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

V. SALINO[1,2], D. ROCHMAN[3], E. DUMONTEIL[2], F. MALVAGI[2] and A. HÉBERT[1]

[1] École Polytechnique de Montréal, Institut de Génie Nucléaire, Canada
[2] Institut de Radioprotection et Sûreté Nucléaire (IRSN), PSN-RES/SNC/LN, France
[3] Paul Scherrer Institut (PSI), Laboratory for Reactor Physics and Thermal-Hydraulics (LRT), Switzerland

Joint ICTP-IAEA Workshop on Simulation of Nuclear Reaction Data with the TALYS Code
Trieste, Italy · October 16 – 20, 2023

# Presentation outline

# Sources of errors in neutron transport deterministic simulations

$$
\begin{aligned}
\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{r},E,\boldsymbol{\Omega}) + \Sigma(\boldsymbol{r},E)\phi(\boldsymbol{r},E,\boldsymbol{\Omega}) = \int_0^\infty dE' \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi}\Sigma_{\mathrm{s},\ell}\left(\boldsymbol{r},E\leftarrow E'\right) \sum_{m=-\ell}^{\ell} R_\ell^m(\boldsymbol{\Omega})\phi_\ell^m\left(\boldsymbol{r},E'\right) \\
+\frac{1}{4\pi}\sum_{j=1}^{J^{\mathrm{fiss}}}\chi_j(E)\int_0^\infty dE'\,\overline{\nu}\Sigma_{\mathrm{f},j}\left(\boldsymbol{r},E'\right)\phi\left(\boldsymbol{r},E'\right)
\end{aligned}
$$

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 human 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

Changing the fast diffusion coefficient of the reflector ($D_1$) :

- ➔ “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)

- ➔ “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)

- ➔ Similar to changing/cheating on boundary conditions!

# Uncertainties of deterministic simulations

➔ Knowledge on sources of errors mentioned earlier ➛ unused

➔ Instead, Westinghouse *et al.* (1960's) made the following assumption :

— usual discrepancy between calculations and measurements, and
— universal uncertainty of calculation

are taken as equal ➛ numerous weaknesses ➛ concepts of radically different natures

➔ Fragilities accentuated for adjusted deterministic simulations (residuals) ➛ compensations between errors of different natures, unlikely to be universal

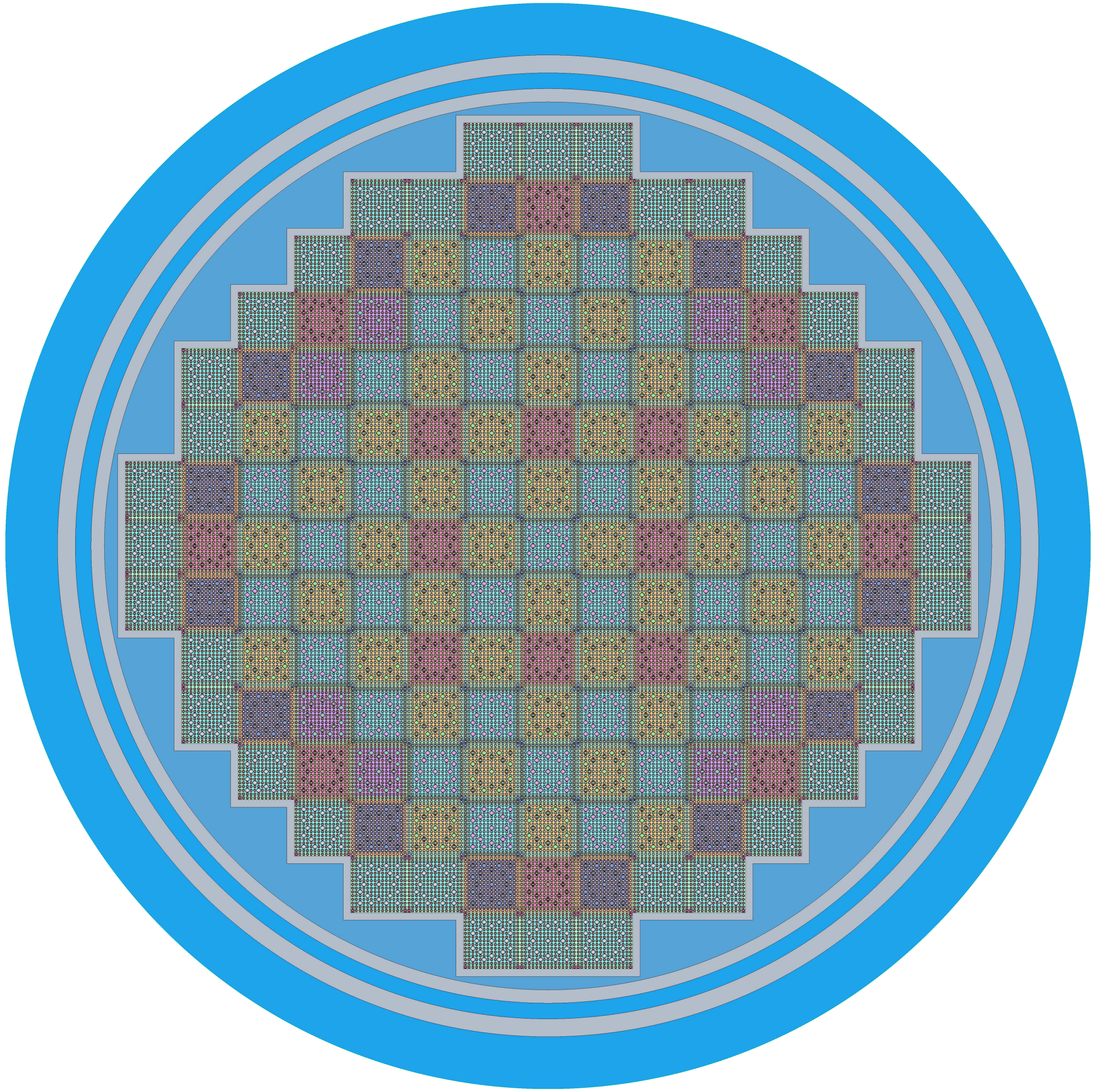
➔ "What adjustments have been made [. . . ] to improve the agreement between calculation and measurement ? How is the uncertainty in this adjustment accounted for in [. . . ] uncertainties ?" (NRC, 1987)

Long-standing and still pending questions, with recently renewed concerns

➔ The French nuclear safety authority "is particularly attentive to feedback from the EPRs [. . . ] in China [. . . ]. This concerns, in particular, [. . . ] anomalies in the power distribution in the core of the Taishan EPRs" (ASN, 2021).

➔ To increase robustness ➛ back to the fundamentals ➛ sources of errors

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



# A deterministic solution, with JEFF-3.3
# Power map in Tihange-1, first start-up

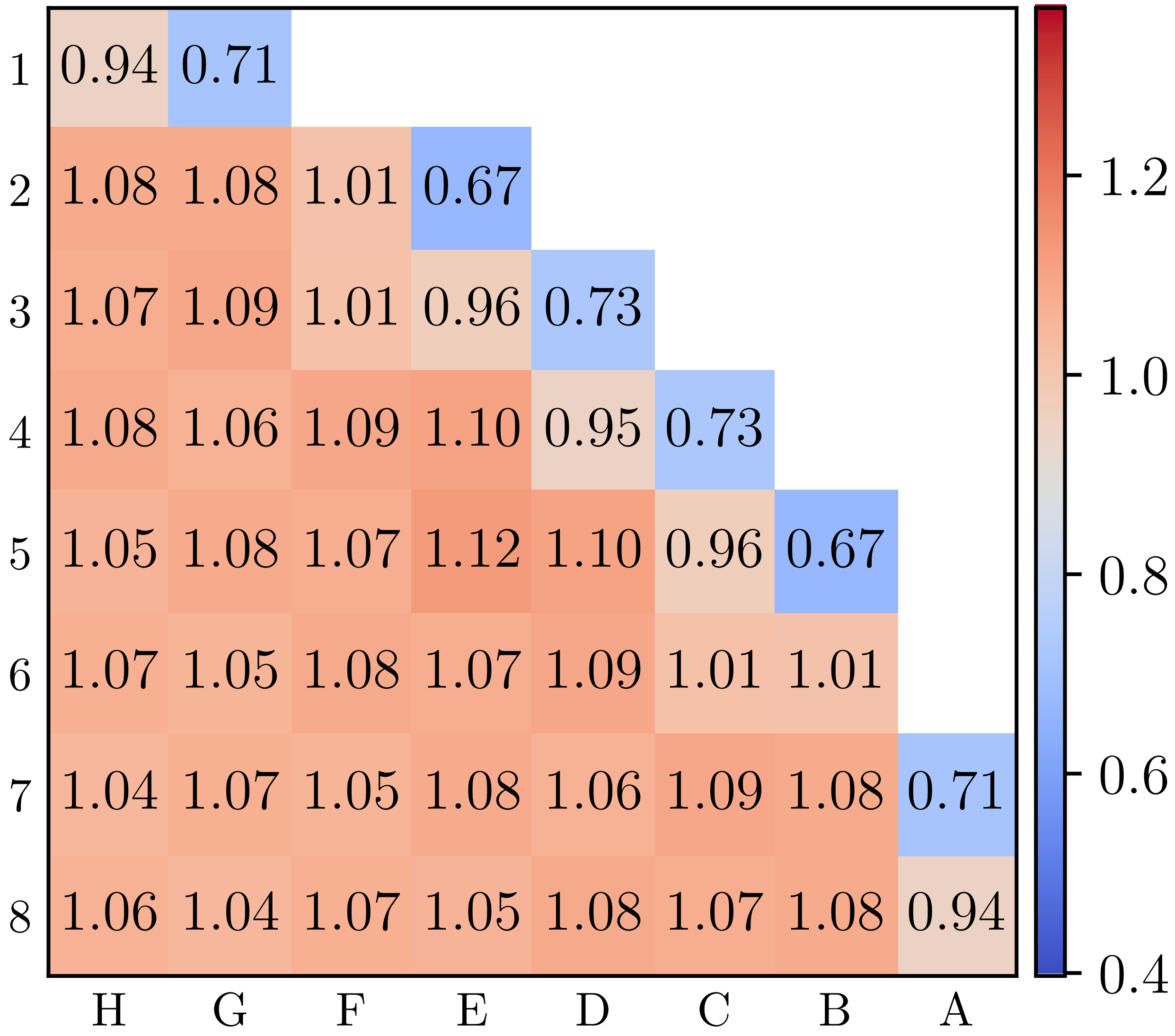
Introduction

Propagation of nuclear data uncertainties

PWR experimental detector responses

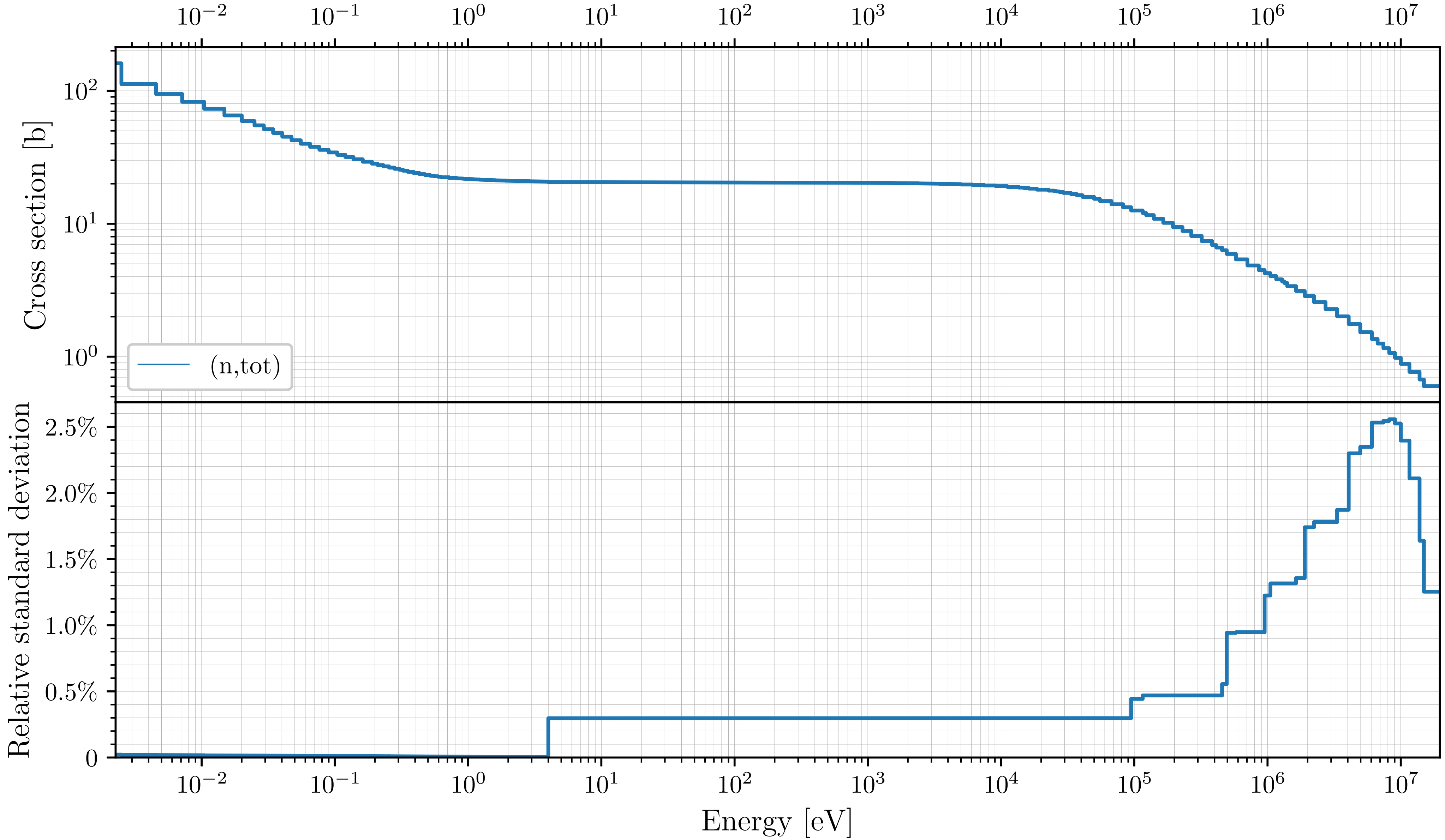
Nuclear data adjustment

Conclusions

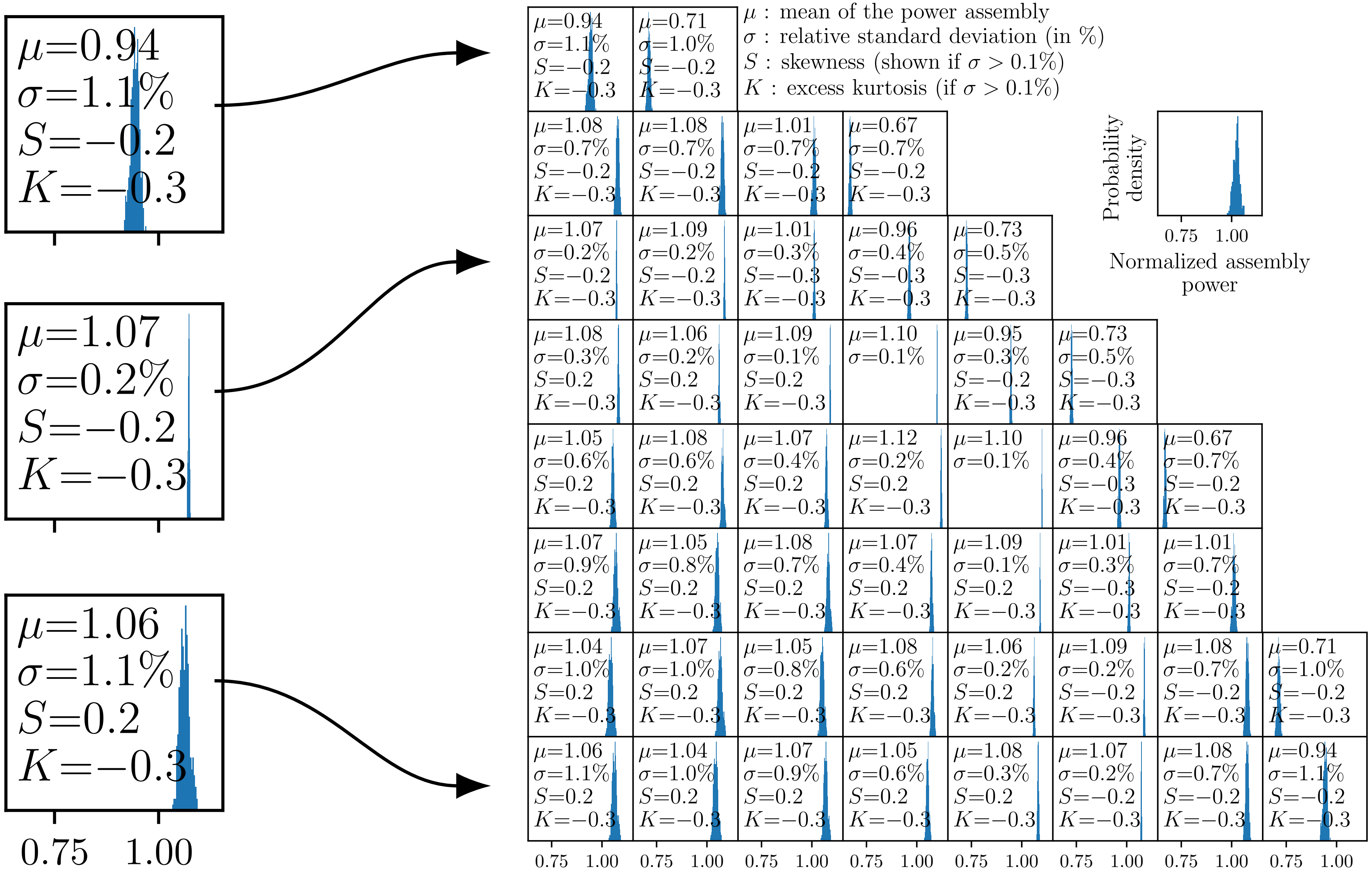


| | H | G | F | E | D | C | B | A |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.94 | 0.71 | | | | | | |
| 2 | 1.08 | 1.08 | 1.01 | 0.67 | | | | |
| 3 | 1.07 | 1.09 | 1.01 | 0.96 | 0.73 | | | |
| 4 | 1.08 | 1.06 | 1.09 | 1.10 | 0.95 | 0.73 | | |
| 5 | 1.05 | 1.08 | 1.07 | 1.12 | 1.10 | 0.96 | 0.67 | |
| 6 | 1.07 | 1.05 | 1.08 | 1.07 | 1.09 | 1.01 | 1.01 | |
| 7 | 1.04 | 1.07 | 1.05 | 1.08 | 1.06 | 1.09 | 1.08 | 0.71 |
| 8 | 1.06 | 1.04 | 1.07 | 1.05 | 1.08 | 1.07 | 1.08 | 0.94 |

# Uncertainties on cross sections of hydrogen bound in $H_2O$
# Source : JEFF-3.3

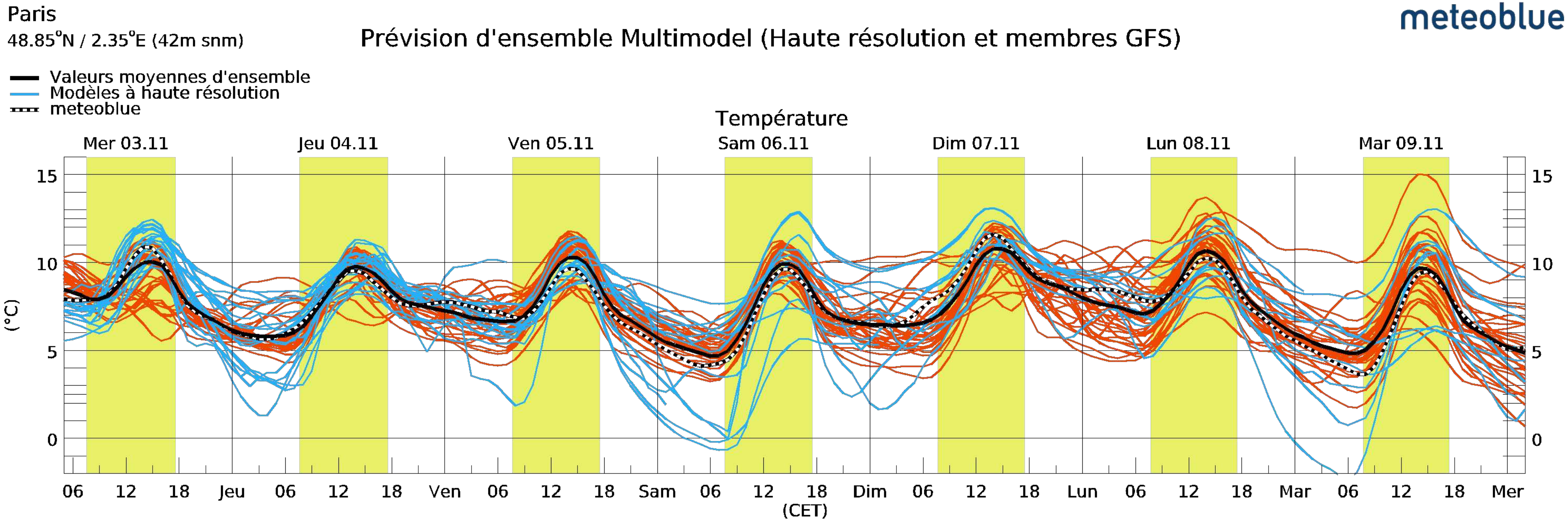


# Propagation of hydrogen uncertainties through deterministic methods
# Total Monte-Carlo : 300 samples of nuclear data (with SANDY)



# Weather prediction analogy and "ensemble forecasting"

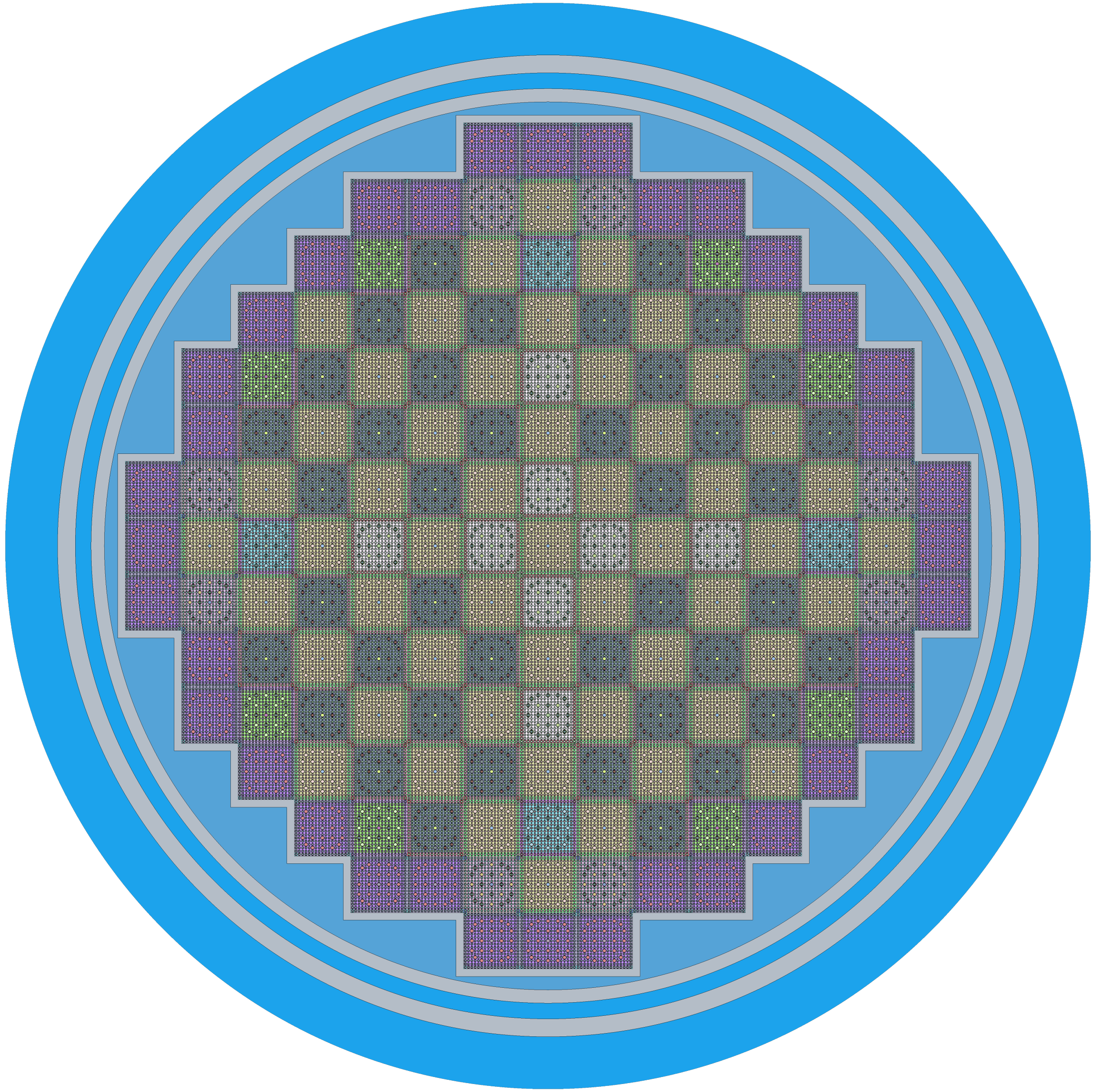
- ➔ Meteorological uncertainties estimated by sampling within plausible uncertainties on initial measured values, then propagated independently in meteorological models
- ➔ Dispersion ➛ confidence score, shown on weather report
- ➔ Common point : propagation of uncertainties using the Monte-Carlo method



