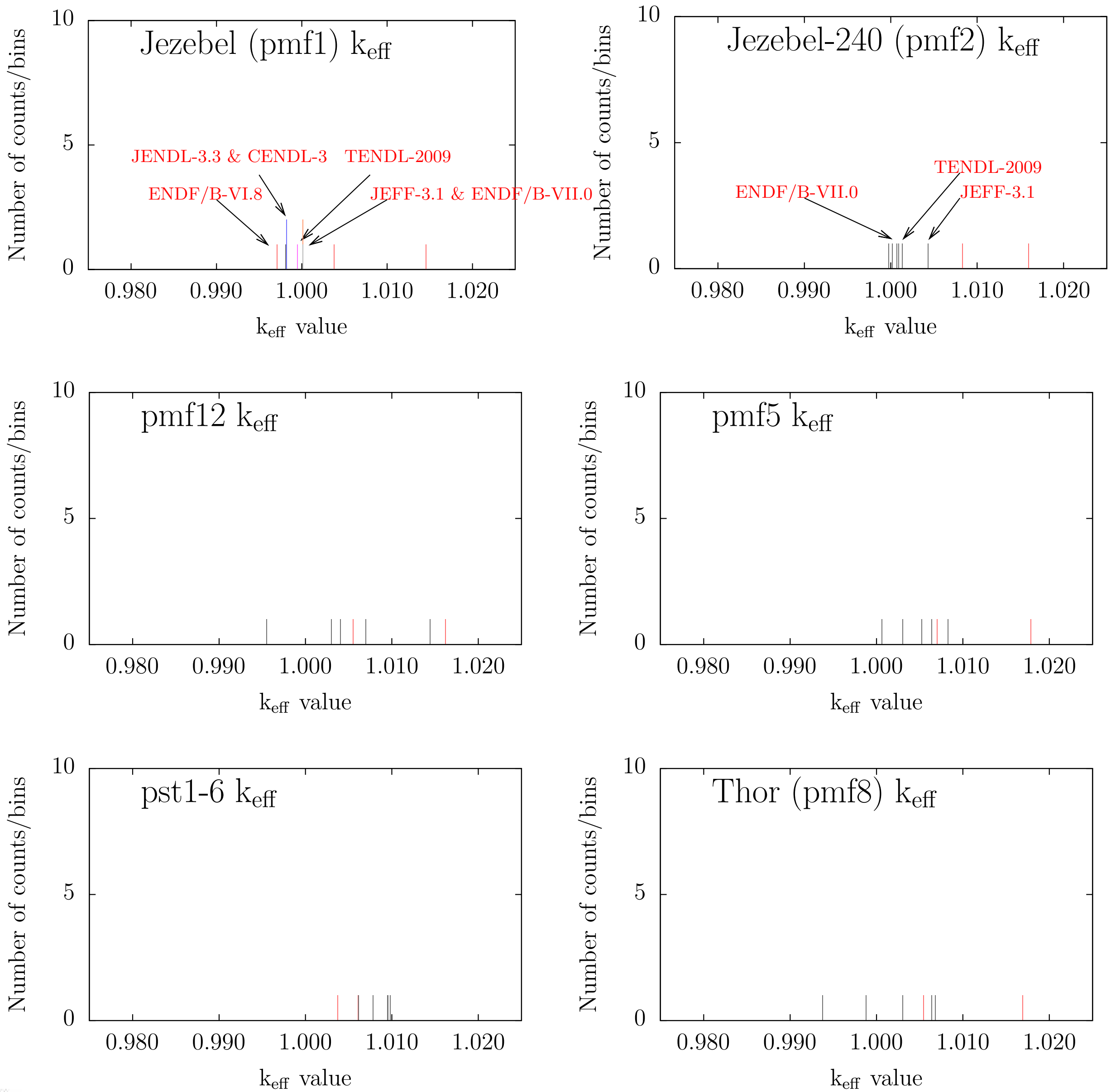


α

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