TMC adjustment of nuclear data libraries using integral benchmarks

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SG46: Definition of the project and of proposed activities

- ” Performing new generalized adjustments to provide unambiguous feedbacks. Some approaches has been proposed (Yokoyama, Palmiotti, and Ivanov) but not yet finalized or widely used. **Other approaches could be proposed** and compared. The use of reaction cross correlations and of covariance data for angular distributions, secondary energy distribution from inelastic scattering should be done as far as these data will be made available in the different nuclear data projects”

TENDL

Uncertainty reduction using benchmarks

- Idea of using benchmarks for randomfile calibration is not new.
  - Petten method for best estimates
- Here:
  - Multiple correlated benchmarks
  - Multiple isotopes within one benchmark

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On the use of integral experiments for uncertainty reduction of reactor macroscopic parameters within the TMC methodology

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Correlations in nuclear data from integral constraints: cross-observables and cross-isotopes

CW 2017

Eric Bauge : CEA DAM DIF, France
Dimitri Rochman : PSI, Swizerland

Cases used

Benchmarks from ICSBEP Handbook were used in this work.

- Method 1: Pu-Met-Fast
  - Re-evaluation of previously obtained data. (TENDL2012)
- Method 2: IEU-Met-Fast and HEU-Met-Fast
  - Curtesy of Steven Van Der Marck
  - TENDL2014

Benchmark example – ^{239}Pu Jezebel.
Picture taking from the ICSBEP Handbook

Uncertainty reduction

Random nuclear data from the 1st step is used as the prior for the 2nd step.

Physical models parameters: TALYS based system (T6)

1st level of constraint: **Differential data**

A large set of acceptable ND libraries

Simulations: mcnp etc.

Applications: Criticality, burnup, Fuel cycle etc.

2nd level of constraint: **Integral benchmarks**

$$w_i = e^{-\frac{\chi_i^2}{2}}$$

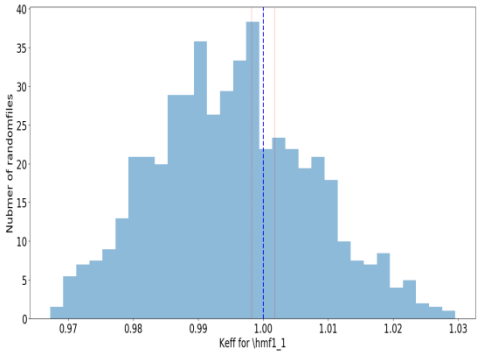
Assign weights to random files

Weighted random files

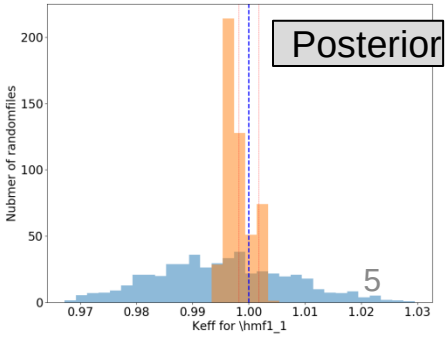
Simulations: MCNP

Validation with a set of benchmarks

Prior k_{eff} distribution



Posterior



The posterior is constrained by both the differential and integral data

Rather complete on uncertainties, correlations and higher moments.

Physical models parameters: TALYS based system (T6)

1st level of constraint: **Differential data**

A large set of acceptable ND libraries

Simulations: mcnp etc.

Applications: Criticality, burnup, Fuel cycle etc.

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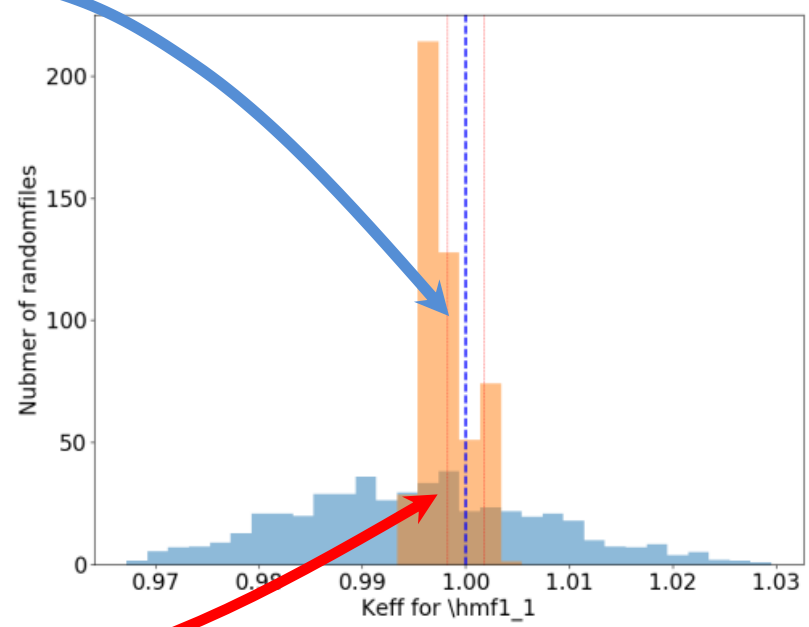

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Benchmark consists of multiple isotopes contributing to the ND uncertainty

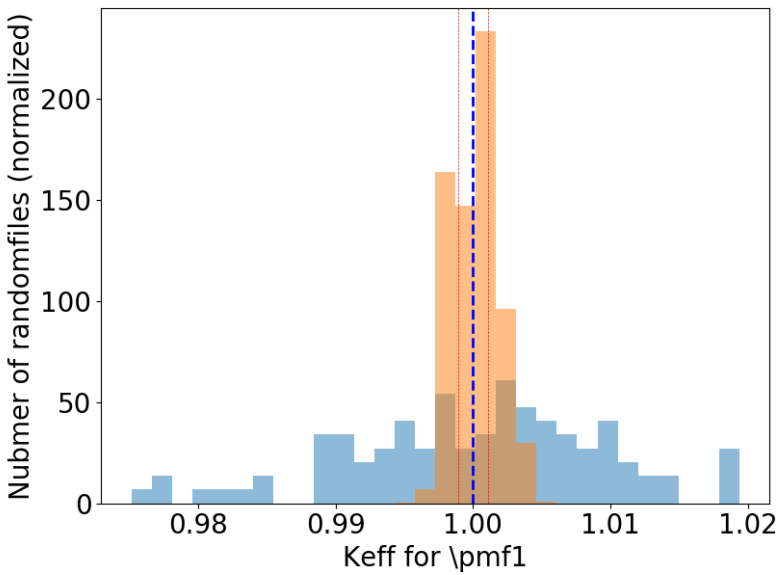
^{239,240,241}Pu nuclear data uncertainties for a set of plutonium sensitive benchmarks computed using the TMC method. Only case one of each benchmark and 300 random nuclear data files were used for all isotopes. Note that, PU-MET-FAST-035 does not contain ^{241}Pu.