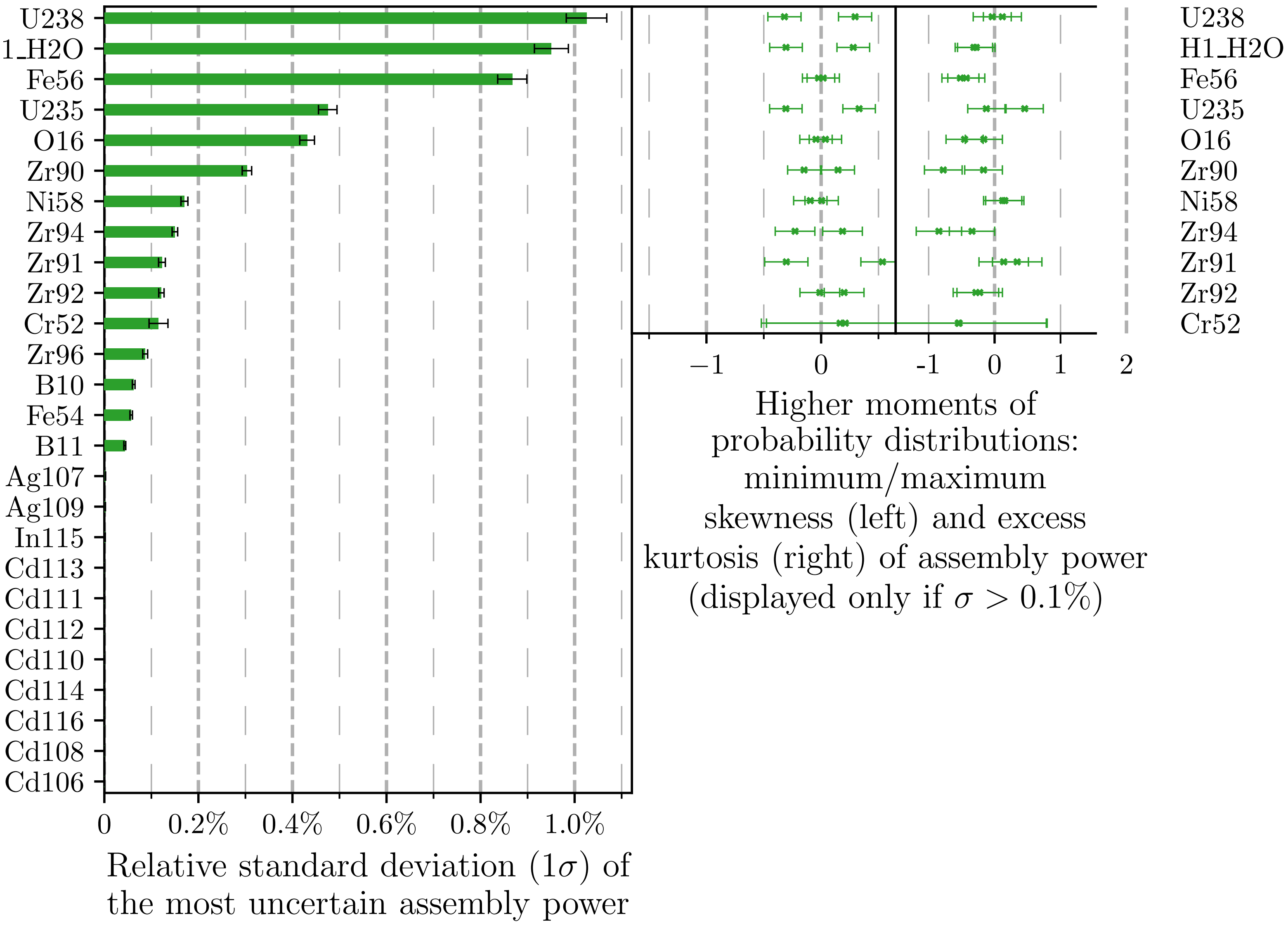
Meteogram of an ensemble model

Credits : `meteoblue.com`, with their kind permission

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

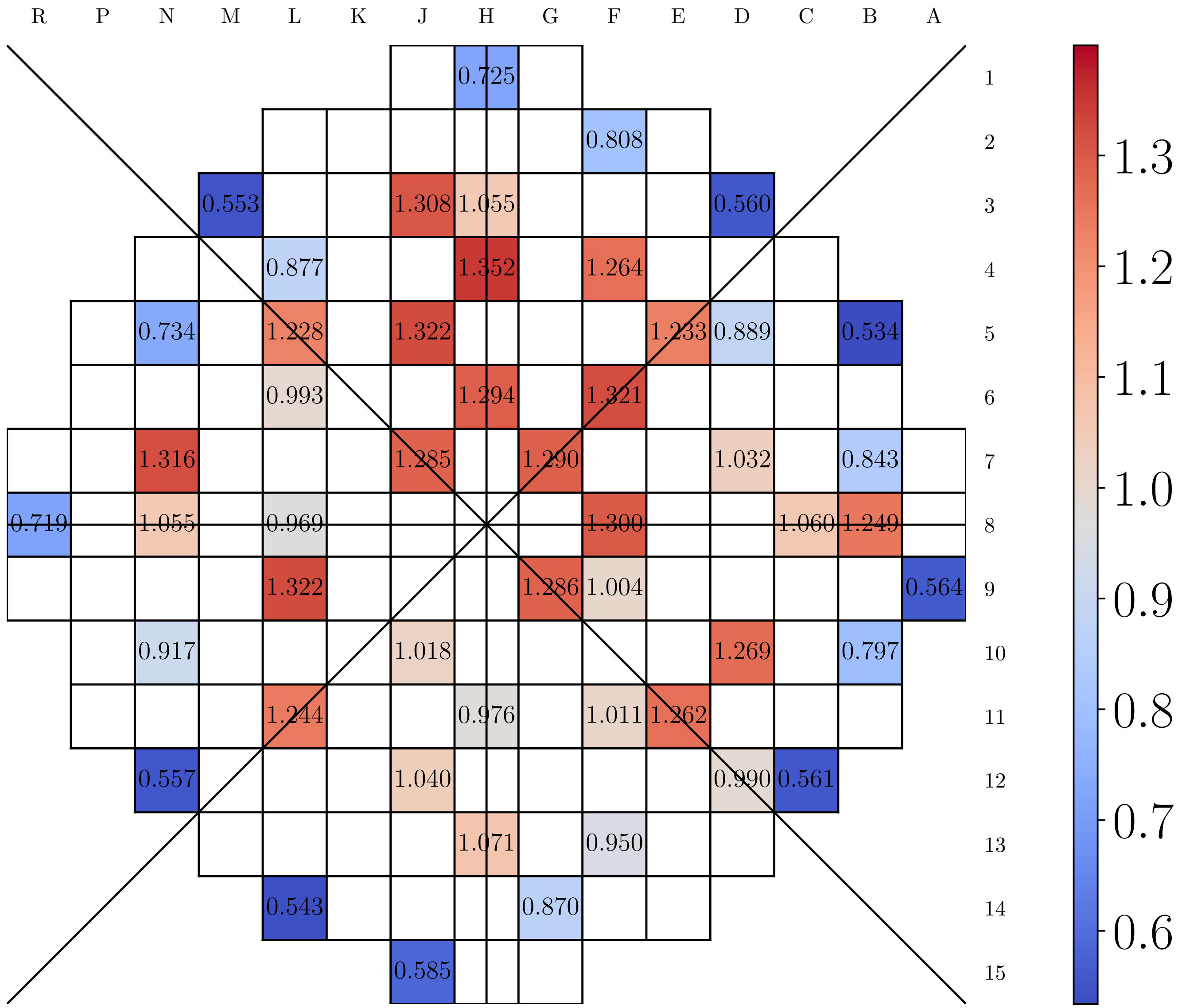


# Ranking of nuclear data uncertainties from TENDL-2019 and JEFF-3.3



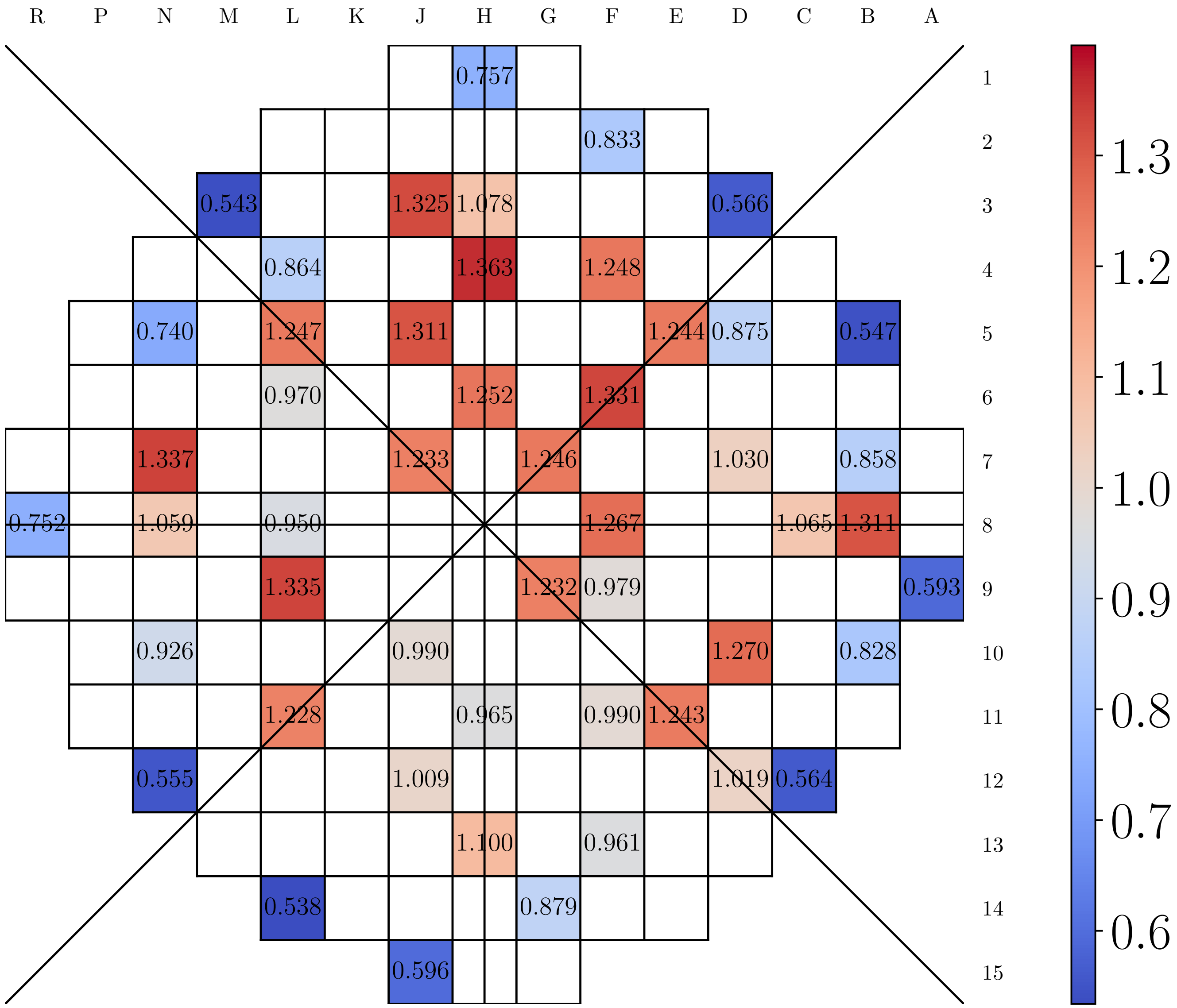
Higher moments of probability distributions: minimum/maximum skewness (left) and excess kurtosis (right) of assembly power (displayed only if $\sigma > 0.1\%$)

# Experimental detector responses during the 1st start-up of Bugey-2



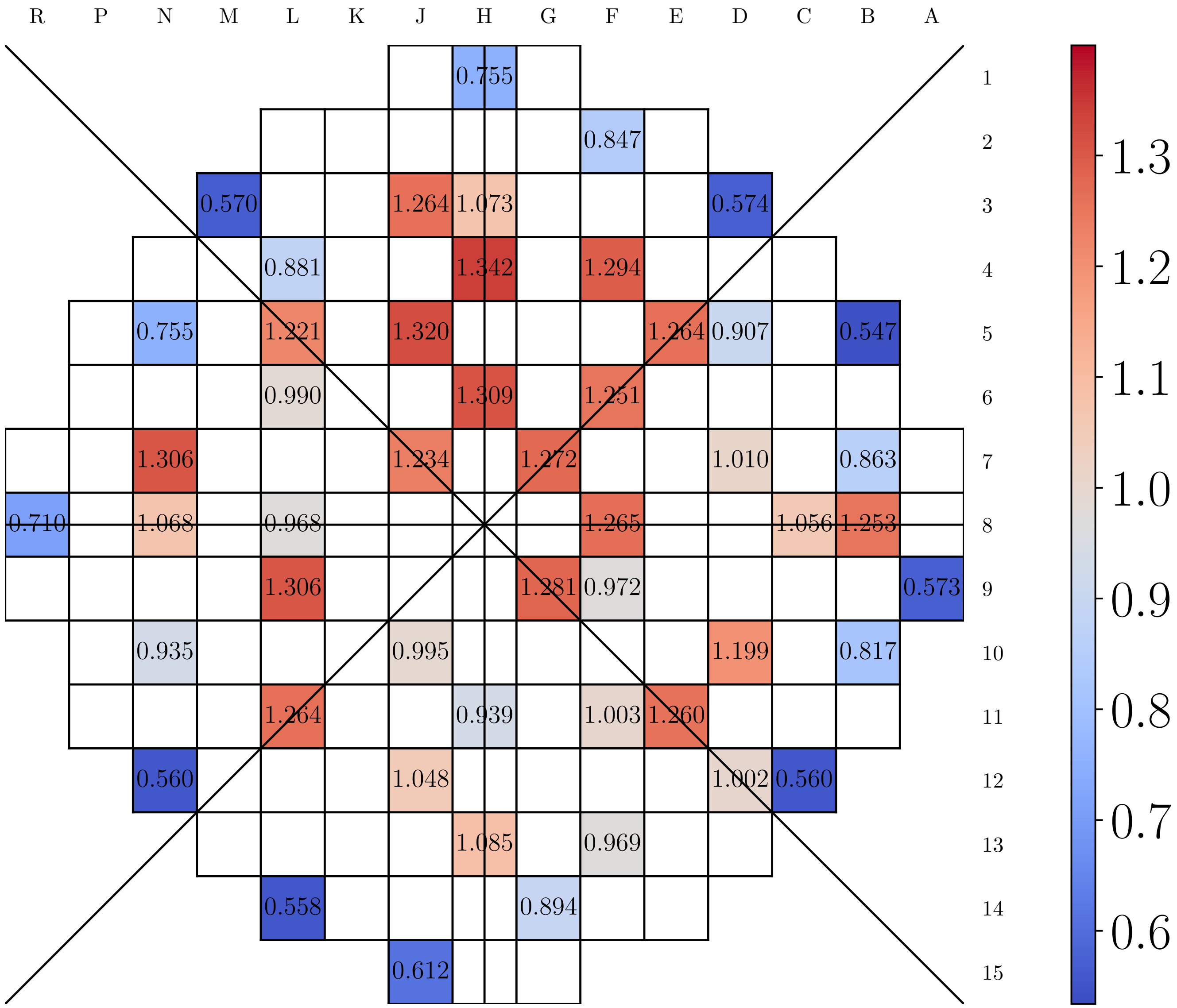
|  | R | P | N | M | L | K | J | H | G | F | E | D | C | B | A |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 |  |  |  |  |  |  |  | 0.725 |  |  |  |  |  |  |  |
| 2 |  |  |  |  |  |  |  |  |  | 0.808 |  |  |  |  |  |
| 3 |  |  |  | 0.553 |  |  | 1.308 | 1.055 |  |  |  | 0.560 |  |  |  |
| 4 |  |  |  |  | 0.877 |  |  | 1.352 |  | 1.264 |  |  |  |  |  |
| 5 |  |  | 0.734 |  | 1.228 |  | 1.322 |  |  |  | 1.233 | 0.889 |  | 0.534 |  |
| 6 |  |  |  |  | 0.993 |  |  | 1.294 |  | 1.321 |  |  |  |  |  |
| 7 |  |  | 1.316 |  |  |  | 1.285 |  | 1.290 |  |  | 1.032 |  | 0.843 |  |
| 8 | 0.719 |  | 1.055 |  | 0.969 |  |  |  |  | 1.300 |  |  | 1.060 | 1.249 |  |
| 9 |  |  |  |  | 1.322 |  |  |  | 1.286 | 1.004 |  |  |  |  | 0.564 |
| 10 |  |  | 0.917 |  |  |  | 1.018 |  |  |  |  | 1.269 |  | 0.797 |  |
| 11 |  |  |  |  | 1.244 |  |  | 0.976 |  | 1.011 | 1.262 |  |  |  |  |
| 12 |  |  | 0.557 |  |  |  | 1.040 |  |  |  |  | 0.990 | 0.561 |  |  |
| 13 |  |  |  |  |  |  |  | 1.071 |  | 0.950 |  |  |  |  |  |
| 14 |  |  |  |  | 0.543 |  |  |  | 0.870 |  |  |  |  |  |  |
| 15 |  |  |  |  |  |  | 0.585 |  |  |  |  |  |  |  |  |

# Experimental detector responses during the $1^{st}$ start-up of Fessenheim-1



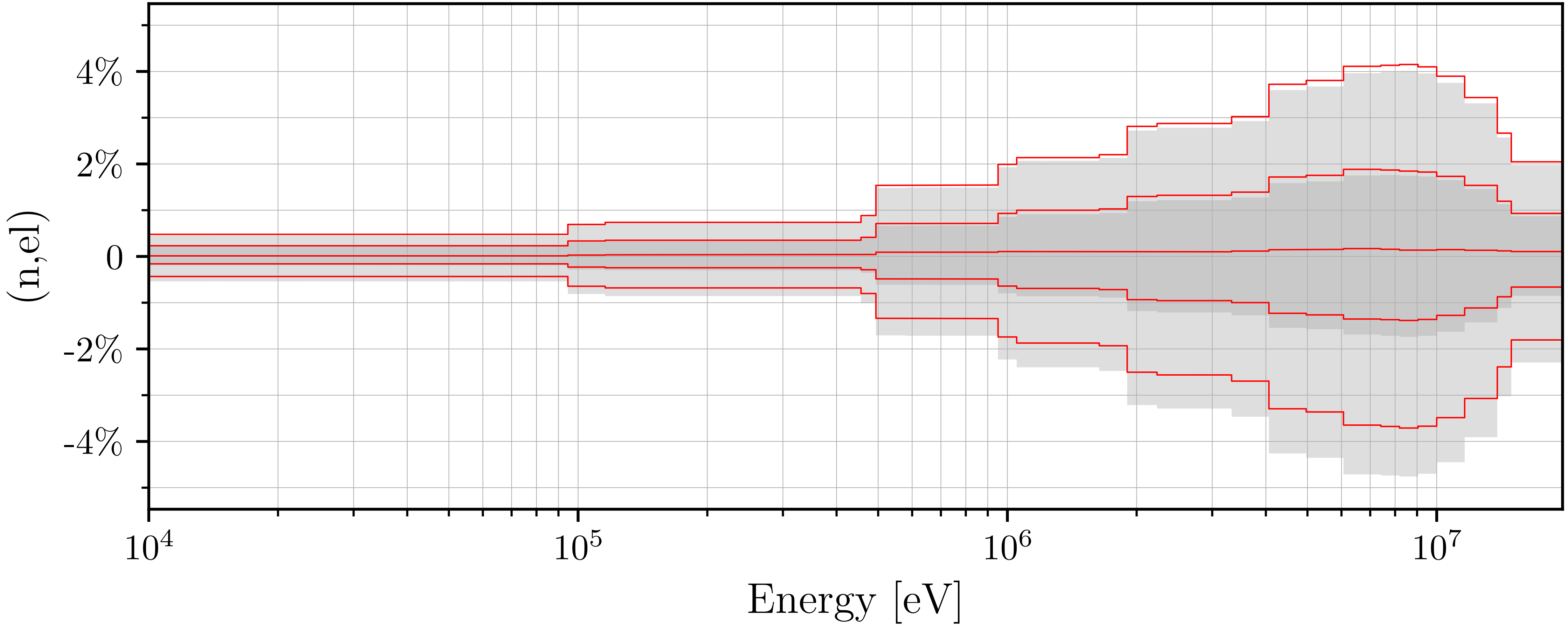
| | R | P | N | M | L | K | J | H | G | F | E | D | C | B | A |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | | | | | | | 0.757 | | | | | | | |
| 2 | | | | | | | | | | 0.833 | | | | | |
| 3 | | | | 0.543 | | | 1.325 | 1.078 | | | | 0.566 | | | |
| 4 | | | | | 0.864 | | | 1.363 | | 1.248 | | | | | |
| 5 | | | 0.740 | | 1.247 | | 1.311 | | | | 1.244 | 0.875 | | 0.547 | |
| 6 | | | | | 0.970 | | | 1.252 | | 1.331 | | | | | |
| 7 | | | 1.337 | | | | 1.233 | | 1.246 | | | 1.030 | | 0.858 | |
| 8 | 0.752 | | 1.059 | | 0.950 | | | | | 1.267 | | | 1.065 | 1.311 | |
| 9 | | | | | 1.335 | | | | 1.232 | 0.979 | | | | | 0.593 |
| 10 | | | 0.926 | | | | 0.990 | | | | | 1.270 | | 0.828 | |
| 11 | | | | | 1.228 | | | 0.965 | | 0.990 | 1.243 | | | | |
| 12 | | | 0.555 | | | | 1.009 | | | | | 1.019 | 0.564 | | |
| 13 | | | | | | | | 1.100 | | 0.961 | | | | | |
| 14 | | | | | 0.538 | | | | 0.879 | | | | | | |
| 15 | | | | | | | 0.596 | | | | | | | | |

# Experimental detector responses during the 1$^{st}$ start-up of Fessenheim-2



| | R | P | N | M | L | K | J | H | G | F | E | D | C | B | A |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | | | | | | | 0.755 | | | | | | | |
| 2 | | | | | | | | | | 0.847 | | | | | |
| 3 | | | | 0.570 | | | 1.264 | 1.073 | | | | 0.574 | | | |
| 4 | | | | | 0.881 | | | 1.342 | | 1.294 | | | | | |
| 5 | | | 0.755 | | 1.221 | | 1.320 | | | | 1.264 | 0.907 | | 0.547 | |
| 6 | | | | | 0.990 | | | 1.309 | | 1.251 | | | | | |
| 7 | | | 1.306 | | | | 1.234 | | 1.272 | | | 1.010 | | 0.863 | |
| 8 | 0.710 | | 1.068 | | 0.968 | | | | | 1.265 | | | 1.056 | 1.253 | |
| 9 | | | | | 1.306 | | | | 1.281 | 0.972 | | | | | 0.573 |
| 10 | | | 0.935 | | | | 0.995 | | | | | 1.199 | | 0.817 | |
| 11 | | | | | 1.264 | | | 0.939 | | 1.003 | 1.260 | | | | |
| 12 | | | 0.560 | | | | 1.048 | | | | | 1.002 | 0.560 | | |
| 13 | | | | | | | | 1.085 | | 0.969 | | | | | |
| 14 | | | | | 0.558 | | | | 0.894 | | | | | | |
| 15 | | | | | | | 0.612 | | | | | | | | |

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



# Discussion

- ➔ $D_1$ 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

# Conclusions and perspectives

- ➔ First theme : Total Monte-Carlo has been applied to reactor physics
- ➔ It would advantageously replace the traditional uncertainty evaluation, nowadays computed as difference between calculations and measurements
- ➔ 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 questionnable ➛ 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
- ➔ Perspective : depletion ➛ reactivity loss, PIE, decay heat, reactor pressure vessel aging...
  - ■ Requires extending from 26 to ∼ 300 isotopes
  - ■ Freedom on number of samples, typically between 10 to 10000 (for adjustment)
  - ■ Produce sampled Draglib (multigroup) libraries for Dragon, integrating T6 in PyNjoy2016 (an open source wrapper of NJOY2016)

