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Microscopic correlations from integral data through Monte Carlo sampling:

Lessons learned from the past 3 years at PSI and CEA

SG44 meeting, NEA, Paris, 26 November 2019

Summary

- Motivation
- Short description on BFMC/BMC
- Inter-isotope covariance found from EXFOR
- Inter-isotope covariance found from fast criticality benchmarks (keff + spectral indexes)
- Inter-isotope covariance found from reactor cycles (boron curve)
- Conclusion

References used in this presentation

- E. Bauge, P. Dossantos-Uzarralde, “*Evaluation of the Covariance Matrix of 239Pu Neutronic Cross Sections in the Continuum Using the Backward-Forward Monte-Carlo Method*”, J. Kor. Phys. Soc. 59 (2011) 1218.

- D. Rochman, E. Bauge, A. Vasiliev and H. Ferroukhi, “*Correlation nu-sigma-chi in the fast neutron range via integral information*”, EPJ/N 3 (2017) 14.

- D. Rochman, E. Bauge, A. Vasiliev, H. Ferroukhi and G. Perret, “*Nuclear data correlation between different isotopes via integral information*”, EPJ/N 4 (2018) 7.

- E. Bauge and D. Rochman, “*Cross-observables and cross-isotopes correlations in nuclear data from integral constraints*”, EPJ/ N 4 (2018) 35.

- D. Rochman, E. Bauge, A. Vasiliev, H. Ferroukhi, S. Pelloni, A.J. Koning and J.Ch. Sublet, “*Monte Carlo nuclear data adjustment via integral information*”, EPJ Plus 133 (2018) 537.

- D. Rochman, A. Vasiliev, H. Ferroukhi, S. Pelloni, E. Bauge and A.J. Koning, “*Correlation nu-sigma for U-Pu in the thermal and resonance neutron range via integral information*”, EPJ Plus 133 (2019) 453.

- J.-Ch. Sublet et al., “*Neutron-induced damage simulations: Beyond defect production cross-section, displacement per atom and iron-based metrics*”, EPJ Plus 134 (2019) 350.

BMC/BFMC + differential/integral data

- Motivation 1: integral data are already used during adjustment
- Motivation 2: This should be done at the evaluation level
- Motivation 3: It leads to uncertainty reduction and cross-isotope correlations
- Motivation 4: Modern transport tools can be used (Monte Carlo)
- Motivation 5:nothing new: already done with GLLS by SG… at the OECD

BMC/BFMC + differential/integral data

- Step 1 - Preliminary work: in-depth cross section evaluation (traditional method of parameters/models adjustment)

- Step 2 - BMC: Based on step 1,
  - Generate n=100 000 (or 1000) random files (TMC-way)
  - Calculate n times the benchmarks
  - Assign weights to all realizations *i* with a chi2 and update the parameter distributions

For a random file i and a set of p benchmarks:

$$\chi_i = \sum_j^p \left(\frac{\mathrm{k}_{\mathrm{eff,i}}^{(\mathrm{j})} - \mathrm{k}_{\mathrm{exp}}^{(\mathrm{j})}}{\Delta \mathrm{k}^{(\mathrm{j})}} \right)^2 \quad (1)$$

$$w_i = \exp(-\frac{\chi_i}{2}) \quad (2)$$

$$\begin{cases} \omega = \sum_i^n w_i \\ \omega_\sigma = \sum_i^n w_i \cdot \sigma_i / \omega \end{cases}$$

  - Update the cross sections with the weights.

- BFMC variation compared to BMC:

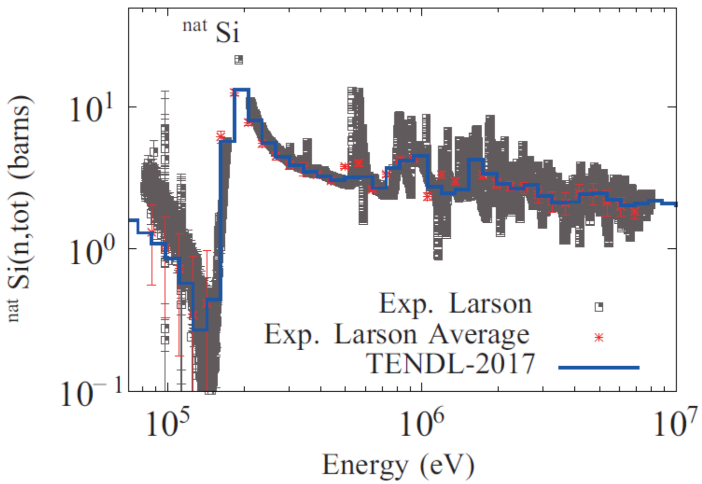
(EPJ/ N 4 (2018) 35,

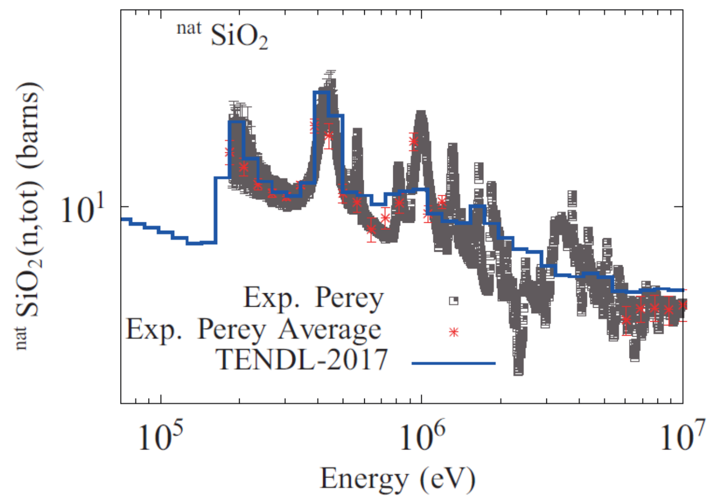
J. Kor. Phys. Soc. 59, 1218 (2011).)

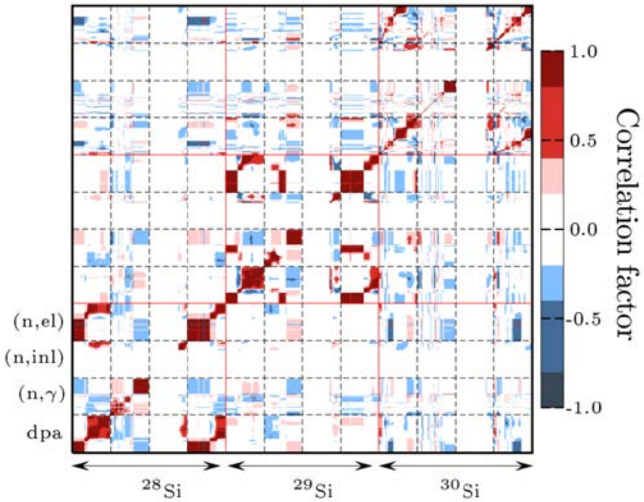
$$w_i = \exp\left[- \left(\frac{\chi_i^2}{\chi_{\min}^2} \right)^2 \right].$$

BMC/BFMC + EXFOR data:

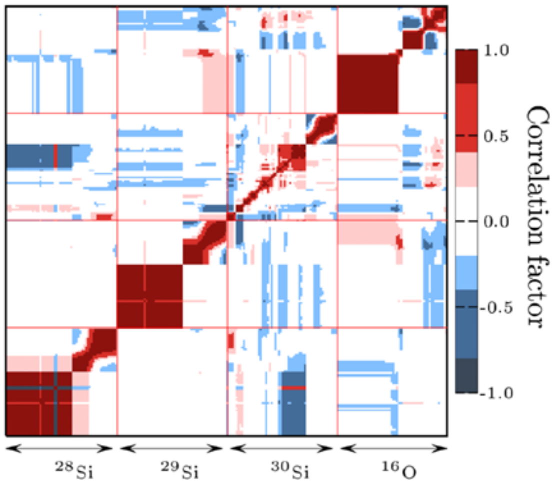
- Based on EXFOR only: Si + SiO_2 + ^{16}O (EPJ Plus 134 (2019) 350)







with SiO_2



(n,tot) only

BMC/BFMC + 1 fast benchmark (pmf1)

- Based on pmf1 : ^{239}Pu (EPJ/N 3 (2017) 14)