Benchmark category	$\sigma_{ND}(^{239}\mathrm{Pu})$	$\sigma_{ND}(^{240}\mathrm{Pu})$	$\sigma_{ND}(^{241}\mathrm{Pu})$
PU-MET-FAST-001	962 ± 42	178 ± 8	36 ± 3
PU-MET-FAST-002	826 ± 36	833 ± 34	254 ± 11
PU-MET-FAST-005	954 ± 42	192 ± 8	31 ± 4
PU-MET-FAST-008	939 ± 41	195 ± 8	28 ± 4
PU-MET-FAST-009	925 ± 41	186 ± 8	33 ± 3

I.e., a deviation between C and E can be due to any of these isotopes.

Important to also include the calculation uncertainty

Method 1: Use benchmarks to calibrate the ND for a specific isotope (here Pu^{239}). Varying a single isotope at a time (here $Pu^{239,240,241}$).



$$\chi^2_{i,j} = \sum_B \frac{(C_{B,i} - E_B)^2}{\sigma^2_{B,j}}, i = randomfile,\ j = isotope, B = benchmark$$

$$\sigma^2_{B,j} = \sigma^2_E + \sigma^2_{C,j} = \sigma^2_E + \sigma^2_{stat} + \sum_{\substack{\text{overall p} \\ \text{where p} \neq \text{j}}} \sigma^2_{ND,p} + \sigma^2_{other}$$

Important to also include the calculation uncertainty

- Main idea: if the calculation deviates from the benchmark value it can be due to σ_E, σ_{stat}, an error in the isotope / (observable) that we are calibrating, any of the other isotopes / (observables) in the benchmark, or other errors not accounted for.

- Note: the σ_E in, e.g., ICSBEP, includes both the actual experimental uncertainty, but also uncertainties in transferring the experiment to a benchmark (e.g., densities).

$$\chi^2_{i,j} = \sum_B \frac{(C_{B,i} - E_B)^2}{\sigma^2_{B,j}}, i = randomfile,\ j = isotope, B = benchmark$$

$$\sigma^2_{B,j} = \sigma^2_E + \sigma^2_{C,j} = \sigma^2_E + \sigma^2_{stat} + \sum_{\substack{\text{overall p} \\ \text{where } p \neq j}} \sigma^2_{ND,p} + \sigma^2_{other}$$

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Benchmark exp. errors are correlated

DICE

File Database=NEA Personal-Keff Window Help

Critical / Subcritical | Alarm / Shielding | Fundamental Physics | Correlation Matrix | Rank Similar | Keff trends plots

Display:

- Uncertainties
- Sensitivities

Filter by...

...Evaluation identifier:

All fissile material

All physical form

All spectrum

...Facilities:

- None selected
- Argentina
  - Centro Atómico Bar
  - National University
- Brazil
  - IPEN

	HMF 008 001	HMF 011 001	HMF 018 001	HMF 020 001	HMF 031 001	HMF 055 001	HMF 060 001	HMF 061 001	HMF 067 001	HMF 067 002	HMF 070 001	HMF 070 002	HMF 070 003	HMF 075 001	HMI 001 001	HMM 012 001
HMF008-001	1000	210														
HMF011-001	210	1000														
HMF018-001			1000	460	320											
HMF020-001			460	1000	460											
HMF031-001			320	460	1000											
HMF055-001						1000	300	250	290	290	260	250	270	210	210	270
HMF060-001						300	1000	510	880	880	840	840	850	430	680	540
HMF061-001						250	510	1000	500	500	440	430	450	870	370	760
HMF067-001						290	880	500	1000	960	930	940	940	420	770	520
HMF067-002						290	880	500	960	1000	940	940	940	420	780	520
HMF070-001						260	840	440	930	940	1000	940	930	370	780	470
HMF070-002						250	840	430	940	940	940	1000	940	360	800	460
HMF070-003						270	850	450	940	940	930	940	1000	380	790	480
HMF075-001						210	430	870	420	420	370	360	380	1000	310	810
HMI001-001						210	680	370	770	780	780	800	790	310	1000	380
HMM012-001						270	540	760	520	520	470	460	480	810	380	1000

Database for the International Criticality Safety Benchmark Evaluation Project (DICE), https://www.oecd-nea.org/science/wpncs/icsbep/dice.html

Working with covariances

How can COV_E be determined?

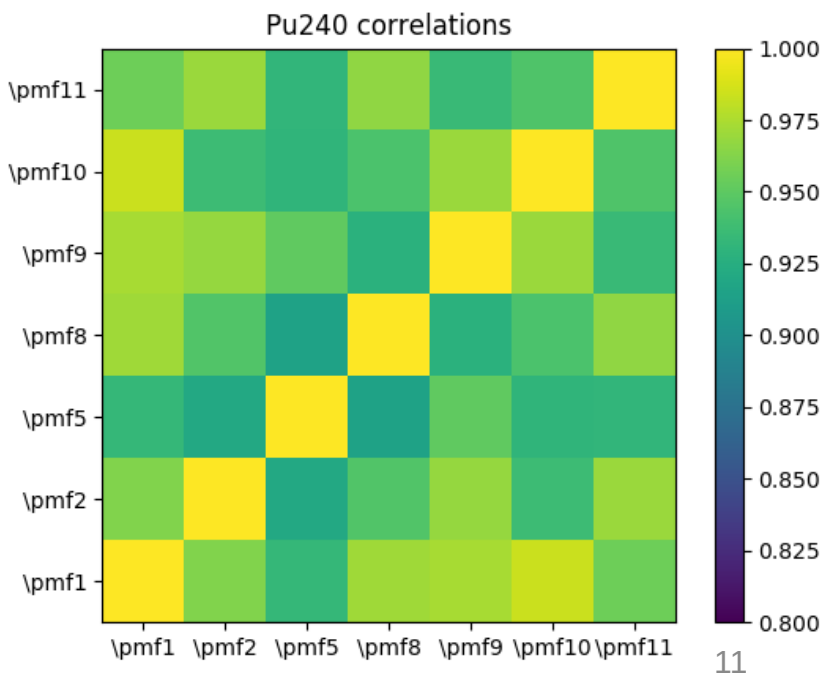
1. Careful analysis of the experiments.
2. Using DICE.
3. Here: checking sensitivity of results, and try to be conservative.