# Reference
# Manifesto for open source software and open data

- ➔ Reference : `https://irsn.hal.science/irsn-04095487/`
- ➔ Totality of developed software and produced data (initial, intermediate and final) available on :

github.com/IRSN/SalinoPhD

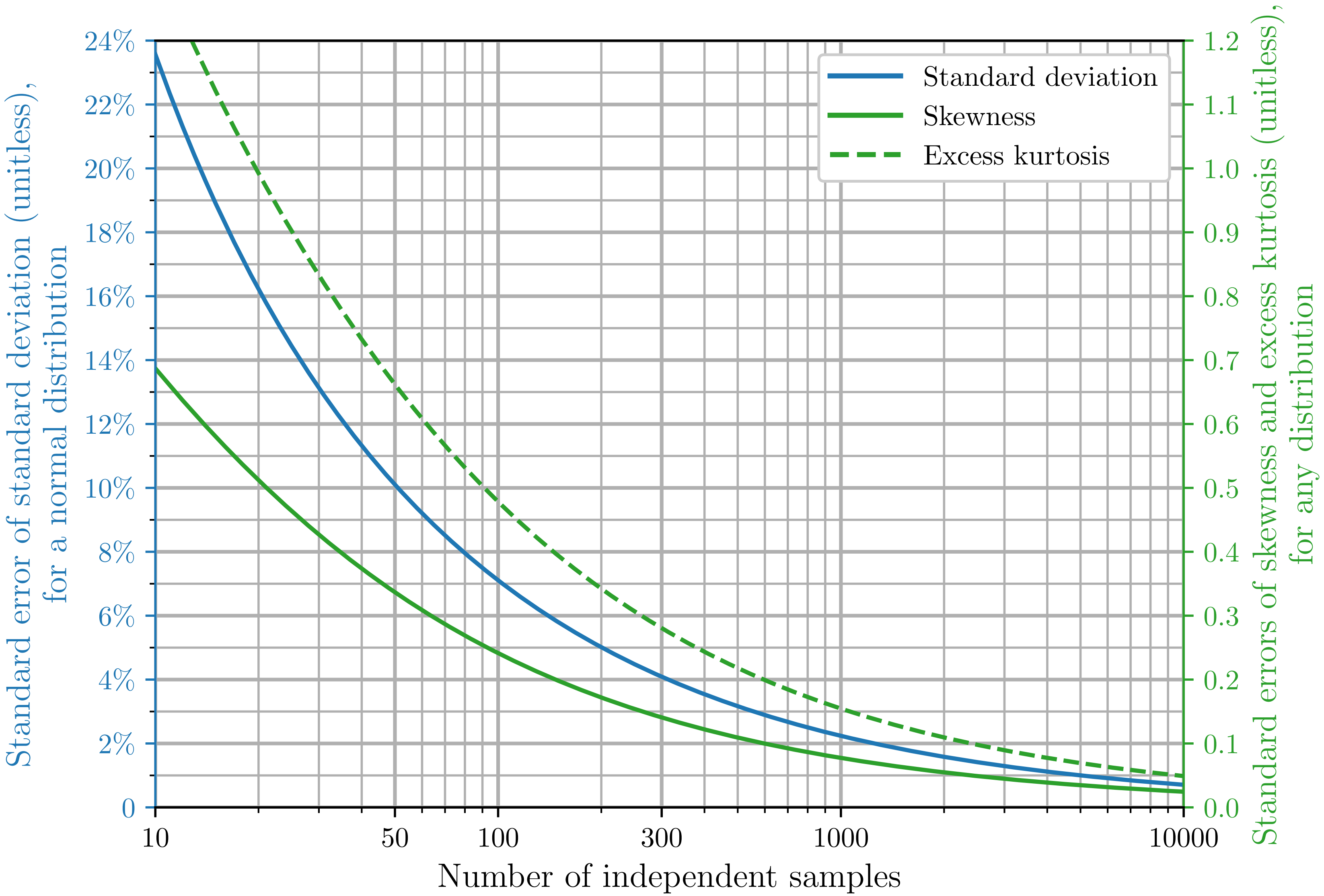
Examples :

- Nuclear data and its processing, from ENDF-6 to ACE, Draglib
- Datasets for Serpent (Monte-Carlo), Dragon and Donjon (deterministic)
- 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

# Backup slides

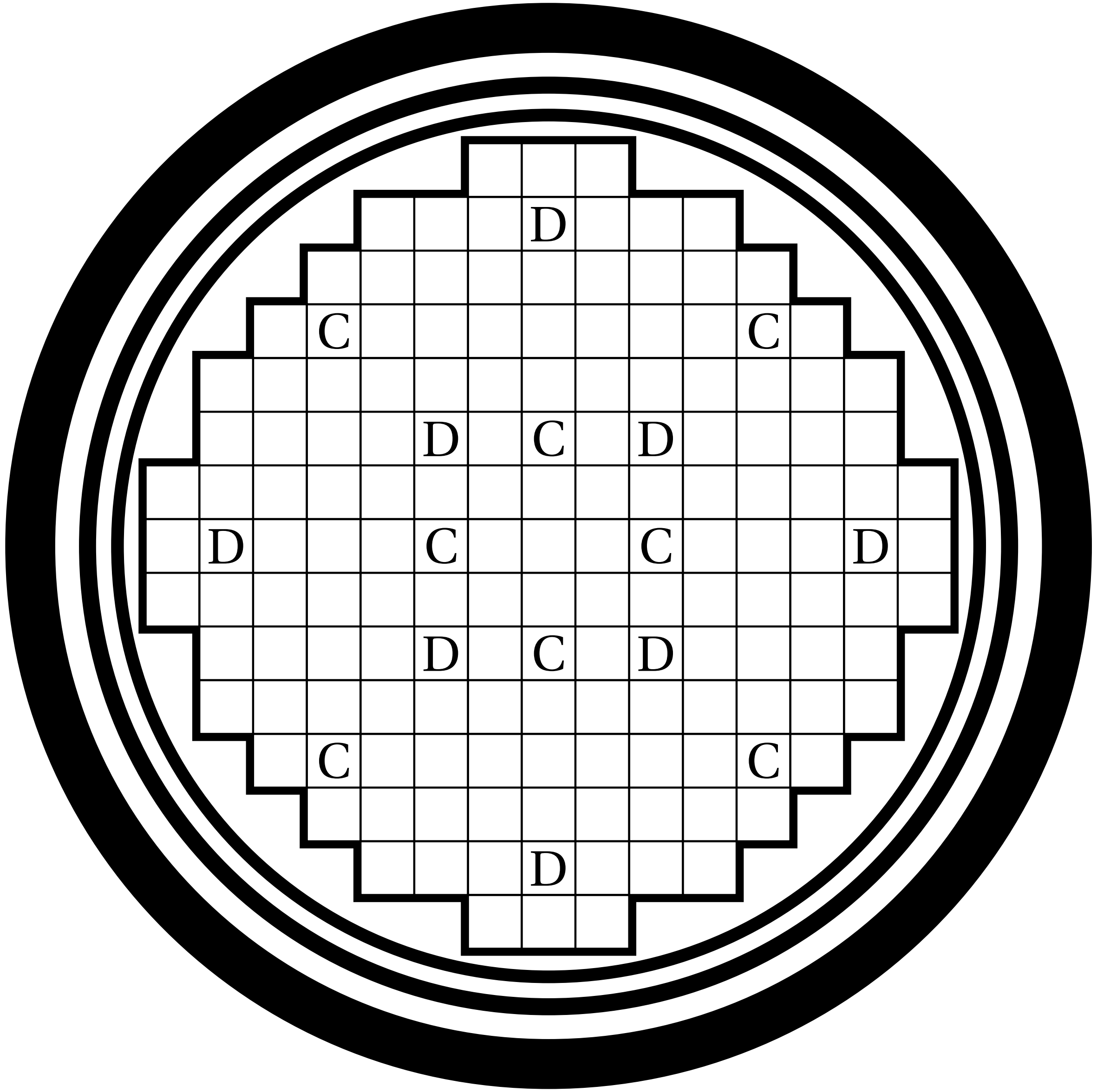
# Standard error on standard deviation (left axis), on skewness and on excess kurtosis (right axis)



# 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)

# C and D control rods banks in Tihange-1



# 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 ($x = 0$)

$$\frac{J_1}{\phi_1} = \sqrt{D_1\left(\Sigma_{a1} + \Sigma_{1\to 2}\right)} \tag{1}$$

and

$$\frac{J_2}{\phi_1} = \frac{\phi_2}{\phi_1}\sqrt{D_2\Sigma_{a2}} - \frac{\Sigma_{1\to 2}\sqrt{D_1 D_2}}{\sqrt{\Sigma_{a2}D_1} + \sqrt{\left(\Sigma_{a1} + \Sigma_{1\to 2}\right) D_2}} \tag{2}$$

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

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

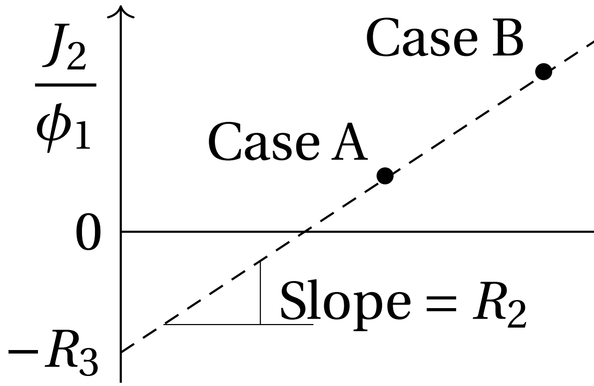
$$R_1 = \frac{J_1}{\phi_1} \tag{3}$$

# Lefebvre-Lebigot method (2/2)

2) Thermal group

➛ $J_2/\phi_1$ depends on the fuel

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



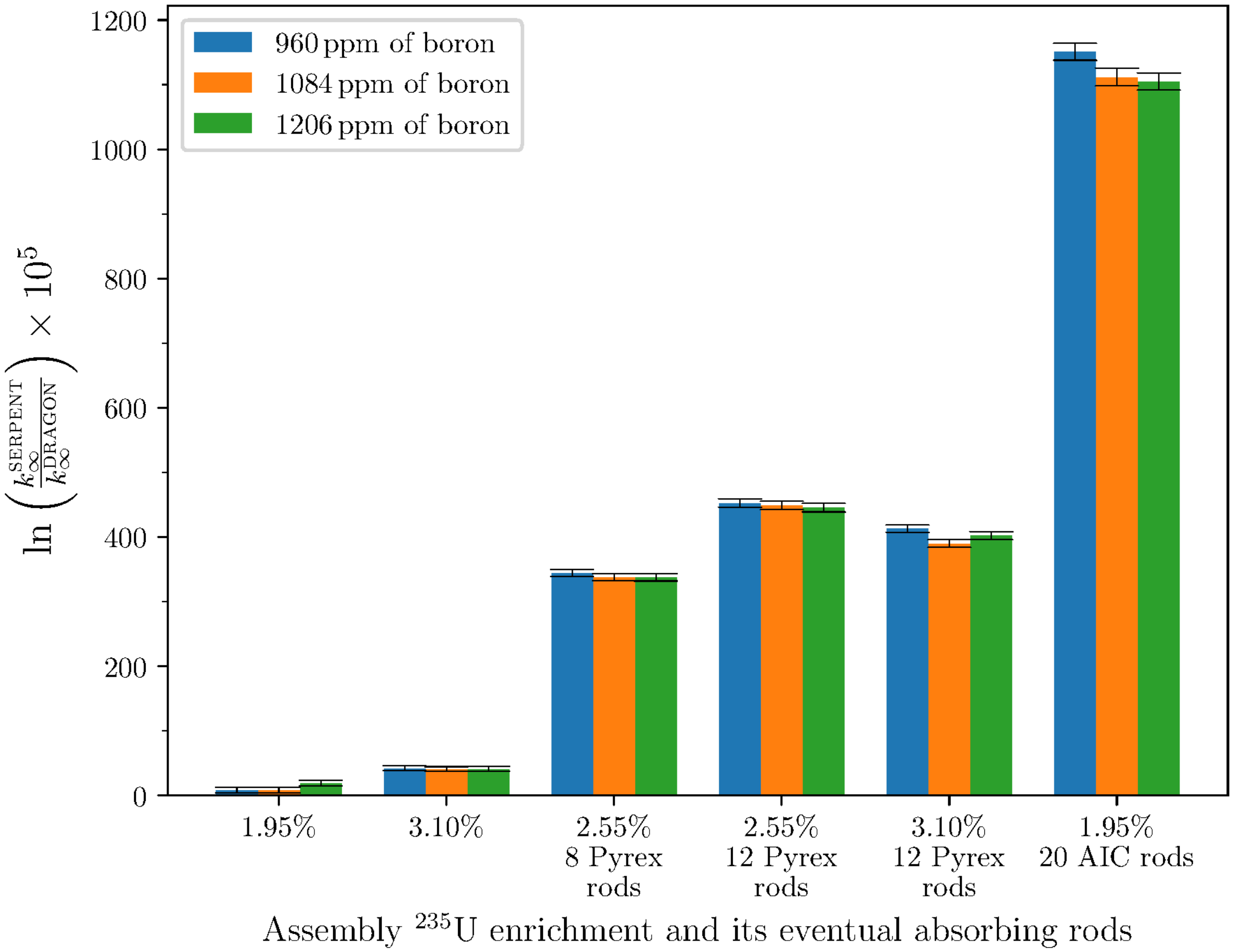
➔ 5 unknowns and 3 parameters ($R_1$, $R_2$ et $R_3$) calculated in $S_N$, Lefebvre and Lebigot suggest to equalize $D_g$ :

$$\begin{aligned} D_1^{\text{fuel}} &\approx 1.3\,\text{cm} & D_1^{\text{reflector}} &= 1.3\,\text{cm} \\ D_2^{\text{fuel}} &\approx 0.4\,\text{cm} & D_2^{\text{reflector}} &= 0.4\,\text{cm} \end{aligned} \quad (5)$$

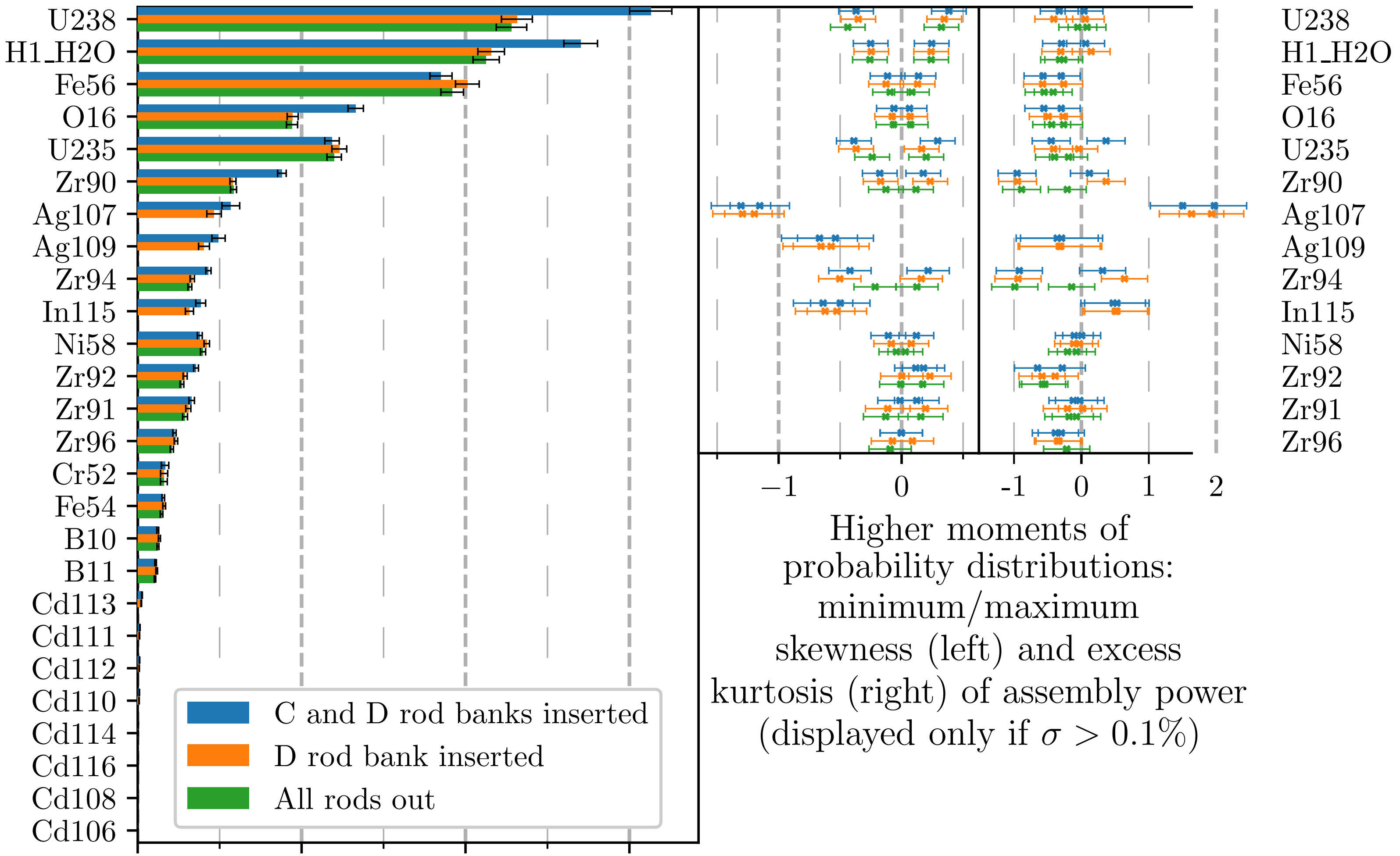
$$\Sigma_{a2} = \frac{(R_2)^2}{D_2} \qquad \Sigma_{1\to 2} = R_3\left(\frac{R_1}{D_1} + \sqrt{\frac{\Sigma_{a2}}{D_2}}\right) \quad (6)$$

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

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



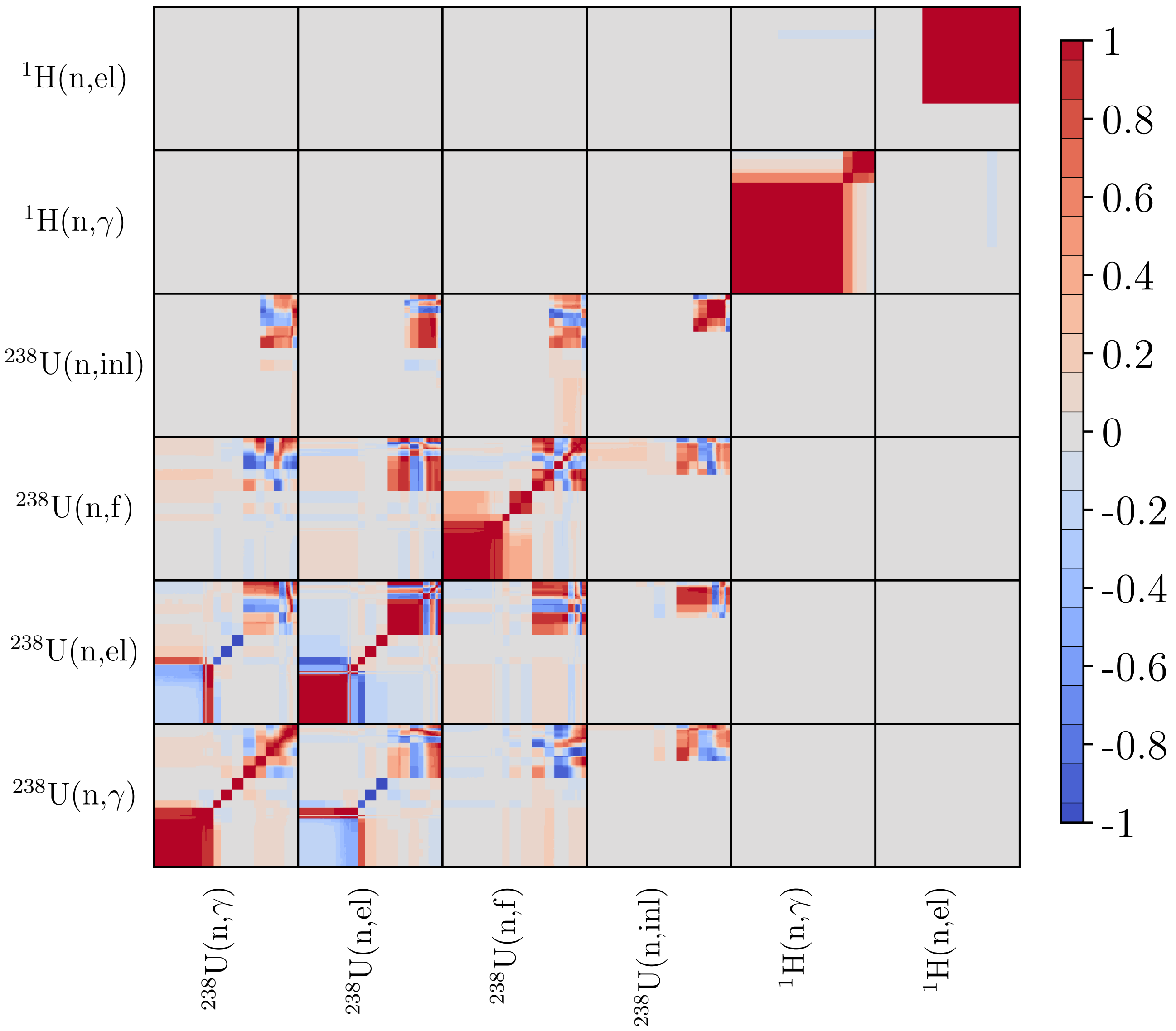
# Ranking of uncertainties in Tihange-1, by isotope



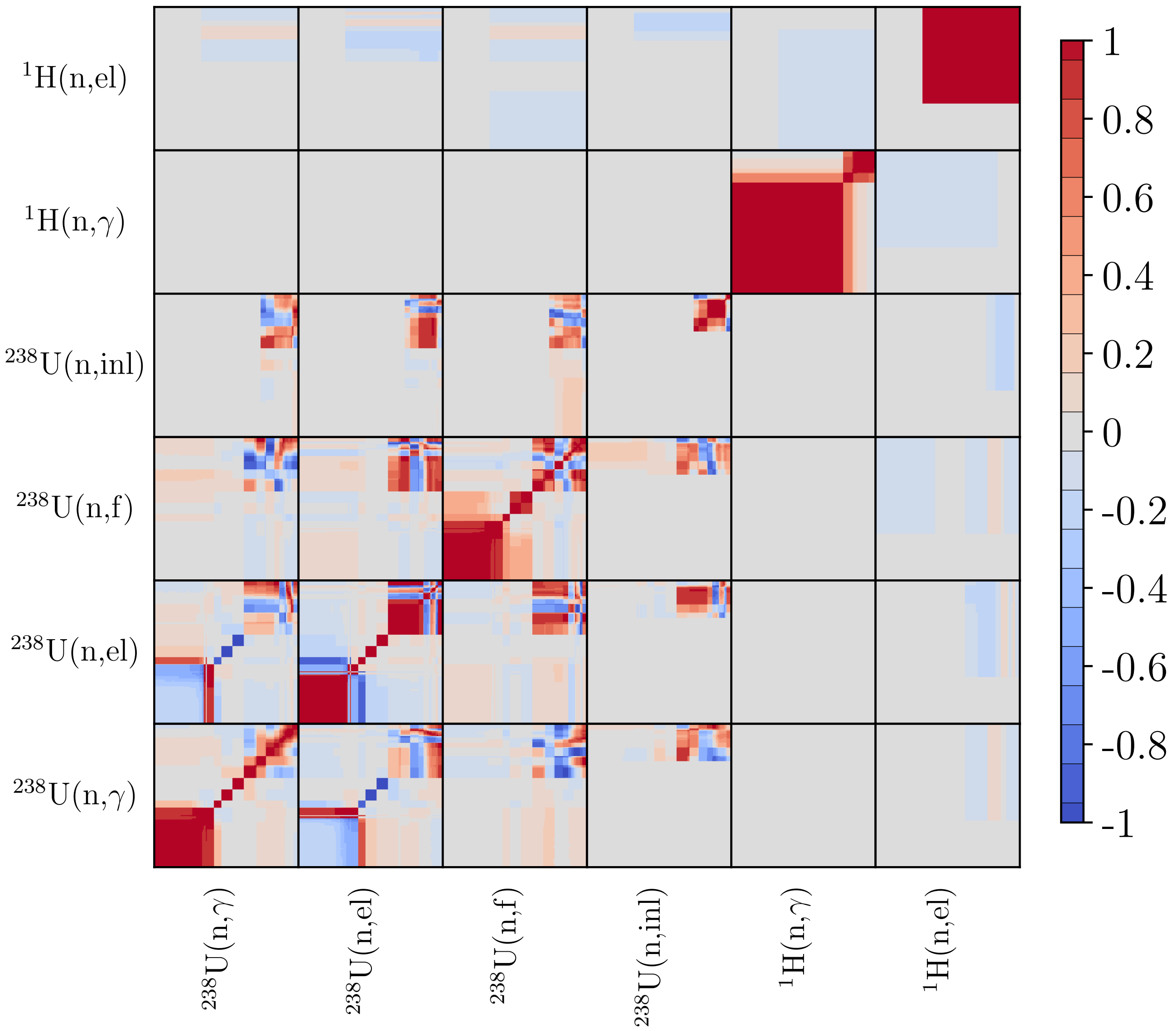
Relative standard deviation (1$\sigma$) of the most uncertain assembly power

Higher moments of probability distributions: minimum/maximum skewness (left) and excess kurtosis (right) of assembly power (displayed only if $\sigma > 0.1\%$)

