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INSTITUT DE RADIOPROTECTION  
ET DE SÛRETÉ NUCLÉAIRE

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# Nuclear Data Uncertainties and Adjustments Using Deterministic and Monte-Carlo Methods along with PWR Measurements

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M&C 2023 - The International Conference on Mathematics and Computational Methods Applied to  
Nuclear Science and Engineering · Niagara Falls, Ontario, Canada · August 13 – 17, 2023

# Presentation outline

(1) Introduction

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(2) Propagation of nuclear data uncertainties

Propagation of  
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(3) PWR experimental detector responses

PWR experimental  
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(4) Nuclear data adjustment

Nuclear data  
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(5) Conclusions

Conclusions

# Sources of errors in deterministic simulations

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**Four** fundamental sources of **errors** (*Neutron Physics*, P. REUSS, 2008) :

- (1) errors related to the **simplified modelling of the physics**
  - models of resonance self-shielding effects,
  - replace transport with diffusion, on full core level, etc.
- (2) errors related to **imperfect numerical schemes** applied to the obtained equations
  - discretizations, computer implementations
- (3) errors due to imperfect knowledge of **nuclear data**
- (4) errors in the system description → dimensions, densities, isotopic compositions
  - **manufacturing tolerances**

The **first two** errors constitute the **deterministic bias** (a systematic error), which can be computed as the **difference with the Monte-Carlo method**

# Adjustment of the power distribution through the reflector (1/2)

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In the 1970s, when full core simulations were performed with 1-group diffusion :

→ “The **albedo** matrices are then often **adjusted** to **experimental results**. The albedo matrix elements are thus used as ‘**tuning**’ constants that may vary, within reasonable limits, around their computed average values.” (STAMM’LER and ABATTE, 1983)

Later, fast diffusion coefficient of the reflector ( $D_1$ ) is used :

→ “The **reflector adjustment** [...] reduces the discrepancies between the calculated and **experimental detector responses** in the peripheral assemblies at the beginning of the cycle by flattening the power distribution. [...] **This adjustment corrects the discrepancy observed but does not constitute a definitive solution**. The latter, currently under development, requires a reference calculation in one and two dimensional geometries.” (our translation from KAMHA, 1981)



## Adjustment of the power distribution through the reflector (2/2)

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- “To fit calculations with respect to real in-core measurements, some reflector parameters can be adjusted. [...] **Adjustment** is done only **on the reflector** description by trying to **decrease calculations-measurements differences**. [...] Fictitious reflector [...] diffusion parameters (and mainly first group diffusion coefficient  $D_1$  and absorption coefficient  $\Sigma_{a1}$ ) can strongly be **changed** (some ten of percent) **to fit in-core measurements.**” (ARGAUD, 1993)
- “The **fast diffusion coefficient** of the radial **reflector** acts on the radial leaks and thus on the bulge of the radial flux distribution. It is **adjusted** to fit more accurately the **experimental** power output distribution over the core.” (JOUTEL, 2015)
- “The fast diffusion coefficient of the reflector **has been set to 1.78 cm instead of 1.3 cm**”, i.e. a 37% increase, “on account of the significant experience of EDF in **improving radial power distribution.**” (MARGUET, 2017)

## Uncertainties of deterministic simulations (1/2)

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- Knowledge on sources of errors mentioned earlier → unused
- Instead, this assumption :
  - usual **discrepancy** between calculations and measurements, and
  - universal **uncertainty** of calculation
- are taken as **equal** → numerous weaknesses
- **Uncertainty** (of calculation) and **discrepancy** (between calculation and measurement) → concepts of **radically different natures**
- Standard deviation (or dispersion)  $\neq$  uncertainty
- Previously measured core, during a similar reloading → expecting similar discrepancy
- Conversely, unmeasured cases may imply more discrepancy
  - new reactors or fuel management, accident simulations
- Fragilities accentuated for **adjusted** deterministic simulations (residuals)
  - **compensations** between **errors** of different **natures**, unlikely to be **universal**

# Uncertainties of deterministic simulations (2/2)

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## Long-standing and still pending questions

- “What **adjustments** have been made to the TURTLE methodology to **improve** the agreement between **calculation** and **measurement**? How is the **uncertainty** in this **adjustment** accounted for in  $F_{\Delta H}$ ,  $F_{xy}(z)$  and  $F_Q(z)$  uncertainties?” (NRC, 1987)

## Recently renewed concerns

- The French **nuclear safety authority** “is particularly attentive to feedback from the EPRs [...] in China, which highlights certain topics requiring specific investigations and instructions. This concerns, in particular, [...] **anomalies in the power distribution** in the core of the **Taishan EPRs**” (ASN, 2021).
- To **increase robustness** → return to the **fundamentals** → **sources of errors**

# First start-up of Tihange-1, 900 MWe PWR

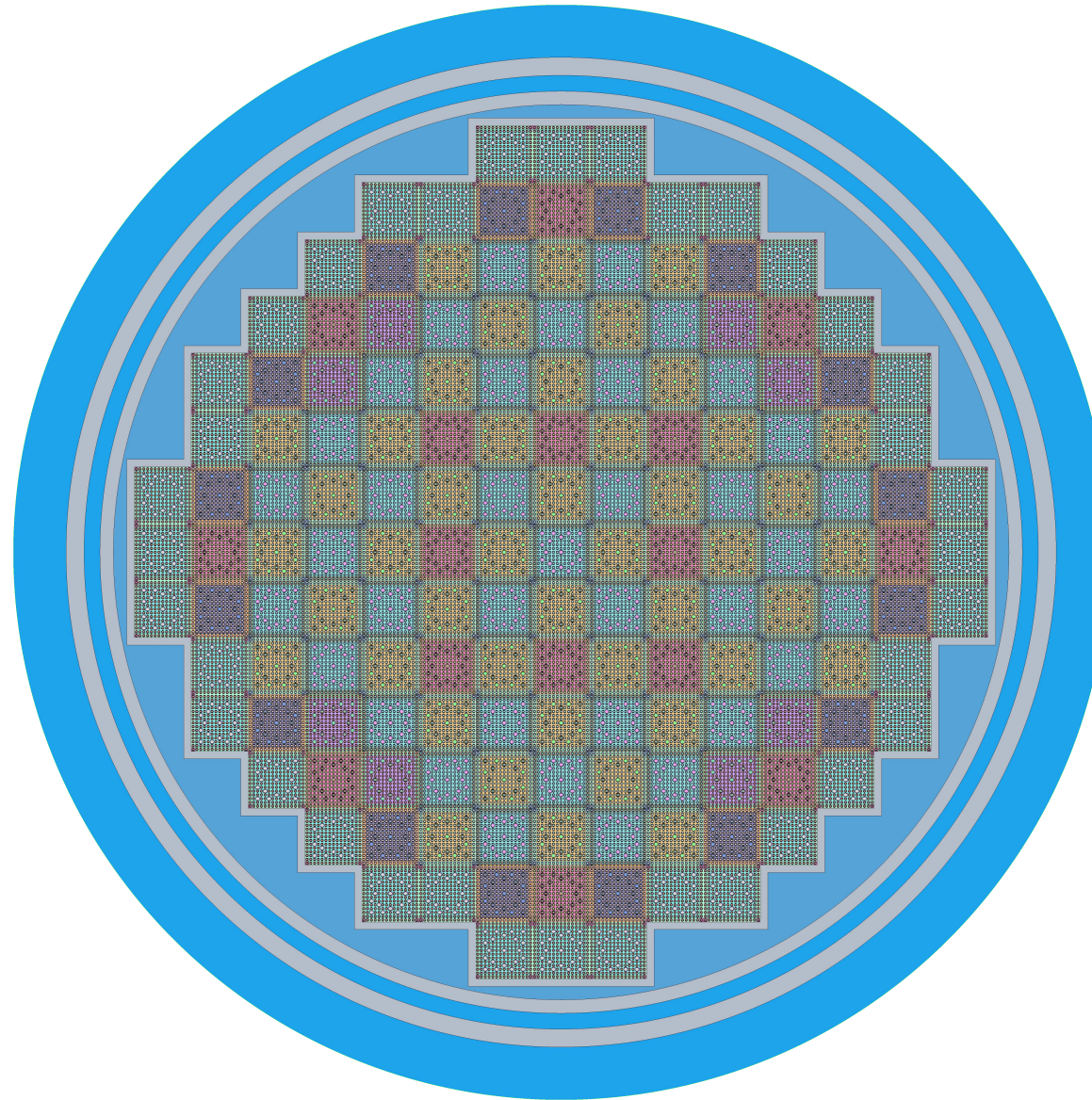
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# A deterministic solution, with JEFF-3.3

## Power distribution in Tihange-1, first start-up

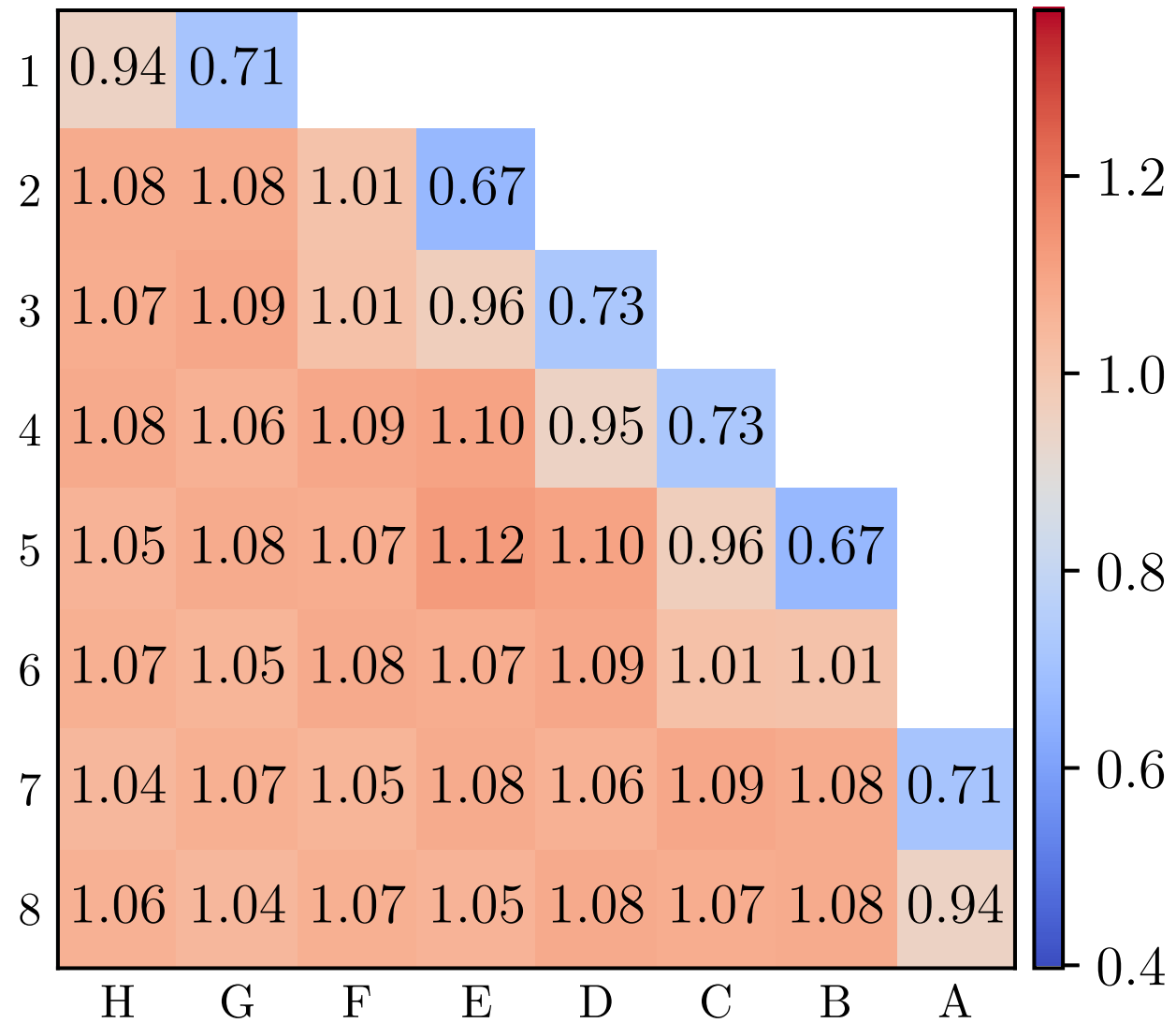
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# Deterministic vs Monte-Carlo $\iff$ deterministic bias

## Power distribution in Tihange-1

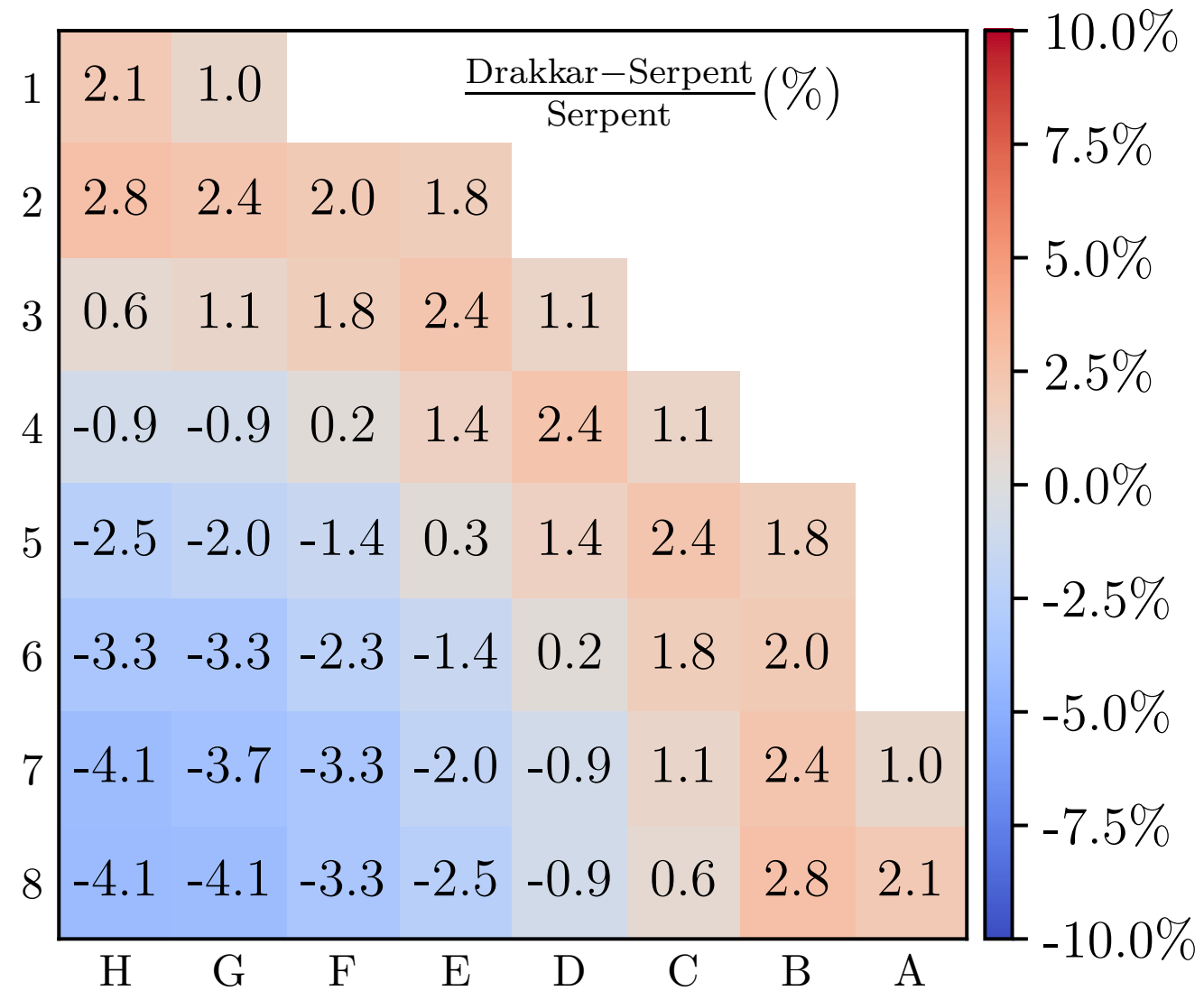
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# Uncertainties on cross sections of **hydrogen** bound in H<sub>2</sub>O

Source : JEFF-3.3

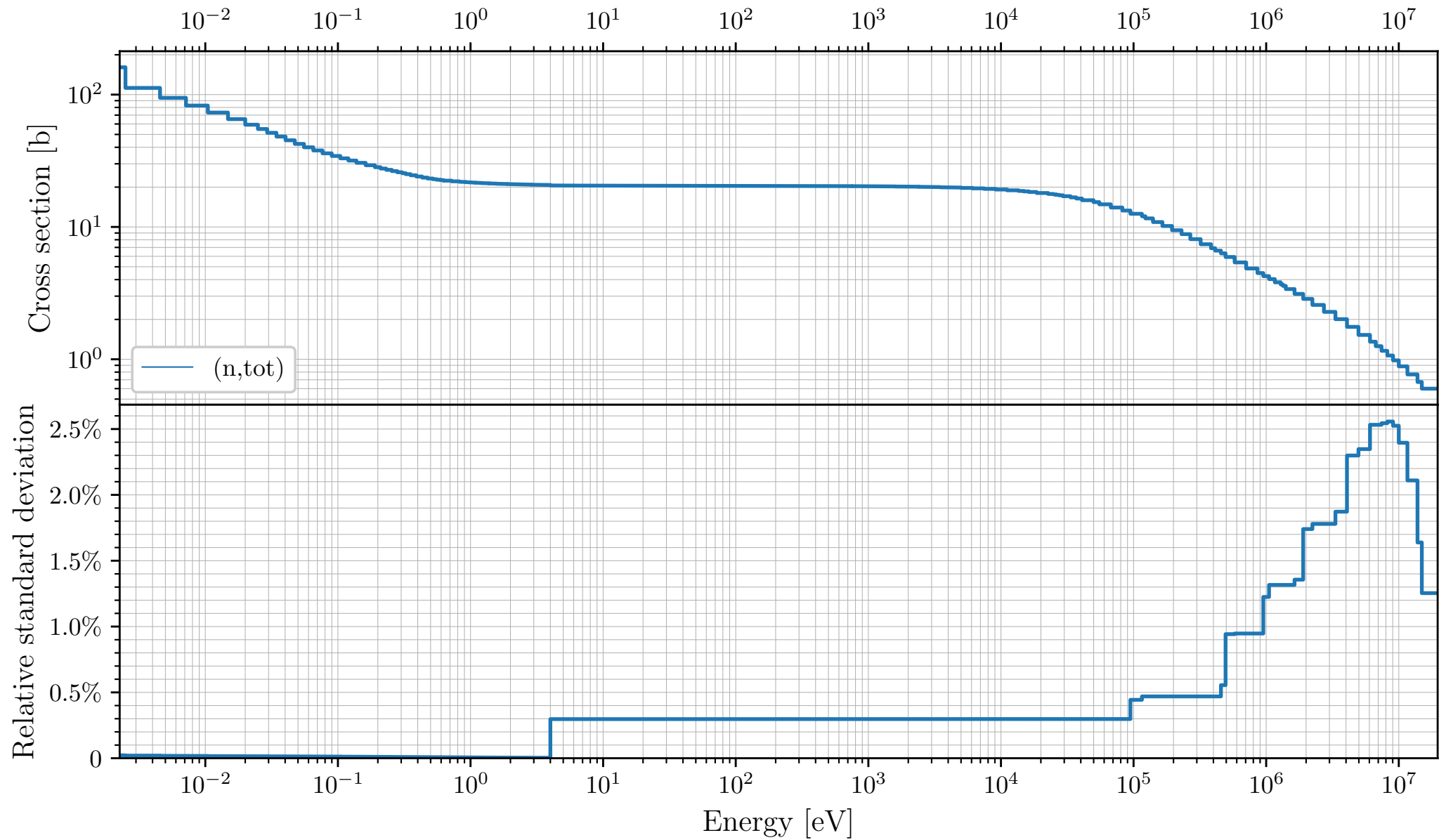
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# Propagation of hydrogen uncertainties through deterministic methods