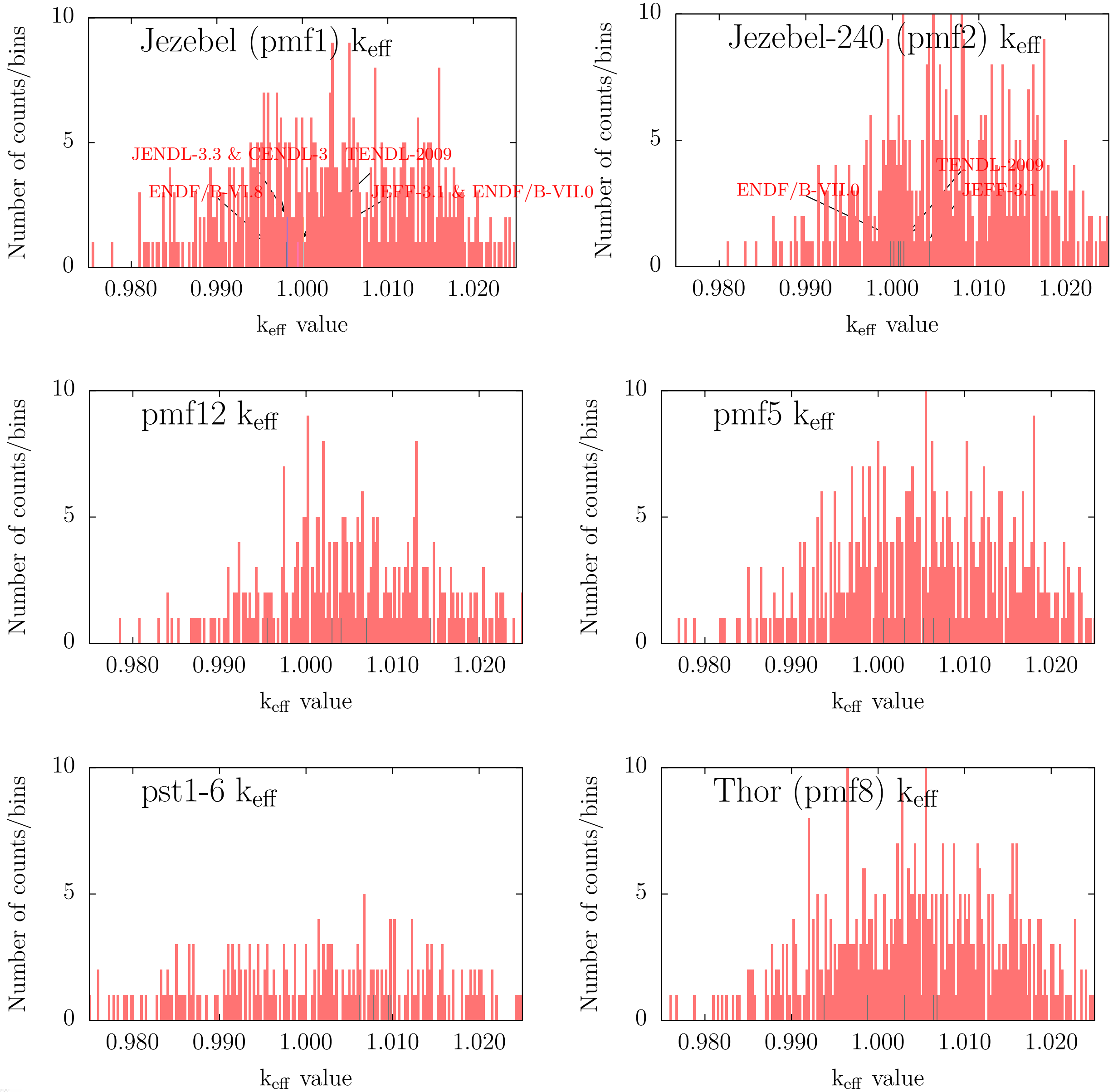
| ENDF/B-VII.0: | $1.69e^{-4}$ |
| random 0: | $2.29e^{-4}$ |
| random 1: | $13.4e^{-4}$ |