# Prior correlations between the uncertainties of hydrogen and uranium 238

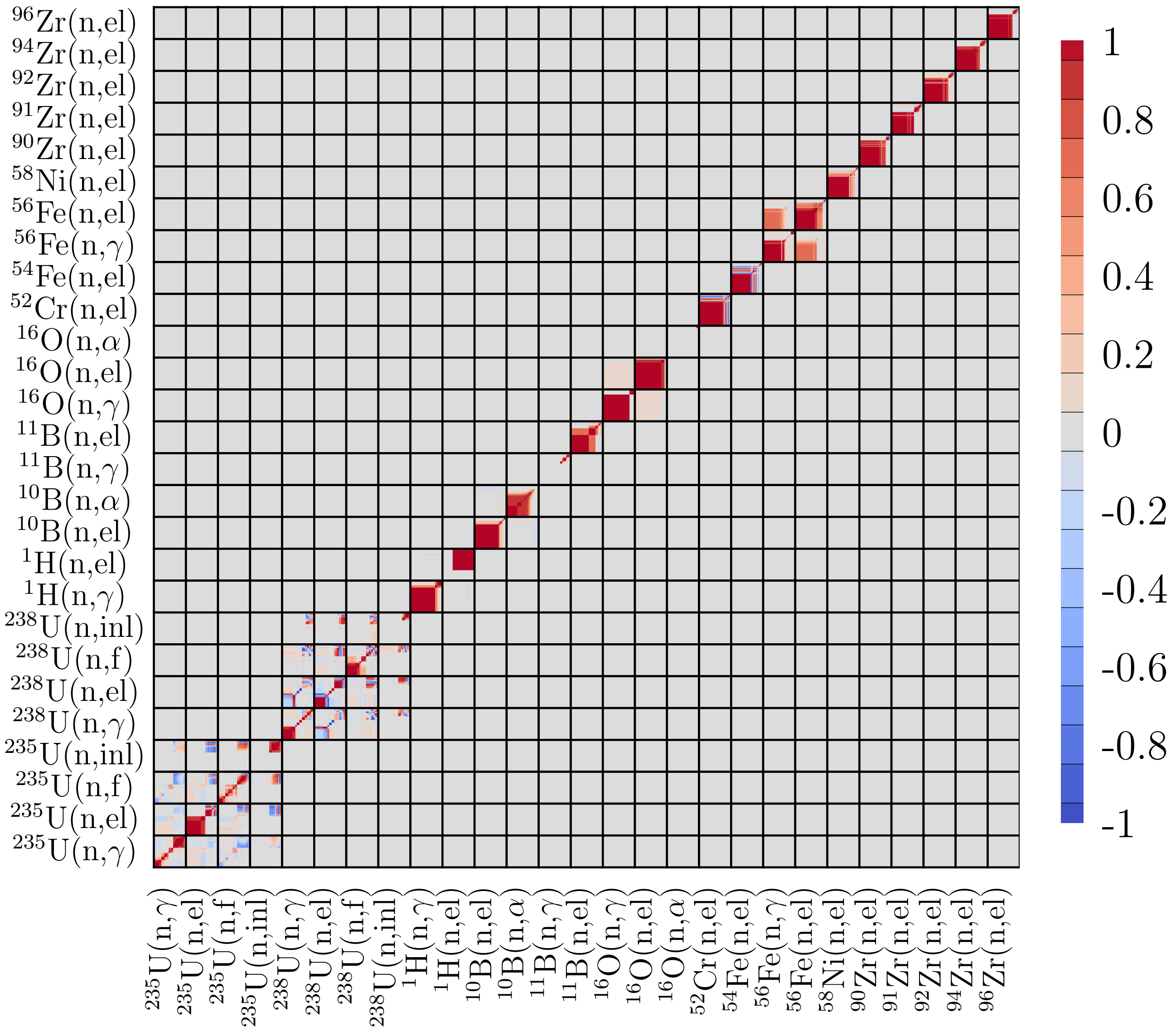


# **Posterior** (BFMC) correlations between the uncertainties of hydrogen and uranium 238

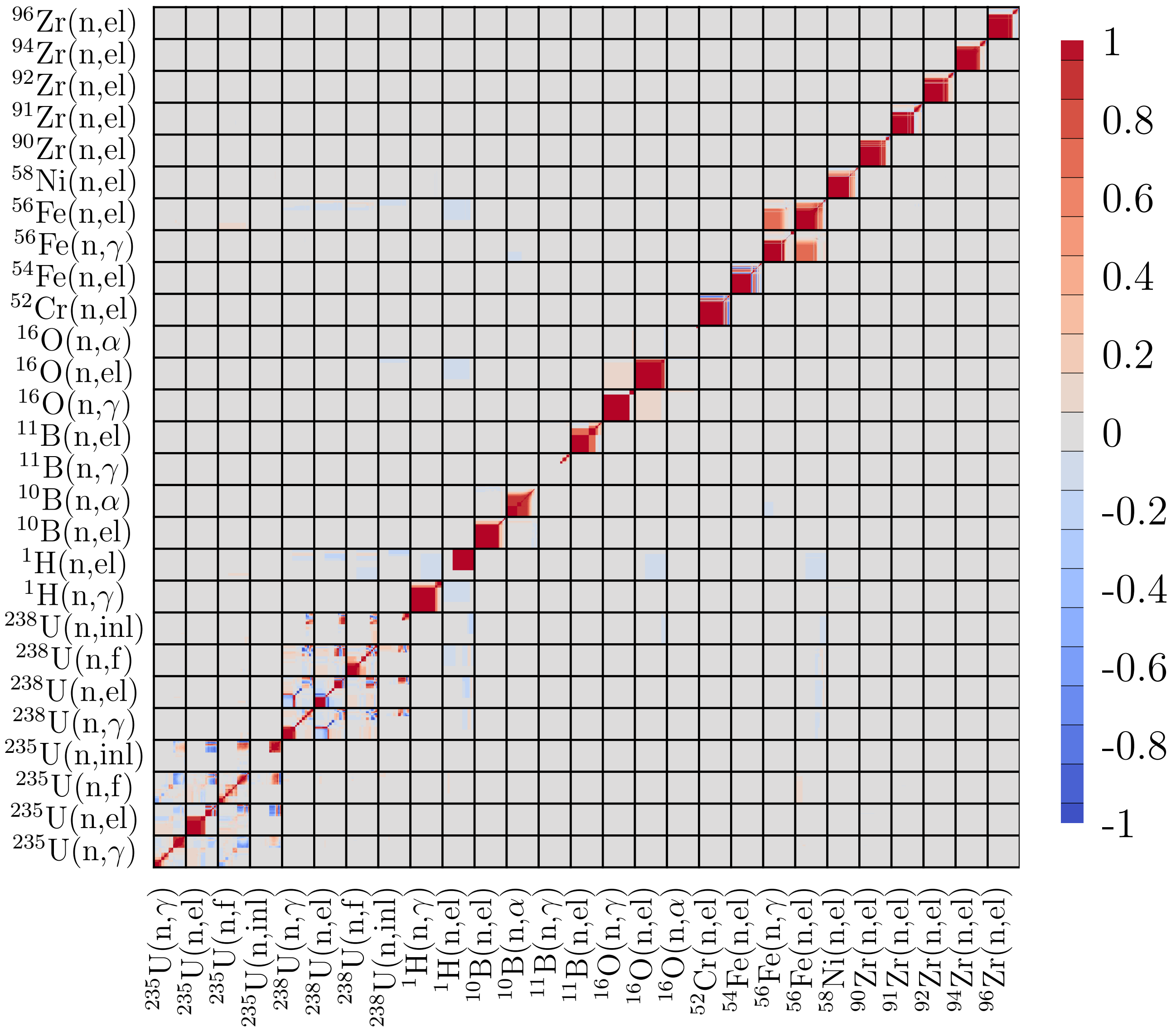


POLYTECHNIQUE
MONTRÉAL

# Prior correlations between the uncertainties of diffrent 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

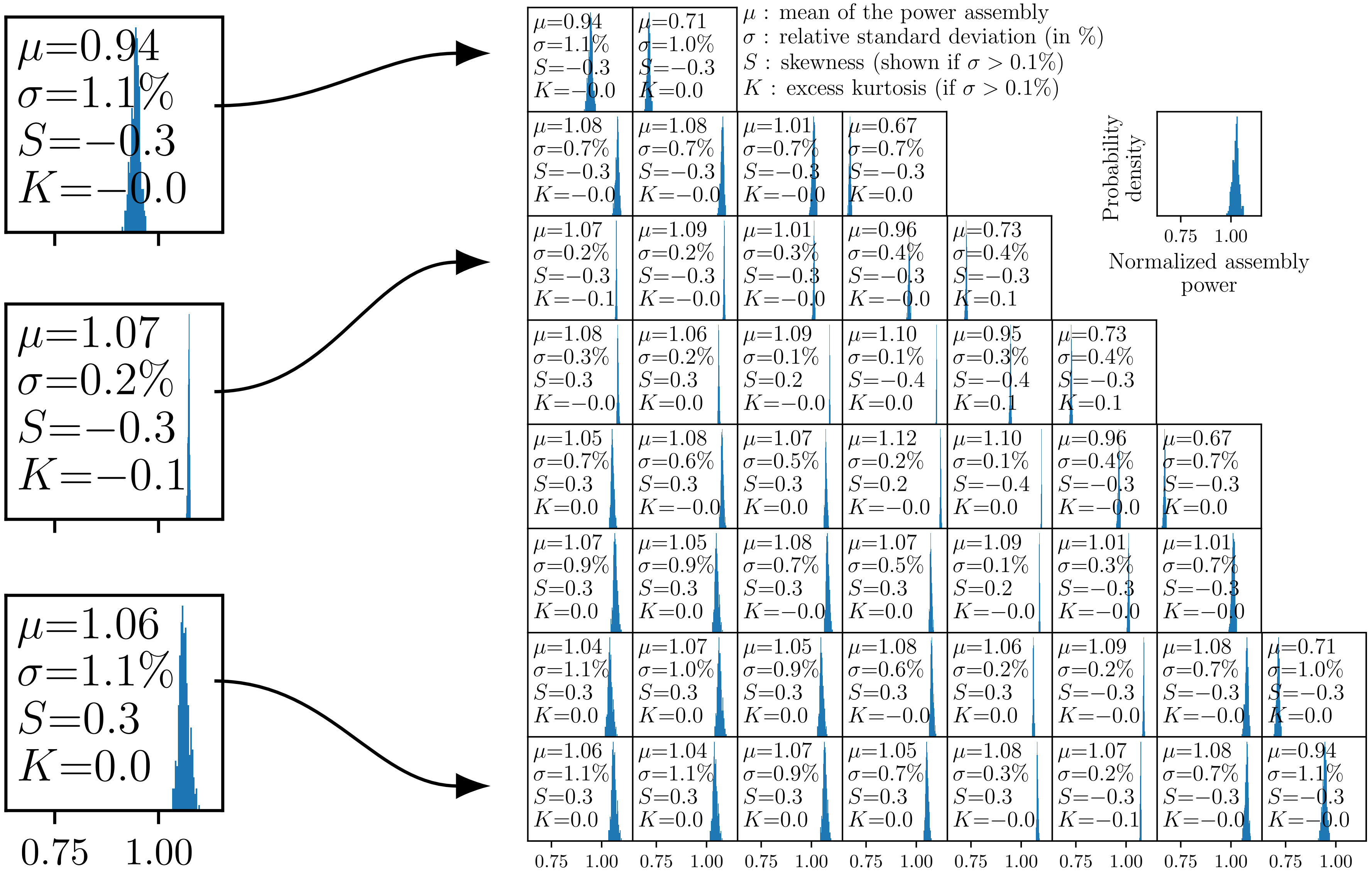
➔ Multigroups ➛ piecewise constant
➔ Sometimes missing or incomplete (minor isotopes)

2) TENDL-2019 evaluation ➛ some various benefits

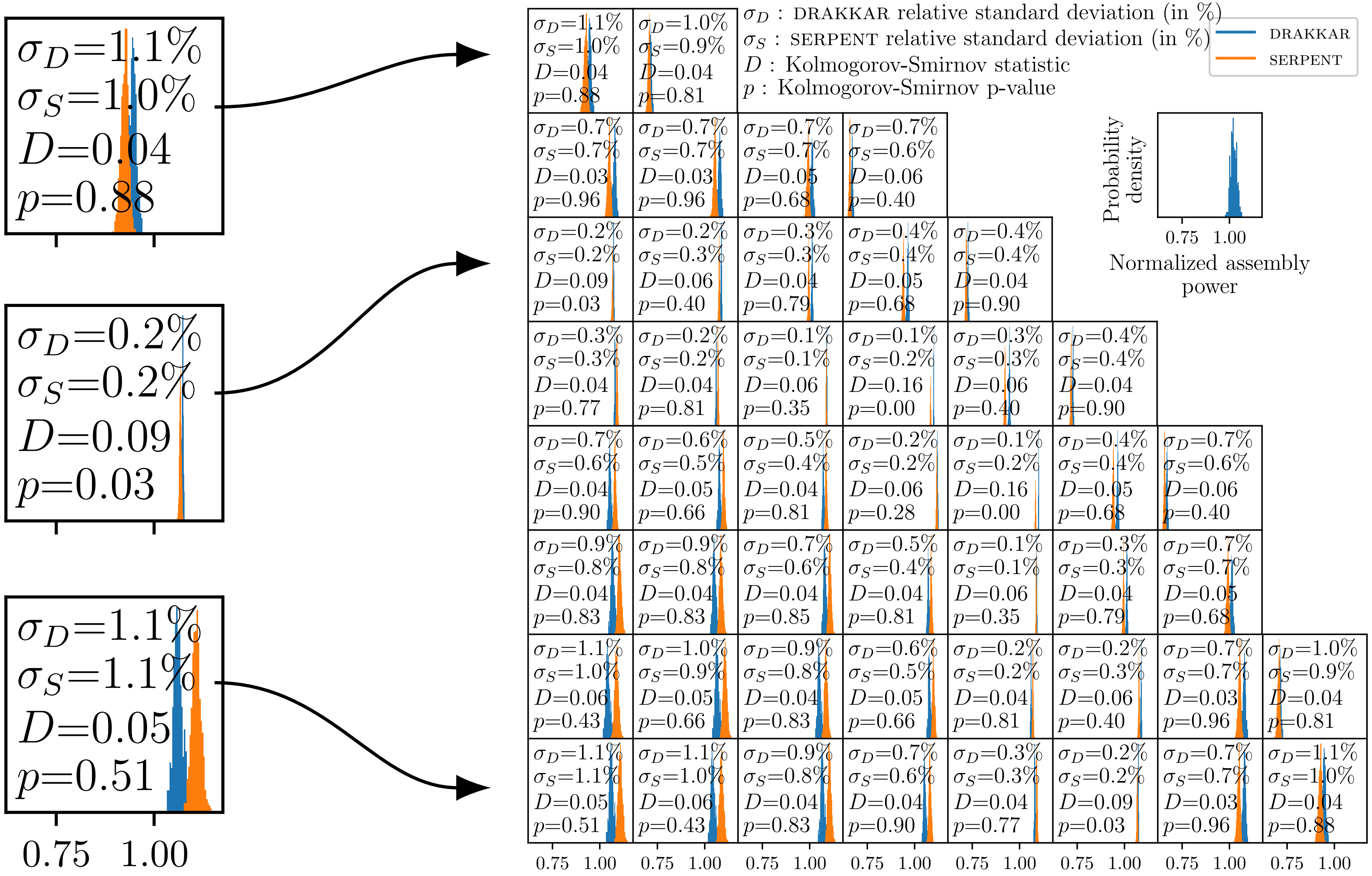
➔ Very complete uncertainties (angular distributions, etc), continuously varying, not necessarily Gaussian
➔ Above all, single code for production ➛high format homogeneity ➛ safer and faster
➔ TALYS optical models ➛ no evaluation for less than 20 nucleons (hydrogen, boron, oxygen. . .) ➛ JEFF-3.3
➔ No 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

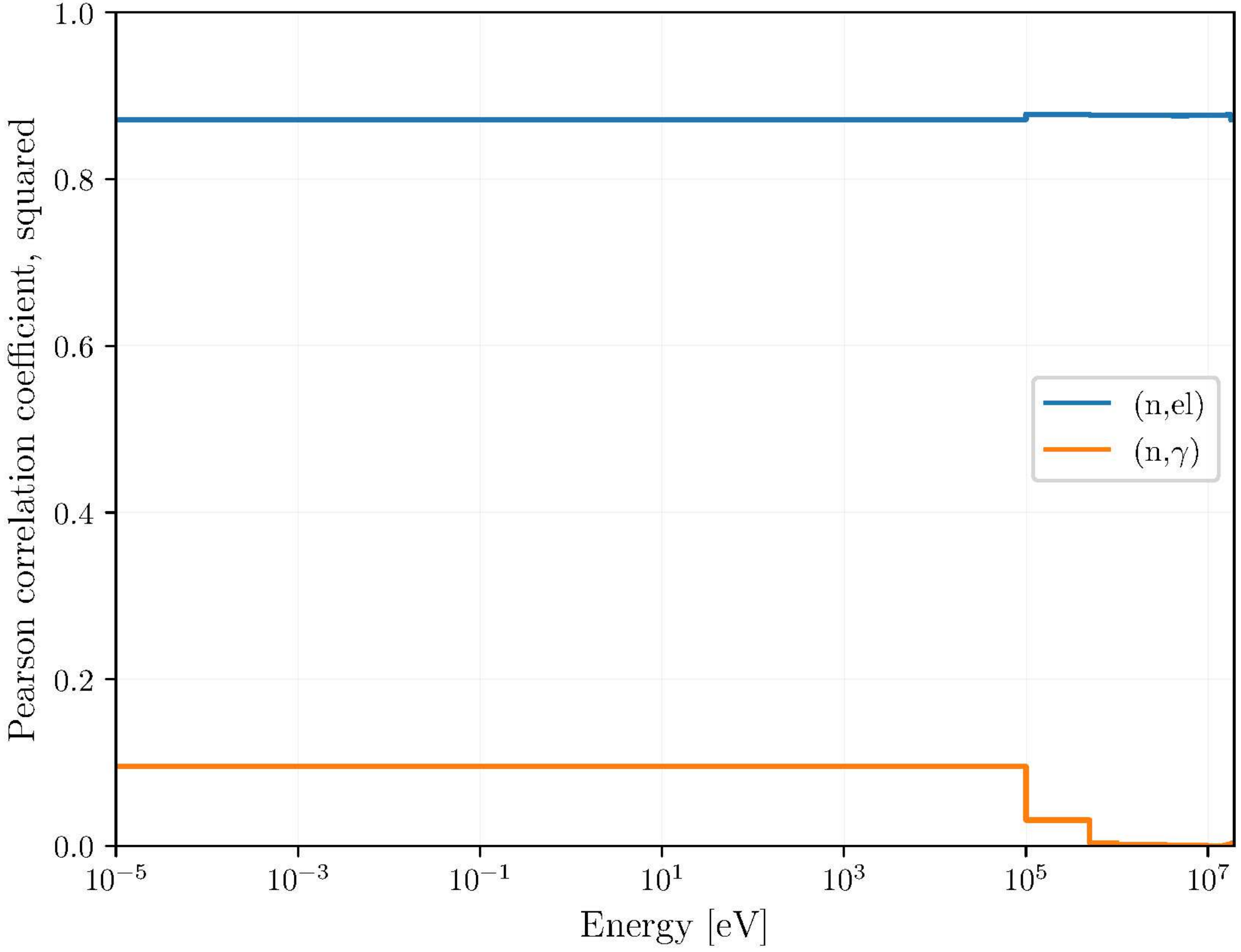
# Propagation of uncertainties from uranium 238, JEFF-3.3
# 300 samples of nuclear data (with SANDY)



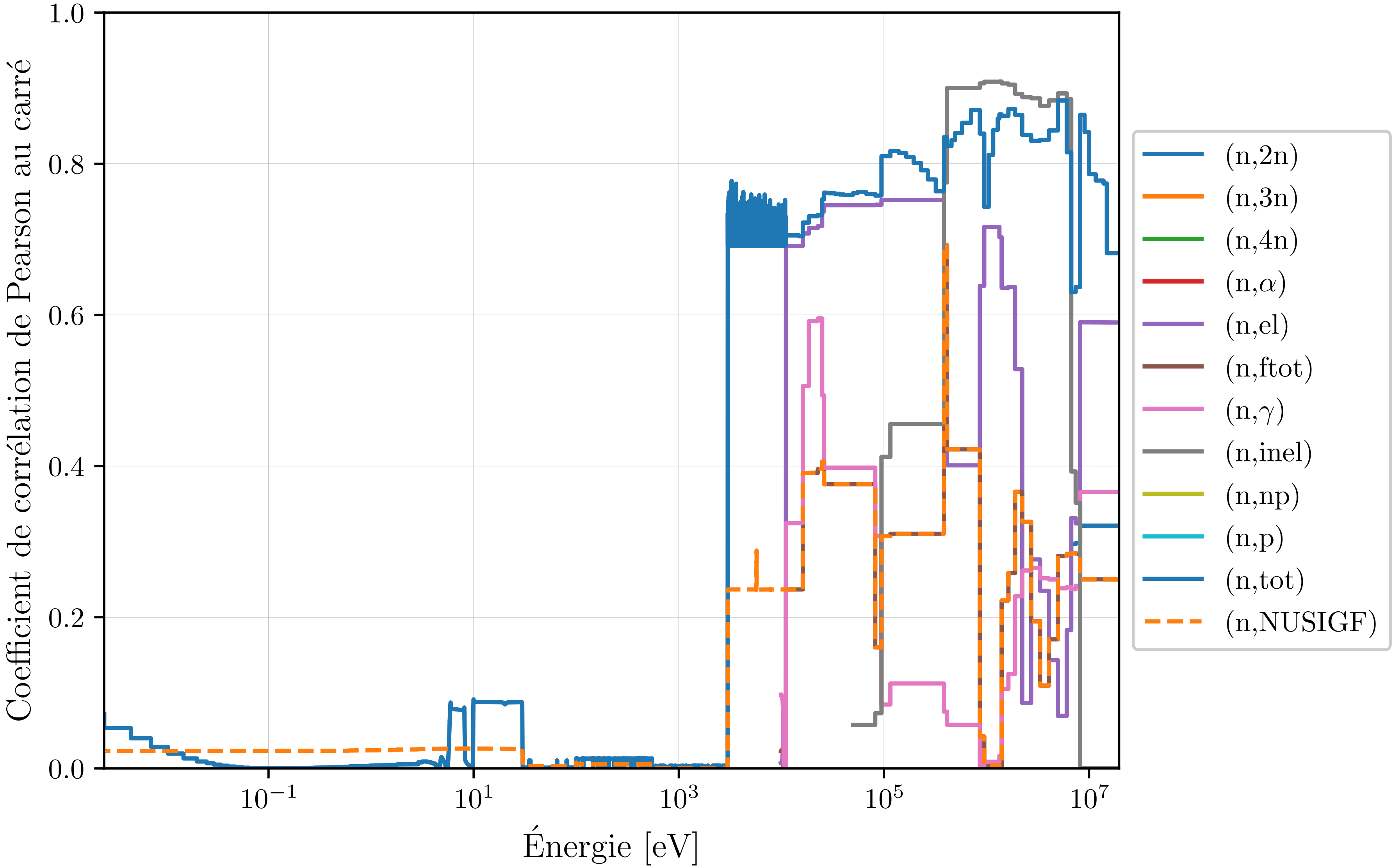
# Propagation of uncertainties from uranium 238, JEFF-3.3 Deterministic and Monte-Carlo comparison



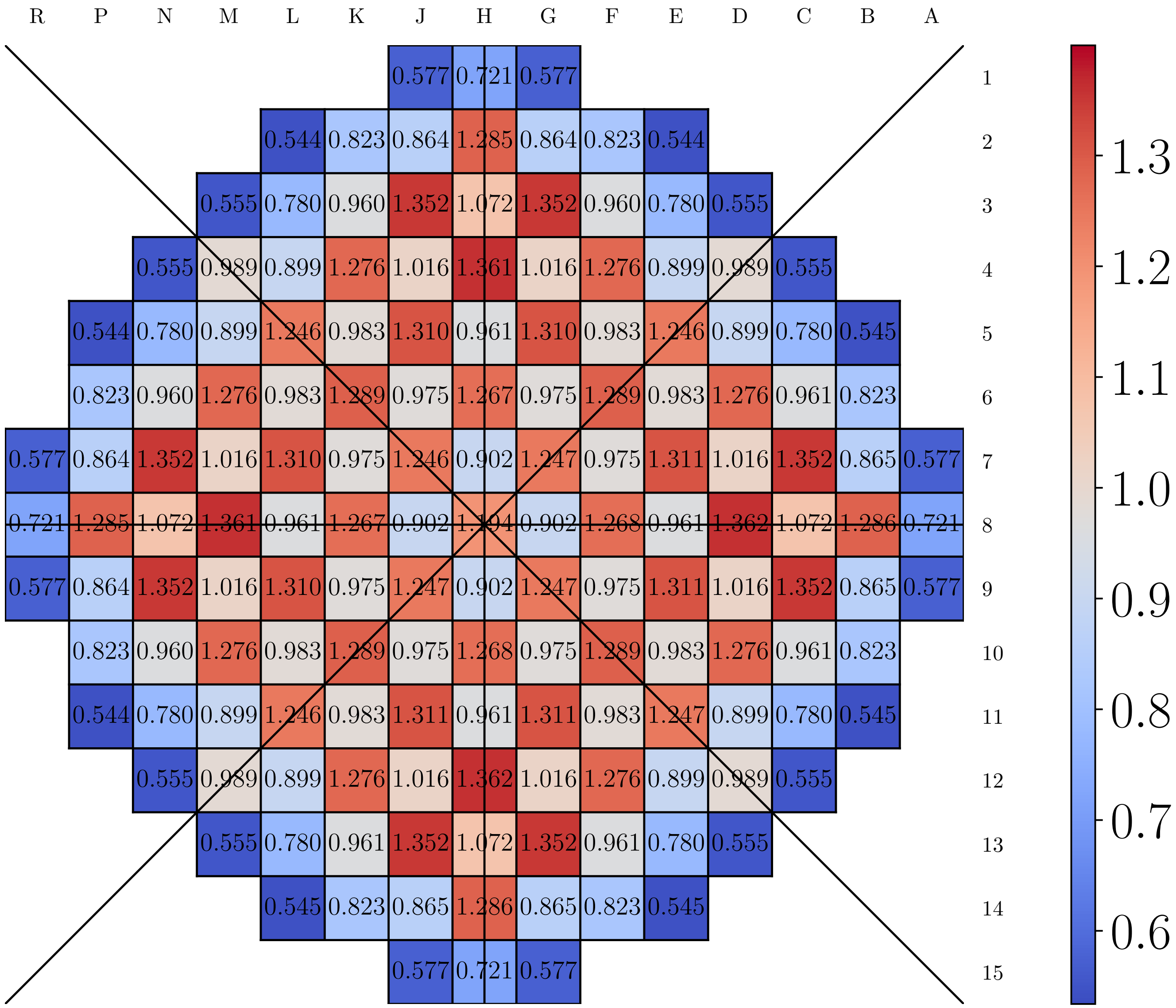
# Hydrogen uncertainty decomposition with respect to reaction and energy