## Total Monte-Carlo : 300 samples of nuclear data (with SANDY)

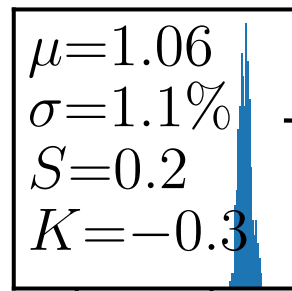
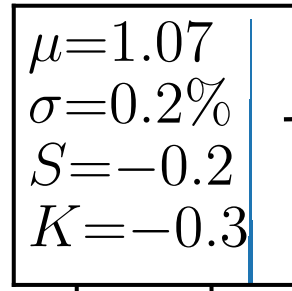
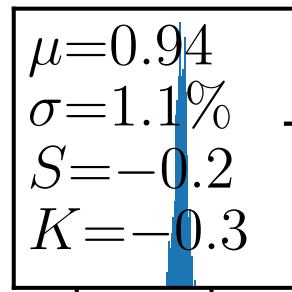
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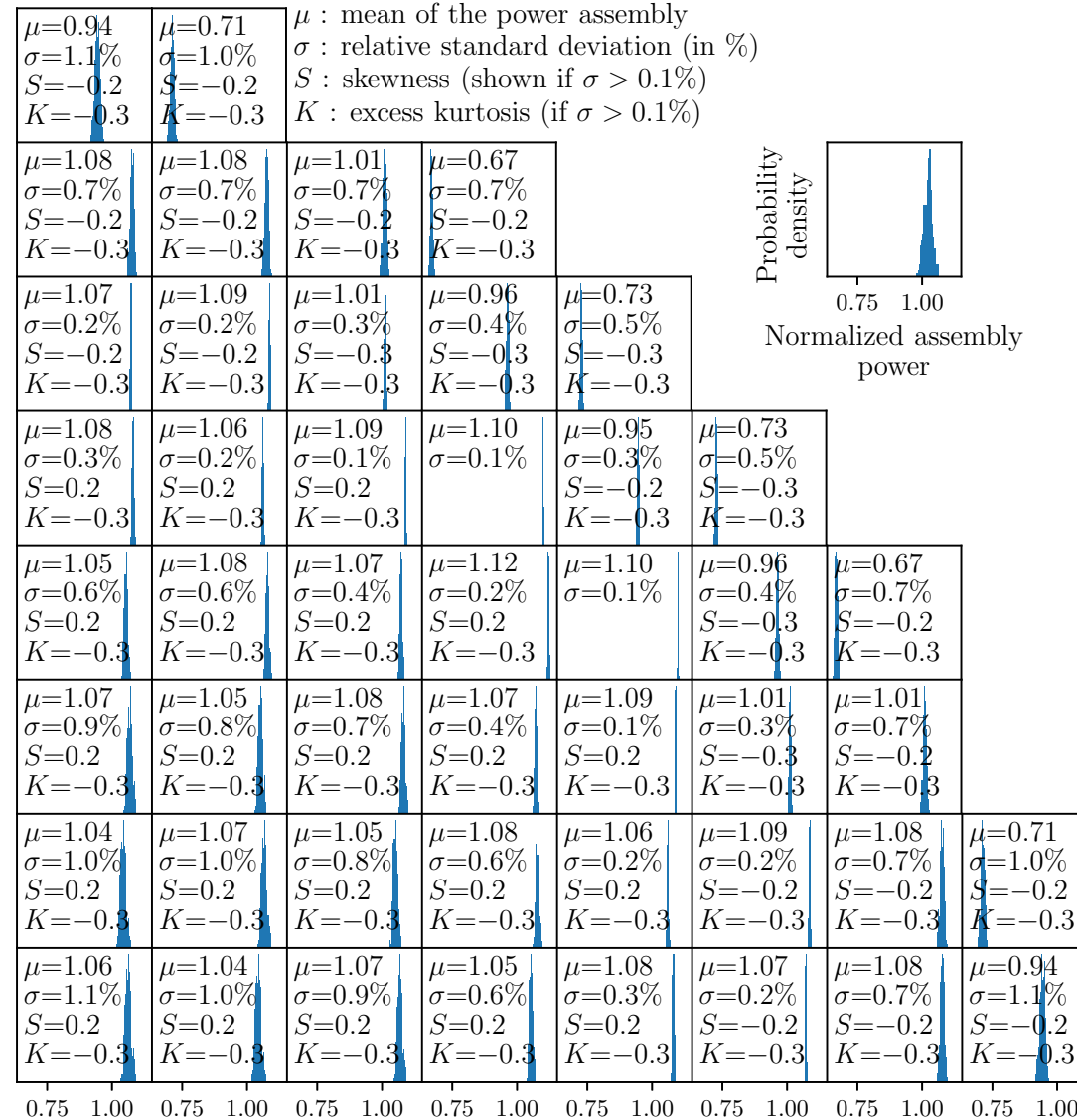
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0.75 1.00





# Propagation of uncertainties from hydrogen, JEFF-3.3

## Deterministic and Monte-Carlo comparison

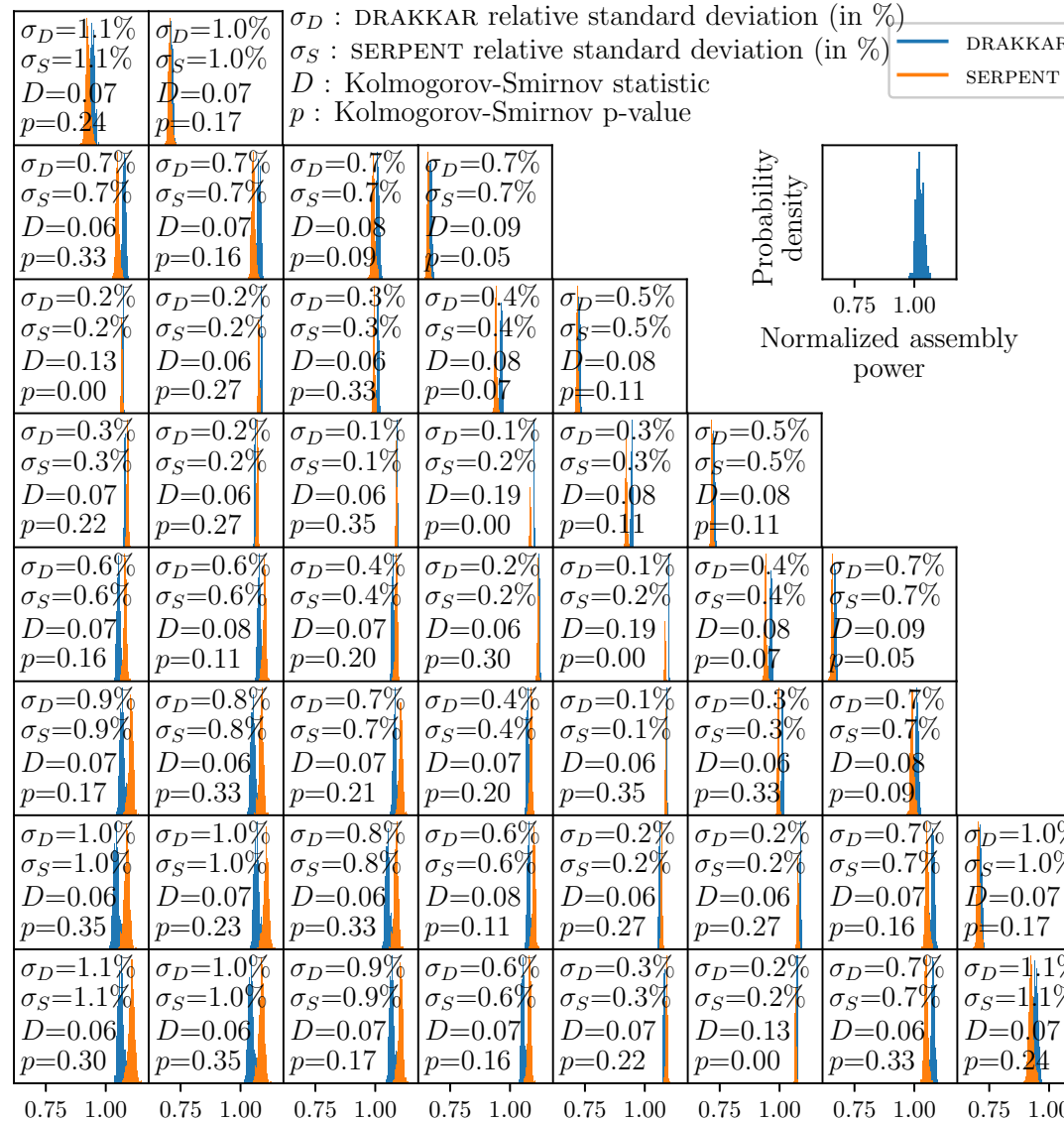
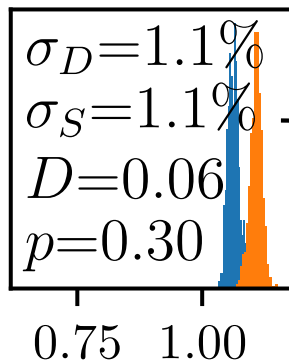
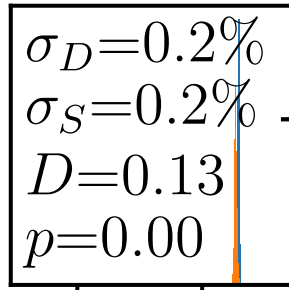
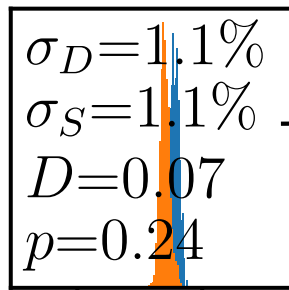
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# First start-ups of Bugey-2, Fessenheim-1 and 2, three identical 900 MWe reactors

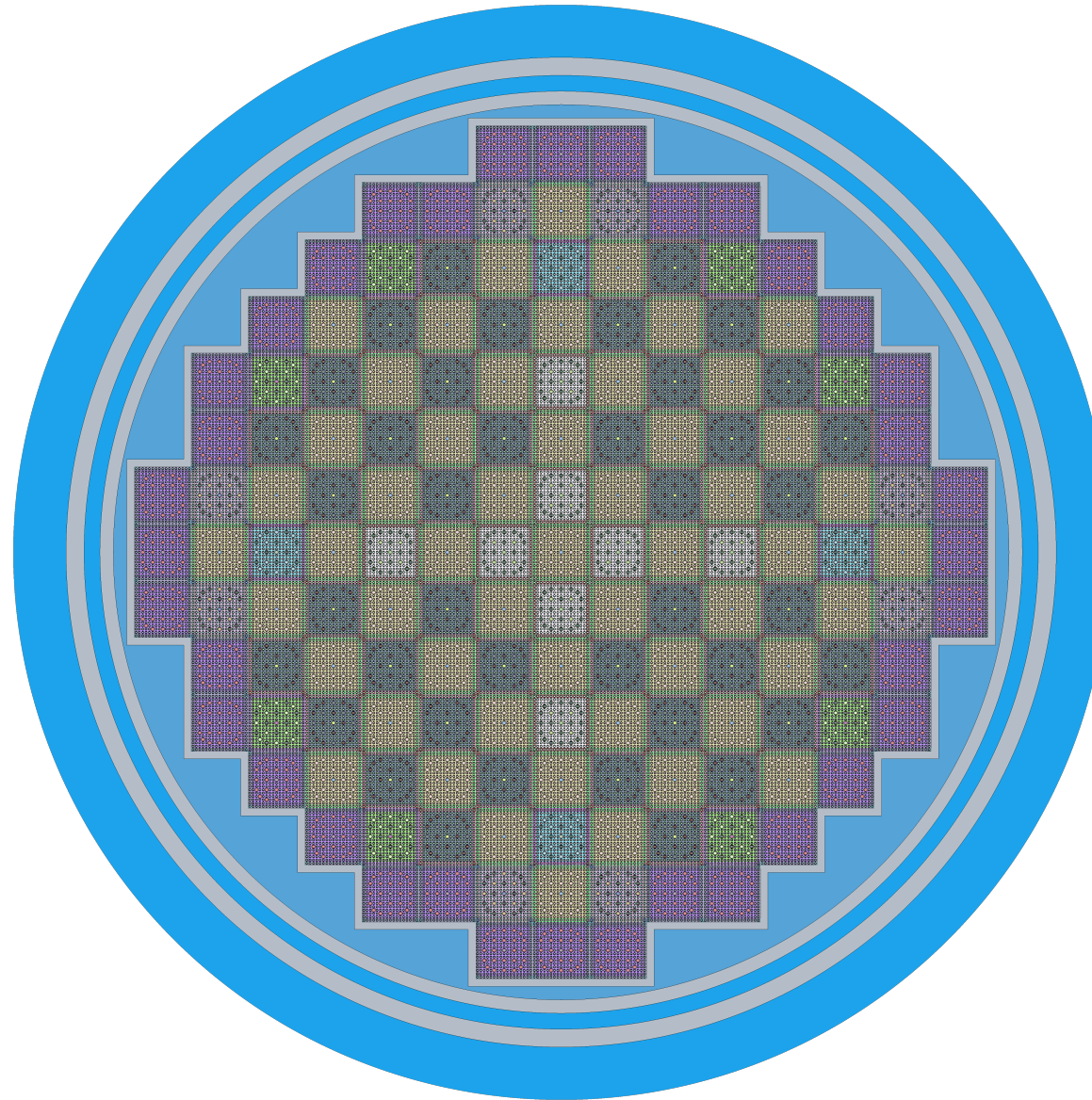
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# Ranking of nuclear data uncertainties

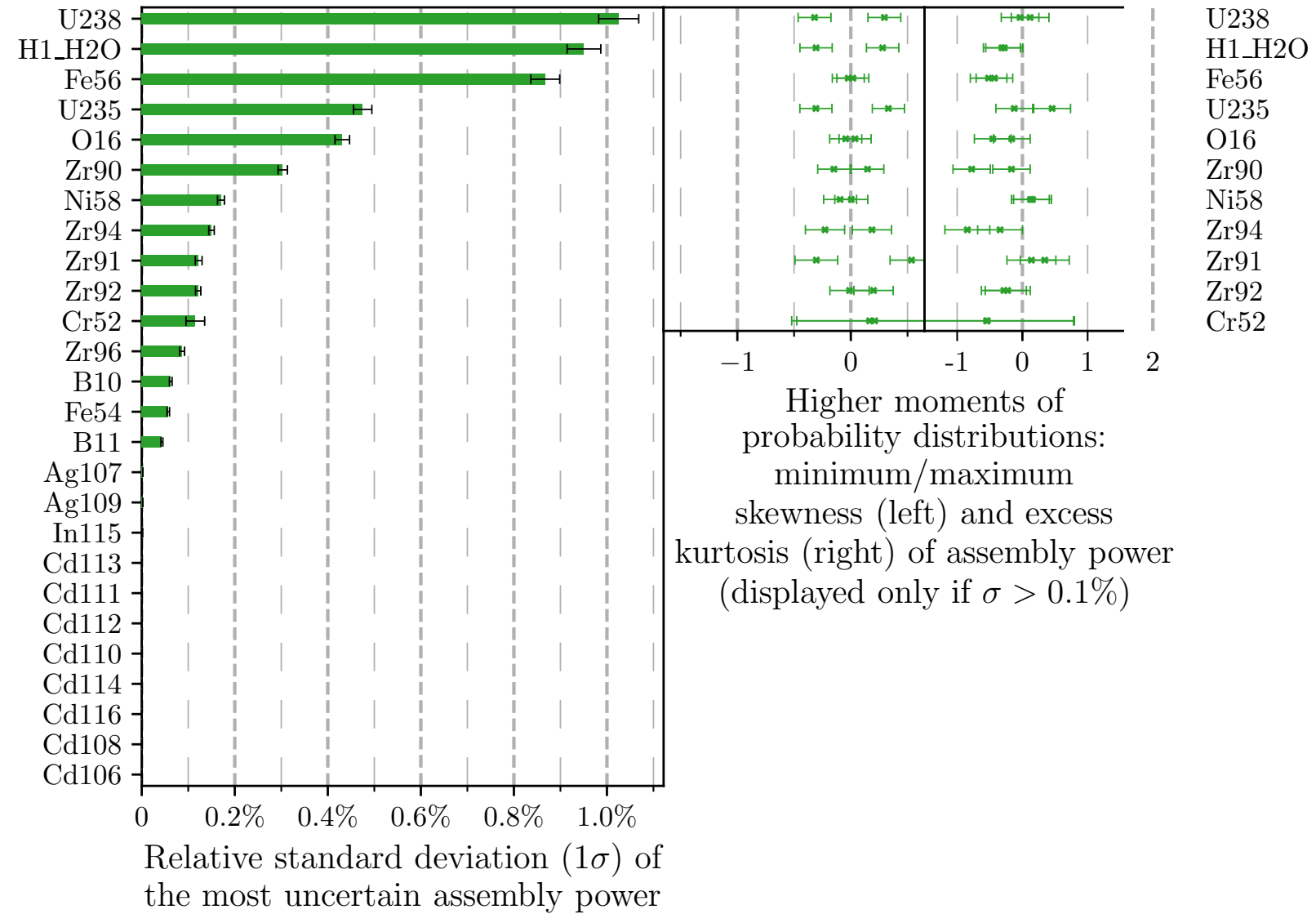
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# Simultaneous sampling : interactions between isotopes

## Detector responses

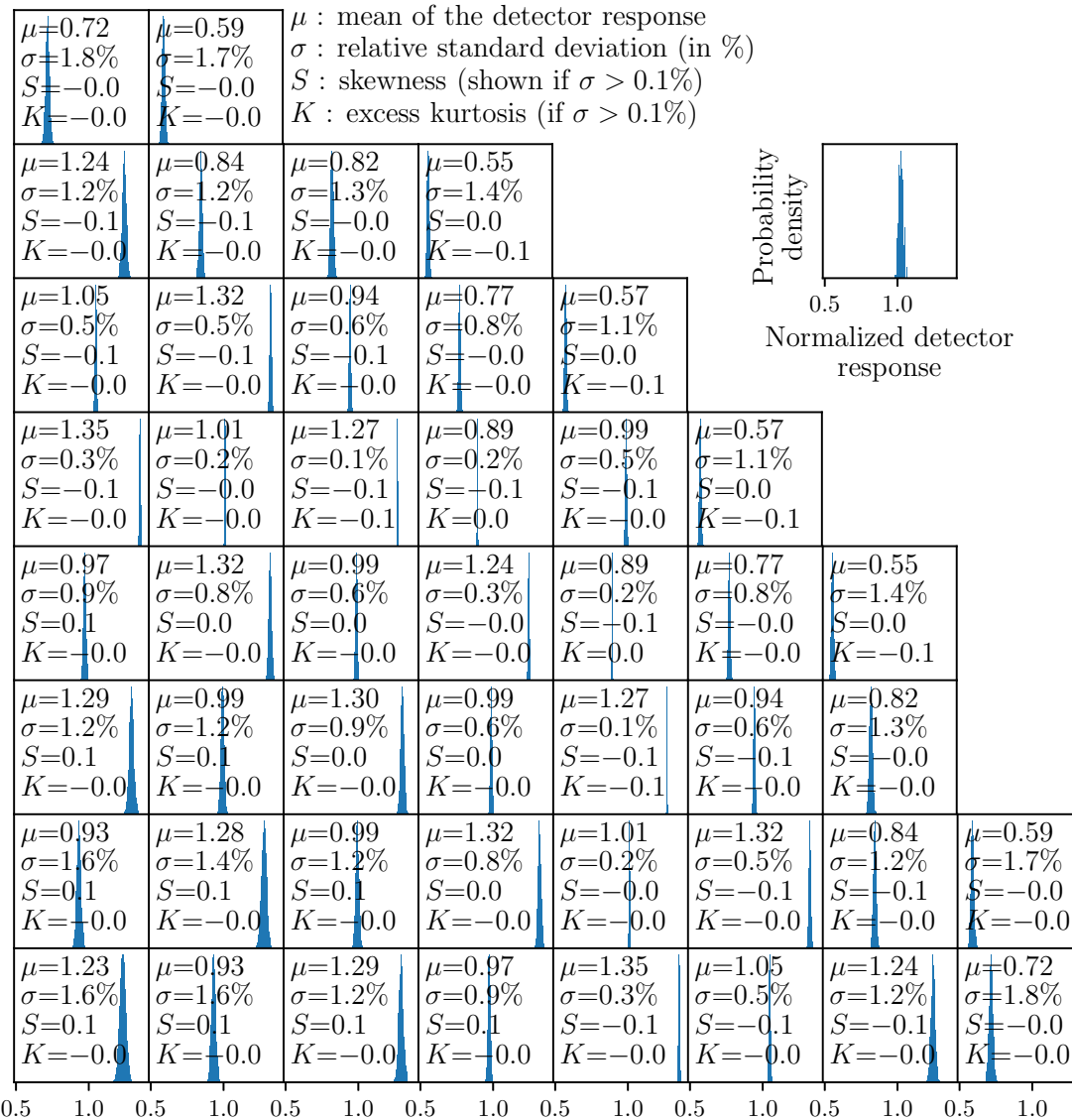
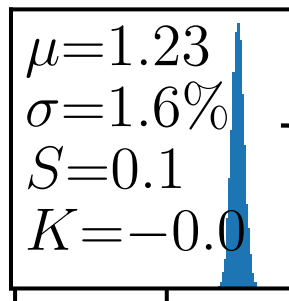
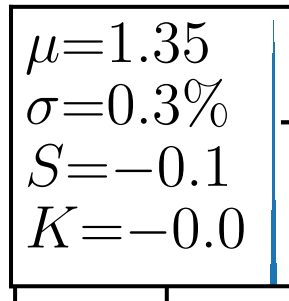
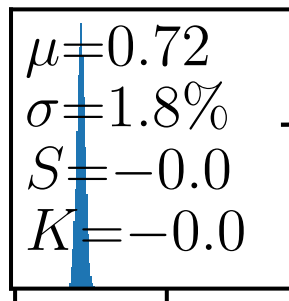
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# Experimental detector responses during the 1<sup>st</sup> start-up of Bugey-2

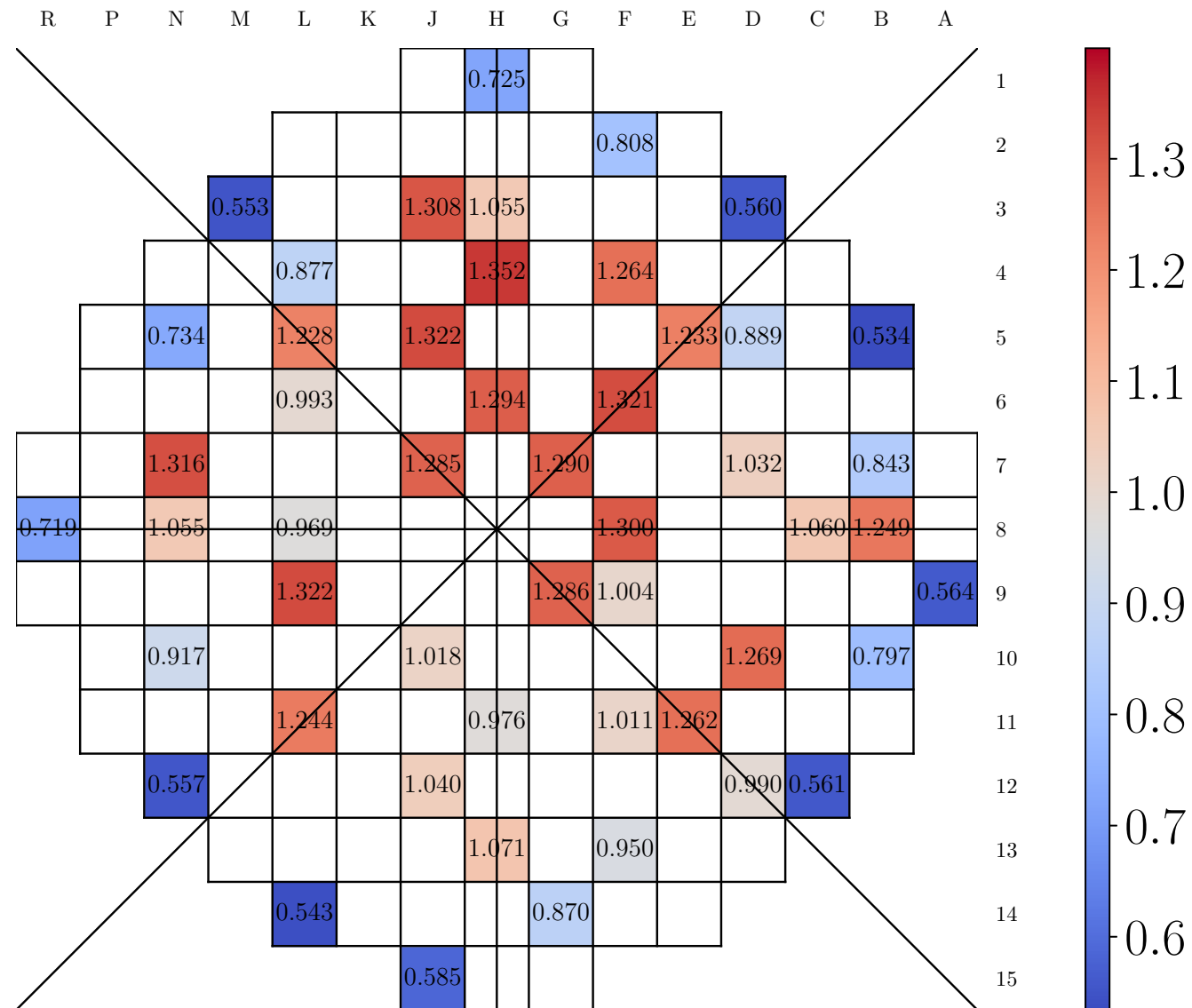
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# Experimental detector responses during the 1<sup>st</sup> start-up of Fessenheim-1