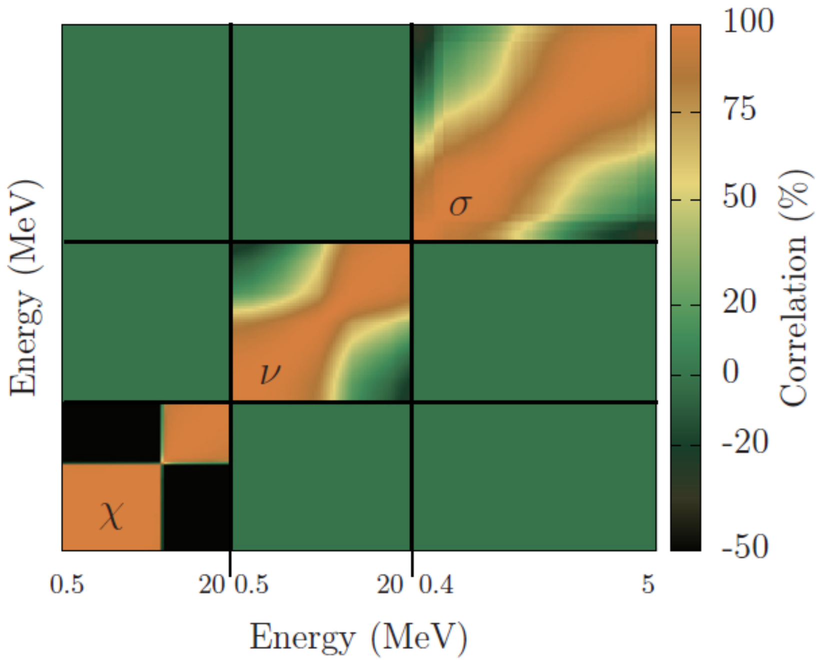


Fig. 2. Prior correlation matrix for ^{239}Pu ν, σ and χ (for the incident neutron energy of 750 keV). The energy axis is for the incident neutrons for ν and σ, and for the outgoing neutron for χ. The X- and Y-axis are in linear scale.

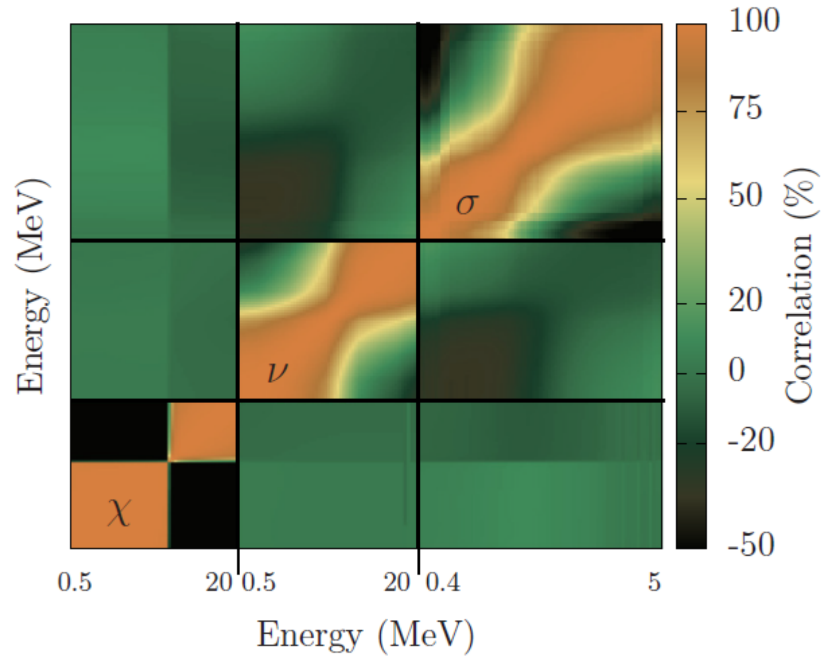


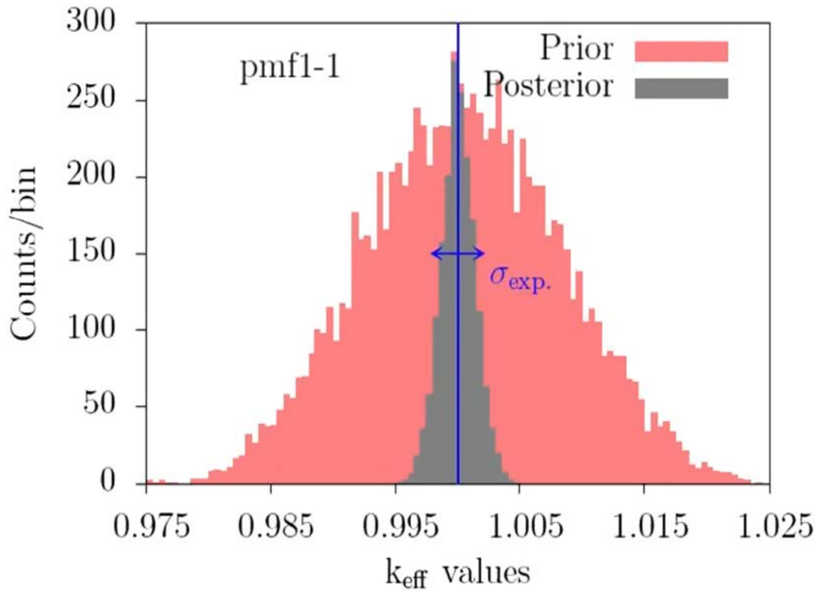
Fig. 5. Posterior correlation matrix for ^{239}Pu ν, σ and χ (for the incident neutron energy of 750 keV). The energy axis is for the incident neutrons for ν and σ, and for the outgoing neutron for χ. The X- and Y-axis are in linear scale.