# Uranium 238 uncertainty decomposition with respect to reaction and energy From Luka Stancev's internship

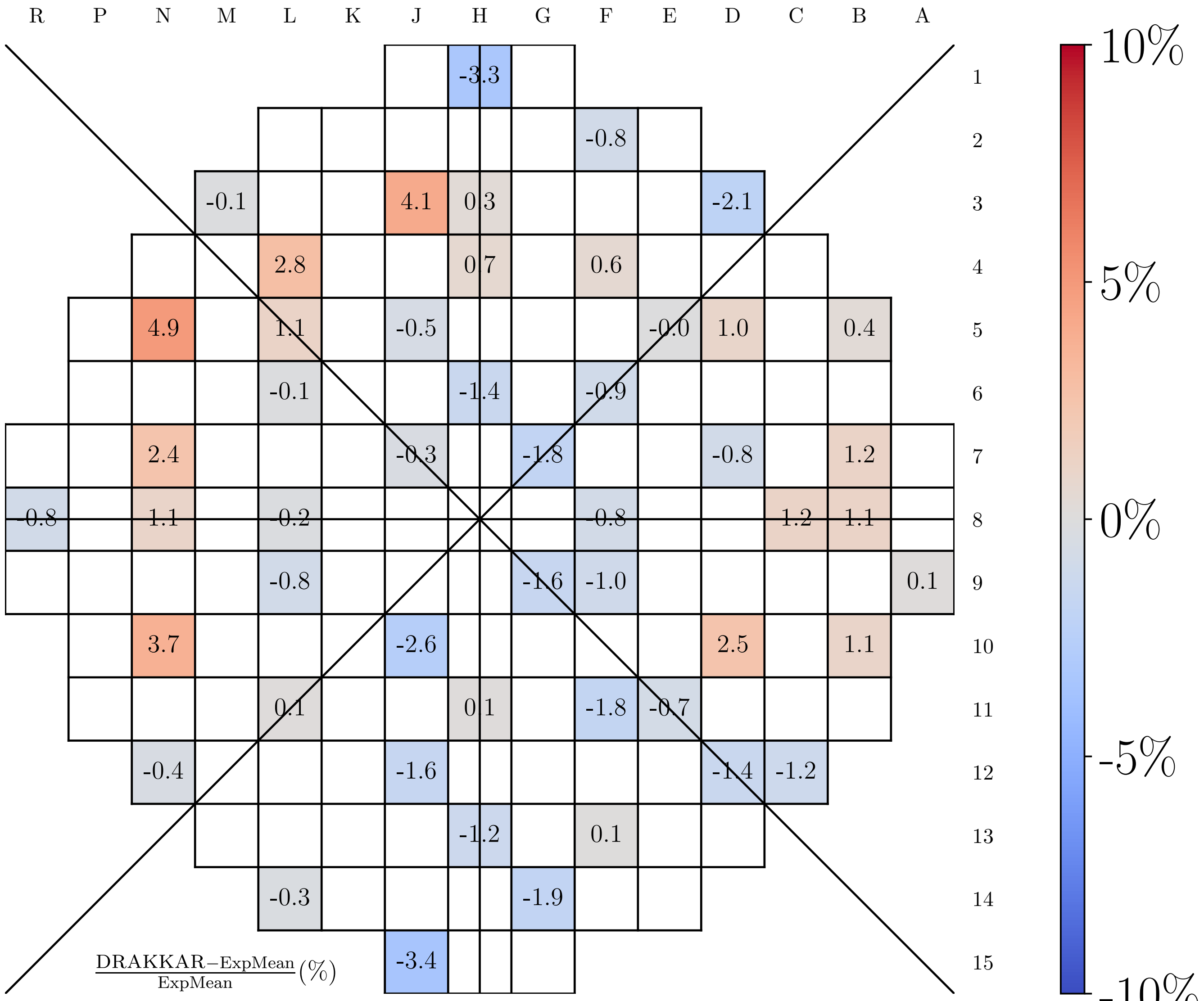


# Drakkar detector responses (JEFF-3.3)



| R | P | N | M | L | K | J | H | G | F | E | D | C | B | A | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | 0.577 | 0.721 | 0.577 | | | | | | | 1 |
| | | | | 0.544 | 0.823 | 0.864 | 1.285 | 0.864 | 0.823 | 0.544 | | | | | 2 |
| | | | 0.555 | 0.780 | 0.960 | 1.352 | 1.072 | 1.352 | 0.960 | 0.780 | 0.555 | | | | 3 |
| | | 0.555 | 0.989 | 0.899 | 1.276 | 1.016 | 1.361 | 1.016 | 1.276 | 0.899 | 0.989 | 0.555 | | | 4 |
| | 0.544 | 0.780 | 0.899 | 1.246 | 0.983 | 1.310 | 0.961 | 1.310 | 0.983 | 1.246 | 0.899 | 0.780 | 0.545 | | 5 |
| | 0.823 | 0.960 | 1.276 | 0.983 | 1.289 | 0.975 | 1.267 | 0.975 | 1.289 | 0.983 | 1.276 | 0.961 | 0.823 | | 6 |
| 0.577 | 0.864 | 1.352 | 1.016 | 1.310 | 0.975 | 1.246 | 0.902 | 1.247 | 0.975 | 1.311 | 1.016 | 1.352 | 0.865 | 0.577 | 7 |
| 0.721 | 1.285 | 1.072 | 1.361 | 0.961 | 1.267 | 0.902 | 1.194 | 0.902 | 1.268 | 0.961 | 1.362 | 1.072 | 1.286 | 0.721 | 8 |
| 0.577 | 0.864 | 1.352 | 1.016 | 1.310 | 0.975 | 1.247 | 0.902 | 1.247 | 0.975 | 1.311 | 1.016 | 1.352 | 0.865 | 0.577 | 9 |
| | 0.823 | 0.960 | 1.276 | 0.983 | 1.289 | 0.975 | 1.268 | 0.975 | 1.289 | 0.983 | 1.276 | 0.961 | 0.823 | | 10 |
| | 0.544 | 0.780 | 0.899 | 1.246 | 0.983 | 1.311 | 0.961 | 1.311 | 0.983 | 1.247 | 0.899 | 0.780 | 0.545 | | 11 |
| | | 0.555 | 0.989 | 0.899 | 1.276 | 1.016 | 1.362 | 1.016 | 1.276 | 0.899 | 0.989 | 0.555 | | | 12 |
| | | | 0.555 | 0.780 | 0.961 | 1.352 | 1.072 | 1.352 | 0.961 | 0.780 | 0.555 | | | | 13 |
| | | | | 0.545 | 0.823 | 0.865 | 1.286 | 0.865 | 0.823 | 0.545 | | | | | 14 |
| | | | | | | 0.577 | 0.721 | 0.577 | | | | | | | 15 |

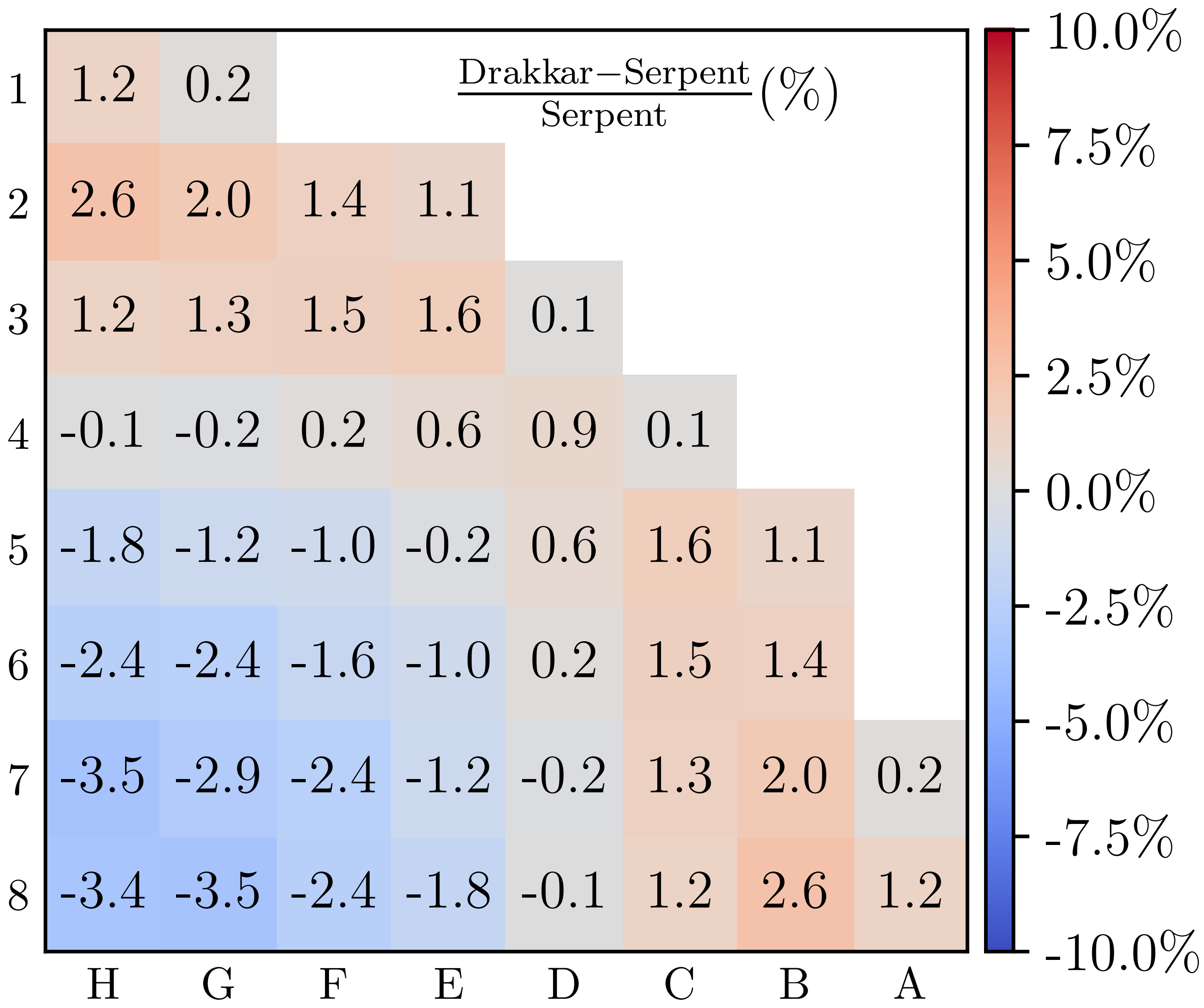
# Discrepancy between Drakkar (JEFF-3.3) and experimental mean



| | R | P | N | M | L | K | J | H | G | F | E | D | C | B | A |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | | | | | | | -3.3 | | | | | | | |
| 2 | | | | | | | | | | -0.8 | | | | | |
| 3 | | | | -0.1 | | | 4.1 | 0.3 | | | | -2.1 | | | |
| 4 | | | | | 2.8 | | | 0.7 | | 0.6 | | | | | |
| 5 | | | 4.9 | | 1.1 | | -0.5 | | | | -0.0 | 1.0 | | 0.4 | |
| 6 | | | | | -0.1 | | | -1.4 | | -0.9 | | | | | |
| 7 | | | 2.4 | | | | -0.3 | | -1.8 | | | -0.8 | | 1.2 | |
| 8 | -0.8 | | 1.1 | | -0.2 | | | | | -0.8 | | | 1.2 | 1.1 | |
| 9 | | | | | -0.8 | | | | -1.6 | -1.0 | | | | | 0.1 |
| 10 | | | 3.7 | | | | -2.6 | | | | | 2.5 | | 1.1 | |
| 11 | | | | | 0.1 | | | 0.1 | | -1.8 | -0.7 | | | | |
| 12 | | | -0.4 | | | | -1.6 | | | | | -1.4 | -1.2 | | |
| 13 | | | | | | | | -1.2 | | 0.1 | | | | | |
| 14 | | | | | -0.3 | | | | -1.9 | | | | | | |
| 15 | | | | | | | -3.4 | | | | | | | | |

$\frac{\text{DRAKKAR}-\text{ExpMean}}{\text{ExpMean}}(\%)$

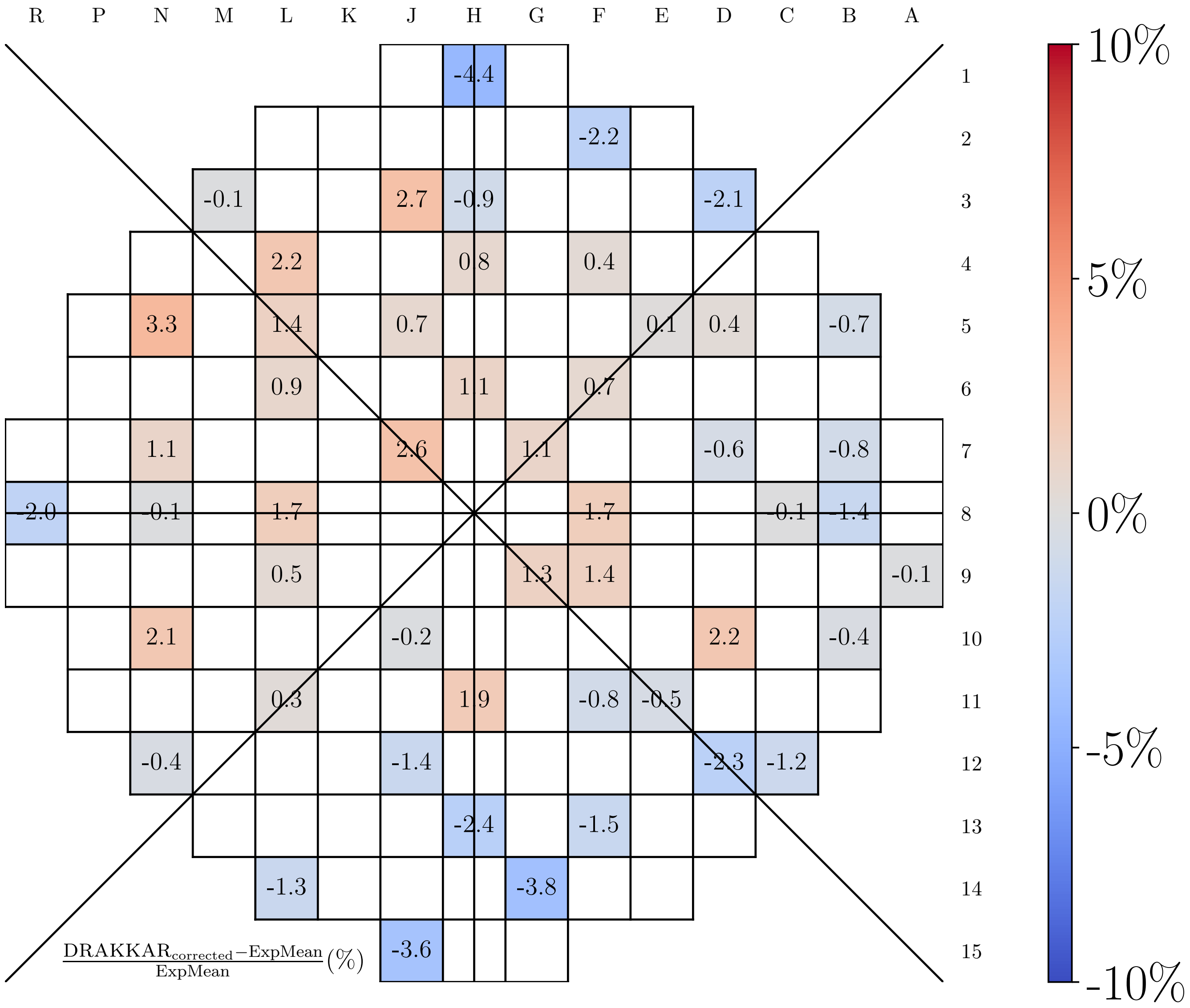
# Power distribution discrepancy between Drakkar and Serpent, on Bugey-2 and Fessenheim-1 and 2



$\frac{\text{Drakkar}-\text{Serpent}}{\text{Serpent}}(\%)$

| | H | G | F | E | D | C | B | A |
|---|---|---|---|---|---|---|---|---|
| 1 | 1.2 | 0.2 | | | | | | |
| 2 | 2.6 | 2.0 | 1.4 | 1.1 | | | | |
| 3 | 1.2 | 1.3 | 1.5 | 1.6 | 0.1 | | | |
| 4 | -0.1 | -0.2 | 0.2 | 0.6 | 0.9 | 0.1 | | |
| 5 | -1.8 | -1.2 | -1.0 | -0.2 | 0.6 | 1.6 | 1.1 | |
| 6 | -2.4 | -2.4 | -1.6 | -1.0 | 0.2 | 1.5 | 1.4 | |
| 7 | -3.5 | -2.9 | -2.4 | -1.2 | -0.2 | 1.3 | 2.0 | 0.2 |
| 8 | -3.4 | -3.5 | -2.4 | -1.8 | -0.1 | 1.2 | 2.6 | 1.2 |

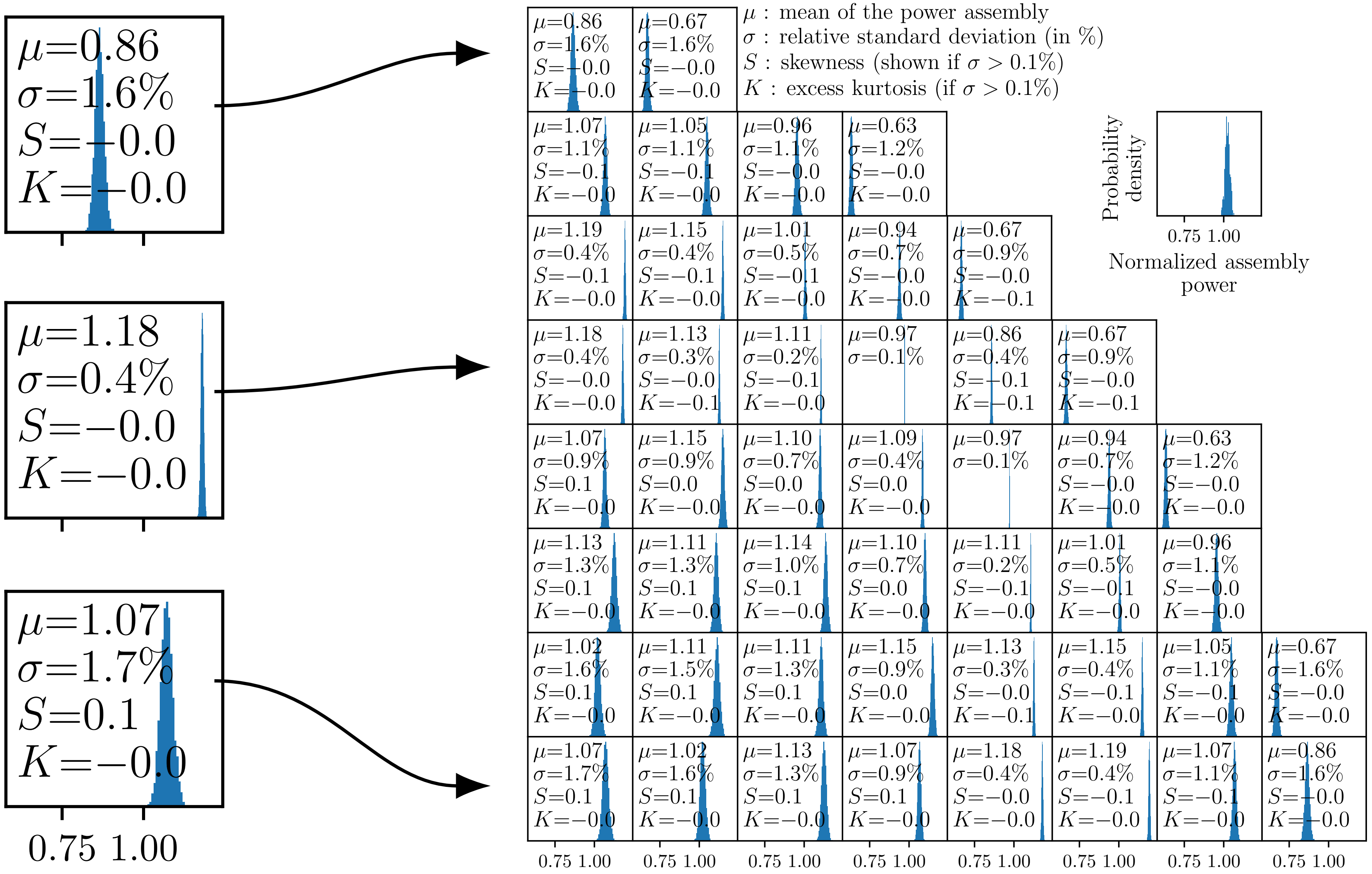
# Discrepancies between Drakkar (corrected from deterministic bias, JEFF-3.3) and experimental mean



| | R | P | N | M | L | K | J | H | G | F | E | D | C | B | A |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | | | | | | | -4.4 | | | | | | | |
| 2 | | | | | | | | | | -2.2 | | | | | |
| 3 | | | | -0.1 | | | 2.7 | -0.9 | | | | -2.1 | | | |
| 4 | | | | | 2.2 | | | 0.8 | | 0.4 | | | | | |
| 5 | | | 3.3 | | 1.4 | | 0.7 | | | | 0.1 | 0.4 | | -0.7 | |
| 6 | | | | | 0.9 | | | 1.1 | | 0.7 | | | | | |
| 7 | | | 1.1 | | | | 2.6 | | 1.1 | | | -0.6 | | -0.8 | |
| 8 | -2.0 | | -0.1 | | 1.7 | | | | | 1.7 | | | -0.1 | -1.4 | |
| 9 | | | | | 0.5 | | | | 1.3 | 1.4 | | | | | -0.1 |
| 10 | | | 2.1 | | | | -0.2 | | | | | 2.2 | | -0.4 | |
| 11 | | | | | 0.3 | | | 1.9 | | -0.8 | -0.5 | | | | |
| 12 | | | -0.4 | | | | -1.4 | | | | | -2.3 | -1.2 | | |
| 13 | | | | | | | | -2.4 | | -1.5 | | | | | |
| 14 | | | | | -1.3 | | | | -3.8 | | | | | | |
| 15 | | | | | | | -3.6 | | | | | | | | |

$$\frac{\text{DRAKKAR}_{\text{corrected}}-\text{ExpMean}}{\text{ExpMean}}(\%)$$

# 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

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

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

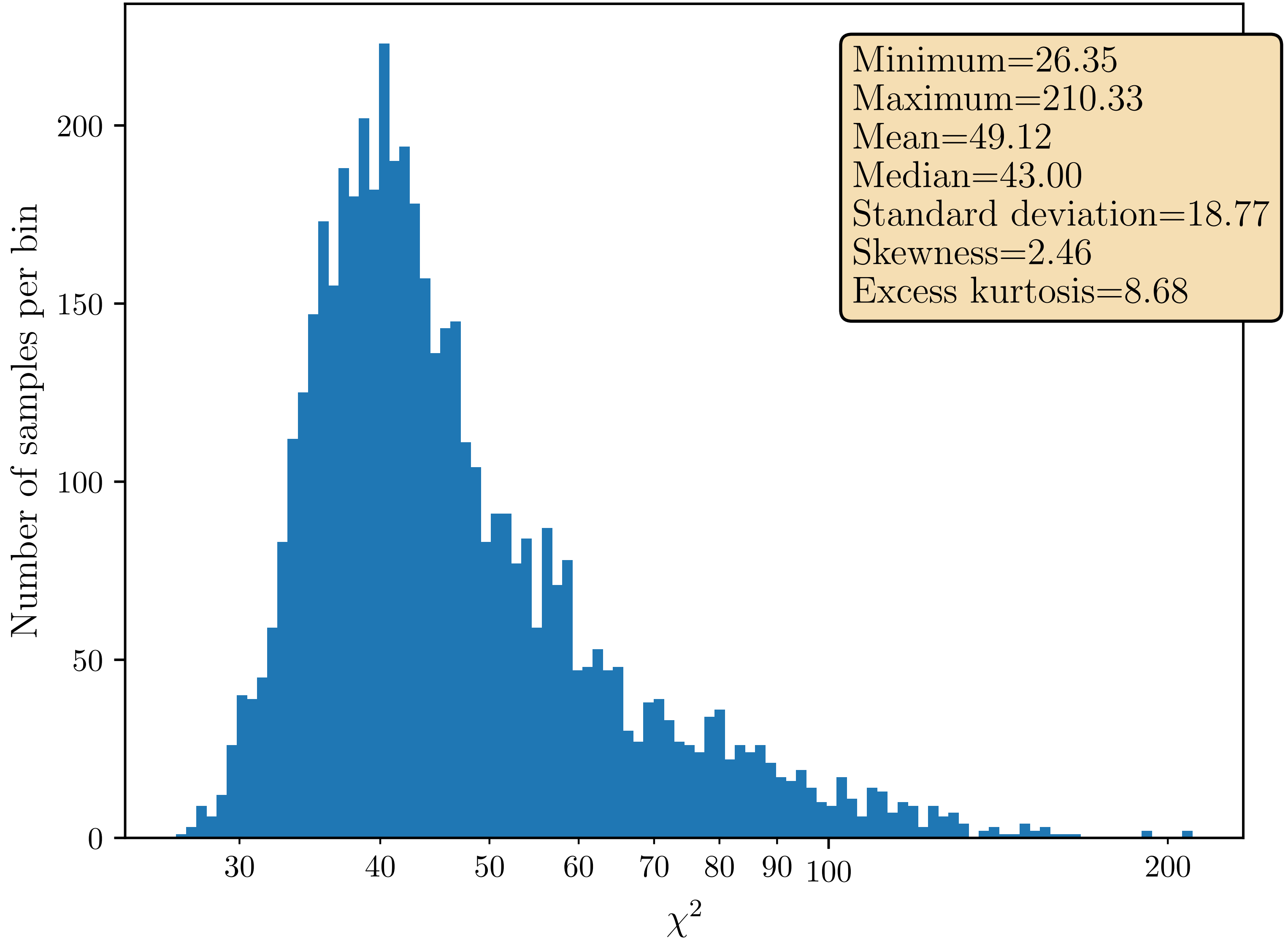
$$\sigma_E = 2\% \tag{9}$$

- ➔ Each nuclear data sample $k$ ➛ weight

$$w_k = \frac{L\left(\mathbf{p}_k, \mathbf{x}\right)}{\sum\limits_{\kappa=1}^{n} L\left(\mathbf{p}_\kappa, \mathbf{x}\right)} = \frac{\exp\left(-\chi_k^2/2\right)}{\sum\limits_{\kappa=1}^{n} \exp\left(-\chi_\kappa^2/2\right)} \tag{10}$$