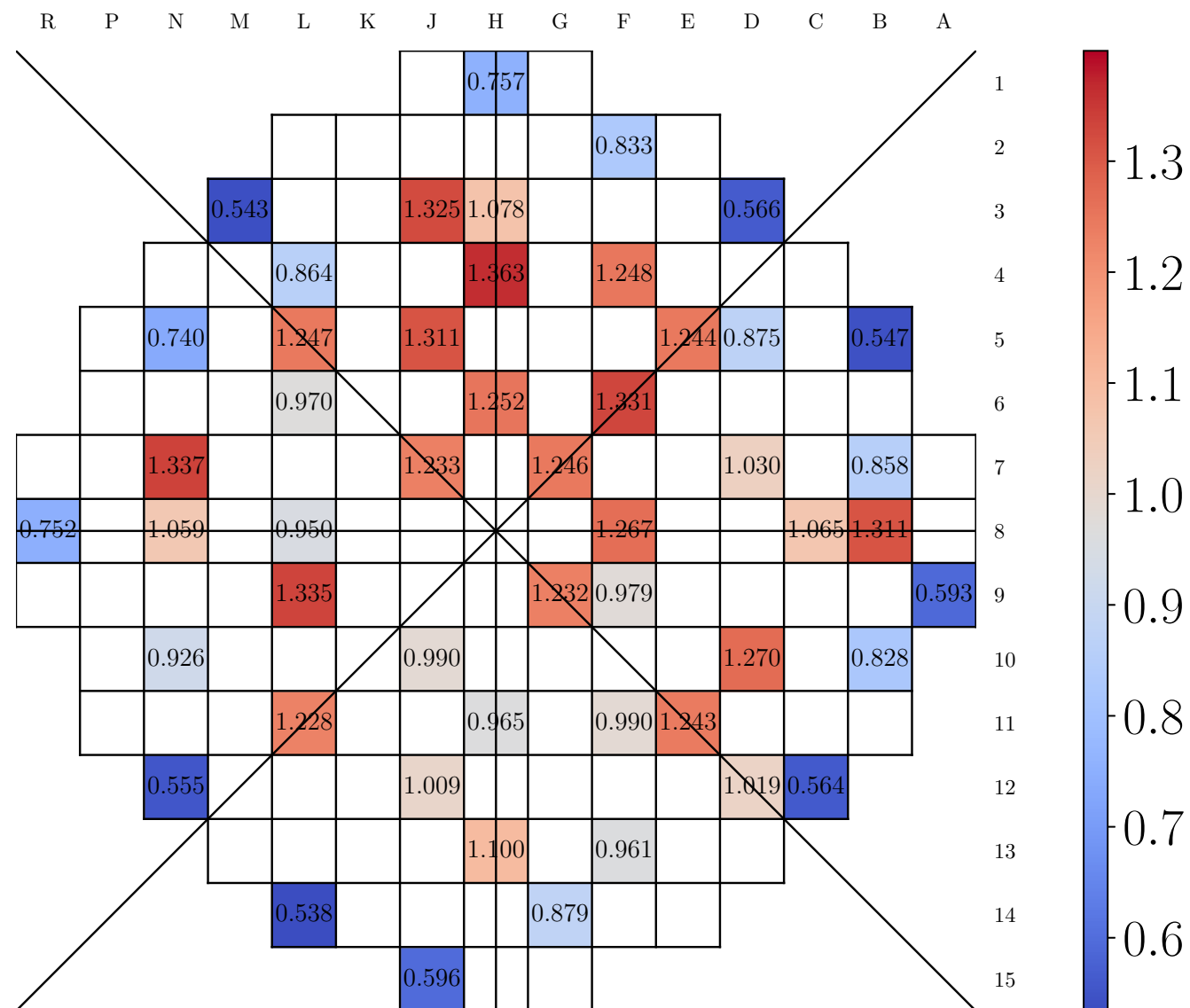
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# Experimental detector responses during the 1<sup>st</sup> start-up of Fessenheim-2

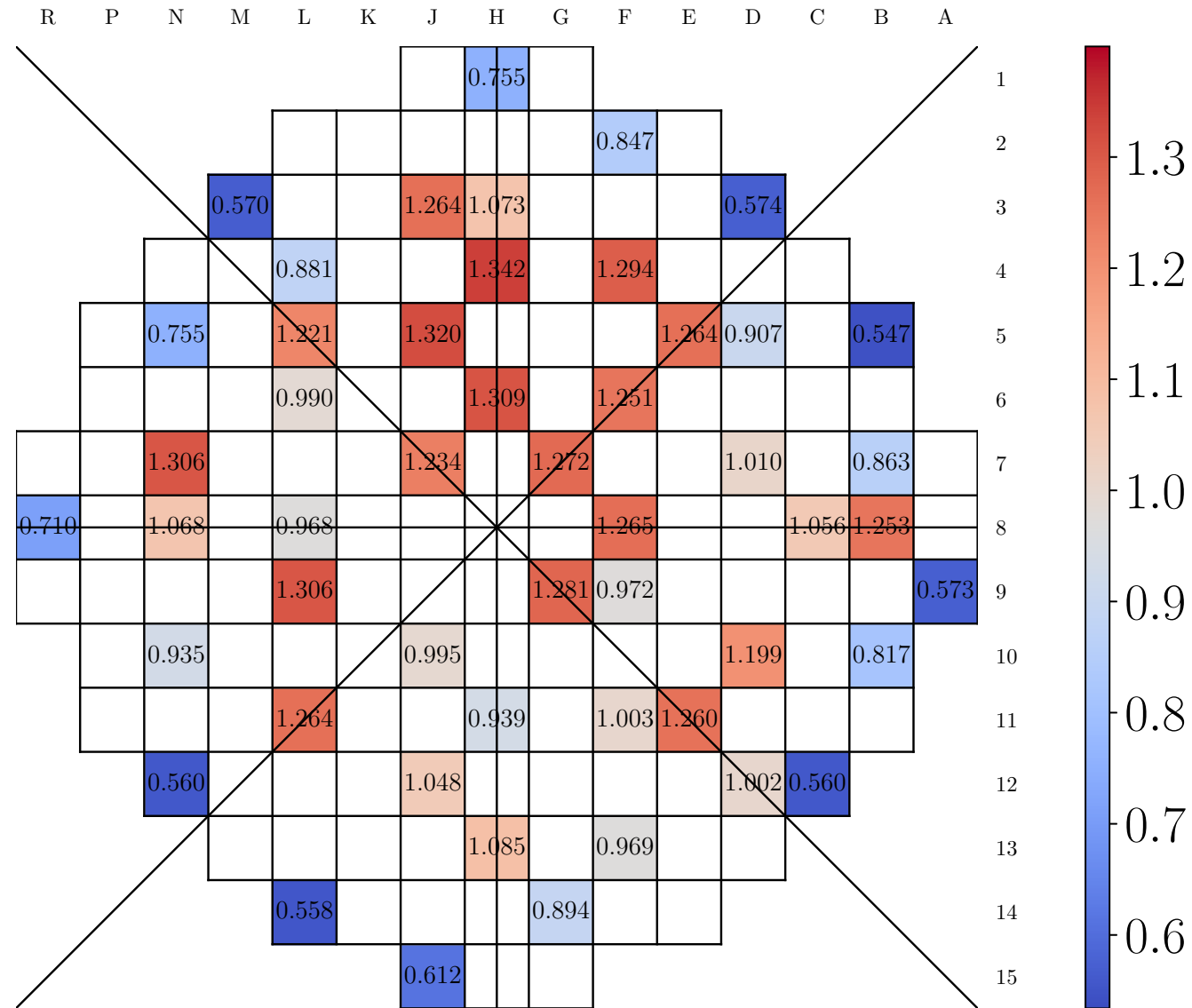
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# Adjustment with BFMC method (Backard-Forward Monte-Carlo)

→ Proximity between the measurement and a sample  $k$  of nuclear data estimated with

$$\chi_k^2 = \sum_{i=1}^{n_{\text{mes}}} \left( \frac{C_{i,k} - E_i}{\sigma_{E_i}} \right)^2 \quad (1)$$

→ Lack of uncertainty estimated by experimentalists  
→ expert opinion, for lack of a better choice

$$\sigma_E = 2\% \quad (2)$$

→ Each nuclear data sample  $k$  → weight

$$w_k = \frac{\exp(-\chi_k^2 / \chi_{\min}^2)}{\sum_{\kappa=1}^n \exp(-\chi_{\kappa}^2 / \chi_{\min}^2)} \quad (3)$$

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# Posterior detector responses (after BFMC)

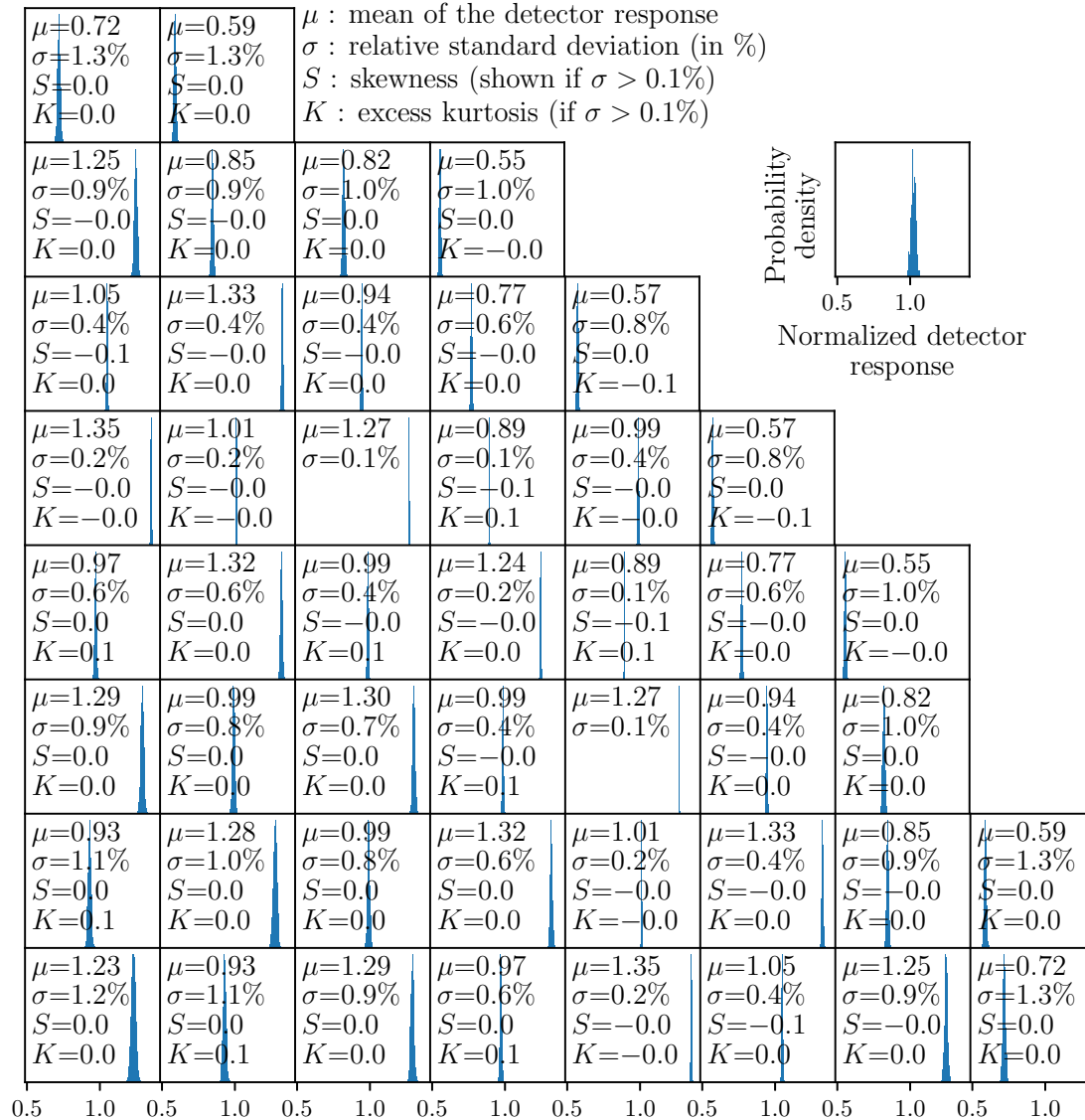
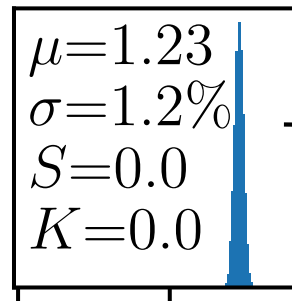
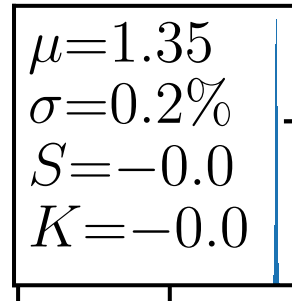
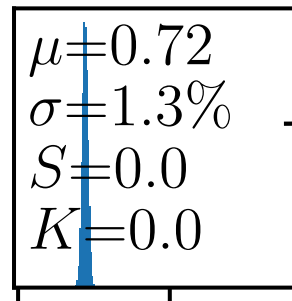
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# Modifications (red) to five prior quantiles (grey) of hydrogen cross sections, with BFMC

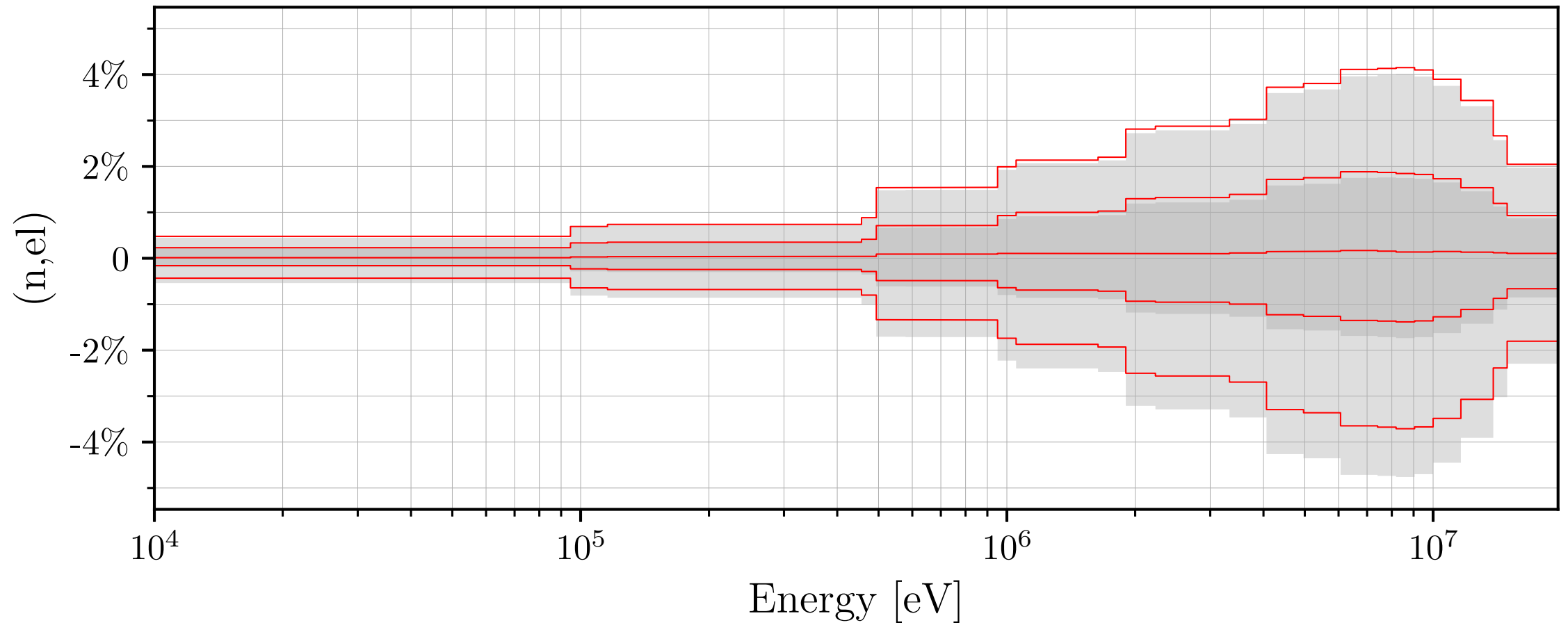
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# Discussion

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- $D_1$  reflector adjustment → depends on the reactor size, fuel loading, etc.
  - transferring information is rather difficult to justify
- Nuclear data are universal, identical for all reactors
  - universal adjustment
  
- $D_1$  reflector adjustment → best estimate only, without any notion of uncertainties, must be estimated afterwards
- Here, nuclear data adjustment also applies to uncertainties
  
- Limit : relies on Monte-Carlo to compute and evict the deterministic bias

# Conclusions

→ For variations in nuclear data typically corresponding to their uncertainties :

**Deterministic bias is constant, identical for  $\neq$  samples**

→ Thus, it is possible to benefit from the “**best of both worlds**” through combination of

- the **best estimate** from the **Monte-Carlo** method (mean) and
- the **uncertainties** obtained with **deterministic** methods (moments of higher orders),

→ Second theme : **adjustments**. Objective : tend toward **better extrapolability** than adjustment on reflector  $D_1$

→ It seems **legitimate** to consider that computations **should reproduce measurements** made experimentally on real reactors. However, the standard adjustment for PWRs is very questionable → **attempt** to improve as much as possible, to remove as much deficiencies as possible

→ Based on a physical knowledge of the underlying causes of errors → **universality** is sought **instead of error compensation**

→ Nevertheless, such an adjustment could still be **questionable**. In your opinion, what is the most convincing **argument against** such **adjustments**?

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# Open source software, open data

- Totality of developed **software** and produced **data** (initial, intermediate and final) available on :

[github.com/IRSN/SalinoPhD](https://github.com/IRSN/SalinoPhD)

## Examples :

- Nuclear data and its processing, from ENDF to ACE, Draglib
- Datasets for Serpent, Dragon and Donjon
- Experimental data (found in public sources) in csv, plots...