BMC/BFMC + 1 fast benchmark (pmf1)

- Based on pmf1 : ^{239}Pu (EPJ/N 3 (2017) 14)

Table 1. Prior and posterior average k_{eff} and uncertainties for selected benchmarks. Uncertainties Δk are given in pcm. C/E values are also indicated.

Benchmark	Prior		Posterior		$C/E-1$ Prior (%)	$C/E-1$ Posterior (%)
	$\bar{k}$	$\pm\Delta k$	$\bar{k}$	$\pm\Delta k$		
pmf1	1.00082	±782	0.99999	±133	0.08	0.00
pmf2	1.00171	±705	1.00023	±143	0.17	0.02
pmf3-1	1.00240	±725	1.00016	±207	0.24	0.02
pmf5-1	1.00056	±782	1.00002	±93	0.06	0.02
pmf6-1	1.00156	±700	1.00018	±218	0.15	0.02
pmf13-1	1.00789	±770	1.00356	±160	0.45	0.01
pmf35-1	0.99755	±760	0.99994	±113	0.25	0.01
pmf44-1	0.99878	±695	0.99772	±144	0.11	0.00
pmi2-1	1.01766	±1018	0.98788	±209	3.11	0.10



BMC/BFMC + 1 fast benchmark (imf7)

- Based on imf7 : ^{235}U- ^{238}U (EPJ/N 4 (2018) 7)