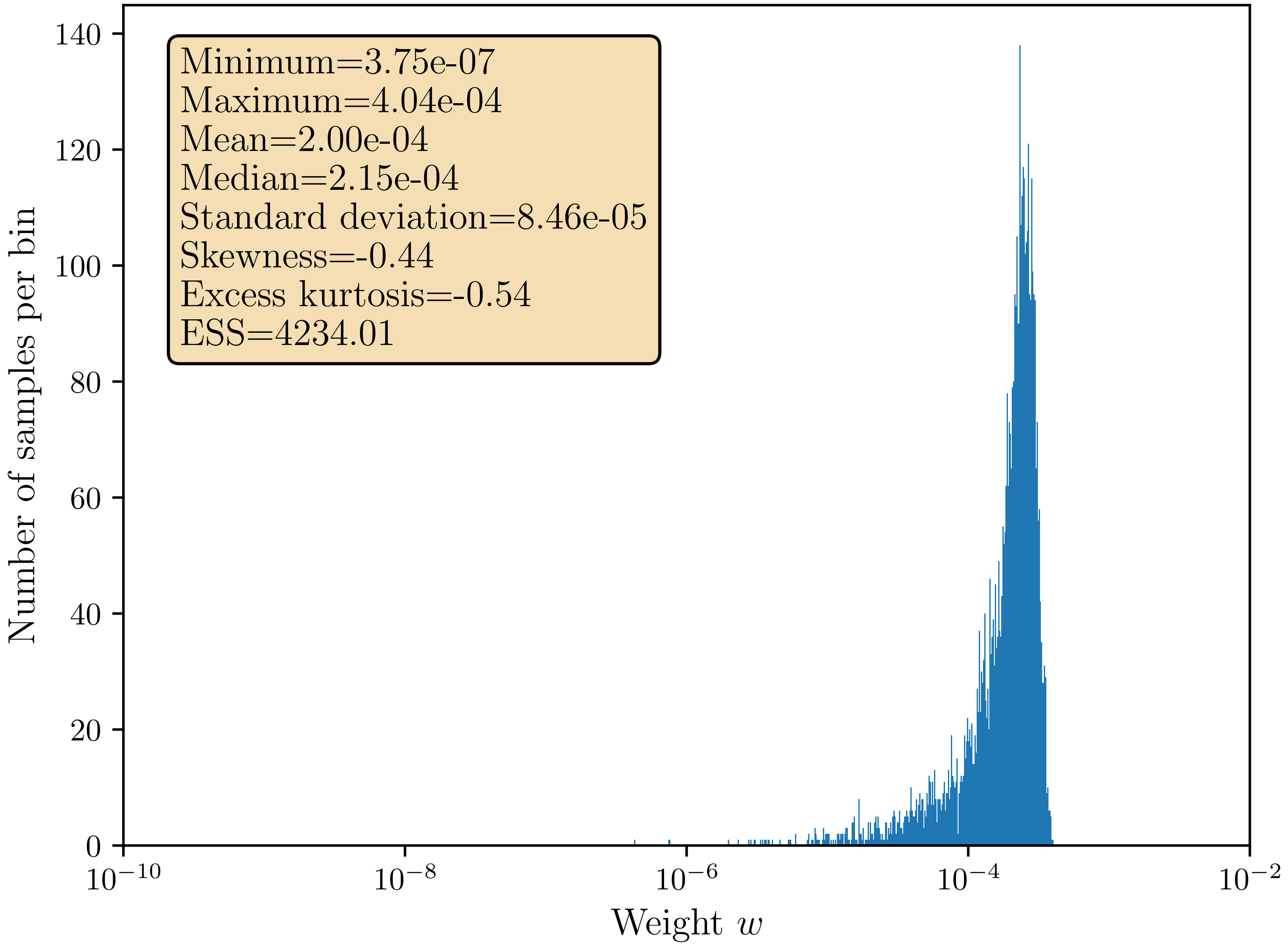
where $L\left(\mathbf{p}_k, \mathbf{x}\right)$ ➛ likelihood of the $\mathbf{x}$ experimental observations for a $k$ sample of $\mathbf{p}$ nuclear data

# $\chi^2$ histogram

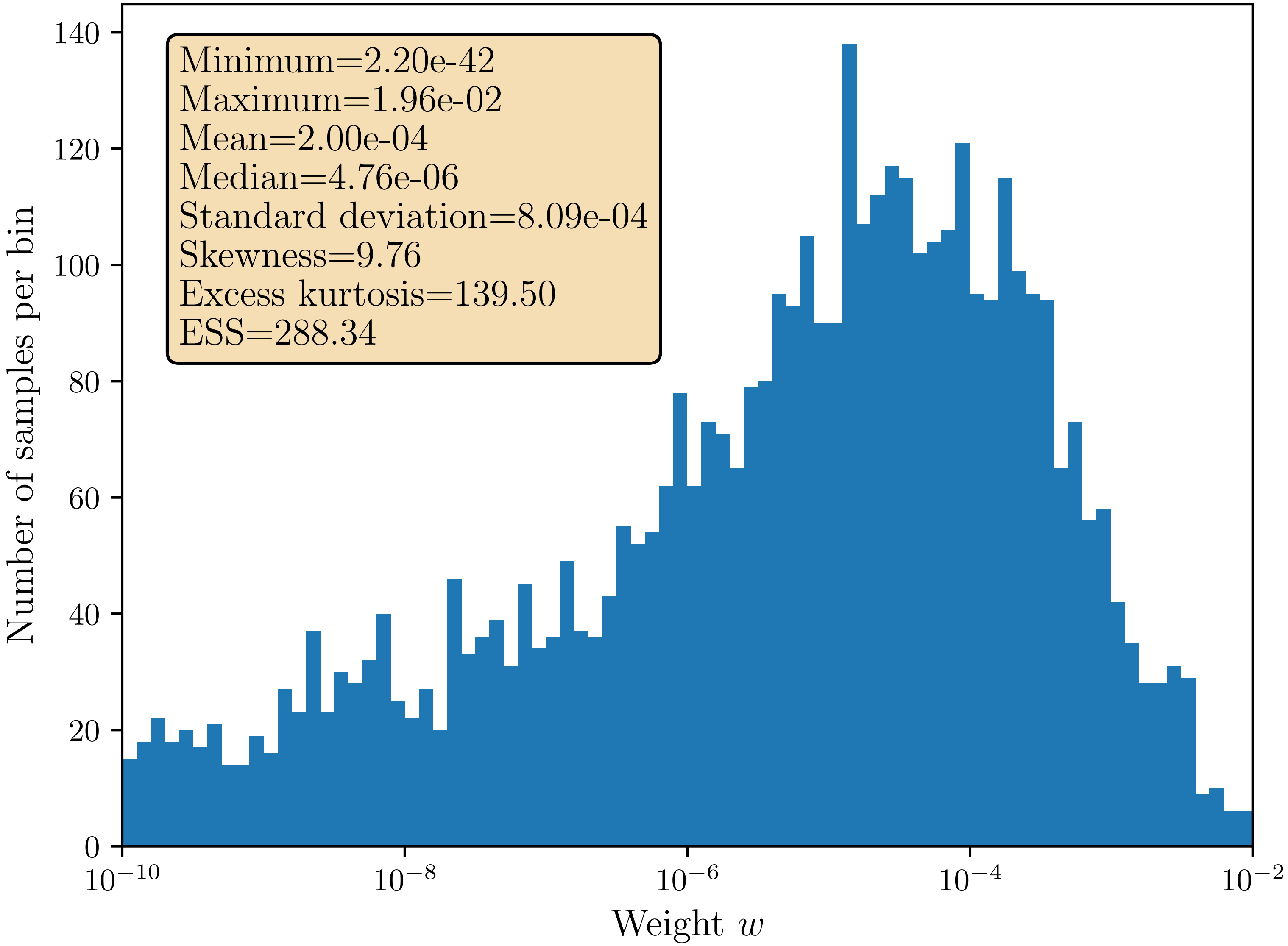


Minimum=26.35
Maximum=210.33
Mean=49.12
Median=43.00
Standard deviation=18.77
Skewness=2.46
Excess kurtosis=8.68

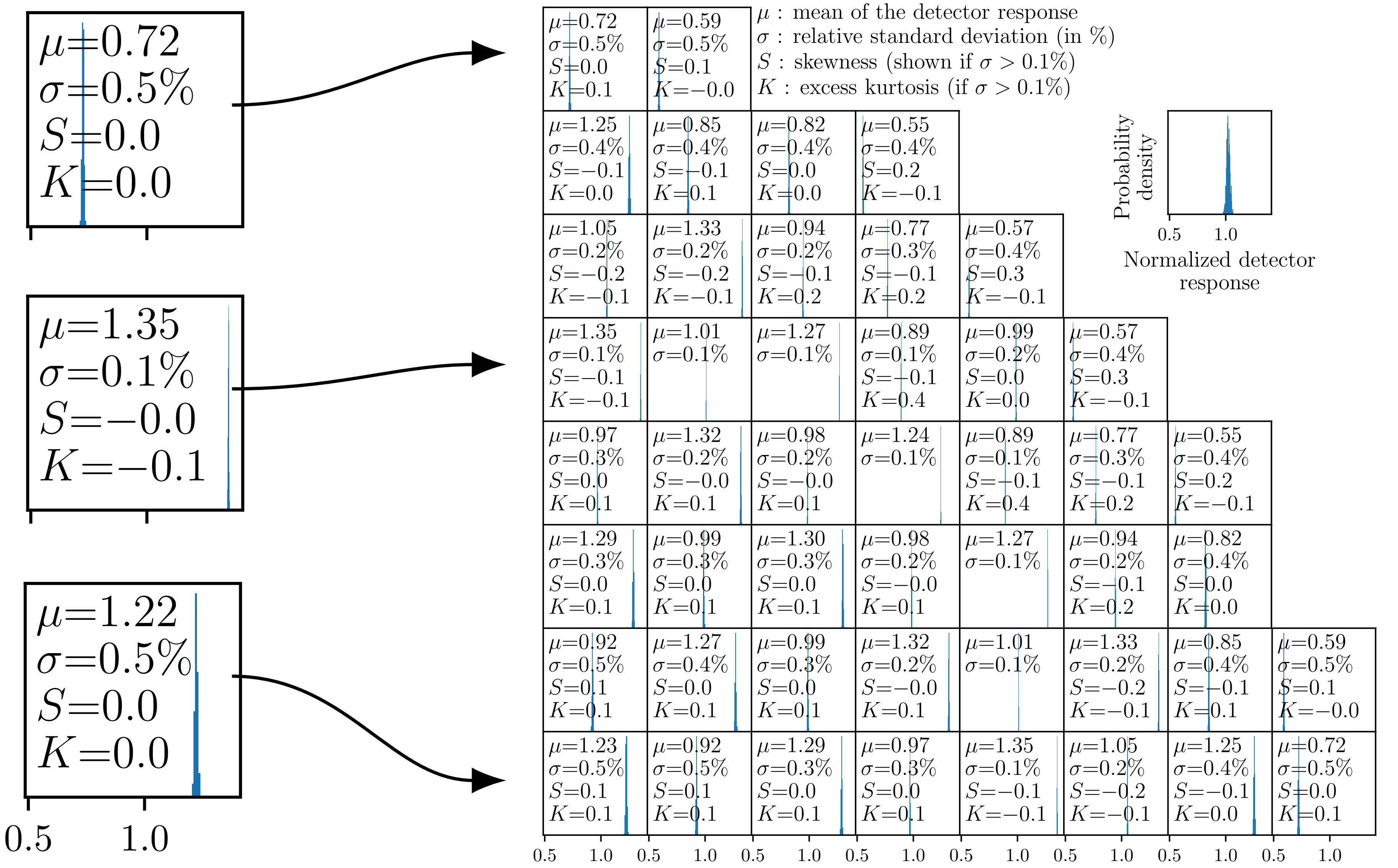
# $w$ weight histogram obtained with BFMC



# $w$ weight histogram obtained with BMC

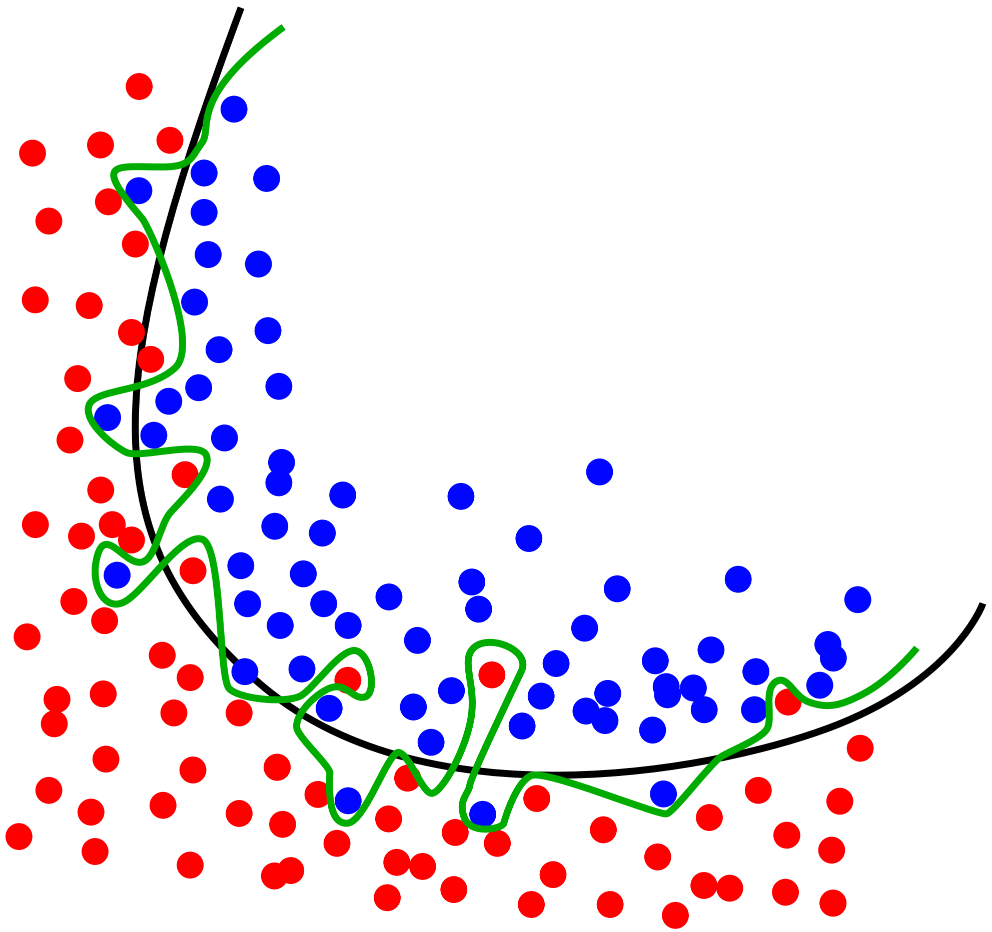


# Posterior (BMC) detector responses



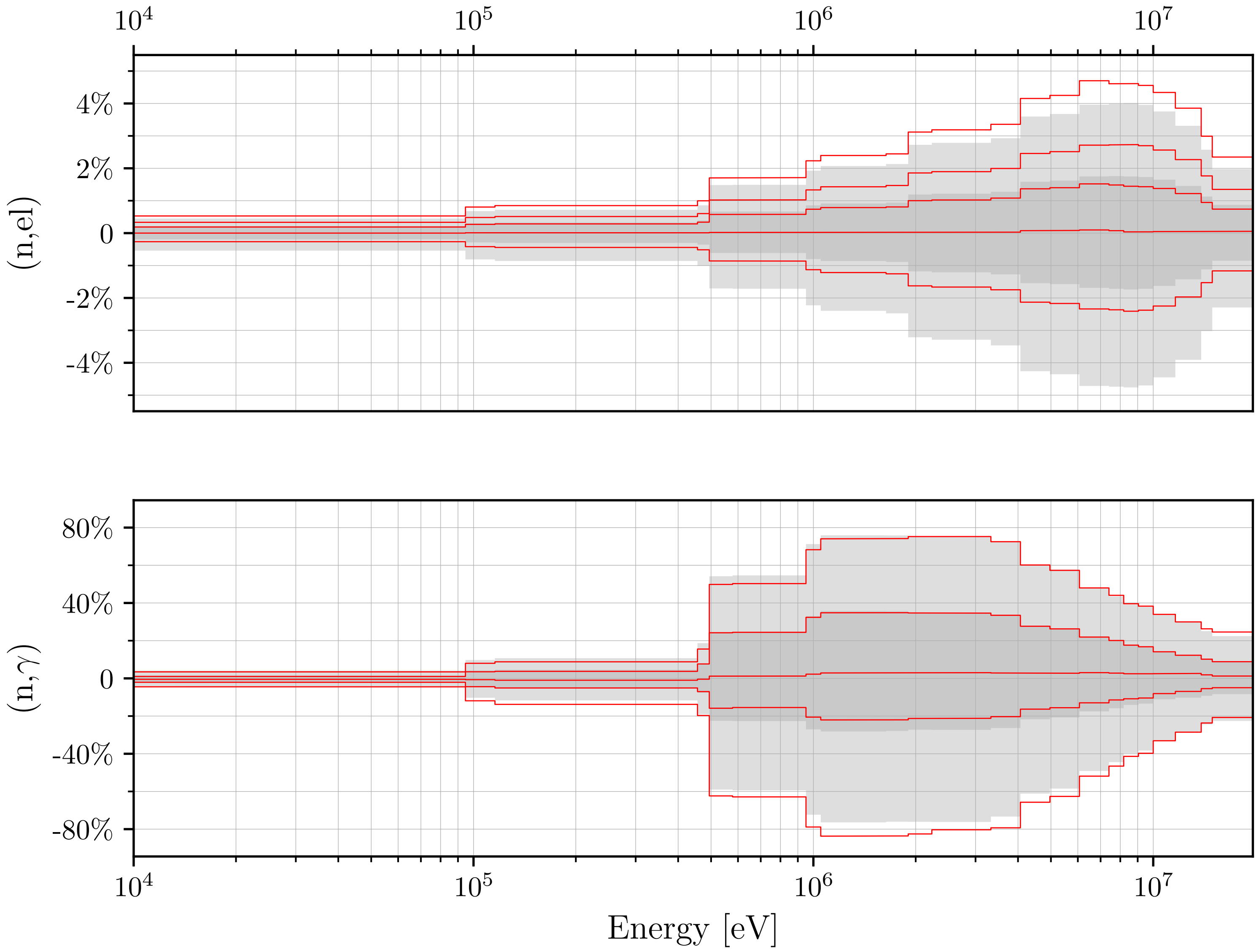
$\mu$ : mean of the detector response
$\sigma$ : relative standard deviation (in %)
$S$ : skewness (shown if $\sigma > 0.1\%$)
$K$ : excess kurtosis (if $\sigma > 0.1\%$)

# Overfitting illustration, in green

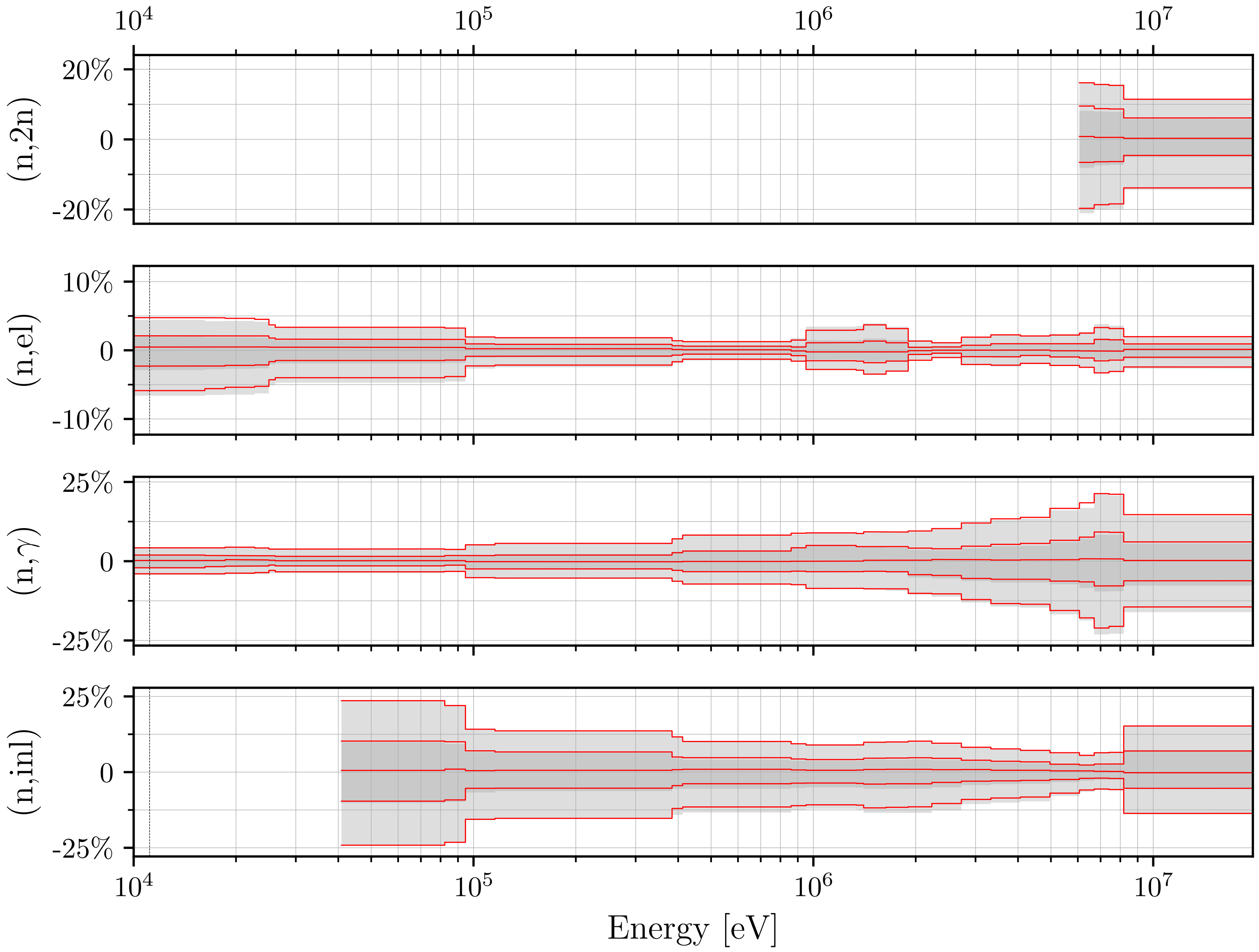


Credits : I. ICKE, Creative Commons BY-SA 4.0 `https://commons.wikimedia.org/wiki/File:Overfitting.svg`