# Benchmarking: 6 $k_{eff}$ benchmarks with random $^{239}$Pu



## Real case: 120 $^{239}$Pu benchmarks

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

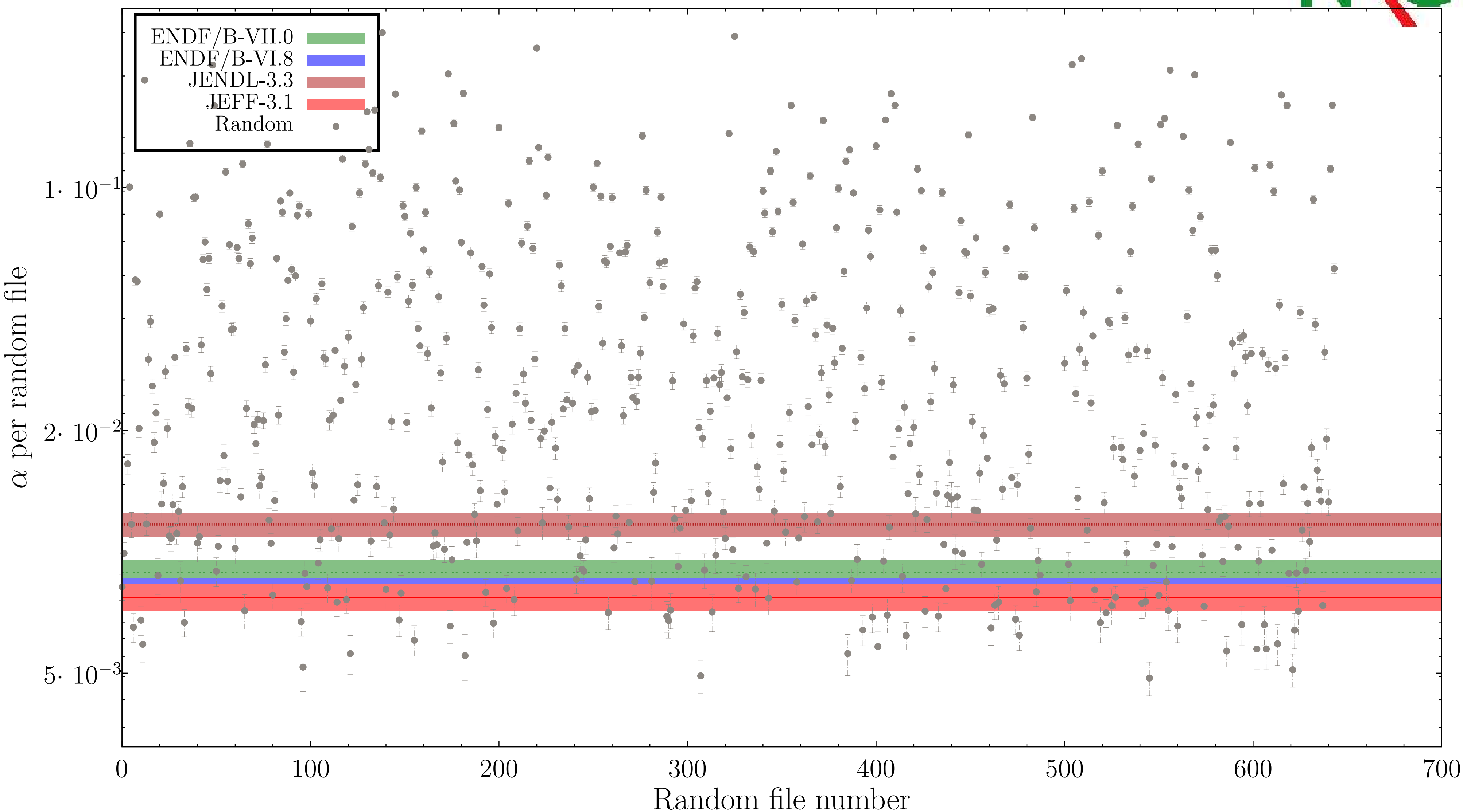
| Name | Cases | Name | Cases | Name | Cases | Name | Cases |
|---|---|---|---|---|---|---|---|
| pmf1 | 1 | pmf2 | 1 | pmf5 | 1 | pmf6 | 1 |
| pmf8 | 1 | pmf12 | 1 | pmf13 | 1 | pci1 | 1 |
| pmi2 | 1 | pst1 | 6 | pst2 | 6 | pst3 | 8 |
| pst4 | 13 | pst5 | 9 | pst6 | 3 | pst7 | 9 |
| pst8 | 29 | pst12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