$$\chi_i^2 = (C - E)^T \, COV_{B,j}^{-1} (C - E)$$

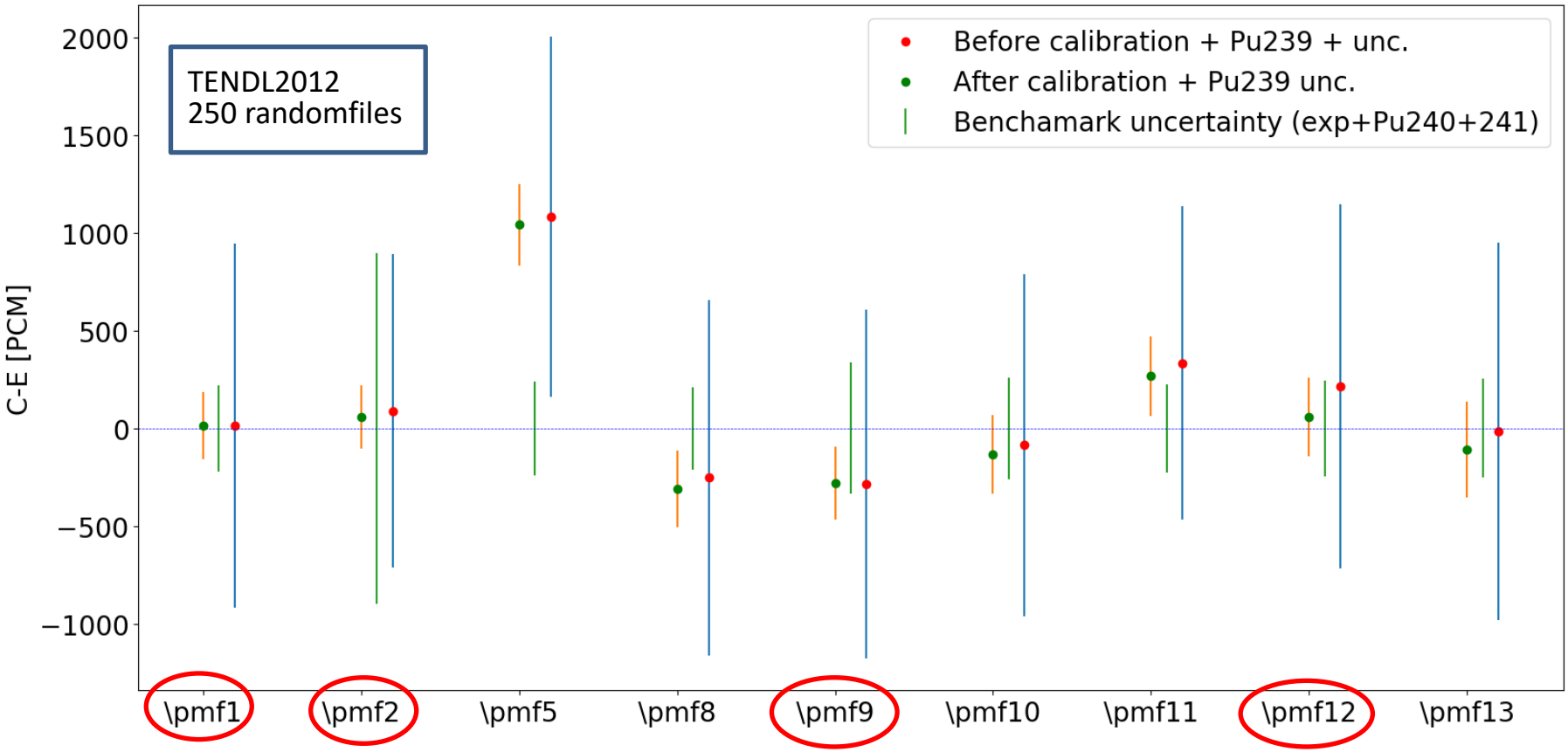
$$COV_{B,j} = COV_E + COV_{C,j}$$

COV_C is also strongly correlated

$$COV_{C,j} = +COV_{stat} + \sum_{\substack{\text{overall p} \\ \text{where p} \neq \text{j}}} COV_{ND,p}$$