- Such a principle of openness is intended to allow, in a pragmatic and effective way :
- the verifiable and complete **reproducibility** of this publicly funded research
  - the **transparency** necessary for a rigorous peer review
  - wide **dissemination** of the developed **ideas**
  - **facilitate** interaction and collaboration

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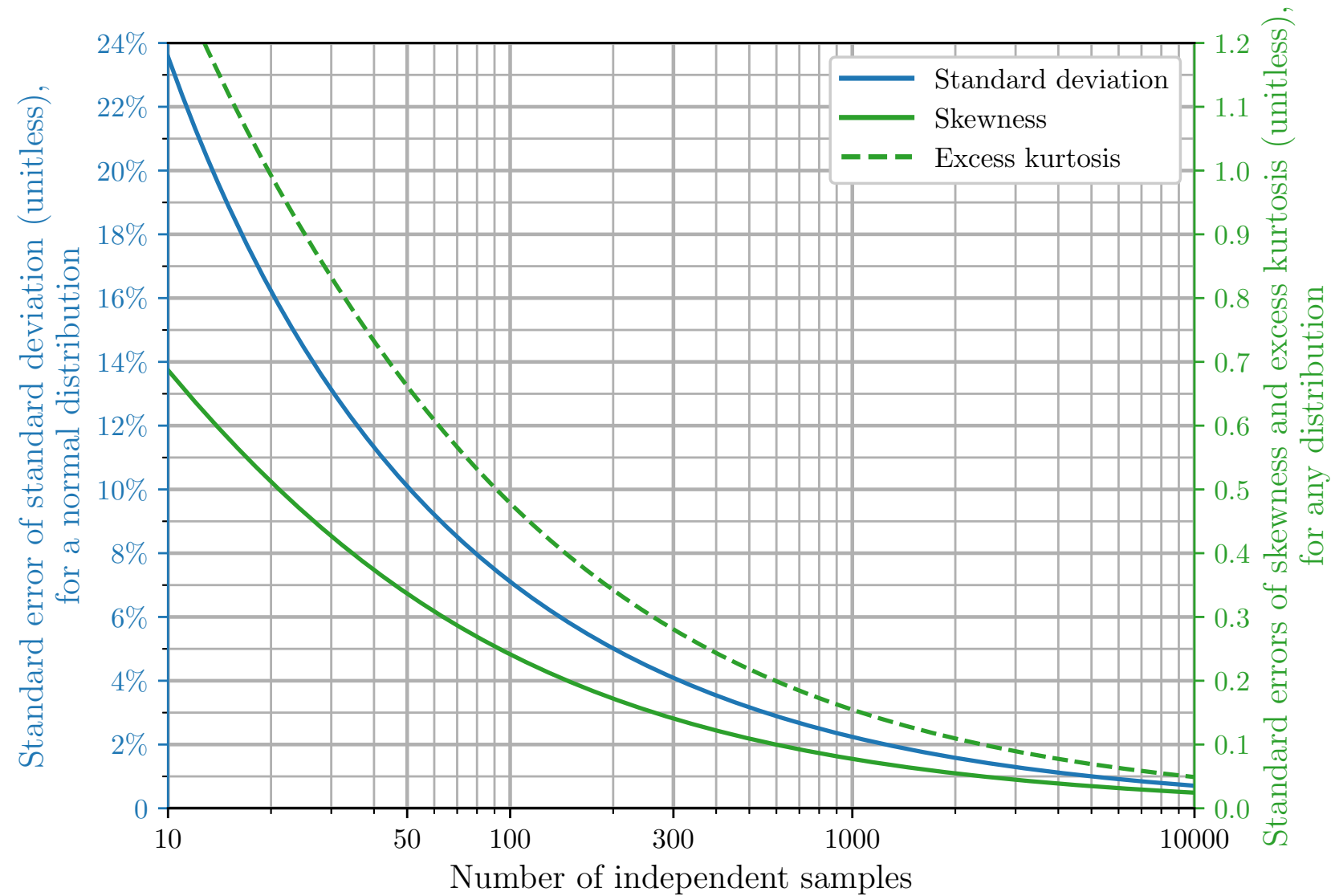


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## Backup slides

# Standard error on standard deviation (left axis), on skewness and on excess kurtosis (right axis)





## Importance of power distribution

- Most of the research in the field of uncertainty is focused on  $k_{\text{eff}}$ , yet, for reactors
  - nuclear safety depends **not much** on it
- Focusing on **power distribution**
  - nuclear safety depends **heavily** on it  
(KERKAR and PAULIN, 2008)





## Equivalence methods for the reflector

- Equivalences used for fuel → not applicable to the reflector, as they typically conserve
  - diffusion properties (diffusion coefficients),
  - reaction rates (SPH)
- Conserving reaction rates **in** the reflector or neutron scattering **in** the reflector is of little interest
- Rather wishes to maintain its reflective properties against an **external source** of neutrons
- Specific equivalences → determining cross sections and diffusion coefficients preserving reflective properties of a (transport) reference

## Lefebvre-Lebigot method (1/2)

→ Analytical solution of the current **at the interface** ( $x = 0$ )

$$\frac{J_1}{\phi_1} = \sqrt{D_1 (\Sigma_{a1} + \Sigma_{1 \rightarrow 2})} \quad (1)$$

and

$$\frac{J_2}{\phi_1} = \frac{\phi_2}{\phi_1} \sqrt{D_2 \Sigma_{a2}} - \frac{\Sigma_{1 \rightarrow 2} \sqrt{D_1 D_2}}{\sqrt{\Sigma_{a2} D_1} + \sqrt{(\Sigma_{a1} + \Sigma_{1 \rightarrow 2}) D_2}} \quad (2)$$

- After analytical study, numerical experiments with a  $S_N$  transport code on a representative heterogeneous traverse
- Reflector applicable for all fuel bundles,  $\forall$  temperature, burnup, etc.
  - reflector response for fuel varying as such

1) Fast group →  $J_1 / \phi_1$  is constant

$$R_1 = \frac{J_1}{\phi_1} \quad (3)$$

## Lefebvre-Lebigot method (2/2)

### 2) Thermal group

→  $J_2/\phi_1$  depends on the fuel

$$\frac{J_2}{\phi_1} = -R_3 + R_2 \frac{\phi_2}{\phi_1} \quad (4)$$

→ **5 unknowns** and **3 parameters** ( $R_1$ ,  $R_2$  et  $R_3$ ) calculated in  $S_N$ ,  
Lefebvre and Lebigot suggest to equalize  $D_g$  :

$$D_1^{\text{fuel}} \approx 1.3 \text{ cm}$$

$$D_1^{\text{reflector}} = \mathbf{1.3 \text{ cm}}$$

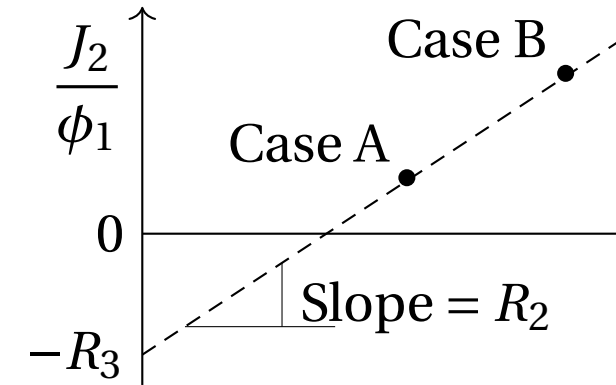
$$D_2^{\text{fuel}} \approx 0.4 \text{ cm}$$

$$D_2^{\text{reflector}} = 0.4 \text{ cm} \quad (5)$$

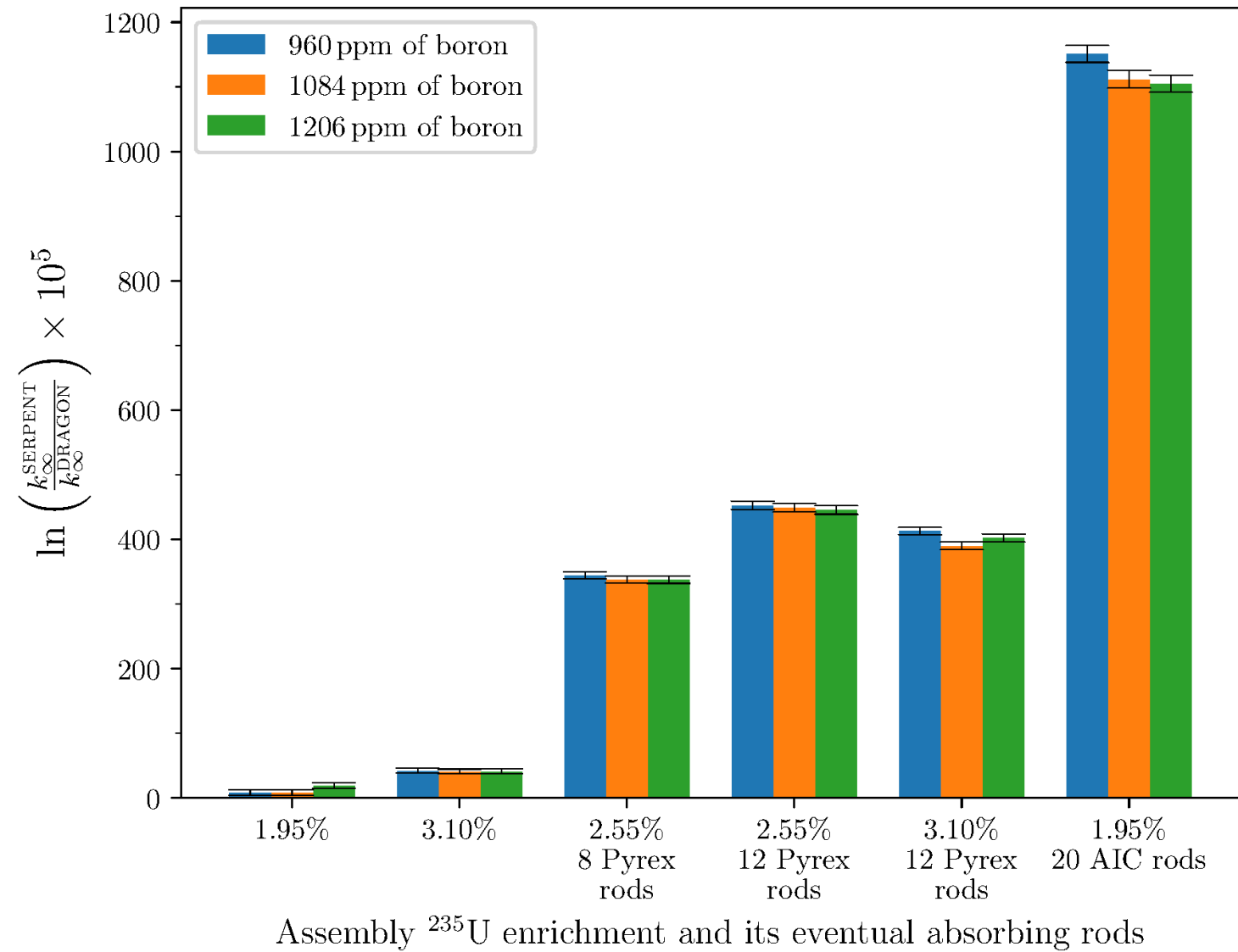
$$\Sigma_{a2} = \frac{(R_2)^2}{D_2}$$

$$\Sigma_{1 \rightarrow 2} = R_3 \left( \frac{R_1}{D_1} + \sqrt{\frac{\Sigma_{a2}}{D_2}} \right) \quad (6)$$

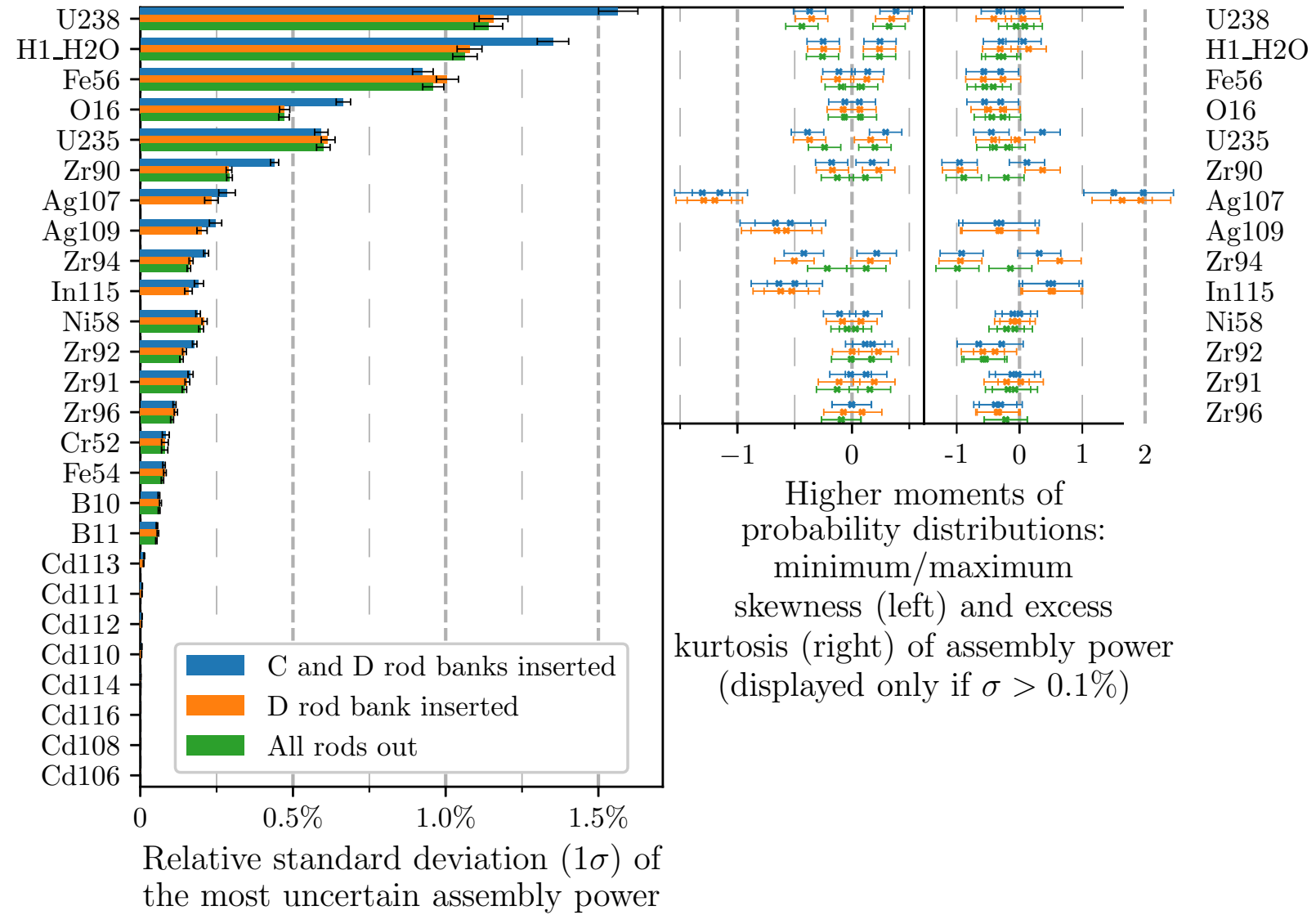
$$\Sigma_{a1} = \frac{(R_1)^2}{D_1} - \Sigma_{1 \rightarrow 2} \quad (7)$$



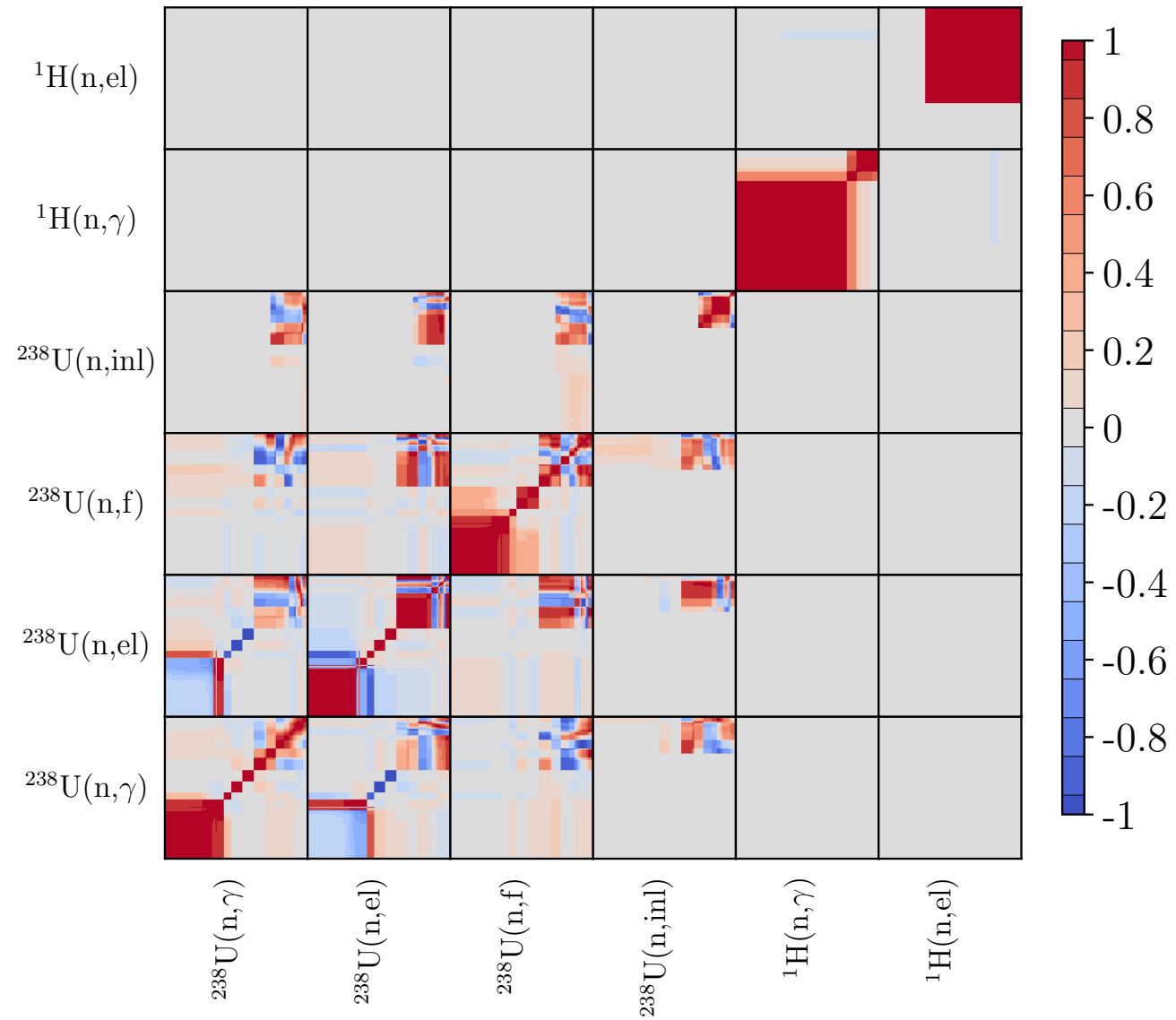
# $k_{\infty}$ discrepancy between Serpent and Dragon (pcm), for assemblies during 1<sup>st</sup> start-up of Tihange-1



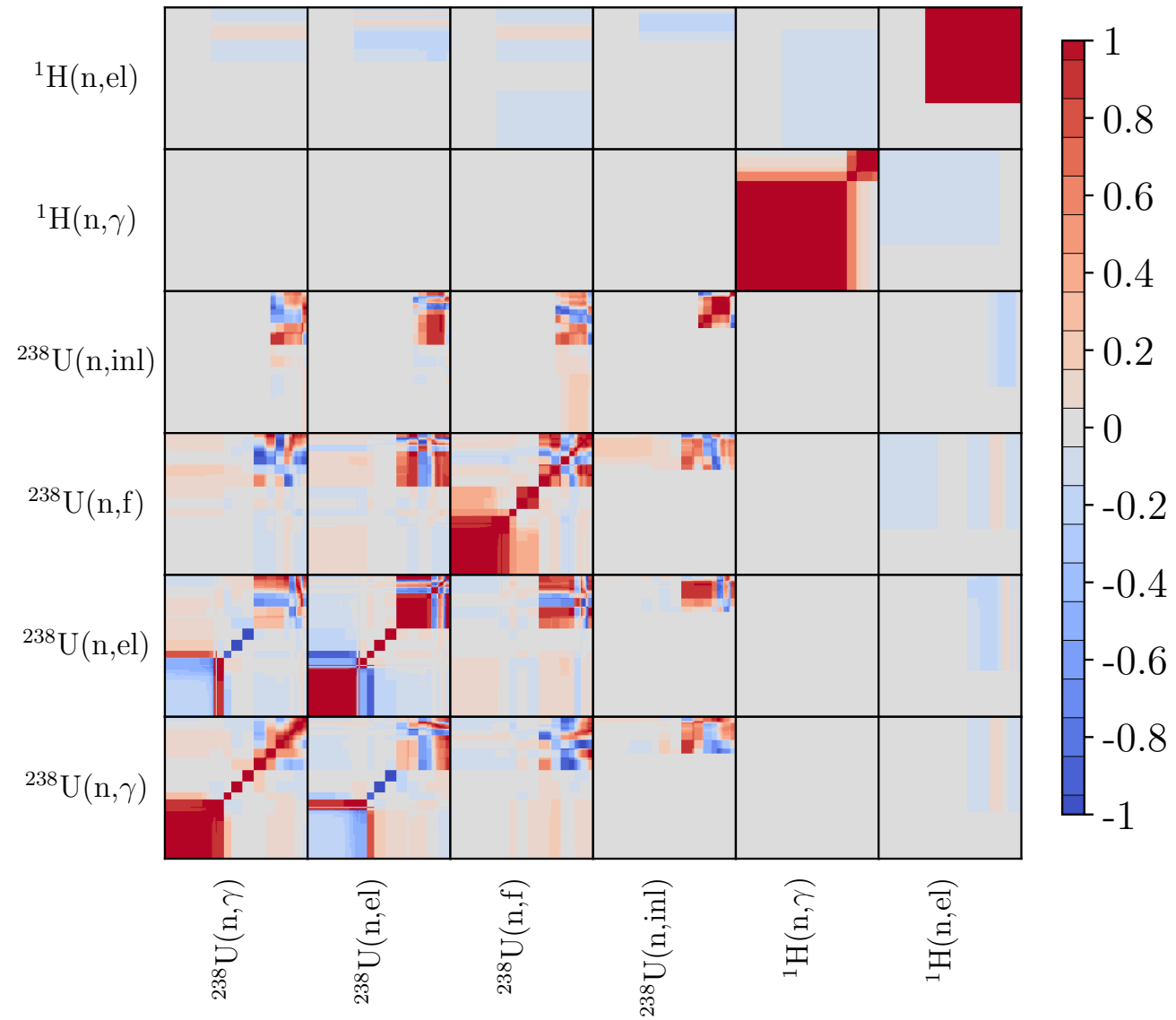
# Ranking of uncertainties in Tihange-1, by isotope