$$\alpha = \sum_{i=0}^{n} \frac{(C_i - E_i)^2}{C_i}, \tag{1}$$

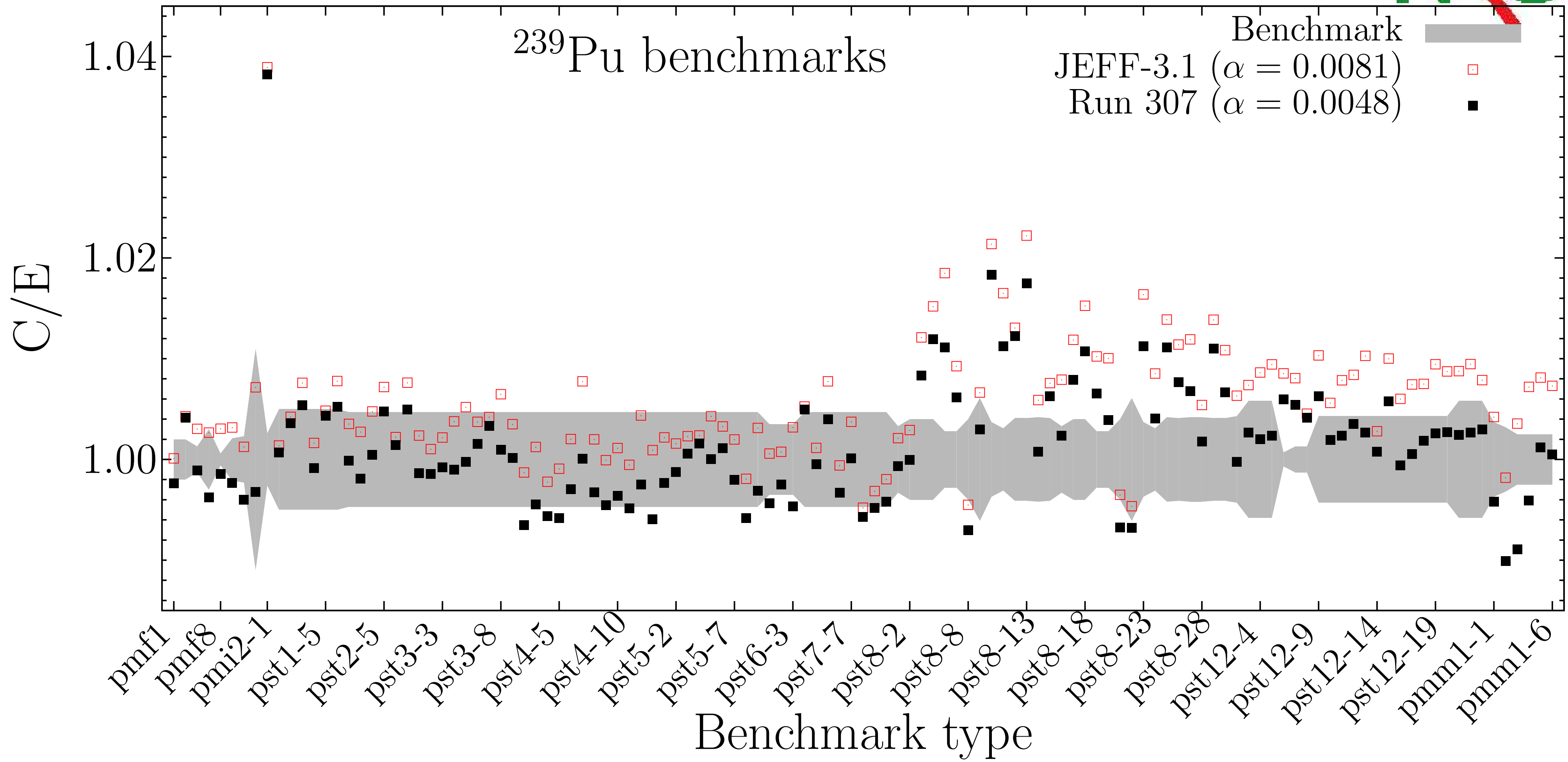
Results independent of the type of factor $\alpha$, $\chi^2$... or