Before and after calibration

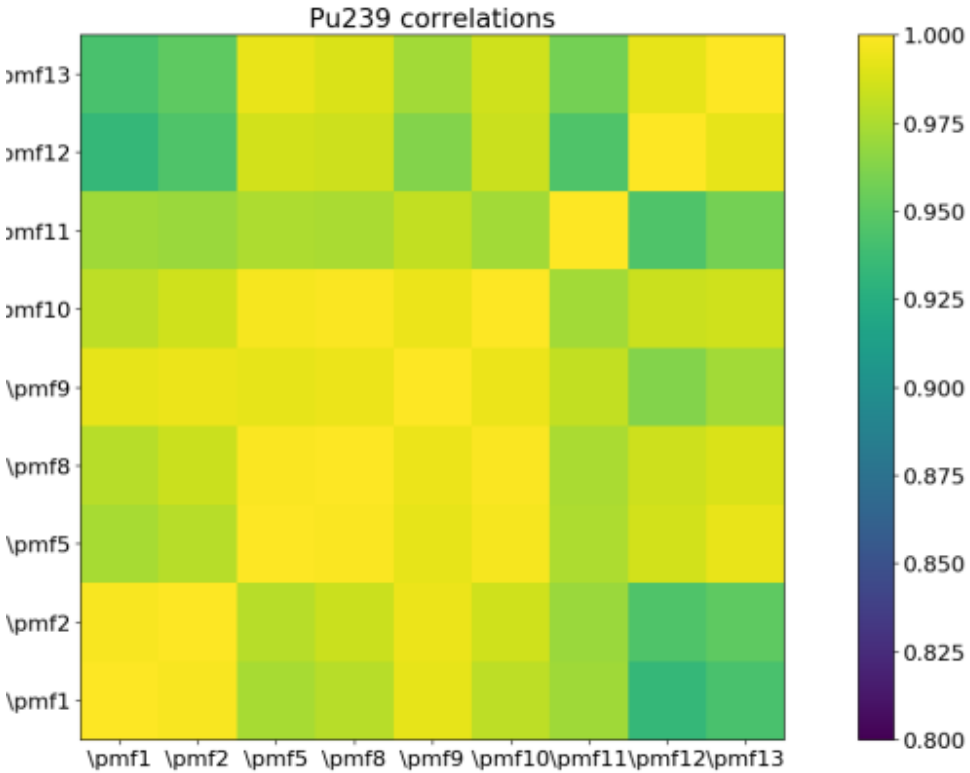


Calibration

Validation

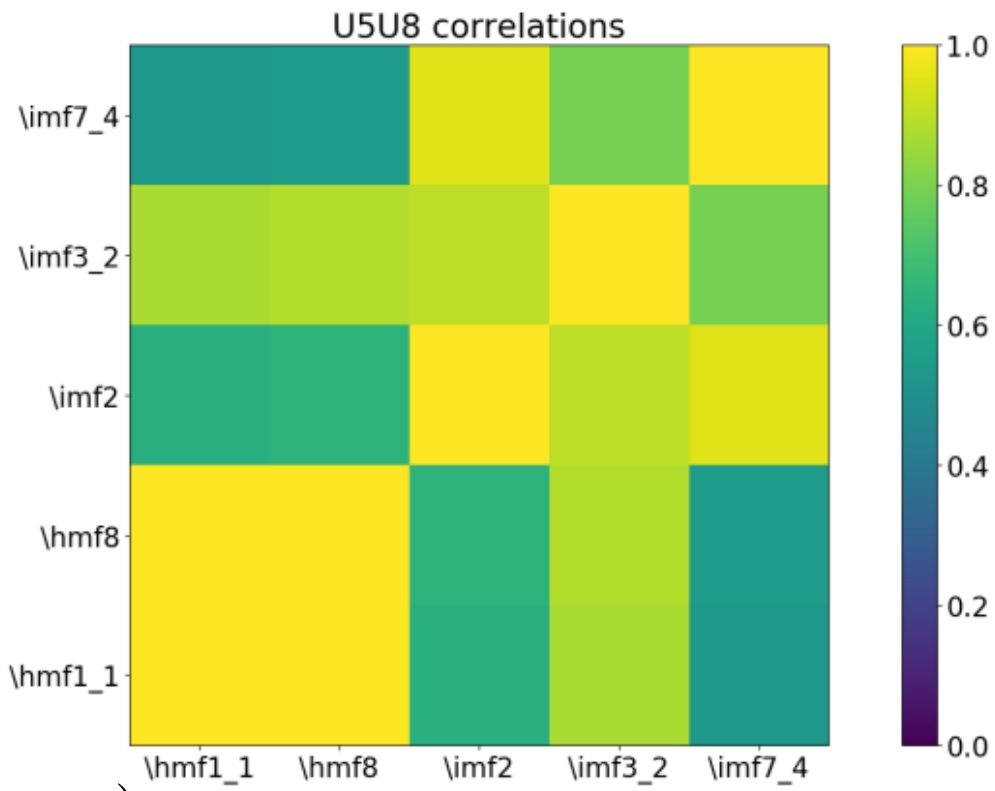
Comment on results

- Decreased ND uncertainty to more ‘realistic values’.
- Small improvement of the best-estimates.
  - Strong correlations
- The inclusion of COV_C and ρ_{exp}=0.5 affects the ND uncertainty but not the mean values.
- Old version of TENDL!



Method 2

- All isotopes of interest are varied simultaneously
- Intrinsically the uncertainty of the different isotopes are taking into account simultaneously
- Investigated for U8 and U5.