# Prior correlations between the uncertainties of hydrogen and uranium 238

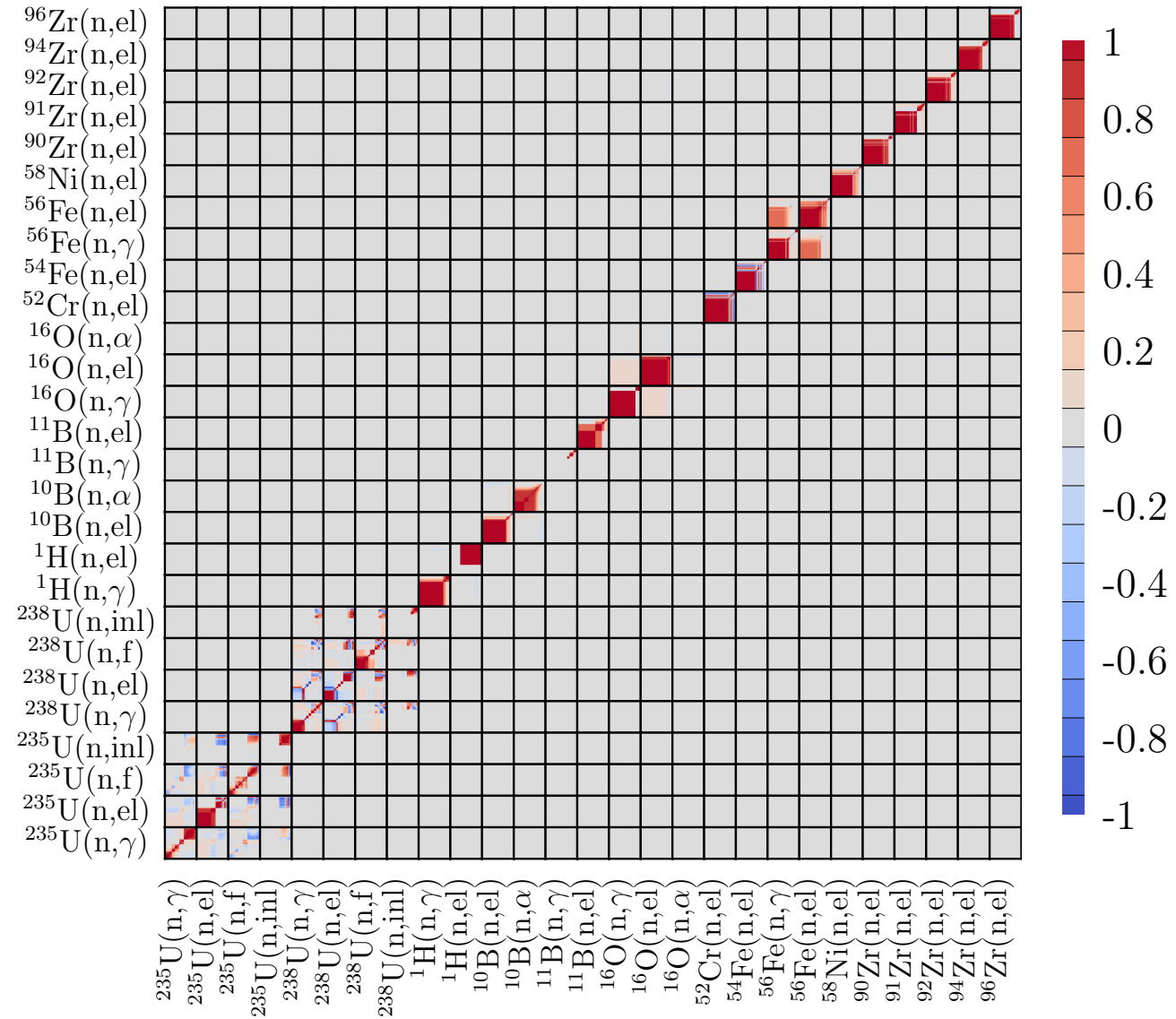


# Posterior (BFMC) correlations between the uncertainties of hydrogen and uranium 238

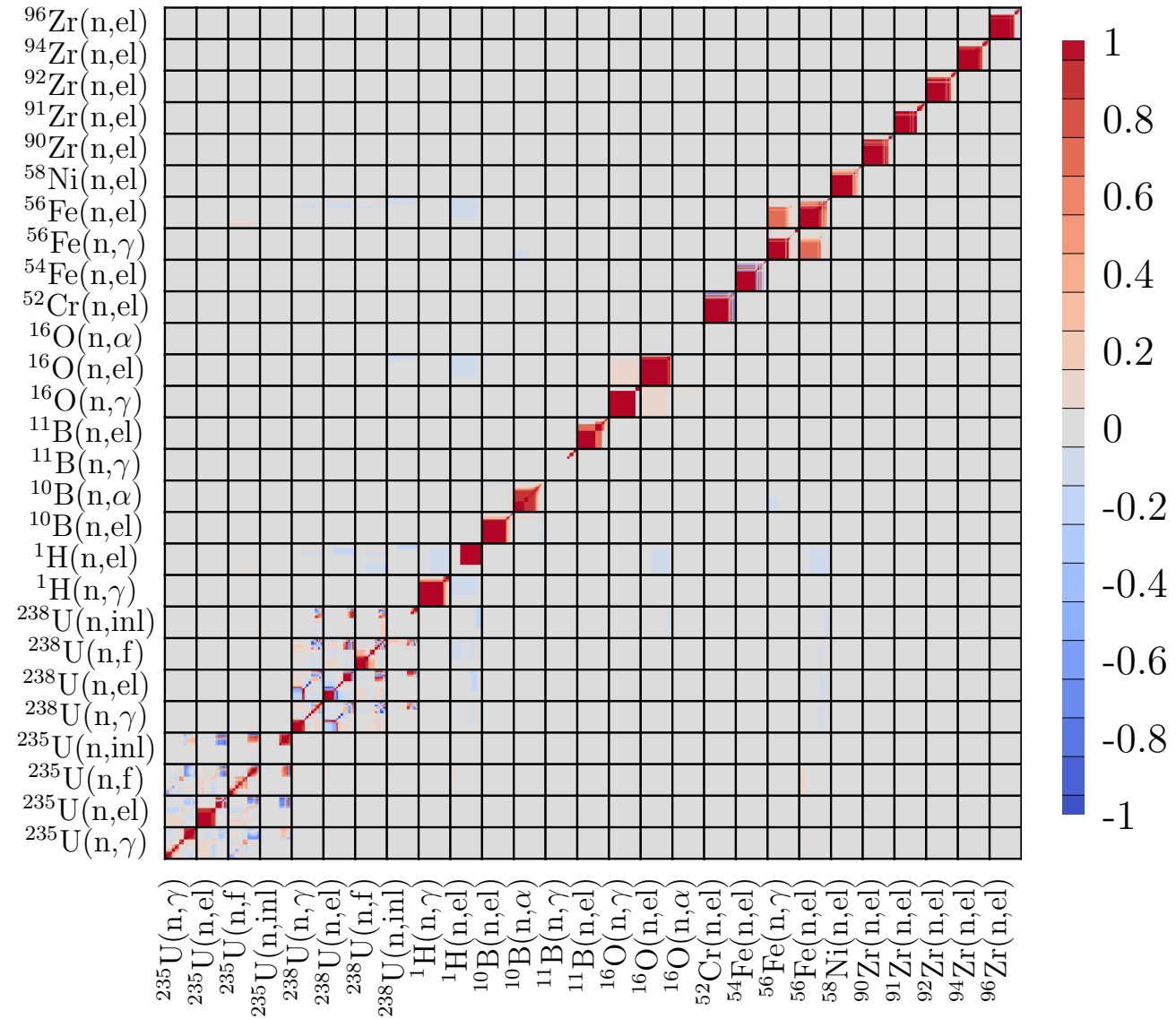




# Prior correlations between the uncertainties of different isotopes



# Posterior (BFMC) correlations between the uncertainties of different isotopes



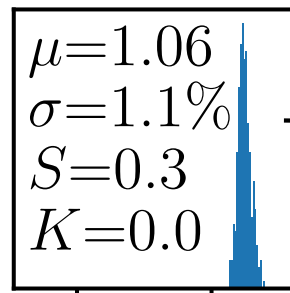
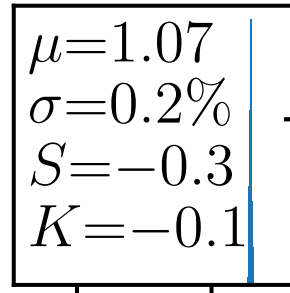
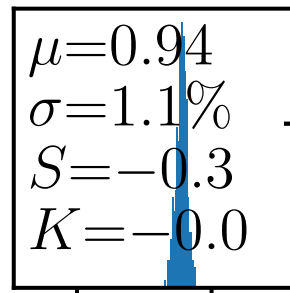
## Evaluation of nuclear data **uncertainties**

- 1) JEFF-3.3 or ENDF-B/VIII.0 evaluations → covariance matrices
  - Multigroups → piecewise constant
  - Sometimes missing or incomplete (minor isotopes)
- 2) TENDL-2019 evaluation → some various benefits
  - Very **complete uncertainties** (angular distributions, etc), continuously varying, not necessarily Gaussian
  - Above all, **single code** for production → high format homogeneity → **safer** and faster
  - TALYS optical models → **no evaluation** for less than 20 nucleons (hydrogen, boron, oxygen...) → JEFF-3.3
  - **No evaluation** either for some heavy isotopes, the most important ones : uranium 235, 238... → JEFF-3.3

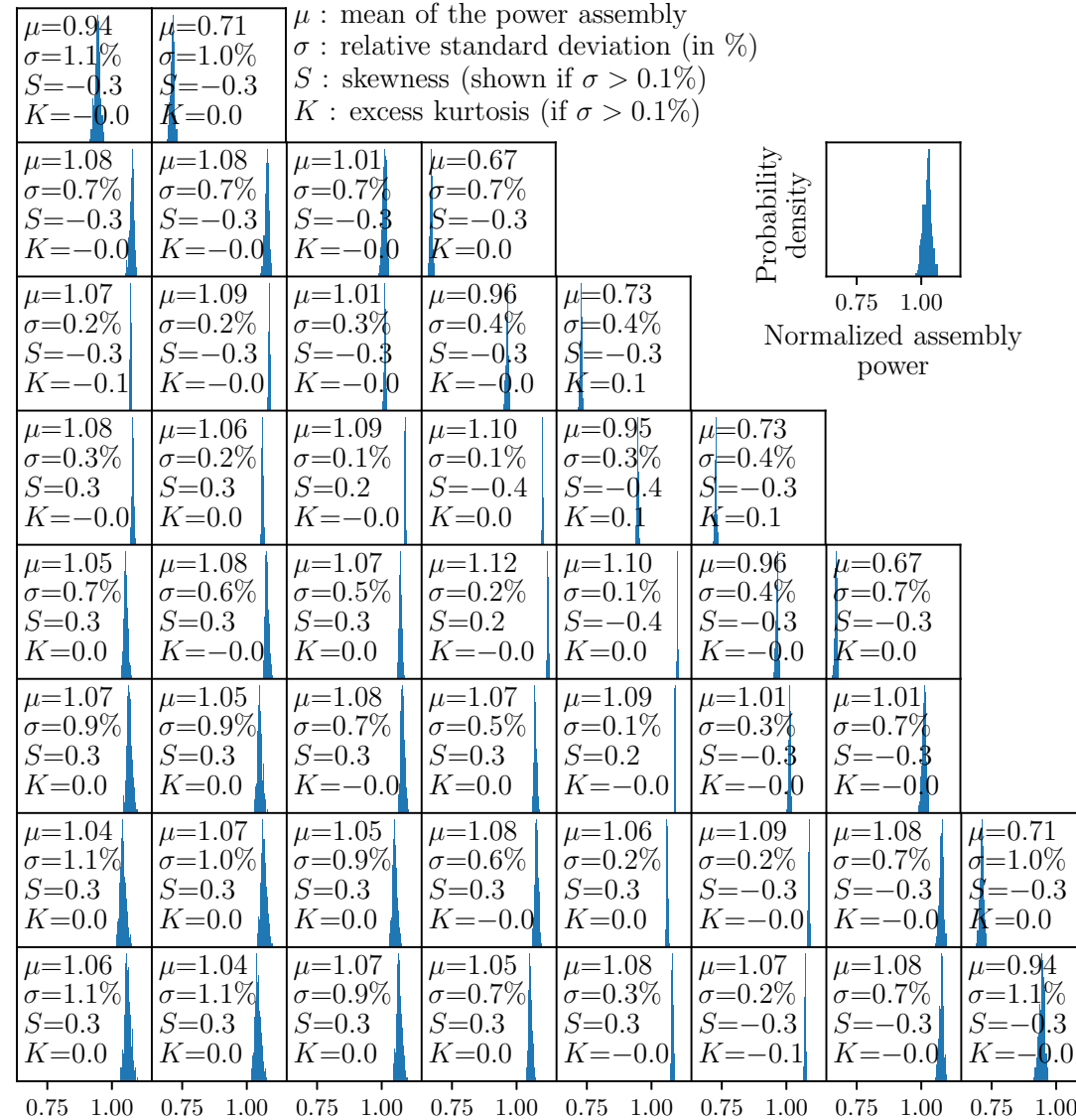
**The idea is not to demonstrate the qualities or defects of JEFF-3.3 or TENDL-2019 : just a choice**

# Propagation of uncertainties from uranium 238, JEFF-3.3

## 300 samples of nuclear data (with SANDY)

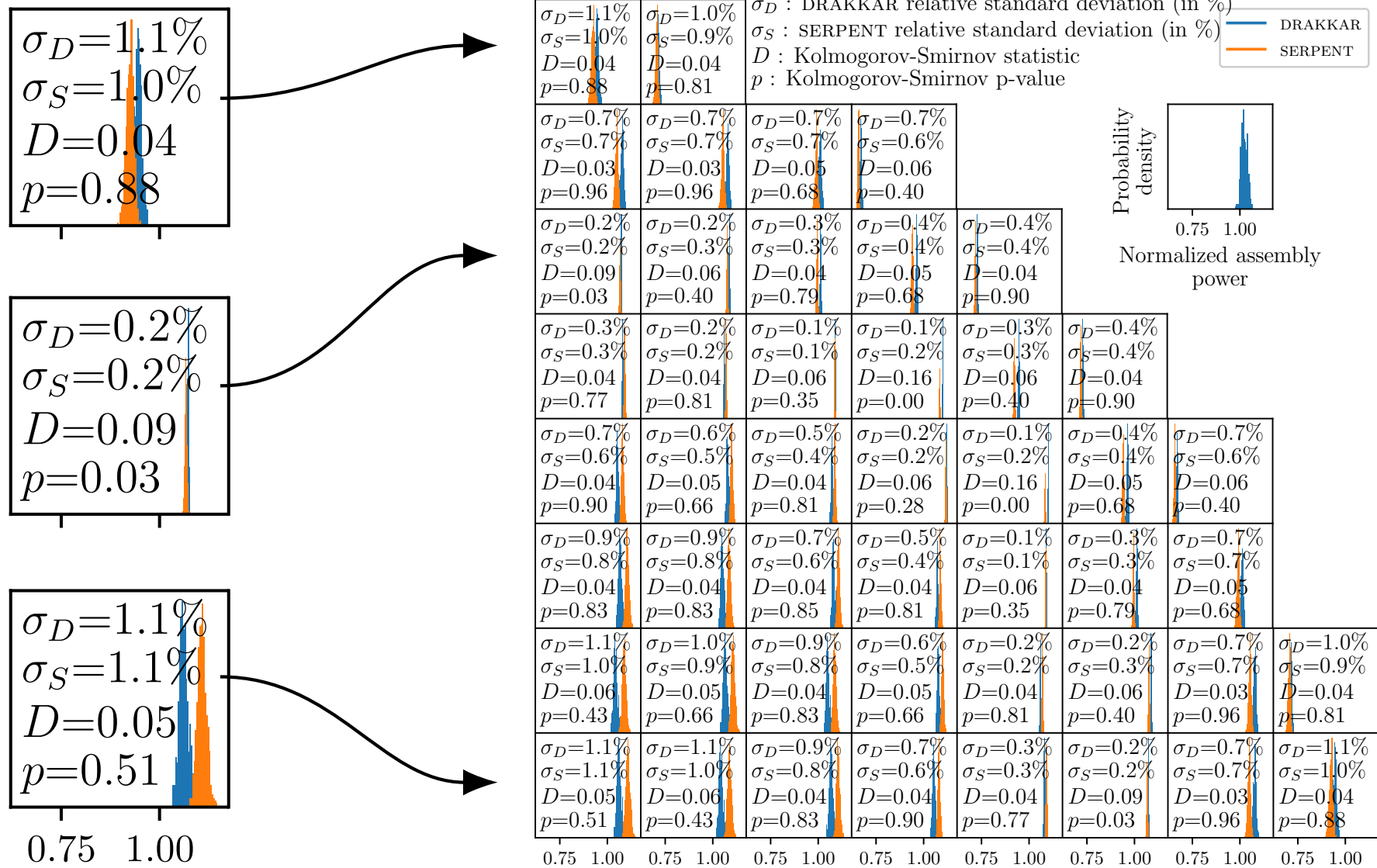


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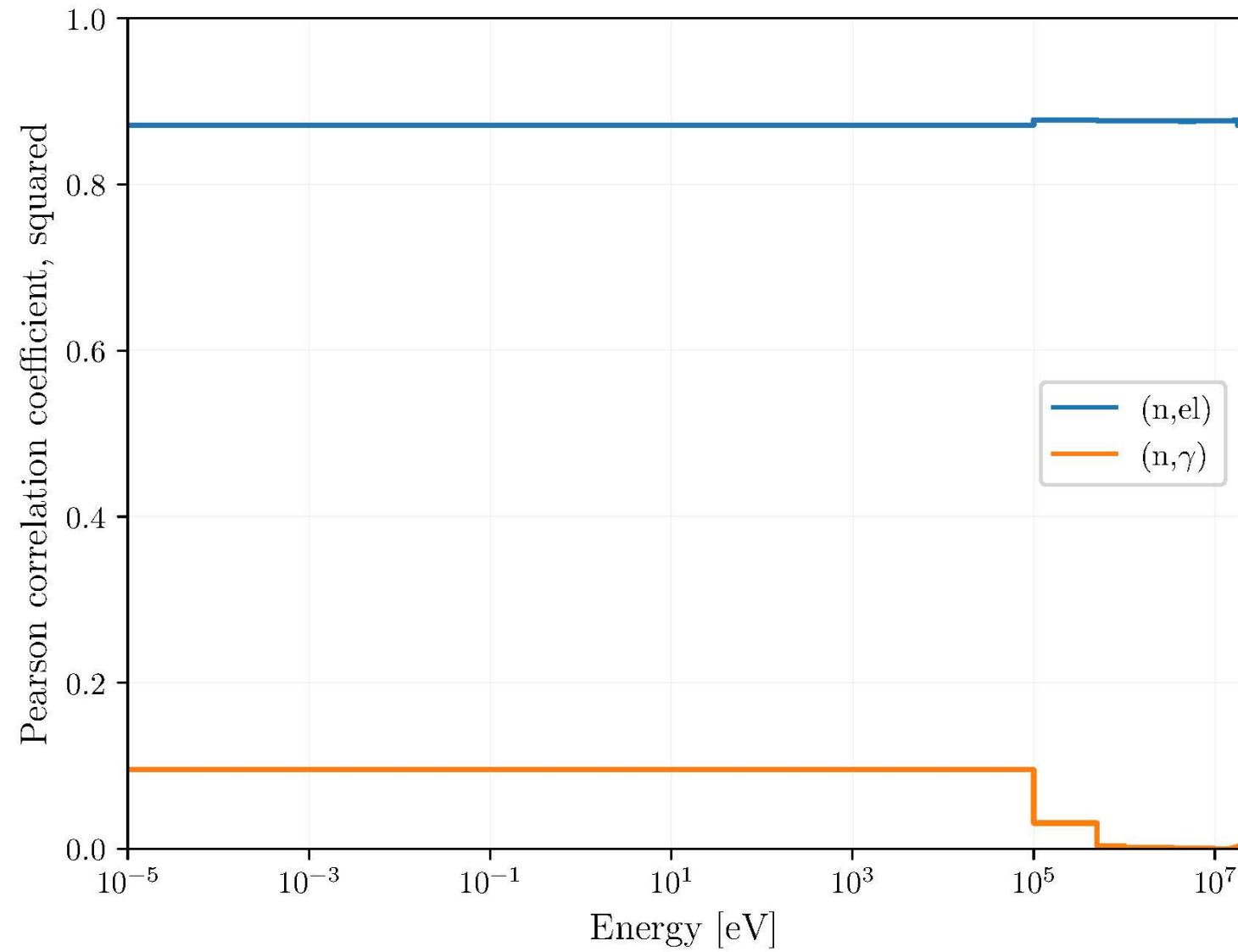