$$F = 1 - 10^{\sqrt{\frac{1}{N}\sum(\log(E_i)-\log(C_i))^2}} \tag{2}$$

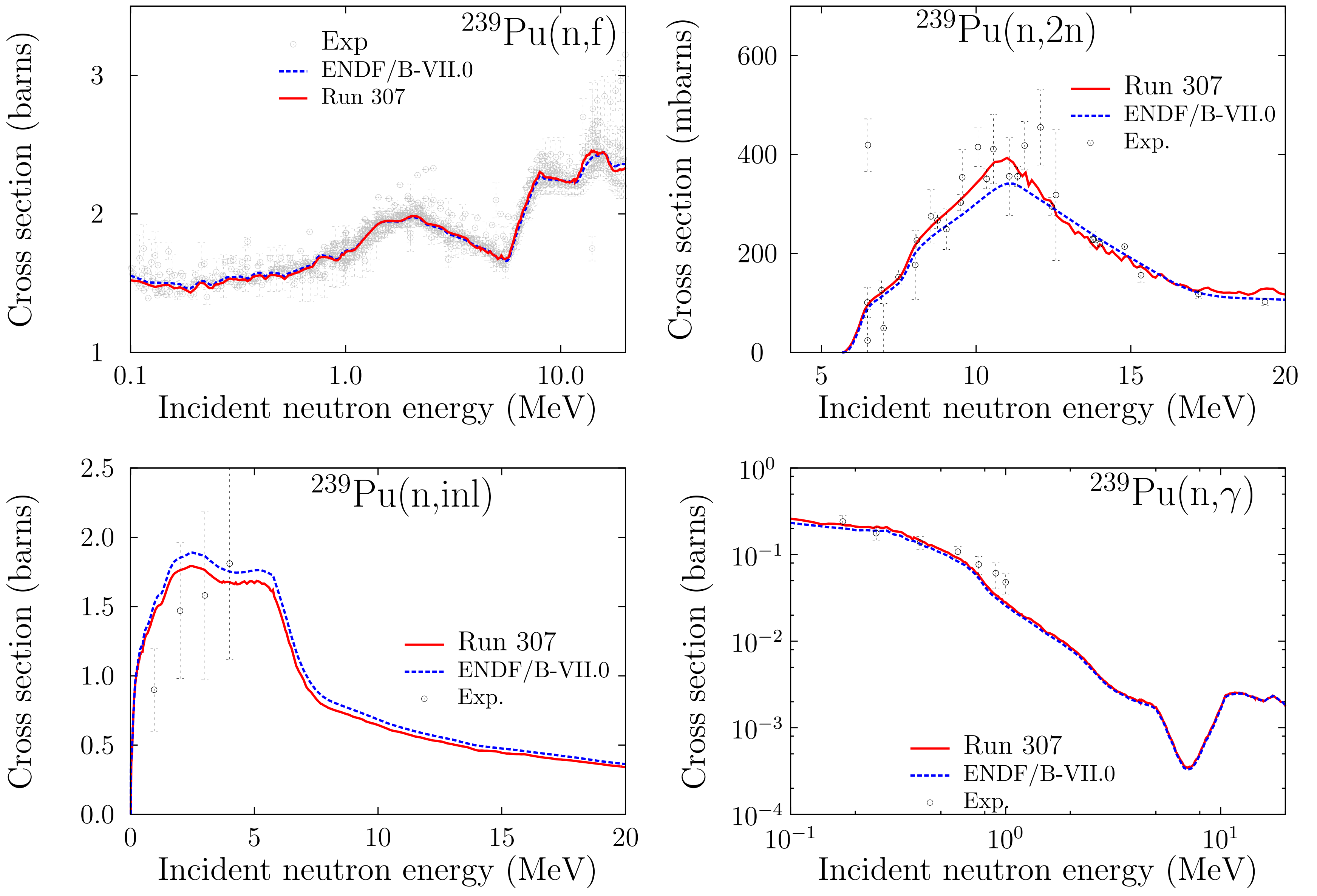
# α values for random $^{239}Pu$ evaluations