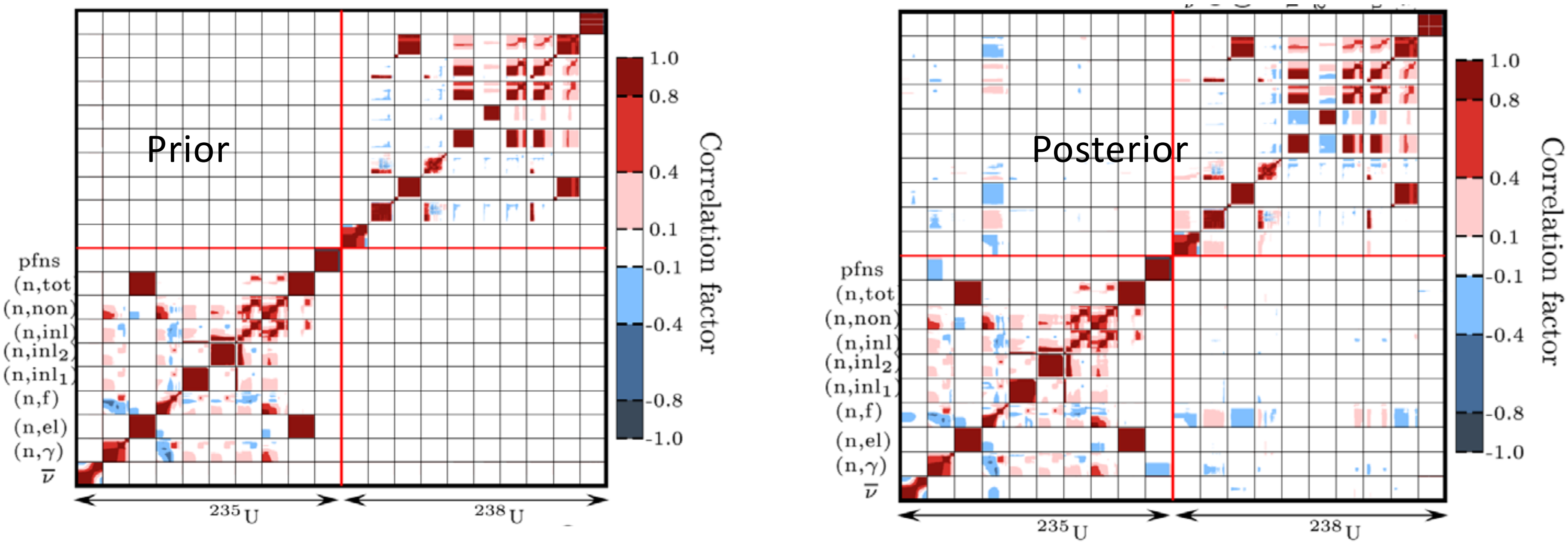


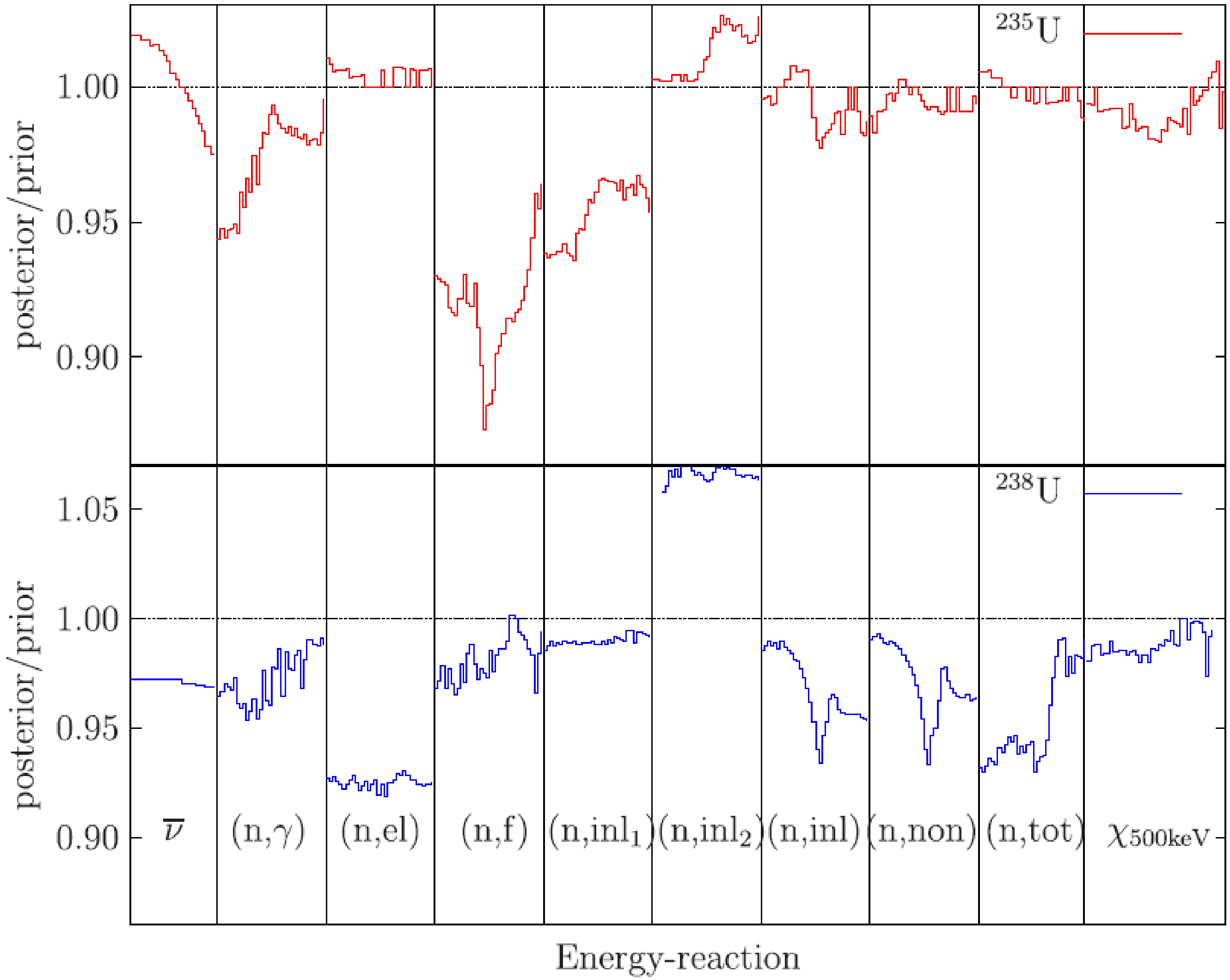
Table 3. Prior and posterior average k_{eff} and uncertainties for four benchmarks. Uncertainties Δk are given in pcm. C/E values are also indicated. The statistical uncertainty for each MCNP6 calculation is in the order of 25 pcm.