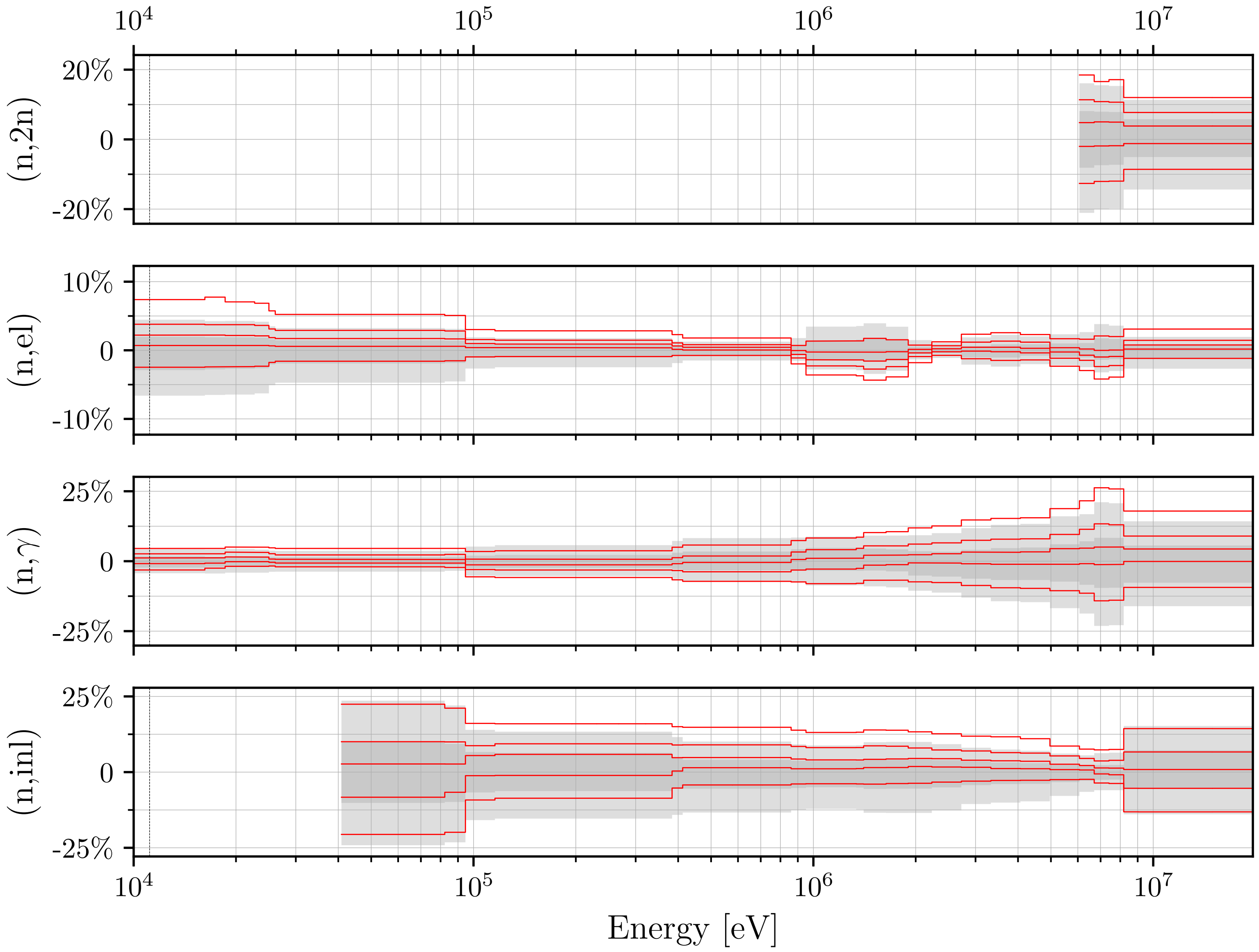
# Modifications (red) to five prior quantiles (grey) of **hydrogen** cross sections, with BMC



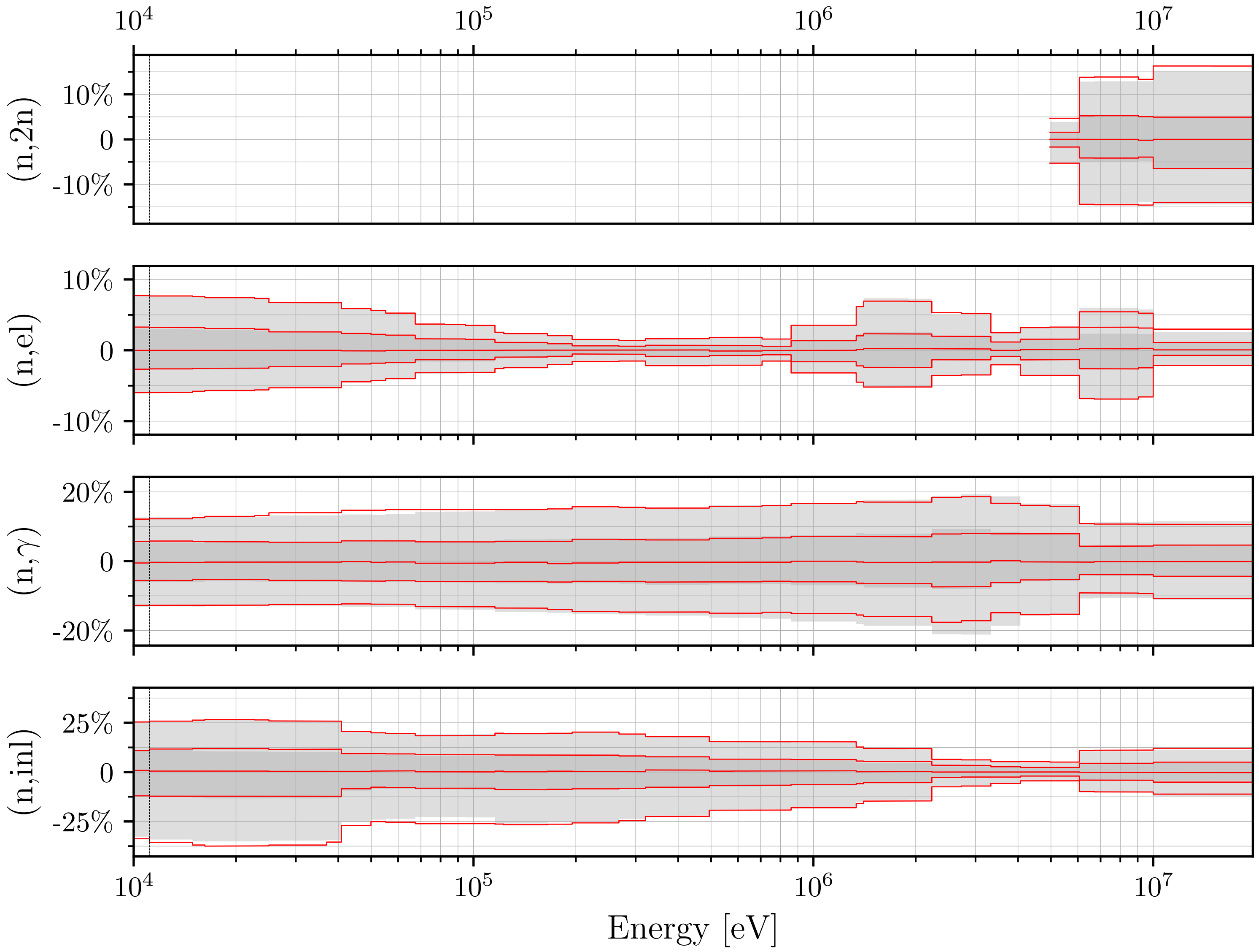
# Modifications (red) to five prior quantiles (grey) of **uranium 238** cross sections, with BFMC



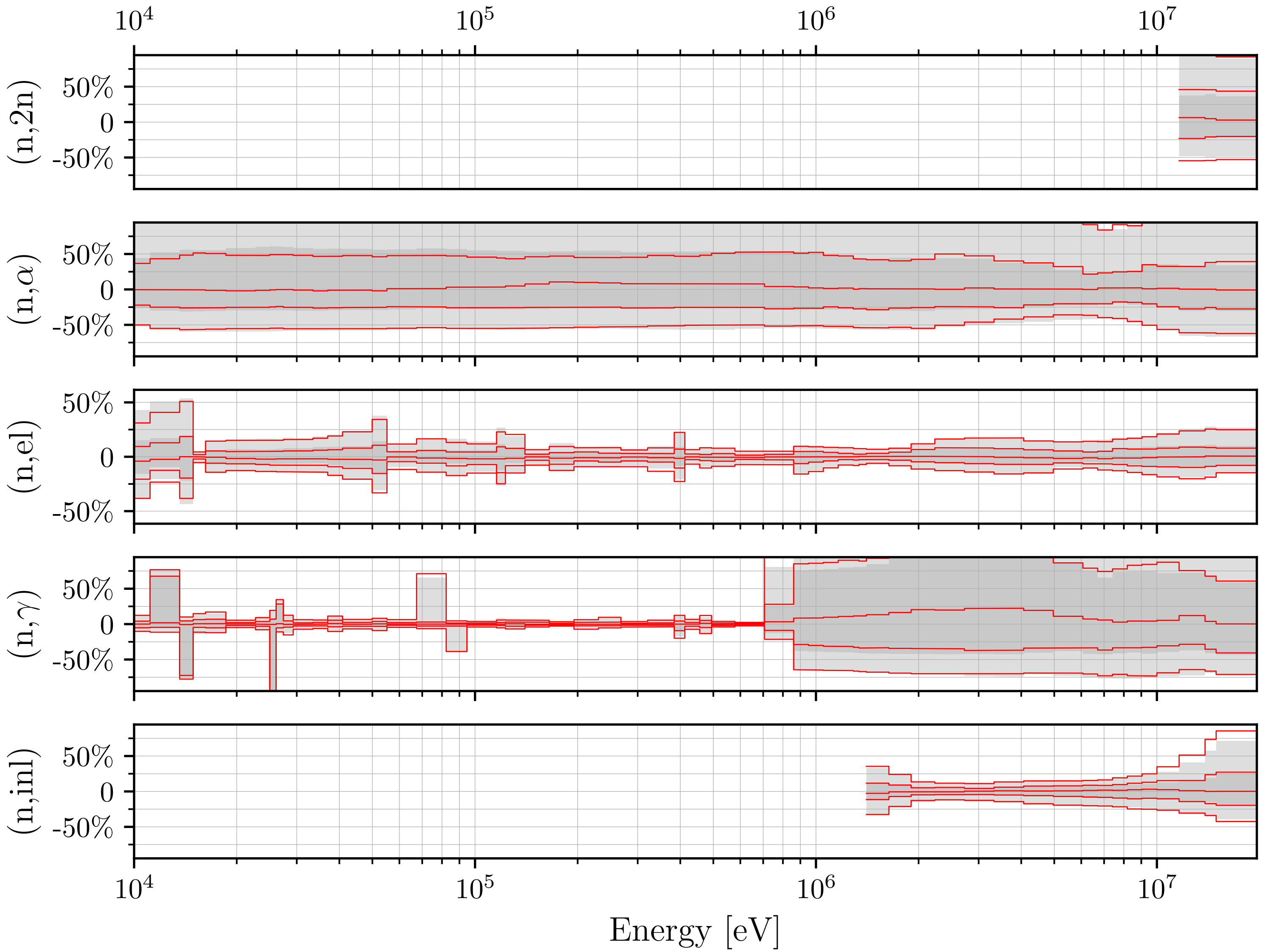
# Modifications (red) to five prior quantiles (grey) of uranium 238 cross sections, with BMC



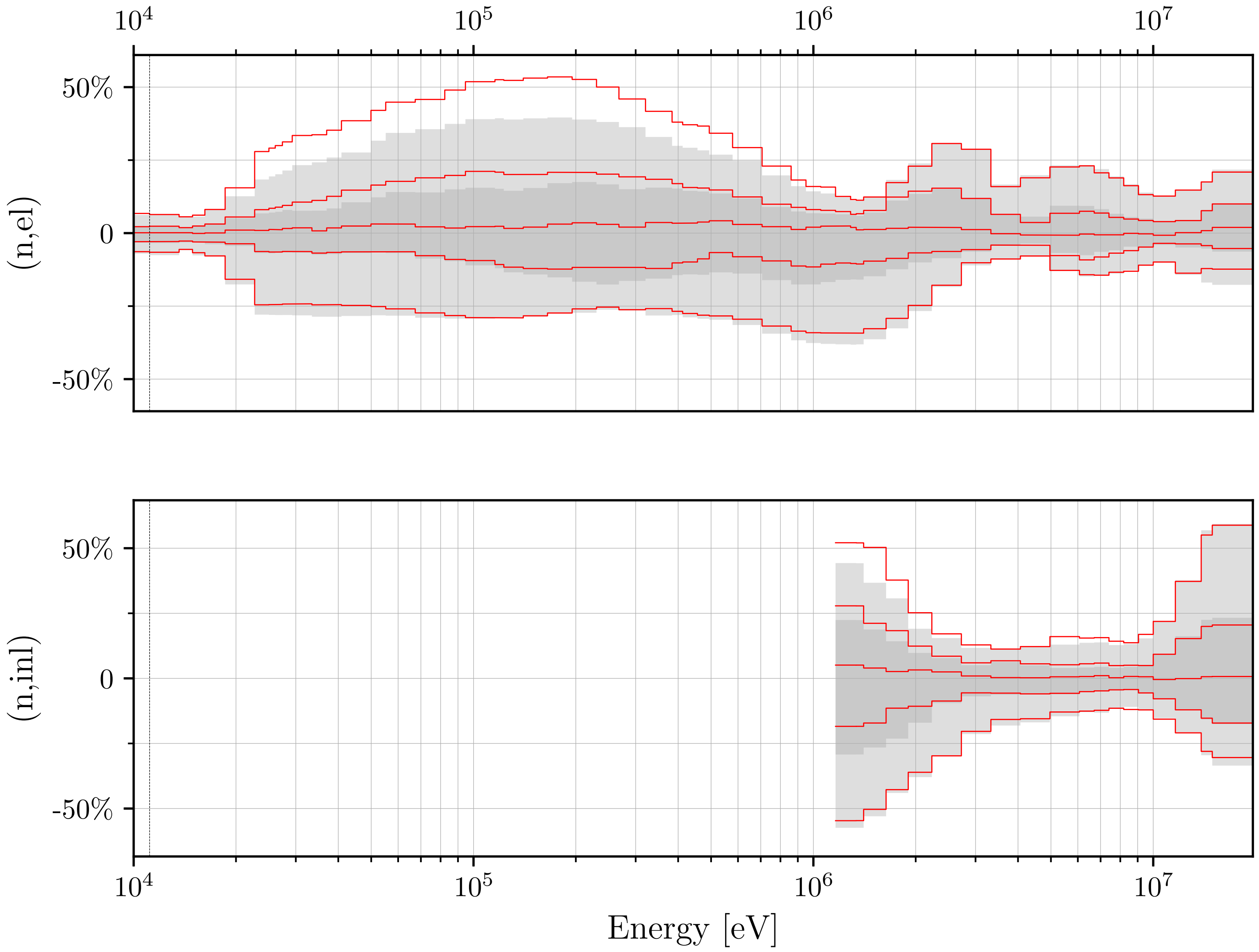
# Modifications (red) to five prior quantiles (grey) of uranium 235 cross sections, with BMC



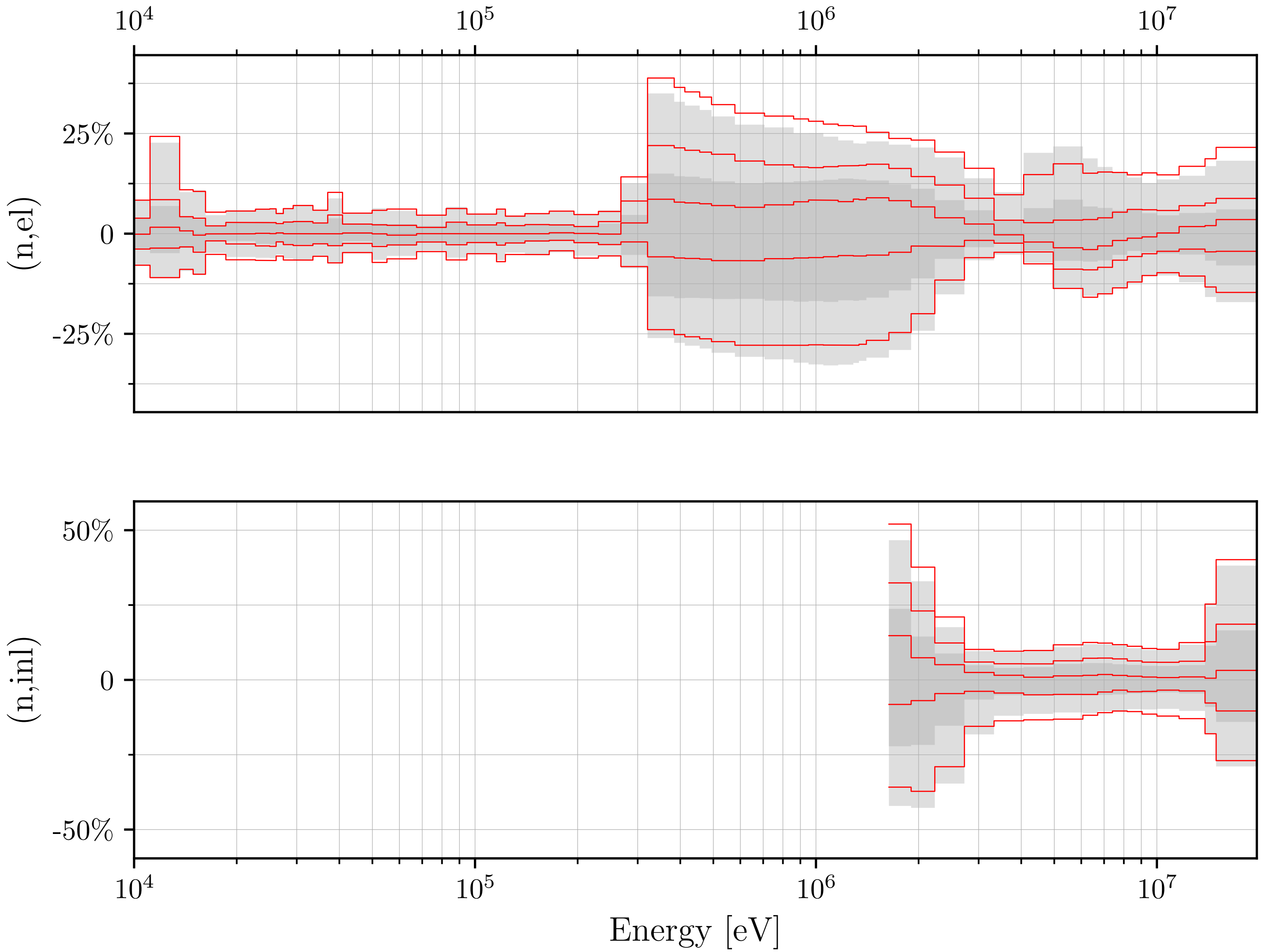
# Modifications (red) to five prior quantiles (grey) of **nickel 58** cross sections, with BMC



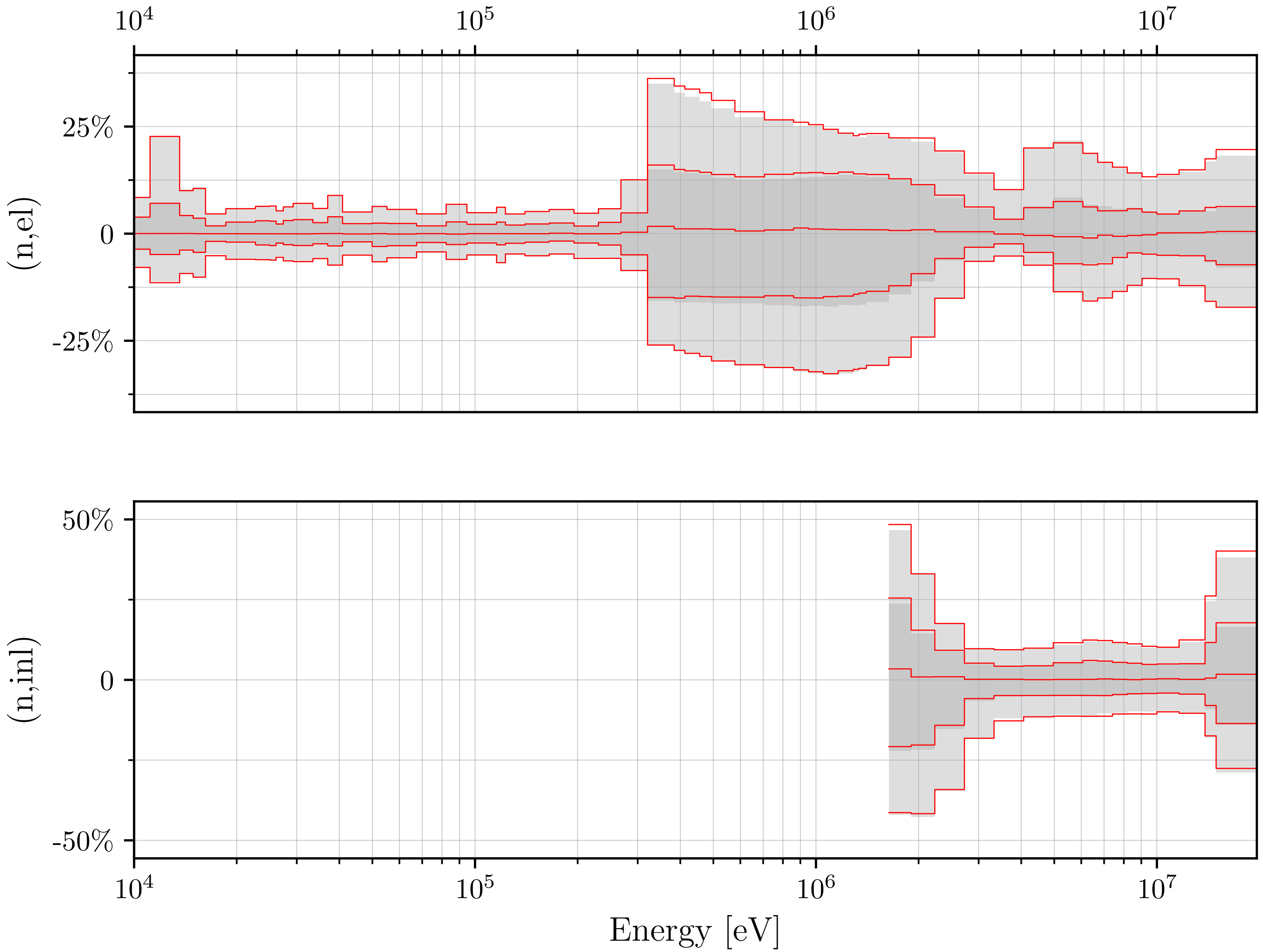
# Modifications (red) to five prior quantiles (grey) of **zirconium 91** cross sections, with BMC



# 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

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

- 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

# PyNjoy2016: an Open Source System for Producing Cross Sections Libraries for DRAGON5 and SERPENT2

V. Salino[1,2] and A. Hébert[1]

[1] École Polytechnique de Montréal, Institut de Génie Nucléaire, Canada
[2] Institut de Radioprotection et Sûreté Nucléaire (IRSN), PSN-RES/SNC/LN, France

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

# Introduction : what is PyNjoy2016 ?

- ➔ Python wrapper around NJOY2016, in a modified and improved version
- ➔ Streamlines processing of complete nuclear data evaluations, producing consistent
  - ➛ multigroup libraries for DRAGON5, in Draglib format
  - ➛ continuous-energy libraries for SERPENT2, in mixed ACE+ENDF-6 format