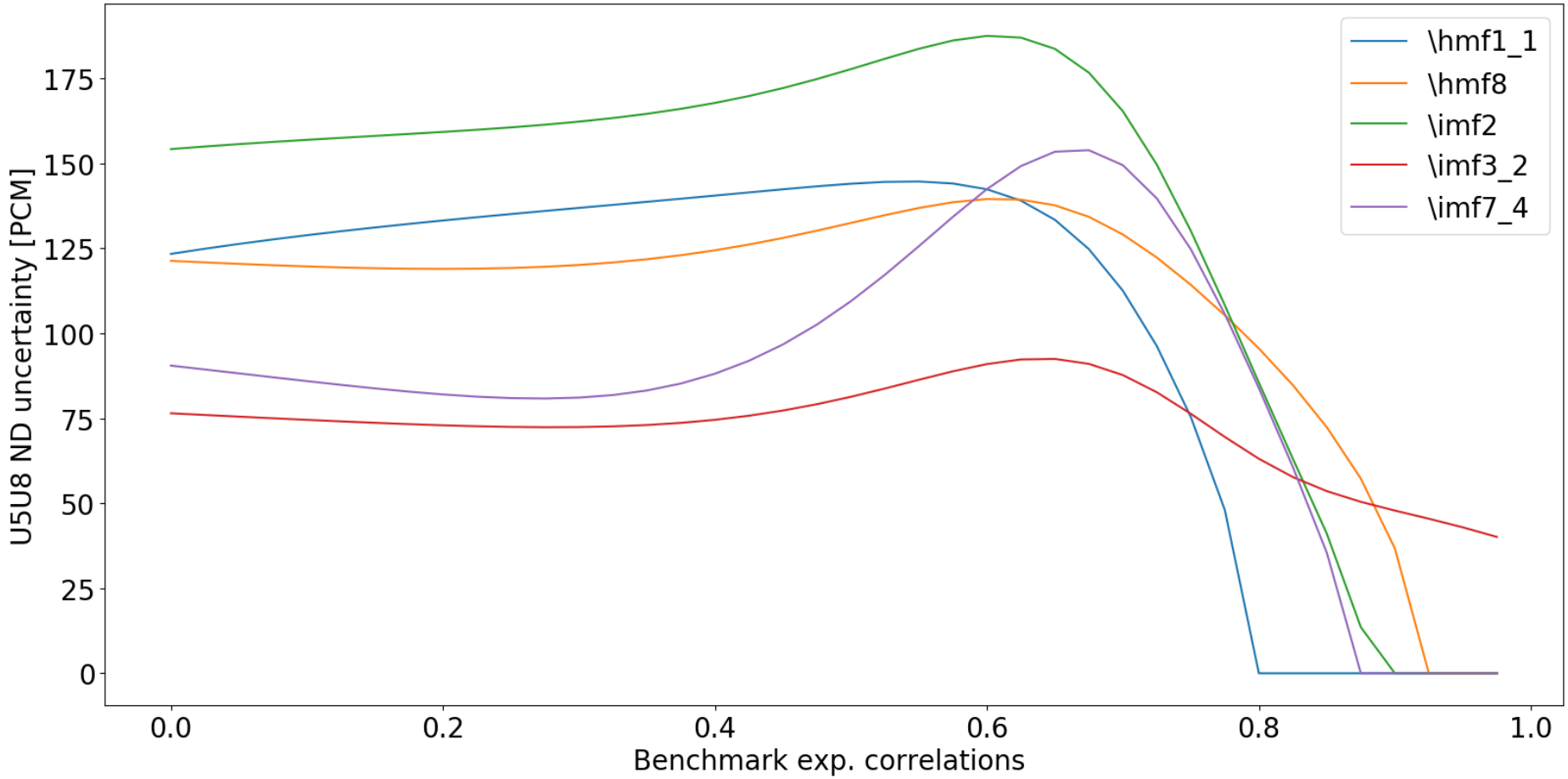


$$w_i = e^{-\frac{\chi_i^2}{2}}$$

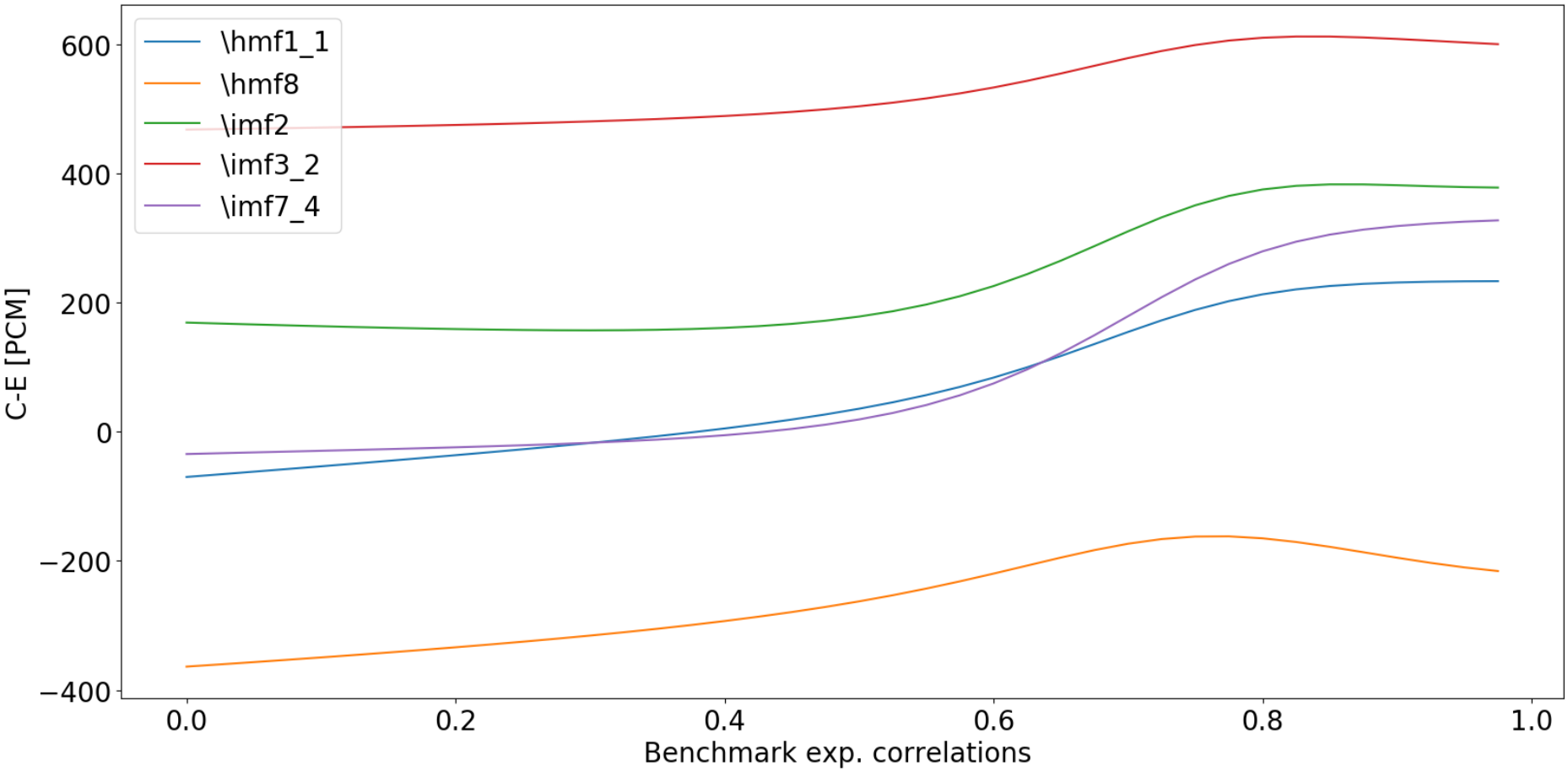
$$\chi_i^2 = (C - E)^T \, COV_{B,j}^{-1} (C - E)$$