# Propagation of uncertainties from uranium 238, JEFF-3.3

## Deterministic and Monte-Carlo comparison

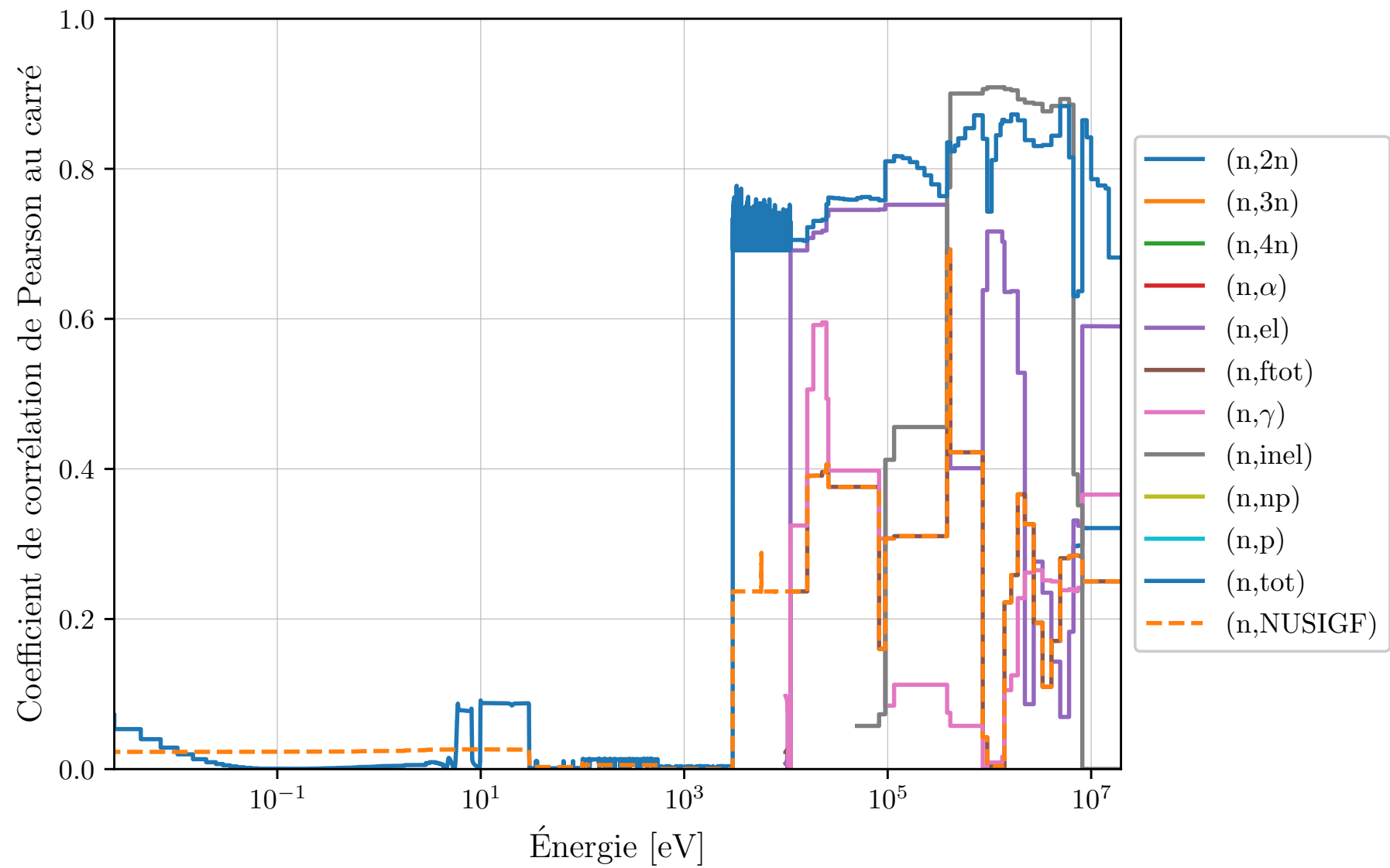


# Hydrogen uncertainty decomposition with respect to reaction and energy

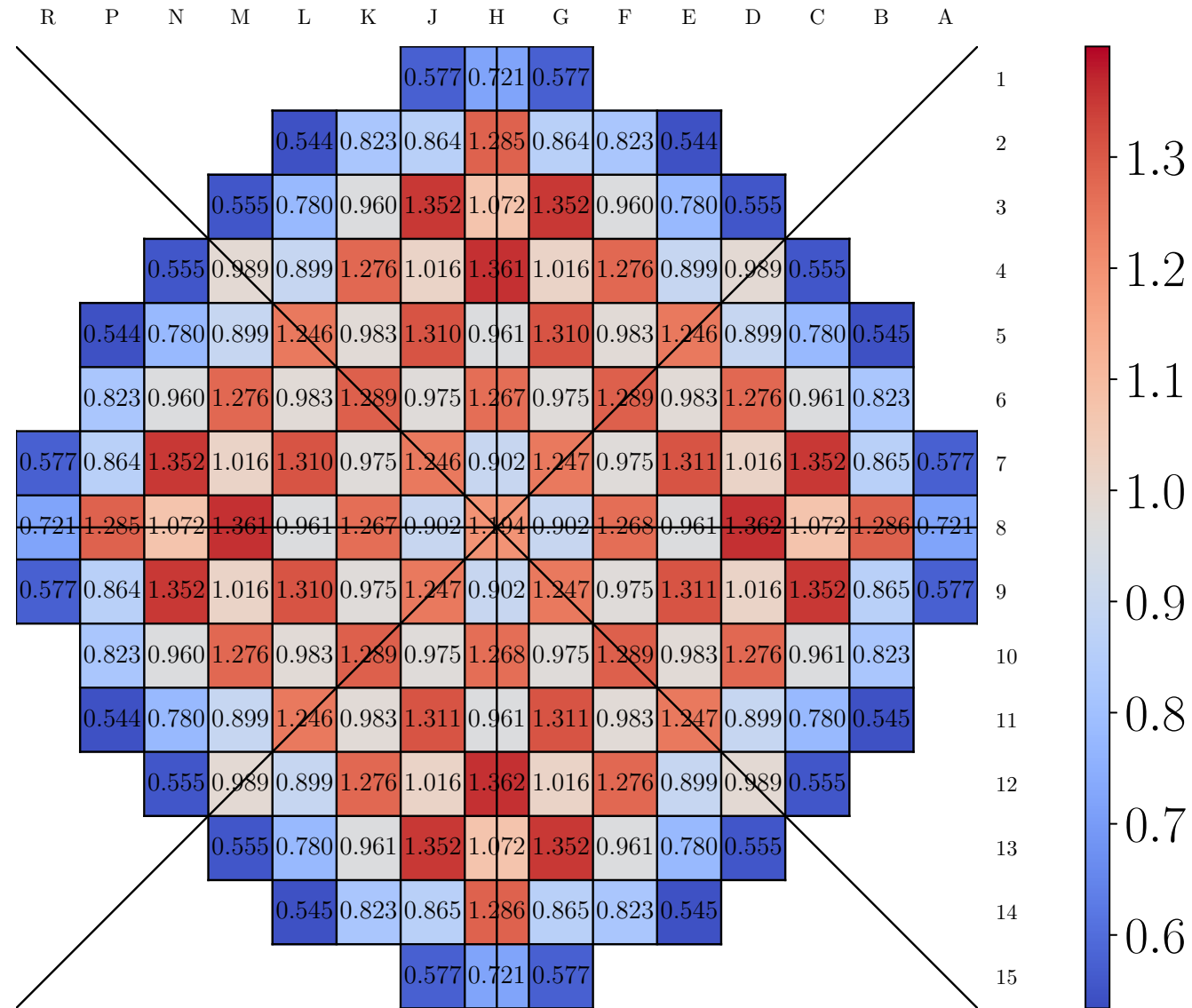


# Uranium 238 uncertainty decomposition with respect to reaction and energy

## From Luka Stancev's internship

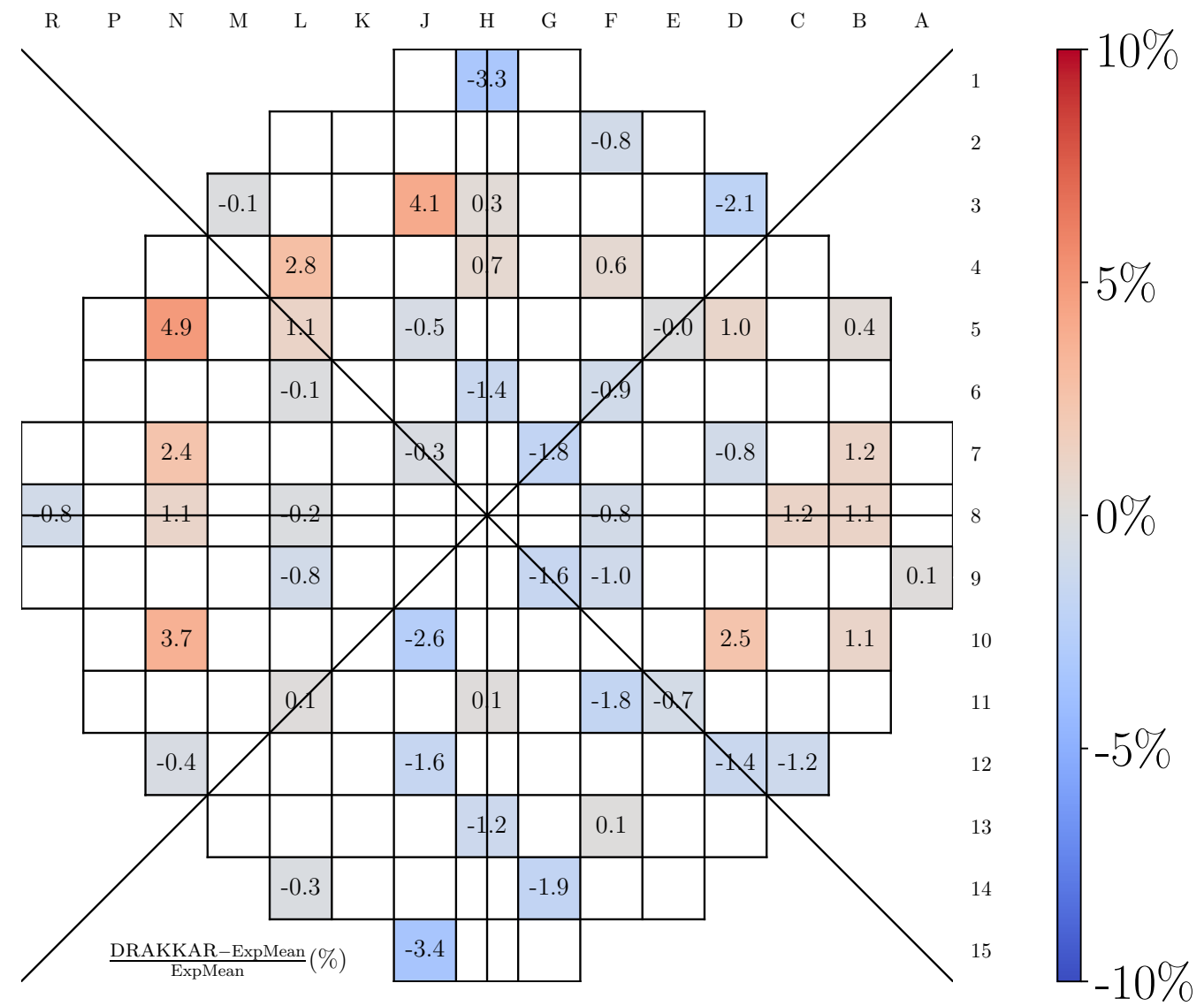


# Drakkar detector responses (JEFF-3.3)

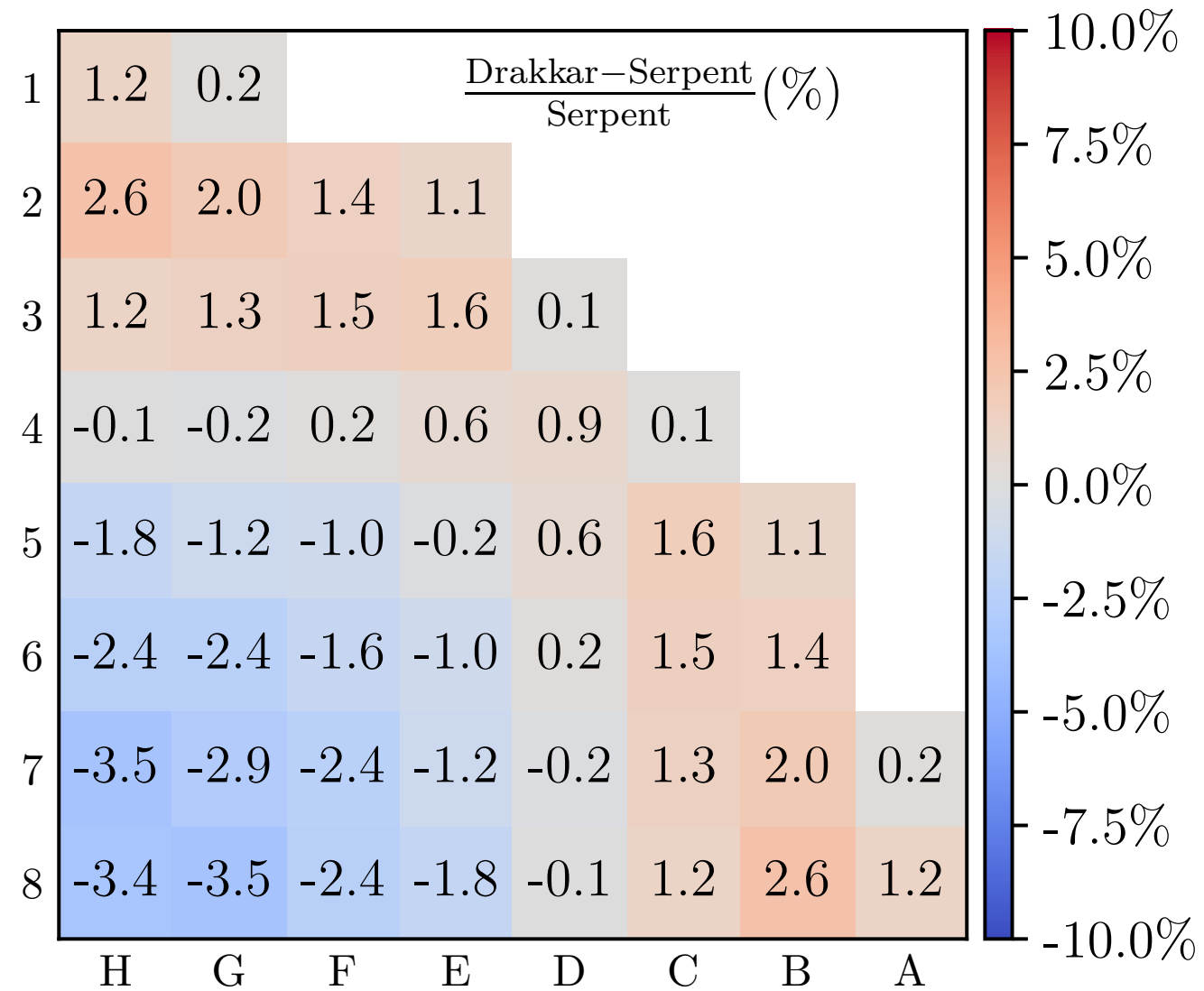




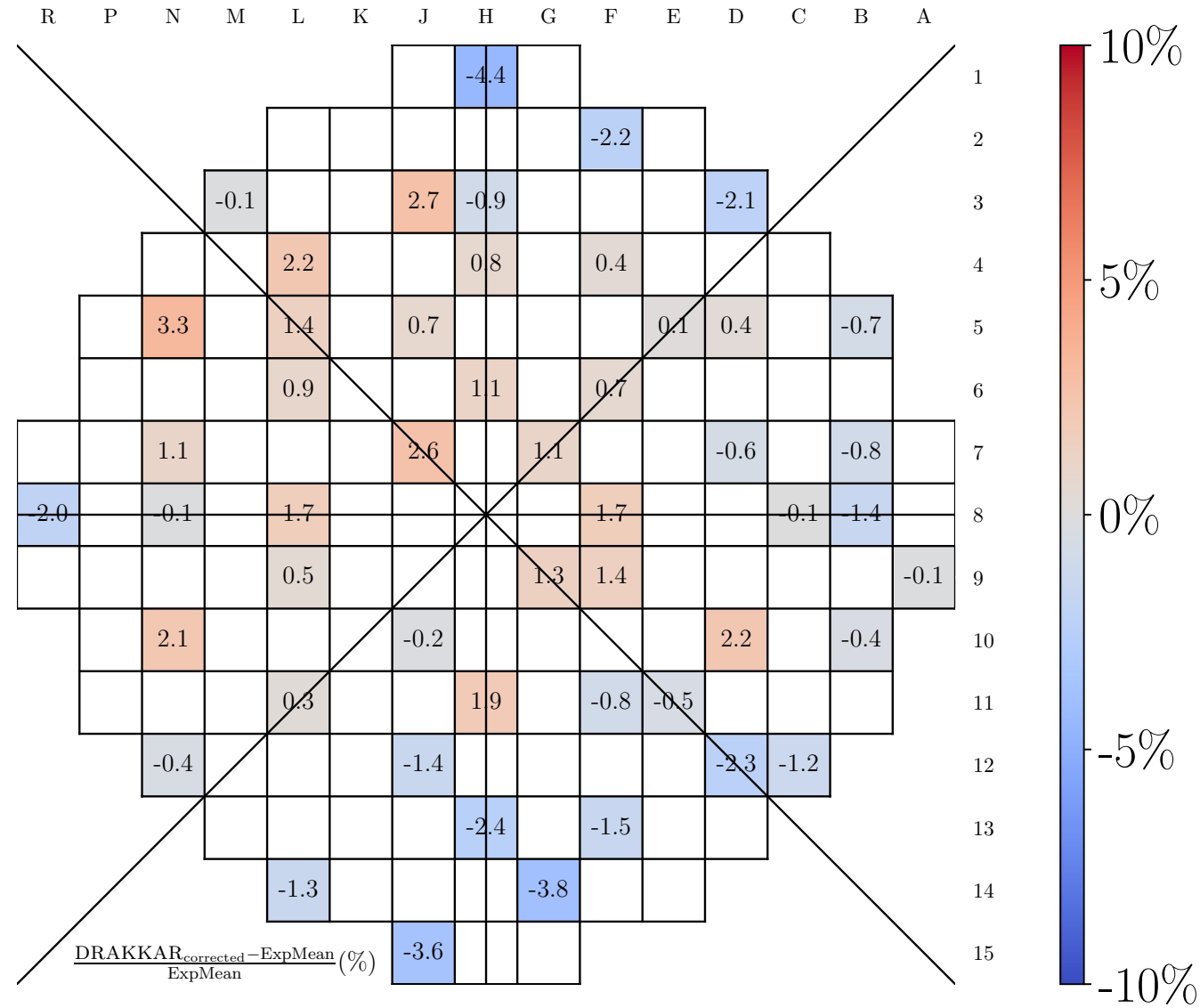
# Discrepancy between Drakkar (JEFF-3.3) and experimental mean



# Power distribution discrepancy between Drakkar and Serpent, on Bugey-2 and Fessenheim-1 and 2

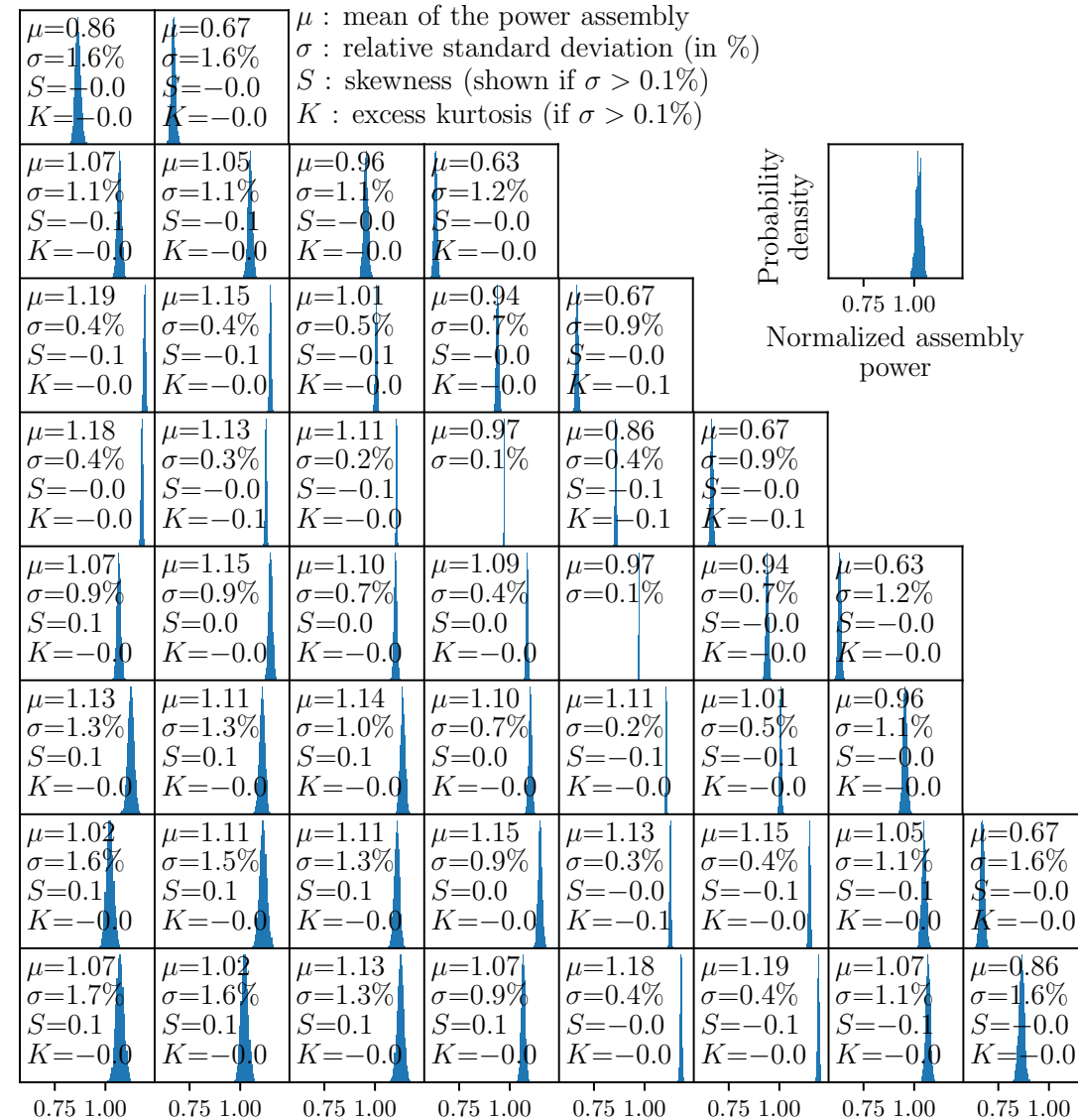
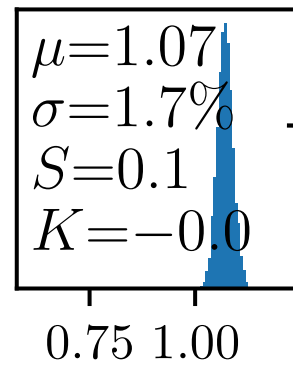
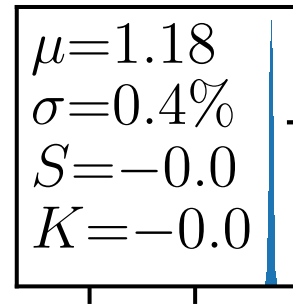
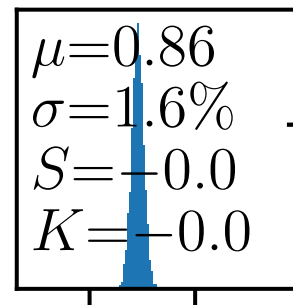


# Discrepancies between Drakkar (corrected from deterministic bias, JEFF-3.3) and experimental mean



# Simultaneous sampling : interactions between isotopes

## Power distribution



## Adjustment with BMC method (Bayesian Monte-Carlo)

- Proximity between the measurement and a sample  $k$  of nuclear data estimated with

$$\chi_k^2 = \sum_{i=1}^{n_{\text{mes}}} \left( \frac{C_{i,k} - E_i}{\sigma_{E_i}} \right)^2 \quad (8)$$

- Lack of uncertainty estimated by experimentalists  
→ expert opinion, for lack of a better choice