# $C/E$ values for the *best* $^{239}$Pu (run 307)



# Optimal cross sections (random file 307)



## Does it work ?

① We have shown that it is possible to ”*improve*” an existing evaluation

② Many questions need to be addressed such as

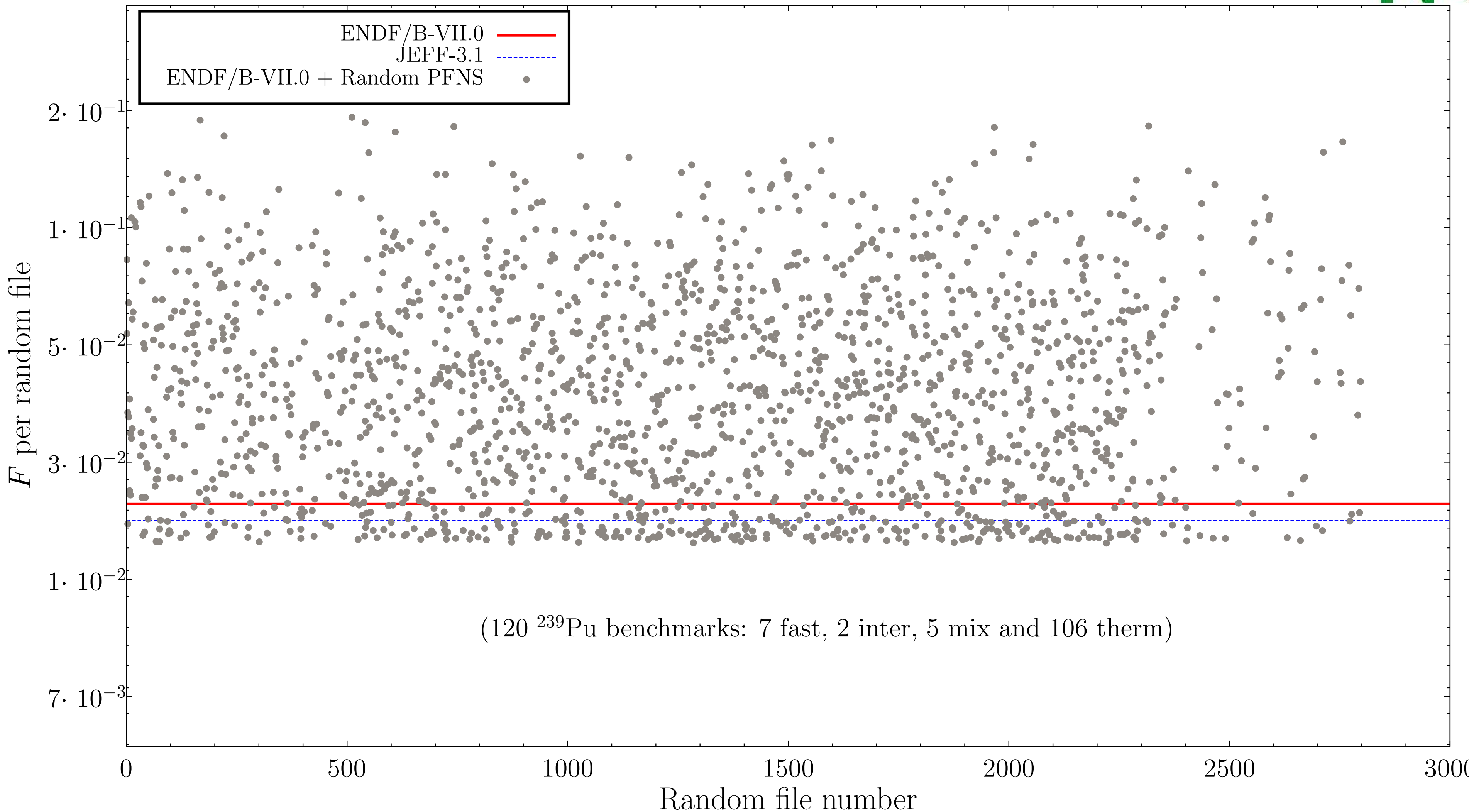
- ➡ Compensation
- ➡ Uncertainty ranges
- ➡ Benchmark list

③ $2^{nd}$ example: fission neutron spectrum for ENDF/B-VII.0 $^{239}$Pu (pfns)

Total Monte Carlo *on pfns*+ selection
$\Longrightarrow$ adjustment *of pfns*

(same benchmarks, keep ENDF/B-VII.0 constant except the pfns, MF5 MT18)