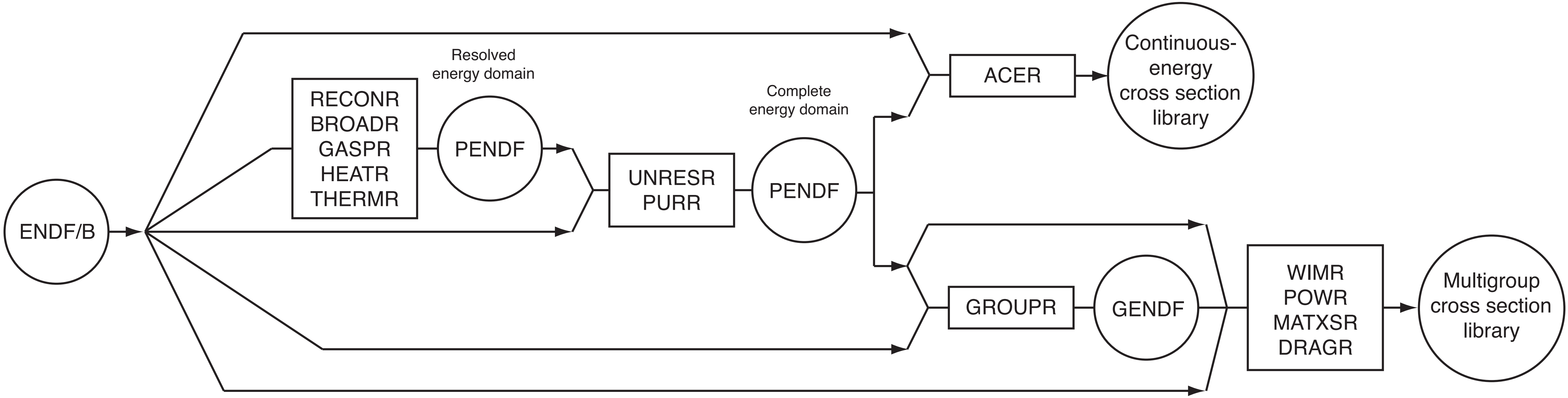


Figure : PyNjoy2016 data flow

# A consistent production of multigroup and continuous-energy libraries

- ➔ Tempting to think that an evaluation can only result in a single ACE file (no multigroup approximation)
- ➔ But it does depend on NJOY version and options
- ➔ Almost inevitably, different NJOY versions and options used for multigroup library and for default ACE files (as delivered with Monte-Carlo codes)
- ➔ Implies inconsistencies when comparing deterministic and Monte-Carlo codes
- ➔ This additionnal error is most often incorrectly attributed to the deterministic code, on account of its deterministic bias, which is then inaccurately evaluated
- ➔ For example, 100 pcm difference on $k_{\mathrm{eff}}$ between

  — ACE files produced with PyNjoy2016

  — ACE files delivered by default with SERPENT2

  based on JEFF-3.1.1 in both cases, on first start-up of Tihange-1
- ➔ Vast majority of comparisons between Monte-Carlo and deterministic codes in public and industrial literature are affected by these inconsistencies
- ➔ Computing deterministic bias requires consistency in nuclear data processing

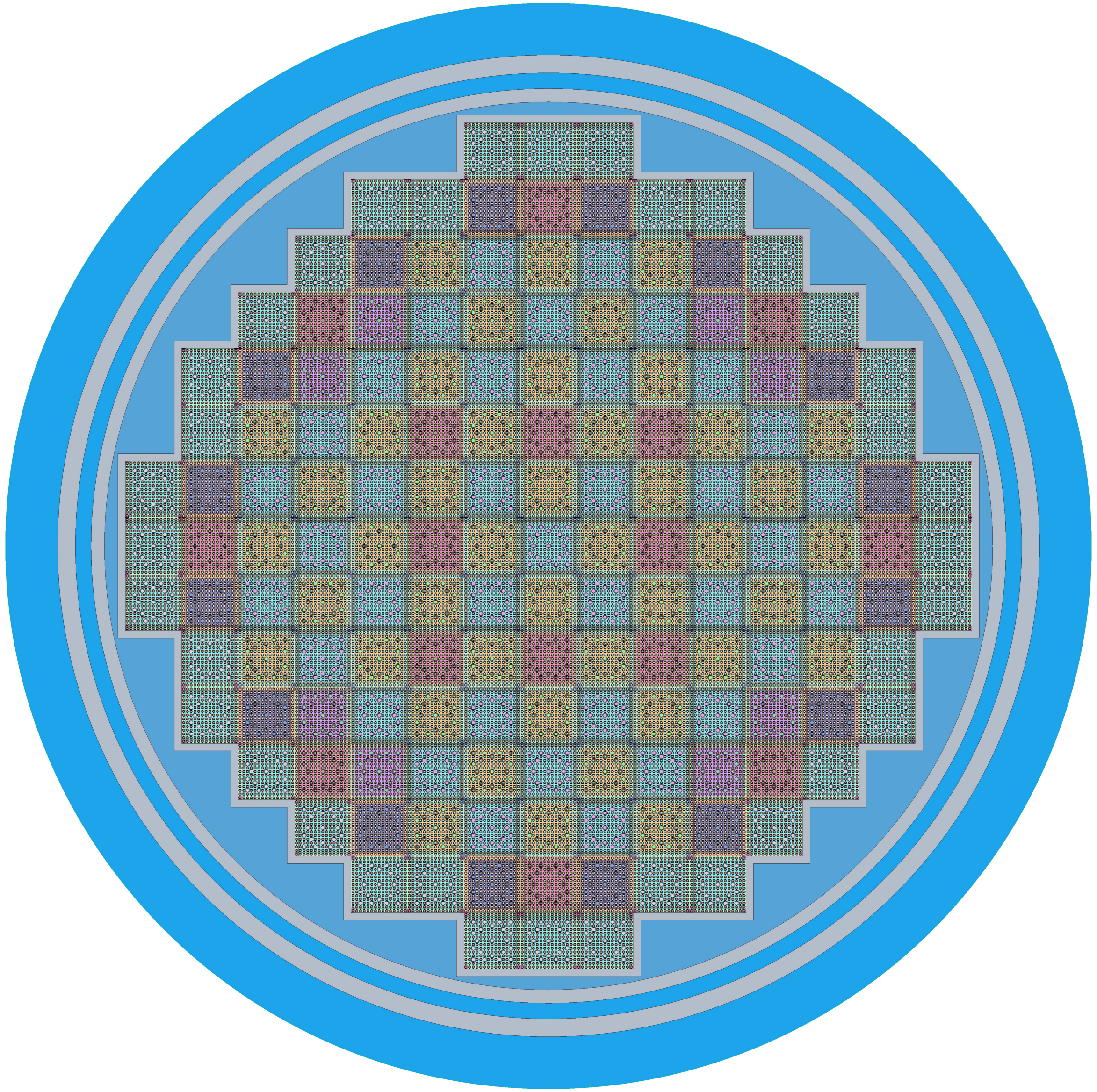
# A lesson learned during non-regression verification : Effective multiplication factor discrepancies, versus PyNjoy2012

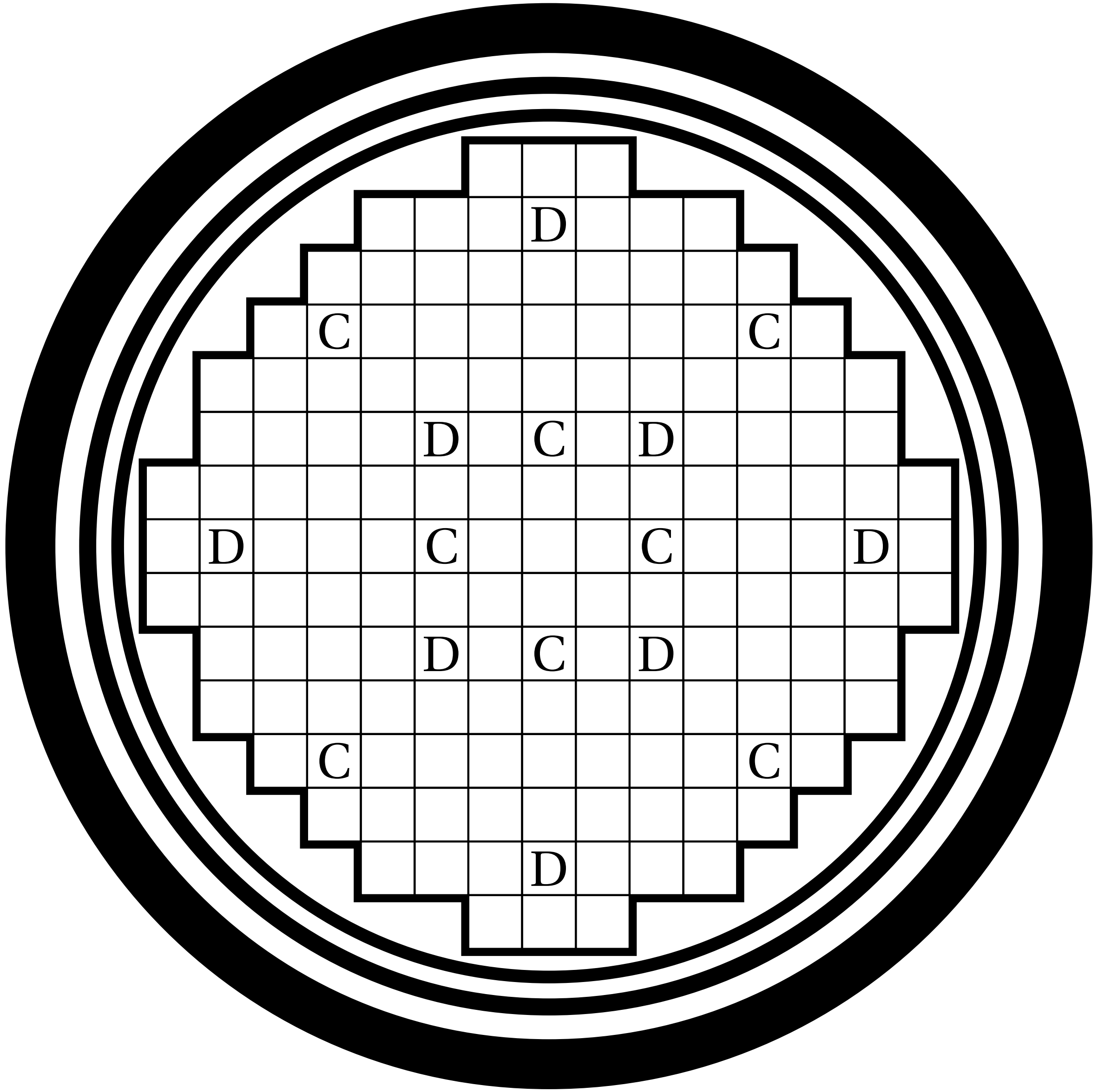
$\Delta \ln k_{\mathrm{eff}}$ (pcm) on Rowland's PWR pincell, with DRAGON5 and 172 energy groups :

| | Burnup (MW·day per ton of initial heavy metal) | 0 | 36,8 | 1000 | 2500 | 5000 |
|---|---|---|---|---|---|---|
| Ⓐ | NJOY2016 with 118 points in THERMR (default) | 15,9 | 15,5 | 4,7 | 8,2 | 10,5 |
| Ⓑ | NJOY2016 with 357 points in THERMR | −0,4 | −0,4 | −0,2 | −0,3 | −0,3 |
| Ⓒ | NJOY2016 with 357 points in THERMR and backporting the universal physical constants from NJOY2012 | 0 | 0 | 0 | 0 | 0 |
| Ⓓ | NJOY99 with 357 points in THERMR | 0 | 0 | 0 | 0 | 0 |

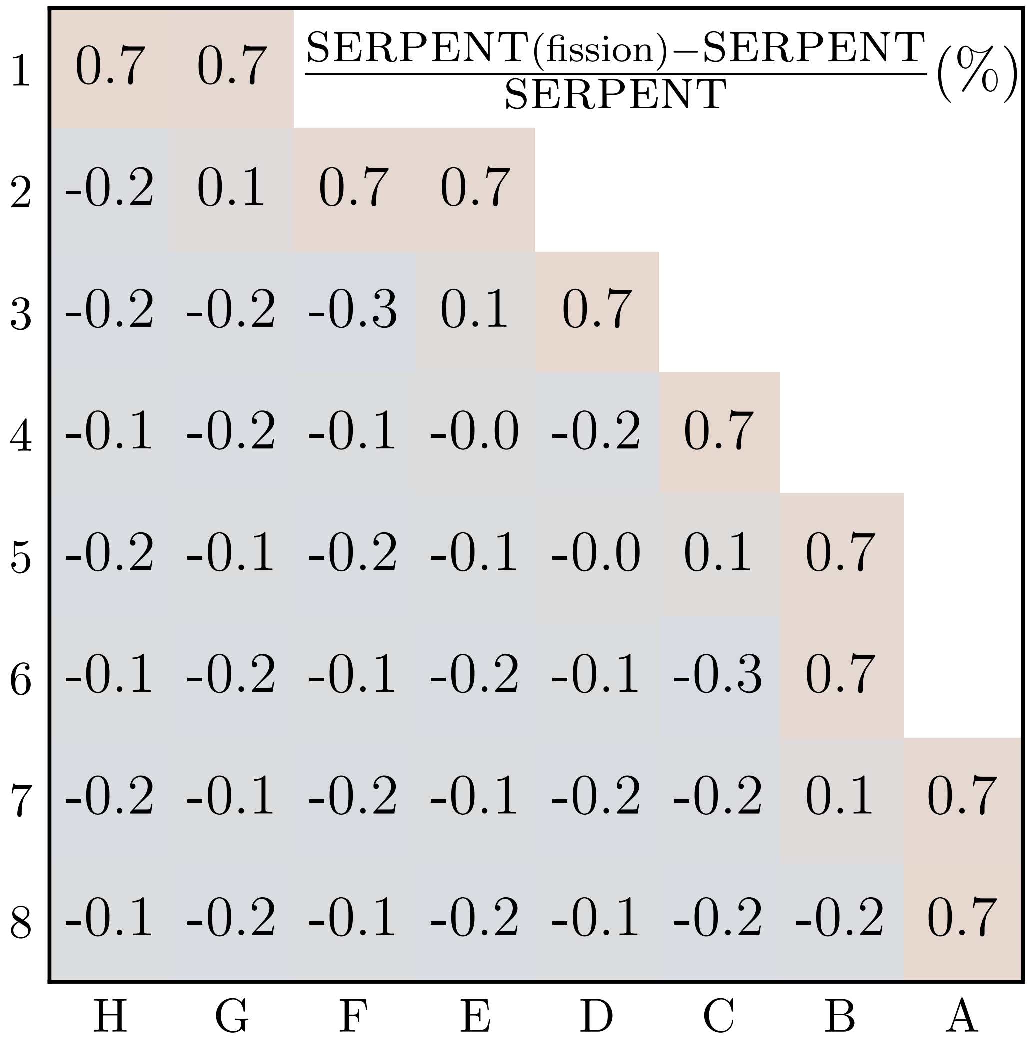
- ➔ Discrepancies mostly due to thermal scattering : NJOY uses an insufficient discretization of the incident energies, in THERMR (`calcem` subroutine)
- ➔ Can reach hundreds of pcm in more thermalized systems (Yamamoto and Sugimura, 2006)
- ➔ Both deterministic and Monte-Carlo codes are affected by this THERMR deficiency
- ➔ Strongly recommend refining this energy grid, without waiting for a complete overhaul of THERMR ➛ meanwhile, NJOY users are getting a biased answer

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





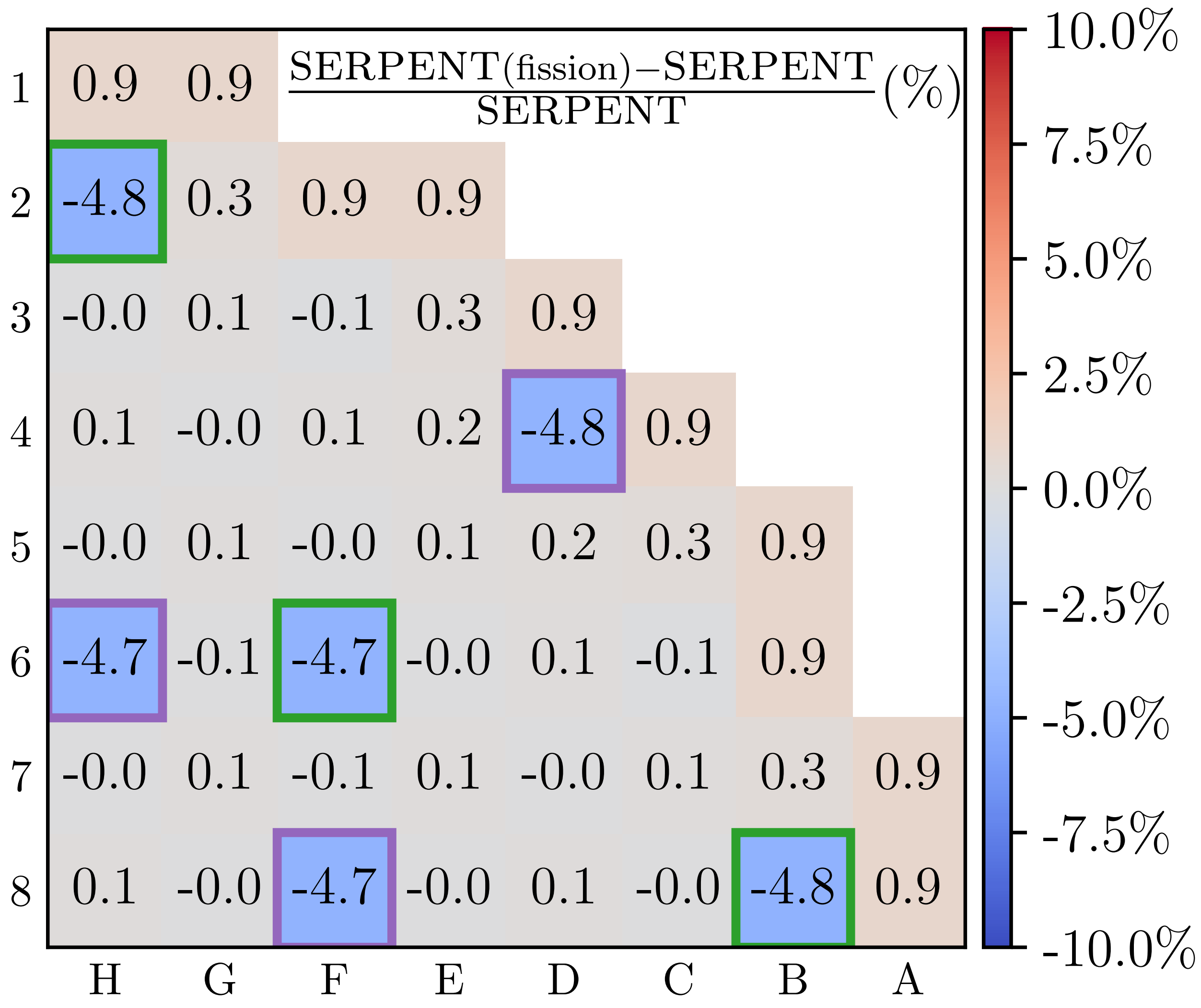
# Impact of energy deposition model (1/2)
## Default in SERPENT2 : an approximate energy is deposited only at fission sites



$\frac{\text{SERPENT(fission)}-\text{SERPENT}}{\text{SERPENT}}$ (%)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.7 | 0.7 | | | | | | |
| 2 | -0.2 | 0.1 | 0.7 | 0.7 | | | | |
| 3 | -0.2 | -0.2 | -0.3 | 0.1 | 0.7 | | | |
| 4 | -0.1 | -0.2 | -0.1 | -0.0 | -0.2 | 0.7 | | |
| 5 | -0.2 | -0.1 | -0.2 | -0.1 | -0.0 | 0.1 | 0.7 | |
| 6 | -0.1 | -0.2 | -0.1 | -0.2 | -0.1 | -0.3 | 0.7 | |
| 7 | -0.2 | -0.1 | -0.2 | -0.1 | -0.2 | -0.2 | 0.1 | 0.7 |
| 8 | -0.1 | -0.2 | -0.1 | -0.2 | -0.1 | -0.2 | -0.2 | 0.7 |
| | H | G | F | E | D | C | B | A |

All rods out



$\frac{\text{SERPENT(fission)}-\text{SERPENT}}{\text{SERPENT}}$ (%)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.9 | 0.9 | | | | | | |
| 2 | -4.8 | 0.3 | 0.9 | 0.9 | | | | |
| 3 | -0.0 | 0.1 | -0.1 | 0.3 | 0.9 | | | |
| 4 | 0.1 | -0.0 | 0.1 | 0.2 | -4.8 | 0.9 | | |
| 5 | -0.0 | 0.1 | -0.0 | 0.1 | 0.2 | 0.3 | 0.9 | |
| 6 | -4.7 | -0.1 | -4.7 | -0.0 | 0.1 | -0.1 | 0.9 | |
| 7 | -0.0 | 0.1 | -0.1 | 0.1 | -0.0 | 0.1 | 0.3 | 0.9 |
| 8 | 0.1 | -0.0 | -4.7 | -0.0 | 0.1 | -0.0 | -4.8 | 0.9 |
| | H | G | F | E | D | C | B | A |

Inserted control rods (purple and green boxes)

# Impact of energy deposition model (2/2)

## SERPENT2 advanced energy deposition model

- When comparing codes, the most common attitude regarding the previous approximate model is to ignore its consequences
- Here again, a deterministic code is often blamed for this error, erroneously labeled as deterministic bias
- SERPENT2 also features an advanced energy deposition model
- For that, relies on files mixing ACE and ENDF-6 formats, but such files are not widely available
- PyNjoy2016 has the ability to produce such ACE+ENDF-6 files, to compute properly
  - Power distribution, even without depletion
  - Depletion, because burnup is an amount of energy deposited (MW·day) per unit mass (ton) ➛ if incorrectly estimated, a drift will appear during depletion, even on $k_{\text{eff}}$
- Unresolved resonance range has no tangible impact on our use case, but is nevertheless properly taken into account in PyNjoy2016 for potential future uses on systems with larger proportions of fast or epithermal neutrons
- PyNjoy2016 also supports energy deposition following photon transport

# Propagation of uncertainties related to nuclear data (1/2)

1) Perturbation theory ➛ some drawbacks

- ➔ Difficult to propagate through self-shielding or a multiphysics coupling (transients, etc)
- ➔ Cannot access the complete distribution, but only the mean and standard deviation

Advantage ➛ very fast and powerful, as long as its drawbacks are not blocking issues for the desired use

2) Total Monte-Carlo (sampling)

- ➔ Propagation through subsequent codes without modification or simplification of any kind (self-shielding, multiphysics. . .)
- ➔ Access the complete distribution on a quantity of interest, without approximation
- ➔ Reference solution, comes with higher computational cost
- ➔ Convergence must be verified

# Propagation of uncertainties related to nuclear data (2/2)

PyNjoy2016 has capability to produce randomly sampled ACE and DRAGLIB files on multiple CPUs (in parallel), taking as a basis either :

1) presampled TENDL files in ENDF-6 format, sampled upstream of its nuclear physics models
   - ➔ Continuously varying uncertainties
   - ➔ Not necessarily Gaussian
   - ➔ But no TENDL files for most important heavy isotopes ($^{233,235,238}$U, $^{239}$Pu, $^{232}$Th) and nor for lightest nuclei, consisting of less than 20 nucleons, due to optical model limitations

2) ENDF-6 files sampled Gaussianly within multigroup covariance matrices, with on-the-fly calls to SANDY (Fiorito, 2017)
   - ➔ More adventurous path, since covariance formats are more heterogeneous than the homogeneous TENDL formats (derived from a single code chain)

See companion presentation on Wednesday evening for such an uncertainty propagation

# Shall we merge DRAGR into NJOY2016 main branch ?

- ➔ NJOY2016 documentation says that "the mission of NJOY is to take basic data from the nuclear data library and convert it into the forms needed for applications"
- ➔ Therefore, we believe DRAGR should be integrated into NJOY2016 main branch
- ➔ Without such an inclusion, the NJOY community may become increasingly divided, having more different versions being used, instead of benefiting from a community effect
- ➔ Added a non-regression test similar to those of NJOY2016, but specific to DRAGR
  - — Using the same ENDF-6 files already used in the non-regression testing of NJOY2016 (does not burden its repository)
  - — As short as possible : does not include all the isotopes of an evaluation (typically between 300 and 800 isotopes), however all possible use cases are covered
- ➔ DRAGR is thoroughly documented, in a LaTeX section following NJOY documentation format

- ➔ Same path should apply to resonant upscattering RESKR module, originally from NECP-Atlas (J. Xu, T. Zu and L. Cao, Xi'an Jiaotong University, China, 2019)

# Conclusions

- ➔ PyNjoy2016 is dedicated to the production of :
  - ➢ multigroup libraries in DRAGLIB format, for the DRAGON5 deterministic code
  - ➢ continuous-energy ACE files, supporting the deposition energy model of SERPENT2
- ➔ Deterministic bias of a calculation scheme based on DRAGON5 can now be precisely calculated by consistently comparing its results with SERPENT2
- ➔ Such a consistency is a rare feature provided by the simultaneous library production : the same NJOY2016 run, in the same version and with the same options are used to produce both libraries
- ➔ As an example of its importance, 100 pcm reactivity difference between ACE files delivered with SERPENT2 and those produced with PyNjoy2016 (for same nuclear data)
- ➔ Open nature of NJOY2016 implies that PyNjoy2016 can be fully open source software (BSD license)

github.com/IRSN/PyNjoy2016

- ➔ Usefully complementing the state-of-the-art DRAGON5 deterministic lattice code, also open source and, in that sense, unique

# Acknowledgments

- ➔ Dimitri Rochman (PSI) for his advices on TENDL, SANDY, covariances and more generally on Total Monte-Carlo
- ➔ Riku Tuominen (VTT) for sharing with us his `runnjoy_kermas.pl` Perl script that enables SERPENT2 precise energy deposition model
- ➔ Nicolò Abrate (Politecnico di Torino) for releasing his NDL software (Nuclear Data Library processing tools) which helped us ordering the NJOY module calls, in particular regarding PURR, HEATR and GASPR
- ➔ Paul Romano (ANL) for his fruitful remarks on THERMR