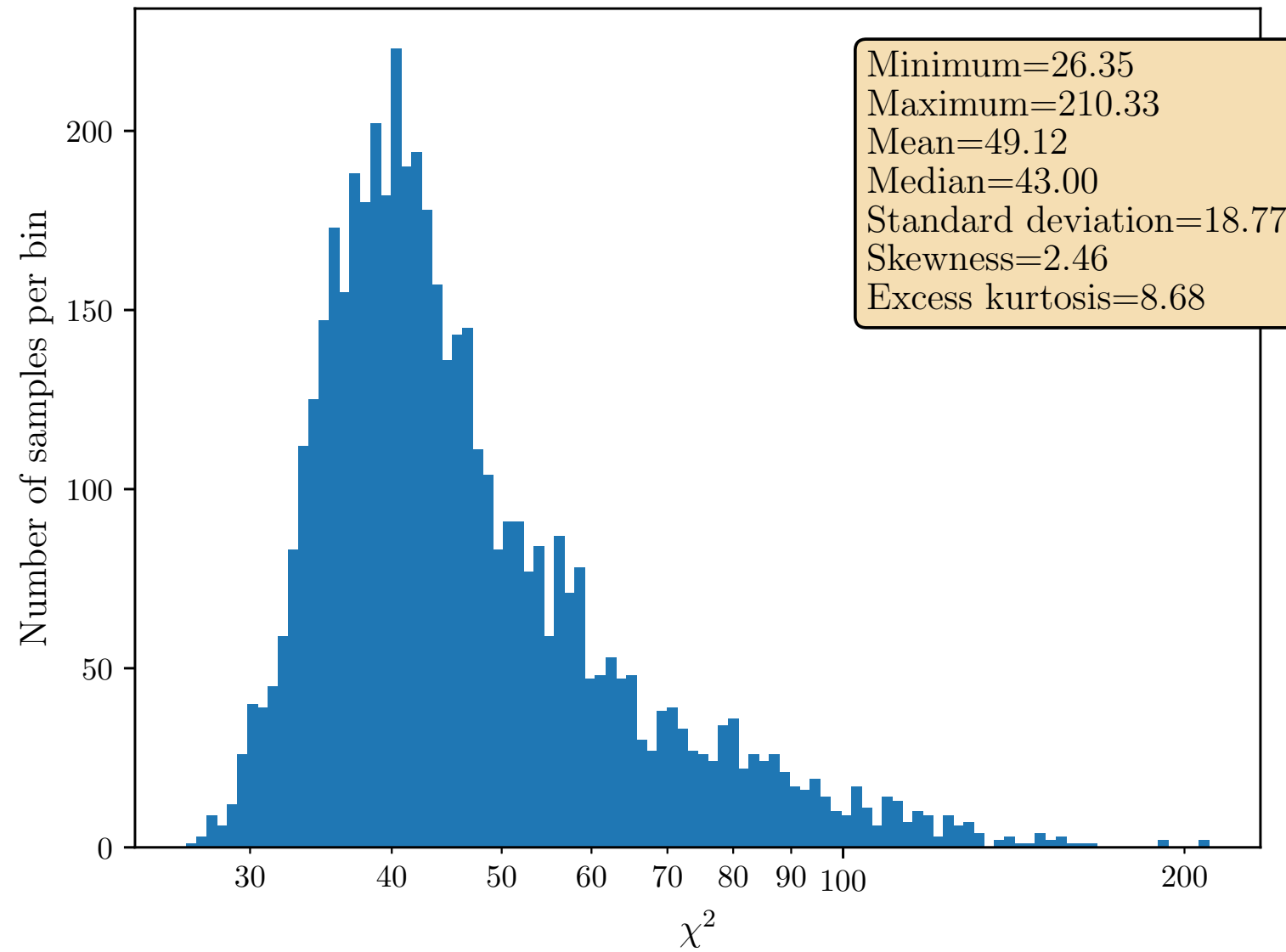
$$\sigma_E = 2\% \quad (9)$$

- Each nuclear data sample  $k$  → weight

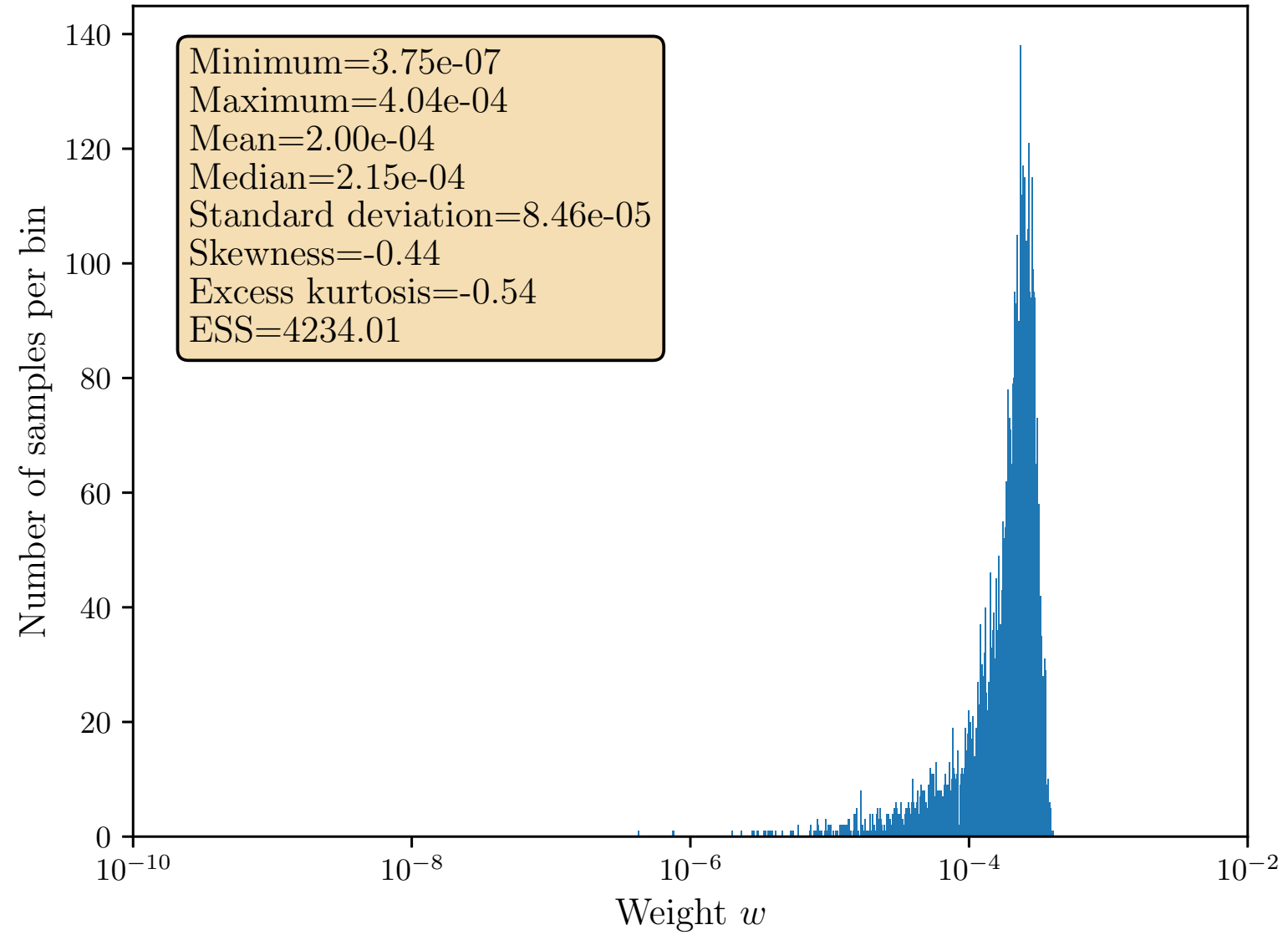
$$w_k = \frac{L(\mathbf{p}_k, \mathbf{x})}{\sum_{\kappa=1}^n L(\mathbf{p}_\kappa, \mathbf{x})} = \frac{\exp(-\chi_k^2/2)}{\sum_{\kappa=1}^n \exp(-\chi_\kappa^2/2)} \quad (10)$$

where  $L(\mathbf{p}_k, \mathbf{x})$  → likelihood of the  $\mathbf{x}$  experimental observations for a  $k$  sample of  $\mathbf{p}$  nuclear data

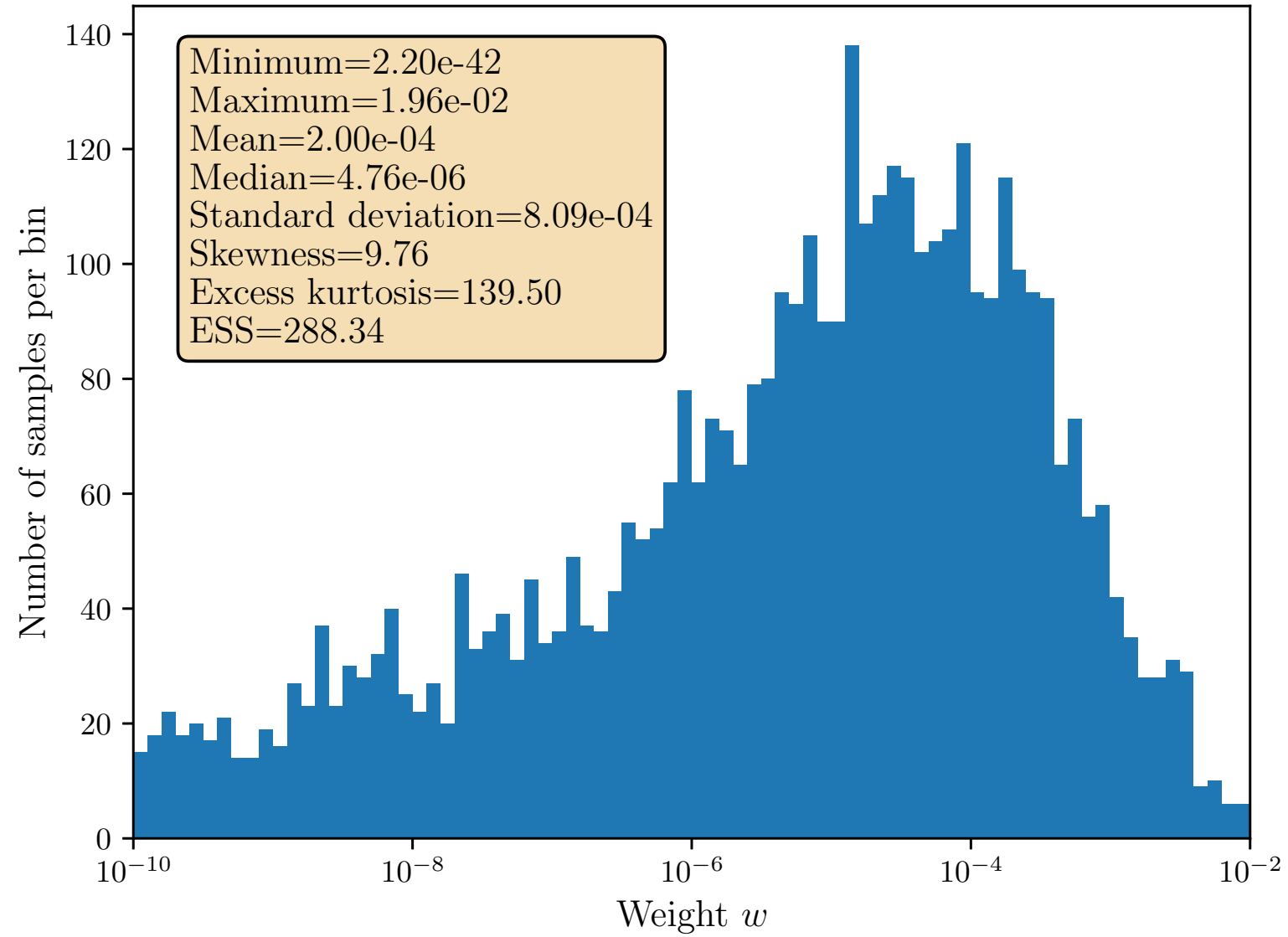
# $\chi^2$ histogram



# $w$ weight histogram obtained with BFMC

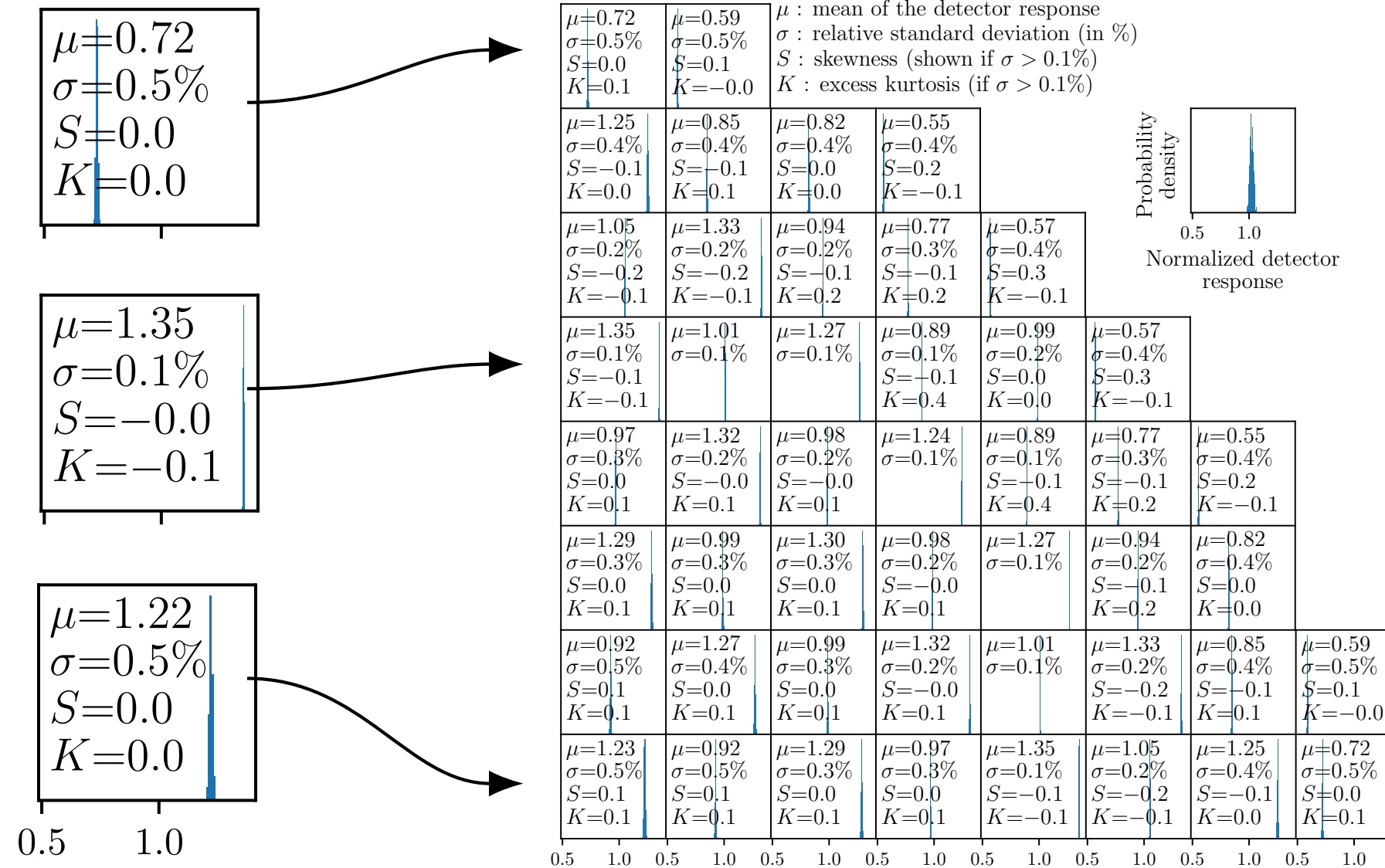


# $w$ weight histogram obtained with BMC

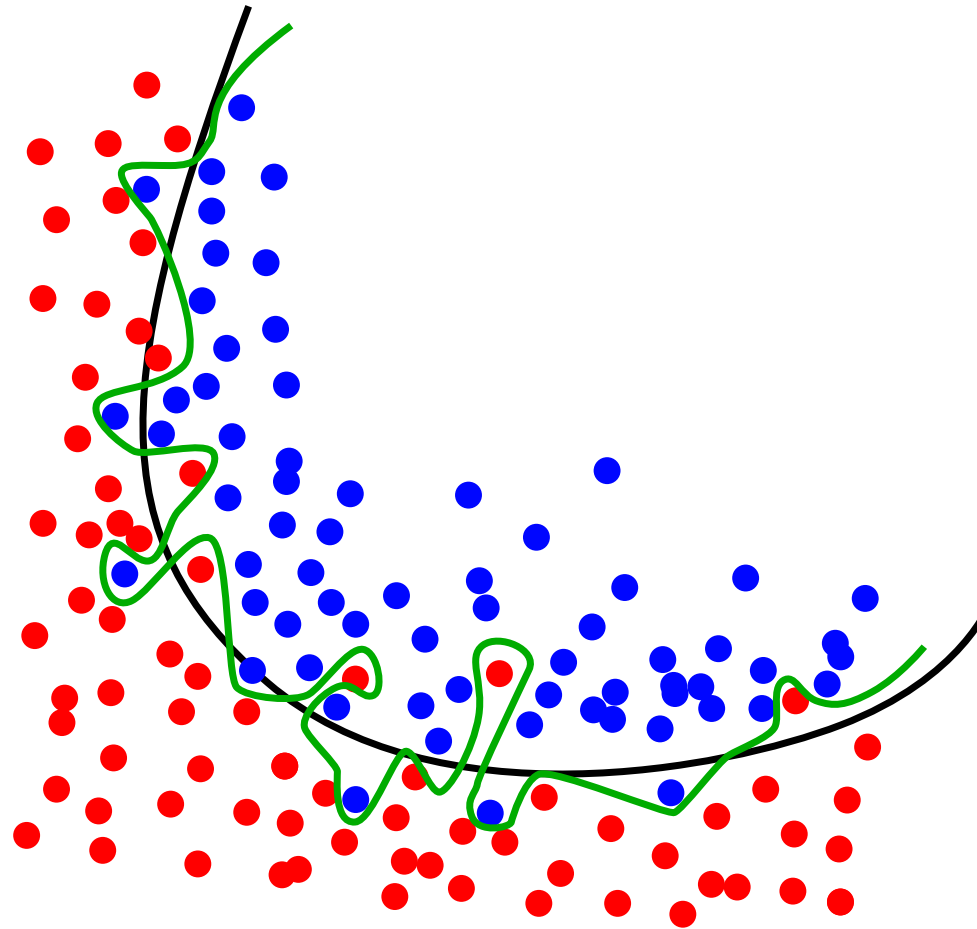




# Posterior (BMC) detector responses

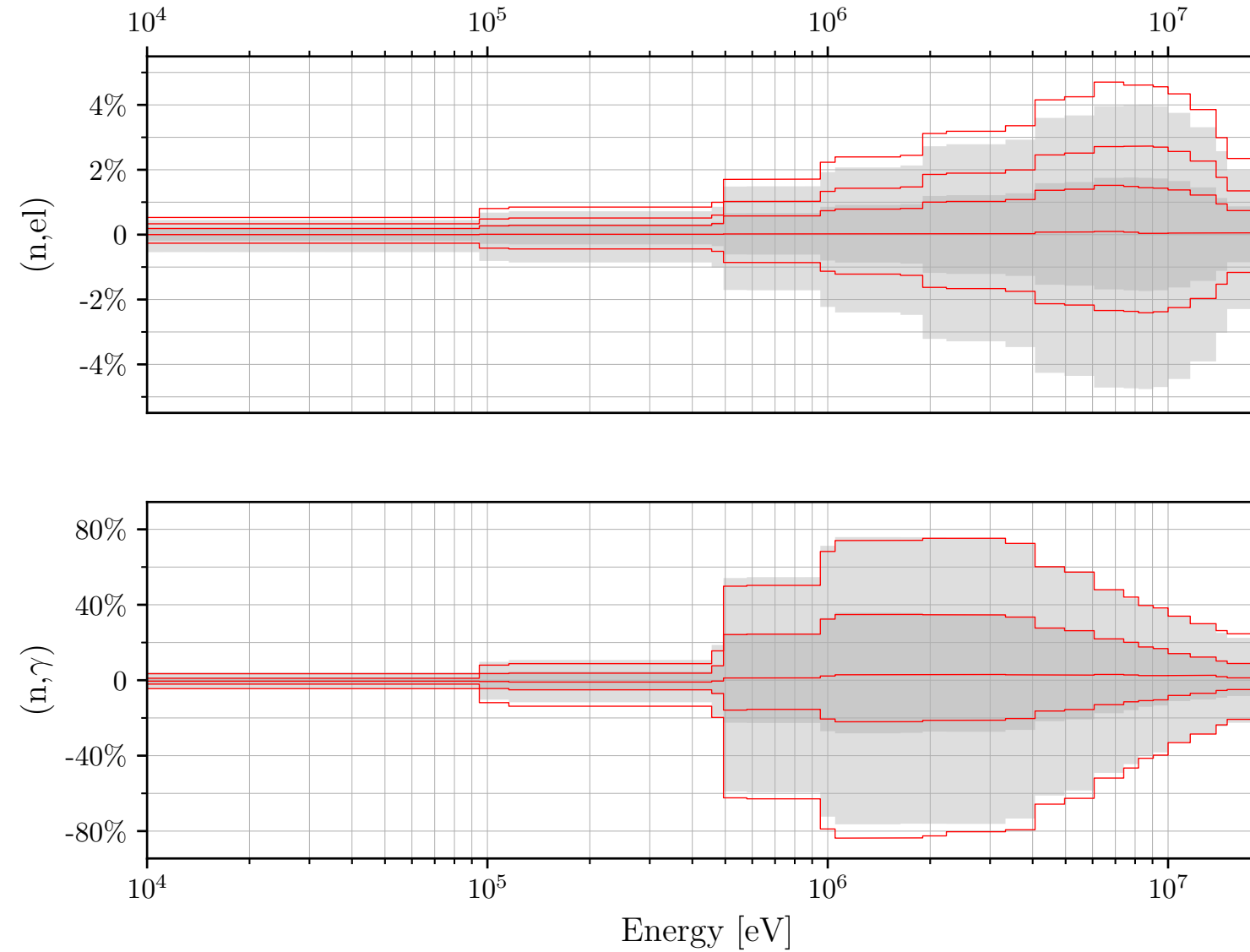


# Overfitting illustration, in green

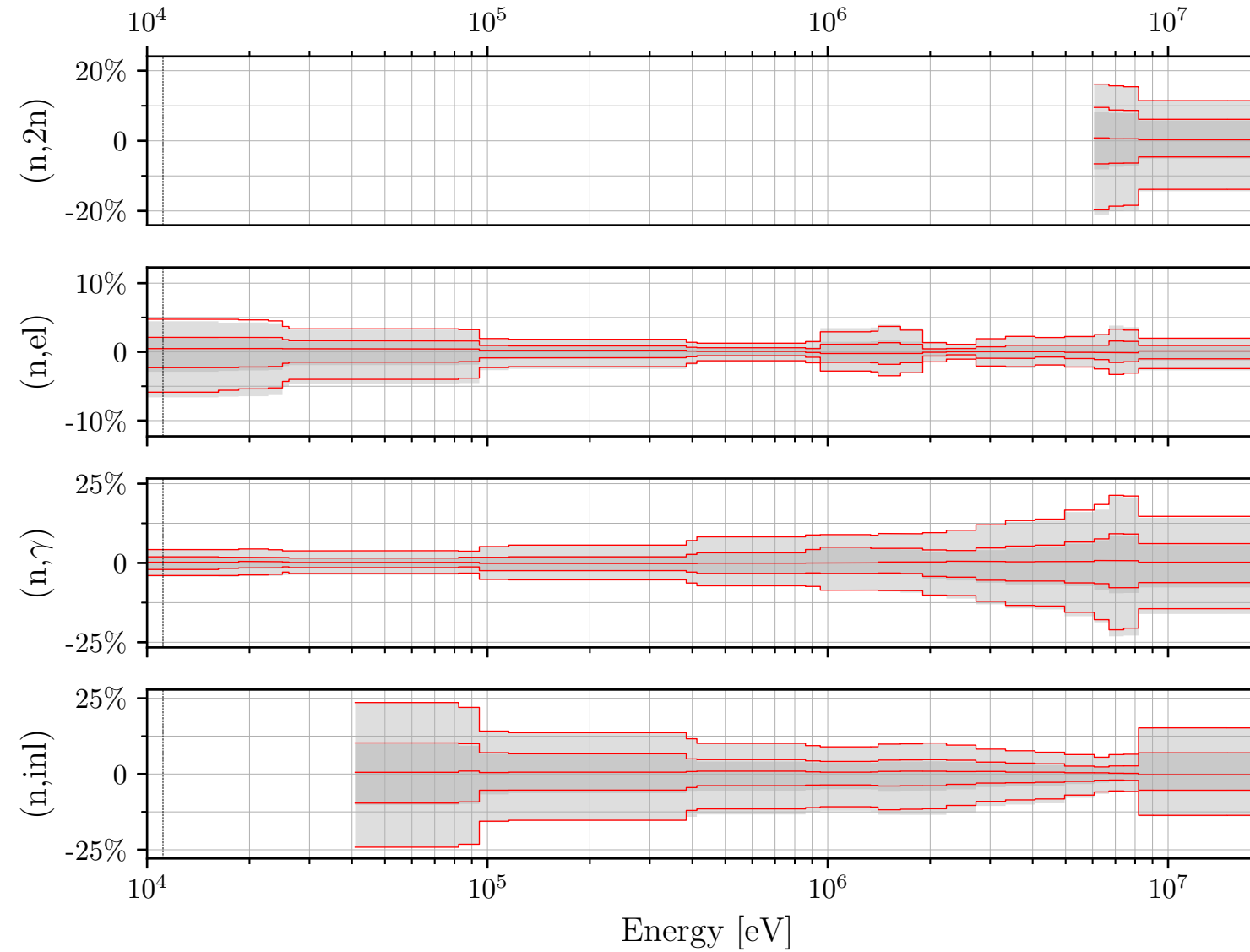


Credits : I. ICKE, Creative Commons BY-SA 4.0 <https://commons.wikimedia.org/wiki/File:Overfitting.svg>