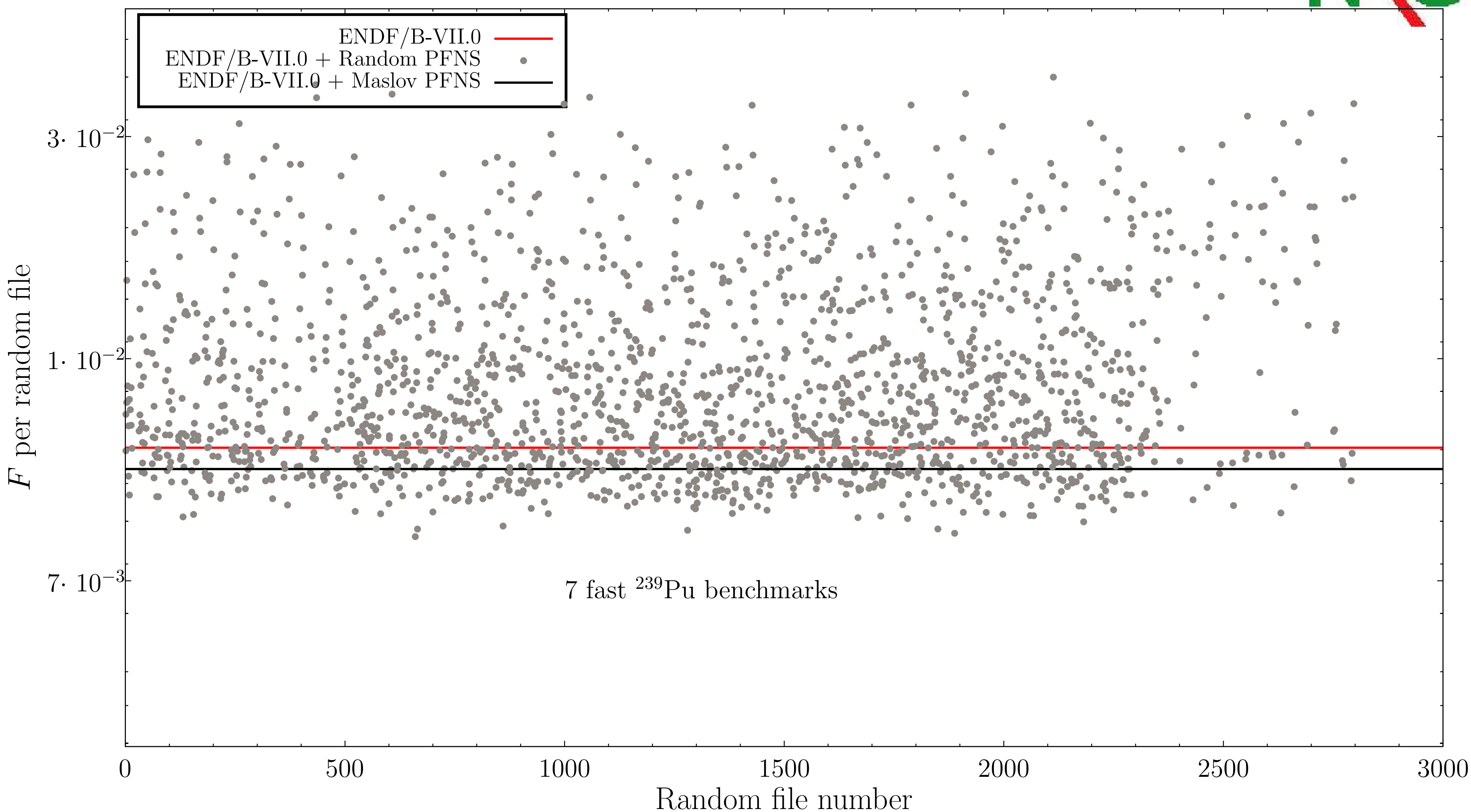
# Example 2 on pfns of $^{239}$Pu



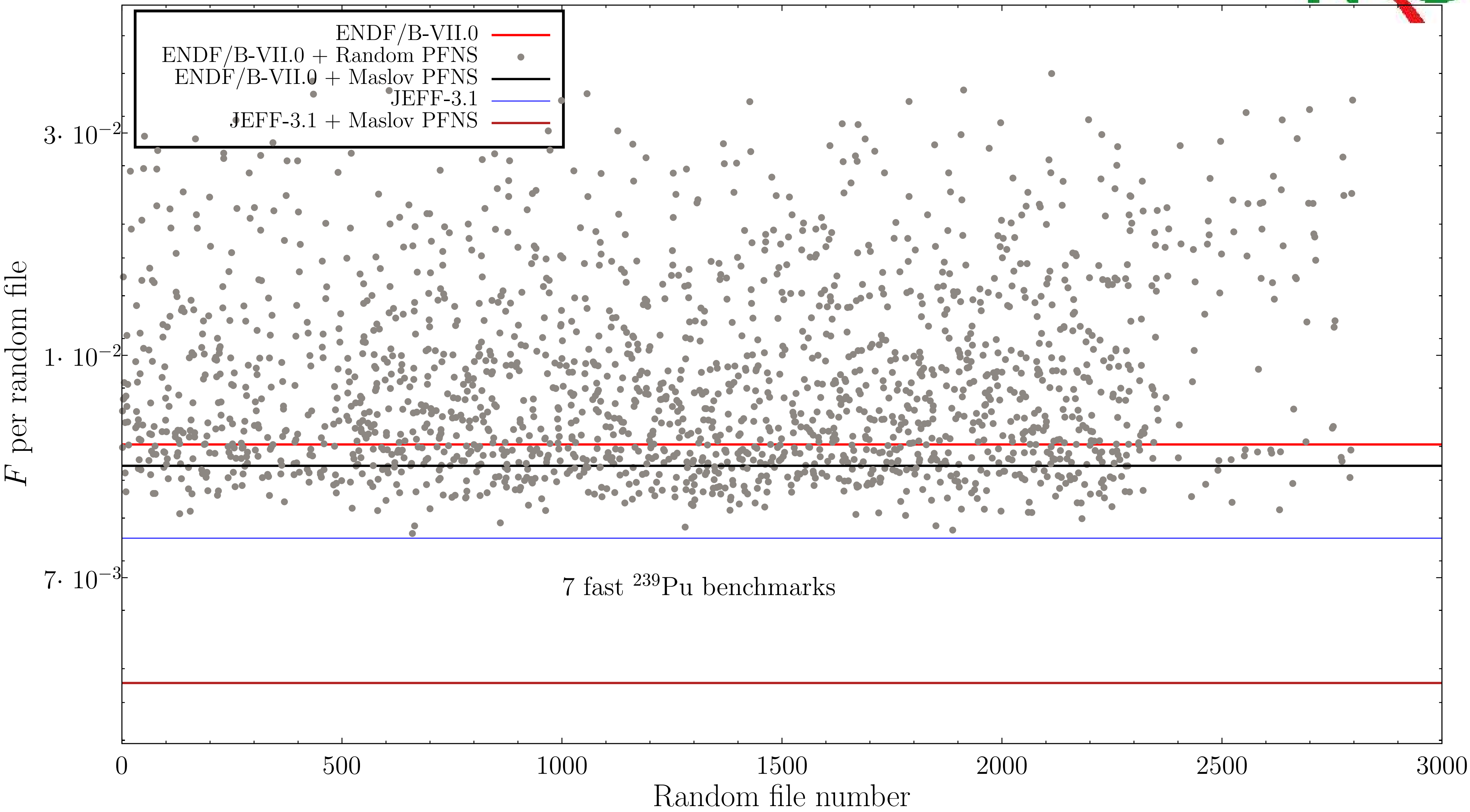

Difference with the previous example (where the whole $^{239}$Pu was random): there is a limit in low $F$

$\Longrightarrow$ like hitting a wall !

# $F$ values for random PFNS $^{239}$Pu evaluations



## $F$ values for random PFNS $^{239}$Pu evaluations



## Generalization

Based on this simple example:

- More random files can be used
- More benchmarks can be included $\Longrightarrow$ JEFF-3.2$\beta$ = JEFF-3.1.1 + New $^{239}$Pu
- Add other actinides (such as $^{235}$U) $\Longrightarrow$ JEFF-3.n$\beta$ = JEFF-3.(n-1)$\beta$ + *i* new isotope
- Apply this method to many (virtually all) isotopes, while improving the agreement with differential data (TALYS) : TENDL

We believe that this approach is condemned to succeed !

# Generalization and (no longer) secret plan

For the next Nuclear Data conference (ND2013) in Manhattan, we want to apply this methodology to produce the first 21$^{st}$ century library (which is different from the first library of the 21$^{st}$ century),

*competing (at least) with any existing library !*

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2010-2013, New library $\Longrightarrow$ A Manhattan Project

## Conclusions

- Clever random search for optimal nuclear data improvement
- What is presented is not about $^{239}$Pu (neither other isotopes)
- It is about
  - propagating current and basic knowledge to applications,
  - using reliable and stable codes,
  - applied for (1) library consistency, robustness
  - and alternatively (2) library optimization without incremental approach
- Not perfect yet (need of more flexible theory, more knowledge...)

None of this would be possible without dependable codes, computer power, systematic approach and a bit of "*brain power*".