$$COV_{B,j} = COV_E + COV_{stat}$$

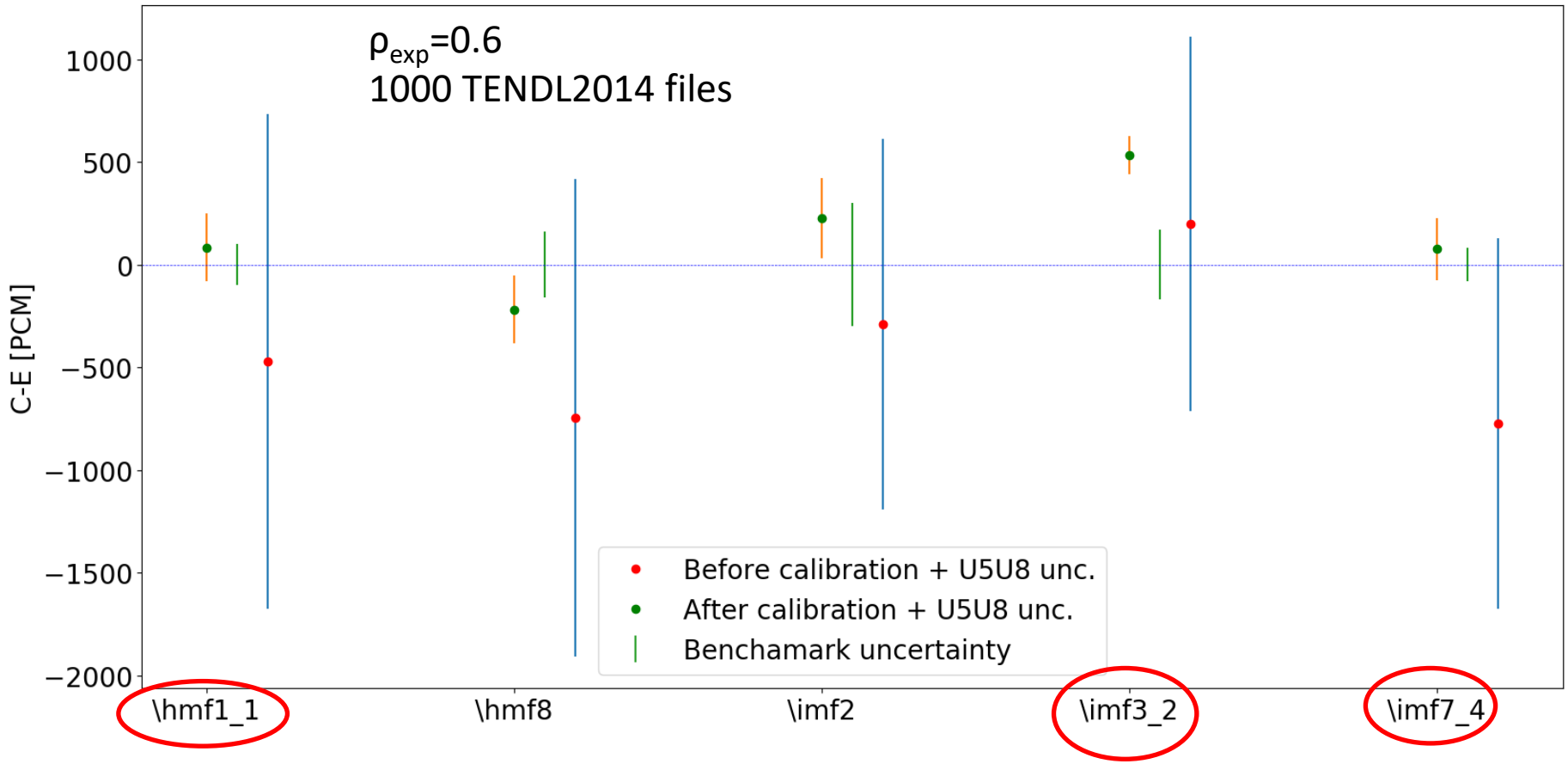
Importance of benchmark exp. correlation