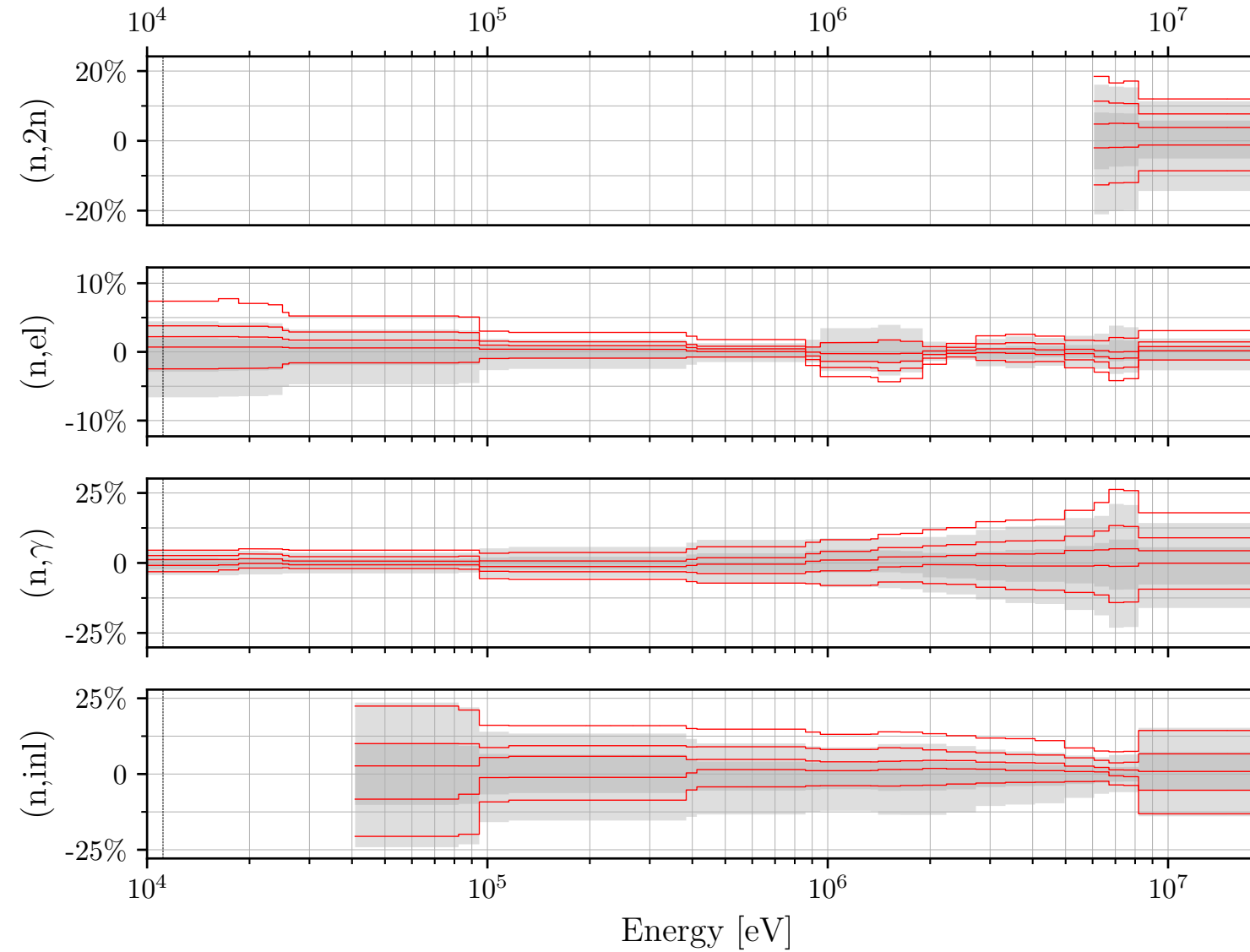
# Modifications (red) to five prior quantiles (grey) of hydrogen cross sections, with BMC



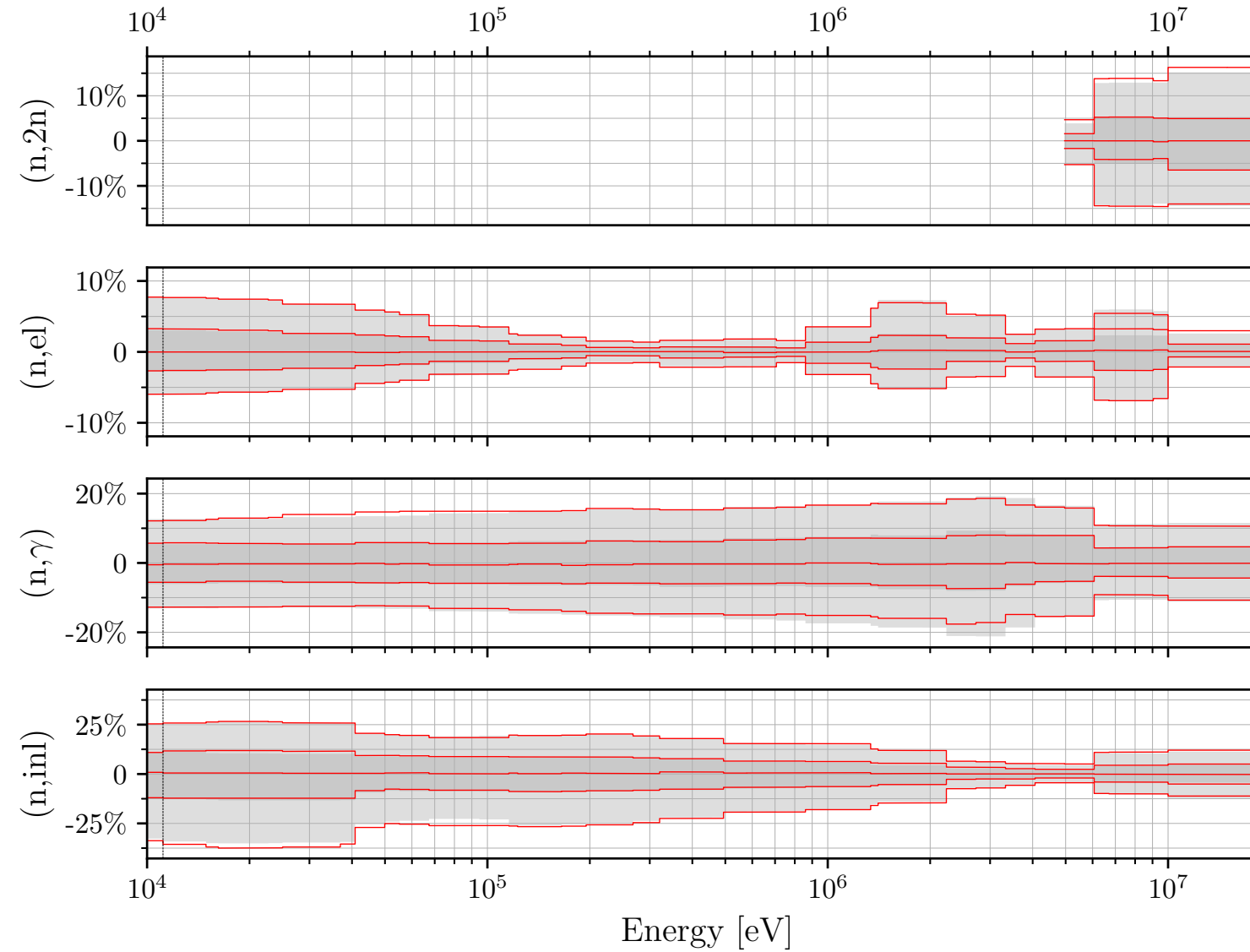
# Modifications (red) to five prior quantiles (grey) of uranium 238 cross sections, with BFMC



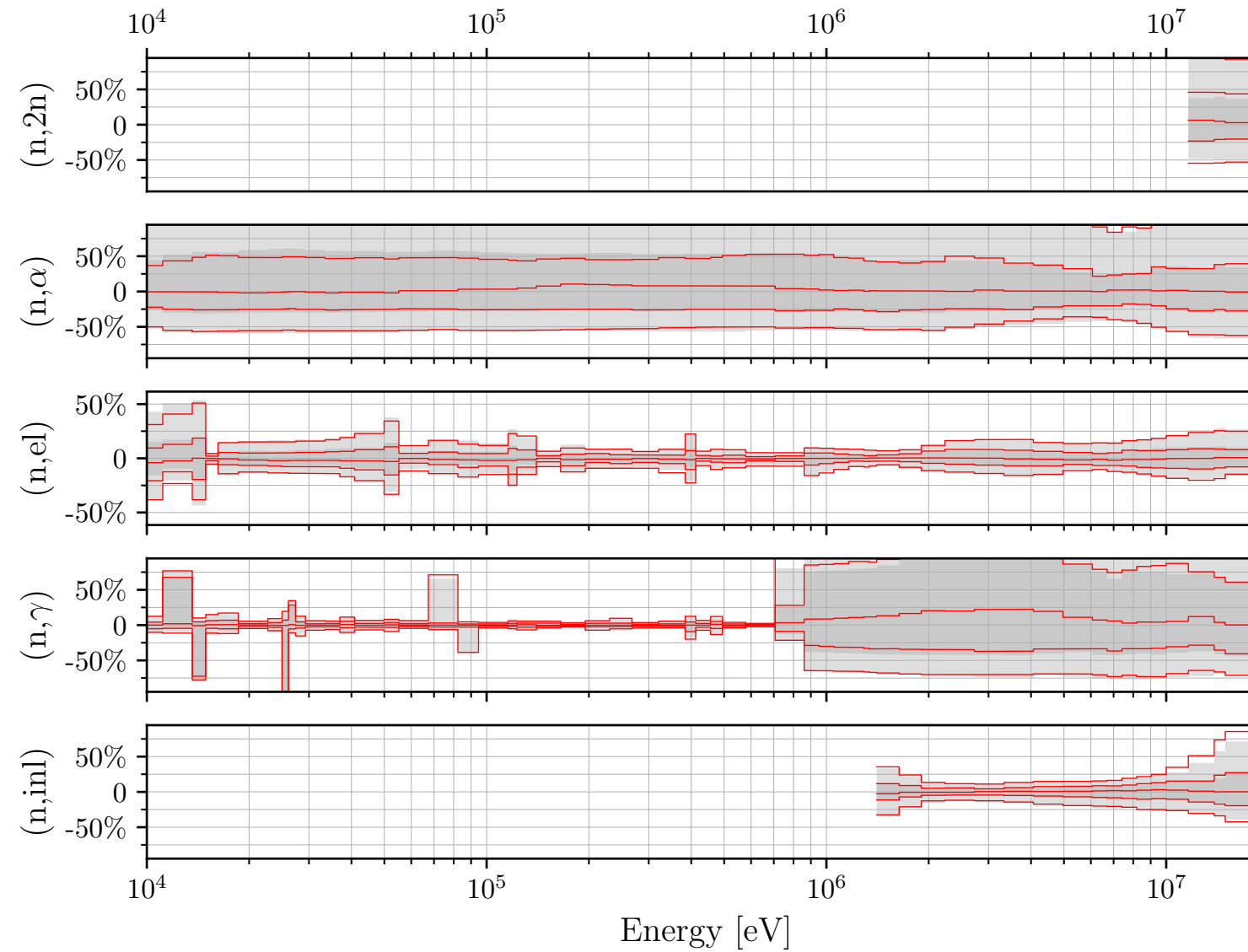
# Modifications (red) to five prior quantiles (grey) of uranium 238 cross sections, with BMC



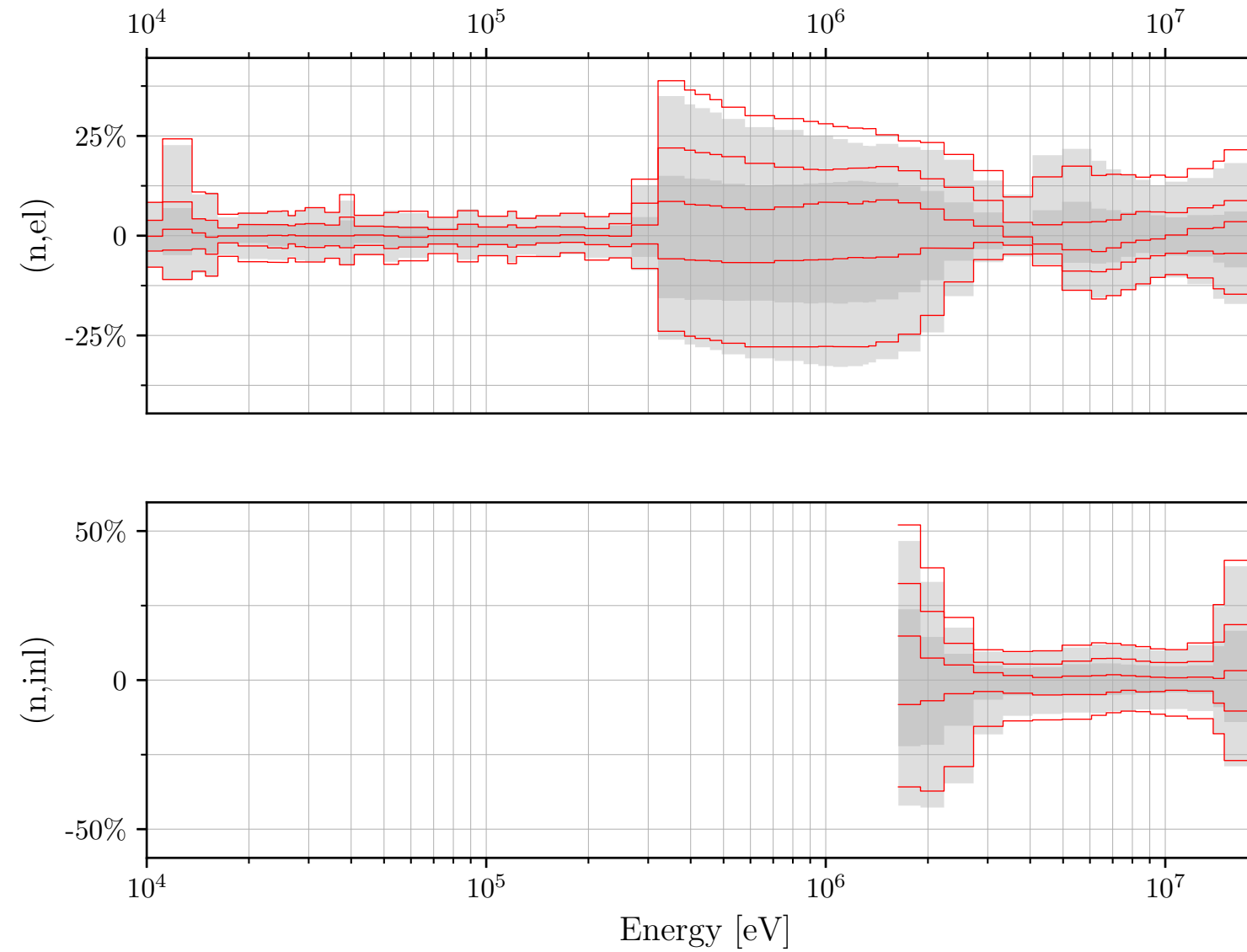
# Modifications (red) to five prior quantiles (grey) of uranium 235 cross sections, with BMC



# Modifications (red) to five prior quantiles (grey) of nickel 58 cross sections, with BMC

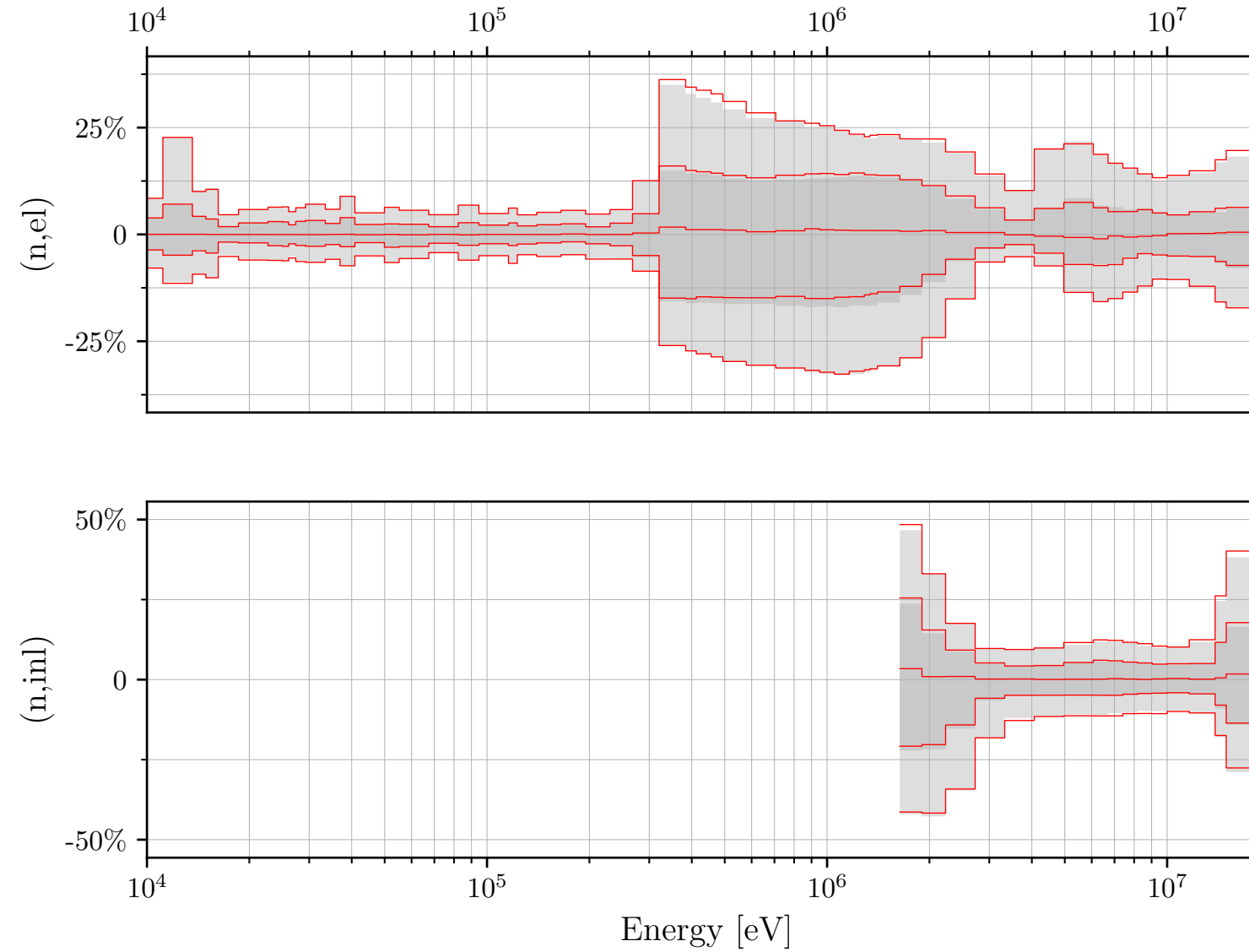


# Modifications (red) to five prior quantiles (grey) of zirconium 90 cross sections, with BMC





# Modifications (red) to five prior quantiles (grey) of zirconium 90 cross sections, with BFMC



# Pseudorandom number generator

- “The generation of random numbers is too important to be left to chance” (COVEYOU)
- Codes such as **SERPENT** (since version 2.1.0) and MCNP5
  - **Linear congruential generator**

$$X_{n+1} = (a \times X_n + c) \mod m \quad (11)$$

- Nuclear data sampling → **SANDY** → NumPy
  - Since NumPy version 1.17, **permuted congruential generator** (PGC64)
  - Before NumPy 1.17, Mersenne Twister
- Random **selection** of nuclear data
  - Here, relies on Python 3.6.9 → **Mersenne Twister**