Importance of benchmark exp. correlation 2



Before and after calibration



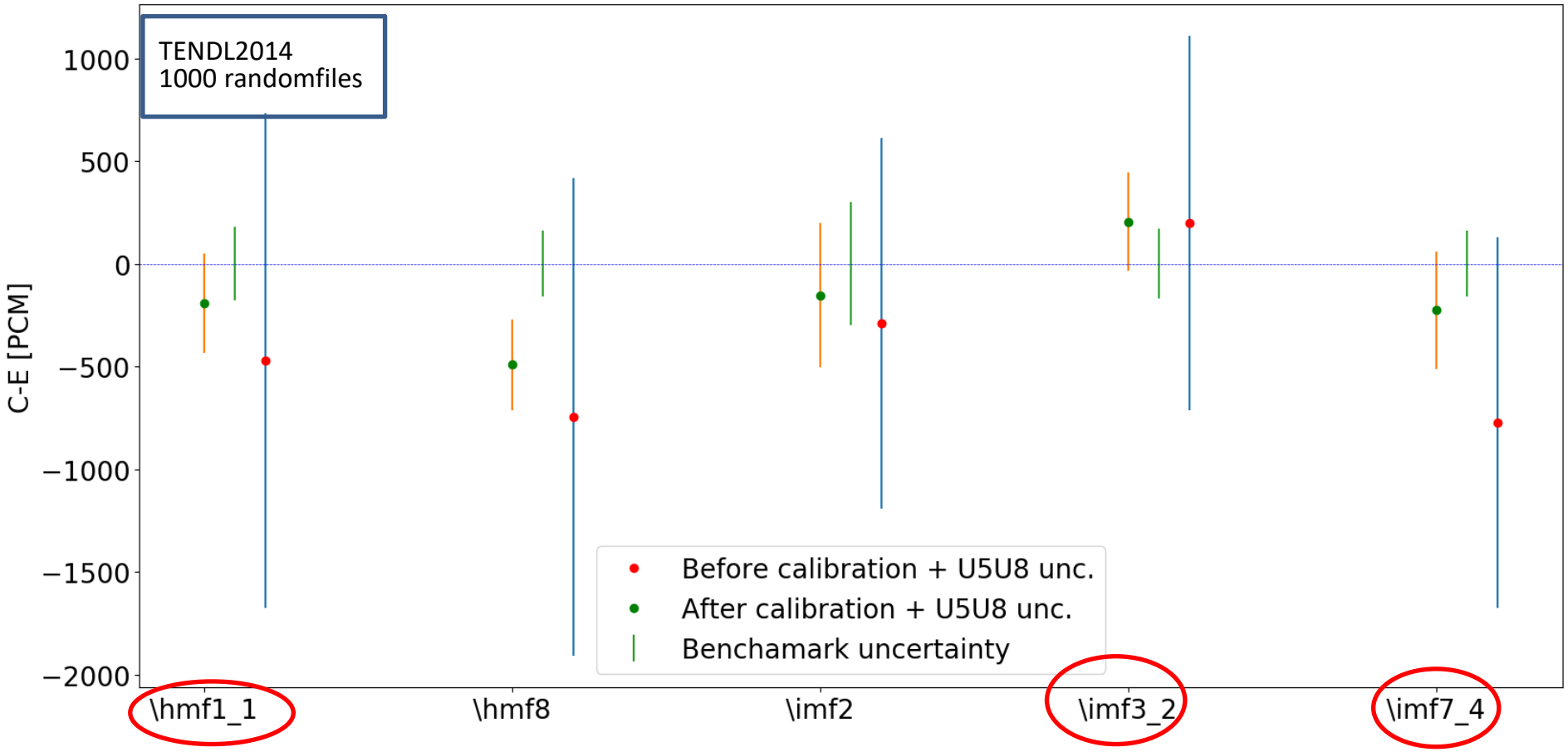
Calibration

Validation

Difficult to fit the experimental data?

- Wrong model parameter distribution?
- Model defects?
- **To small experimental uncertainties or wrong experimental covariance matrix.**

Adding 80 pcm experimental uncertainty to hmf1 and imf7_4



Calibration

Validation

Method 1 vs. Method 2

Method 2 -hypothesis

- Better calibration of the best estimate- due to higher degree of freedom
- Smaller posterior ND uncertainty – negative correlations between isotopes.
- Higher cost in terms of random files needed. I.e., the method produce lower average weights.

Proposal

Use Method 1 to determine the uncertainty for minor isotopes (e.g. ^{234}U) and Method 2 for the major isotopes ($^{235,\ 238}$U).

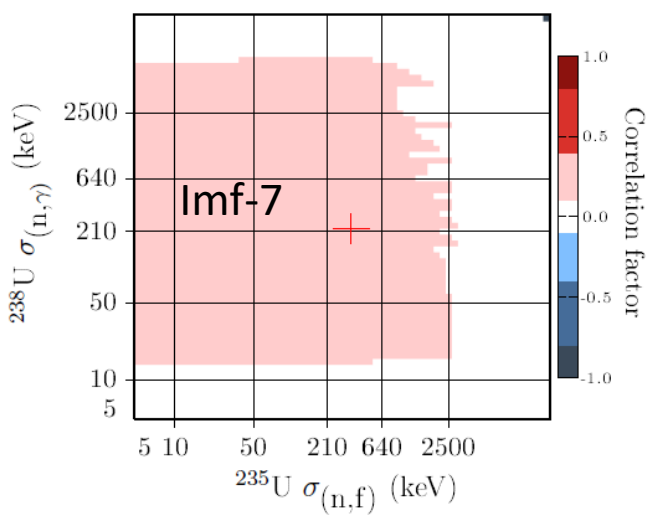
Limitation of this work

- To few effective randomfiles
- ENDF/B-VII.0 used as background library

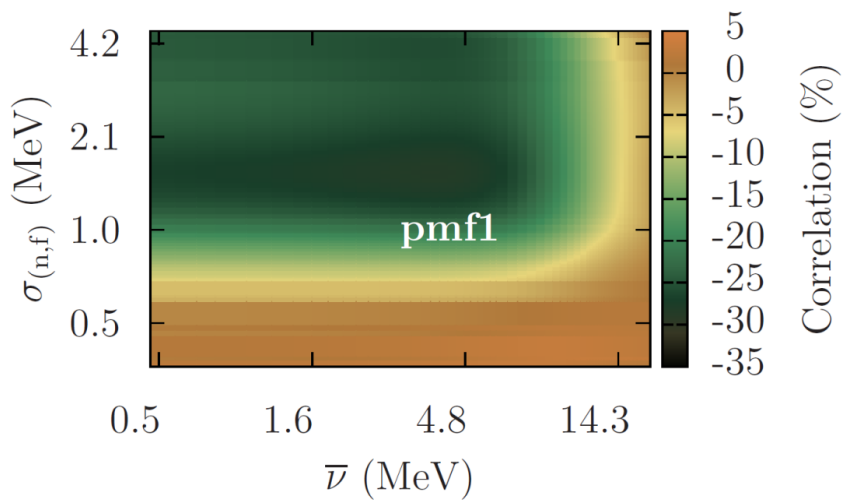
How is the uncertainty reduced?

E.Bauge."*Correlations in nuclear data from integral constraints: cross-observables and cross-isotopes ", CW2017*

- Using integral data introduce correlations: between isotopes and between different parts of the ND file.
- The integral weighing only slightly change the best estimate <1% and std dev < 10%



D. Rochman: Nuclear data correlation between different isotopes via integral information



D. Rochman et al., EPJ Nuclear Sci. Technol. 3, 14 (2017)

Conclusion

- Random file integral calibration possible.
- Results still constrained by differential data and the model.
- Calculation uncertainties should be included
  - e.g., take into account multiple isotopes within the benchmarks (and observables not accounted for).
- The correlation between the benchmarks are important.
- Robust techniques to account for discrepant integral data needs to be developed.

$$\sigma_{C,j}^2 = \sigma_{stat}^2 + \sum_{\substack{\text{overall p} \\ \text{where } p \neq j}} \sigma_{ND}^2$$

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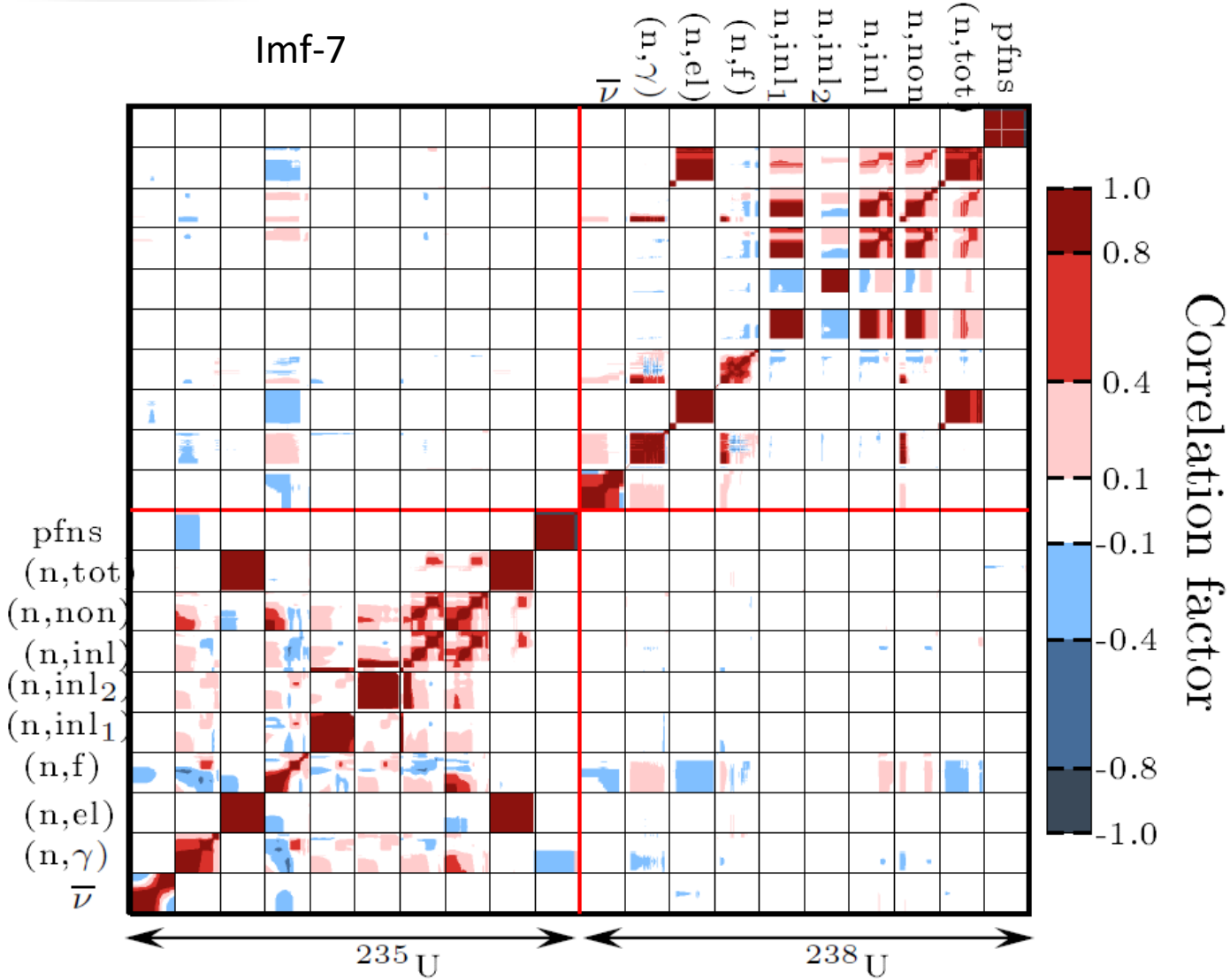
THANK YOU FOR YOUR ATTENTION!

References

1. Alhassan, E., et al. On the use of integral experiments for uncertainty reduction of reactor macroscopic parameters within the TMC methodology, Progress in Nuclear Energy, 88, pp. 43-52. (2016)
2. D. Rochman, et al. Nuclear data correlation between different isotopes via integral information , submitted to *EPJ/N, Sept. 2017*
3. D. Rochman et al., EPJ Nuclear Sci. Technol. 3, 14 (2017)

Cross-isotope correlations



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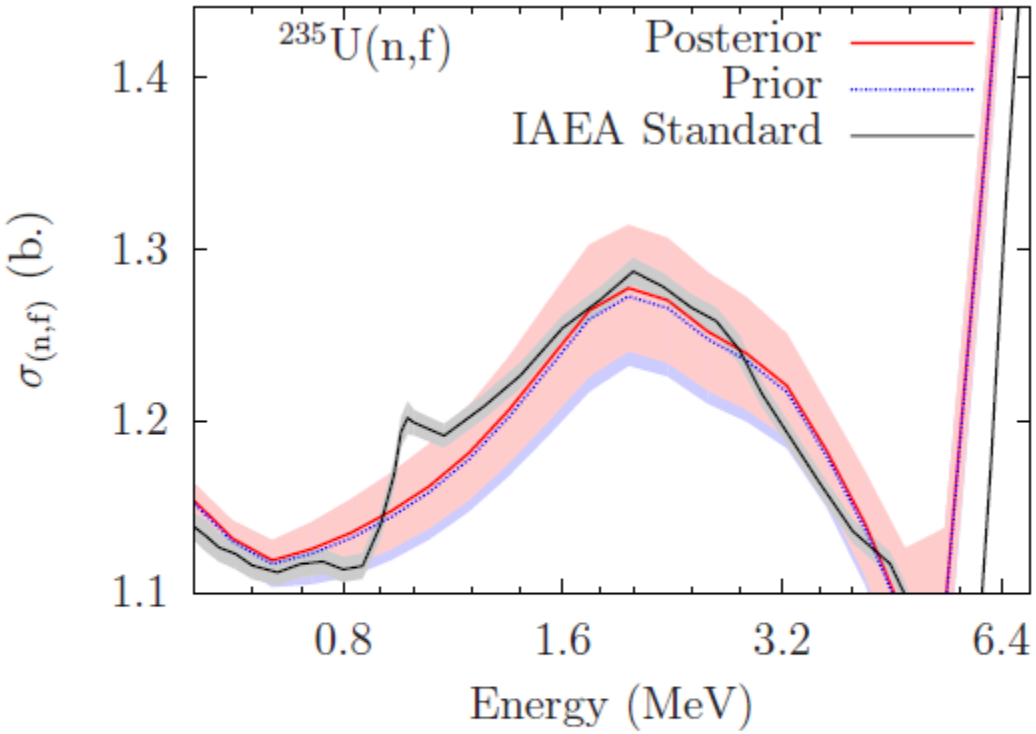

Fig. 11. Comparison between the posterior (weighted), prior (unweighted) and the IAEA standard ^{235}U(n,f) cross section and uncertainties (the lines denotes the cross sections whereas the bands are the uncertainties).