Benchmark	Used in Bayesian update	Exp		Prior		Posterior		Prior C/E-1	Posterior C/E-1
		k_{eff}	$\pm\Delta k$	$\overline{k}$	$\pm\Delta k$	$\overline{k}$	$\pm\Delta k$	(%)	(%)
imf7	yes	1.00450	±70	1.00156	±850	1.00446	±71	−0.29	−0.004
hmf1	no	1.00000	±100	0.99509	±1120	0.99691	±960	−0.49	−0.39
imf1-1	no	0.99880	±90	0.99767	±900	0.99984	±670	−0.11	0.10
lct6-1	no	1.00000	±200	0.99836	±405	0.99879	±440	−0.16	−0.12

BMC/BFMC + 1 fast benchmark (imf7)

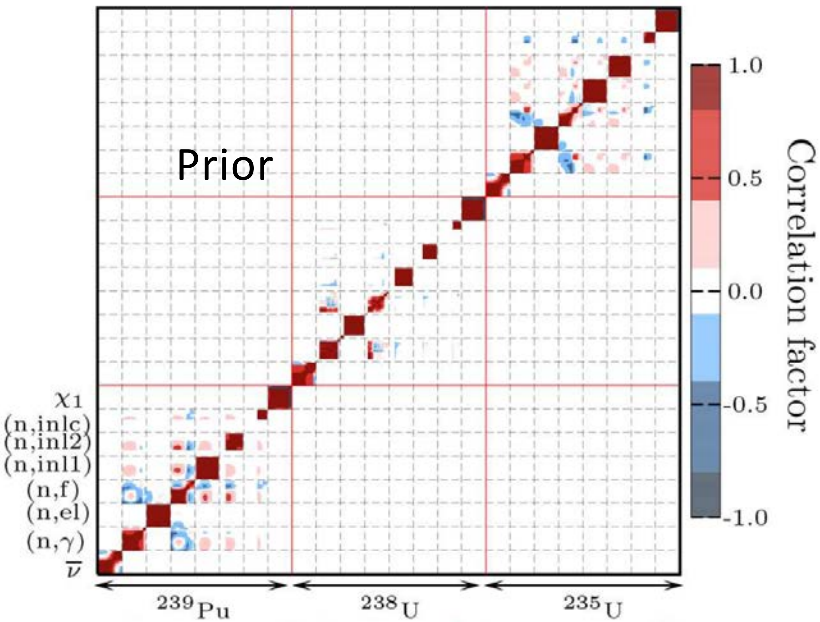
- Based on imf7 : ^{235}U- ^{238}U (EPJ/N 4 (2018) 7)

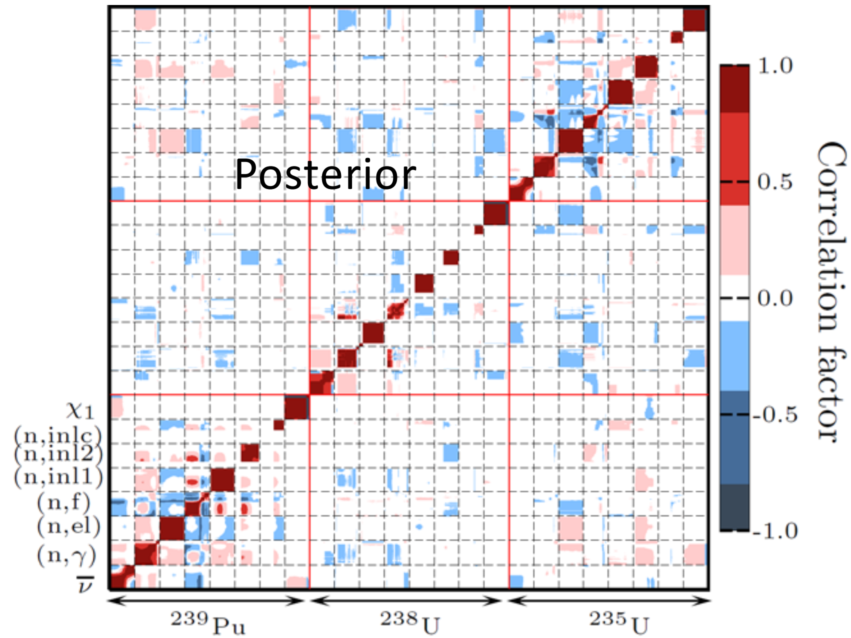
Uncertainty ratios

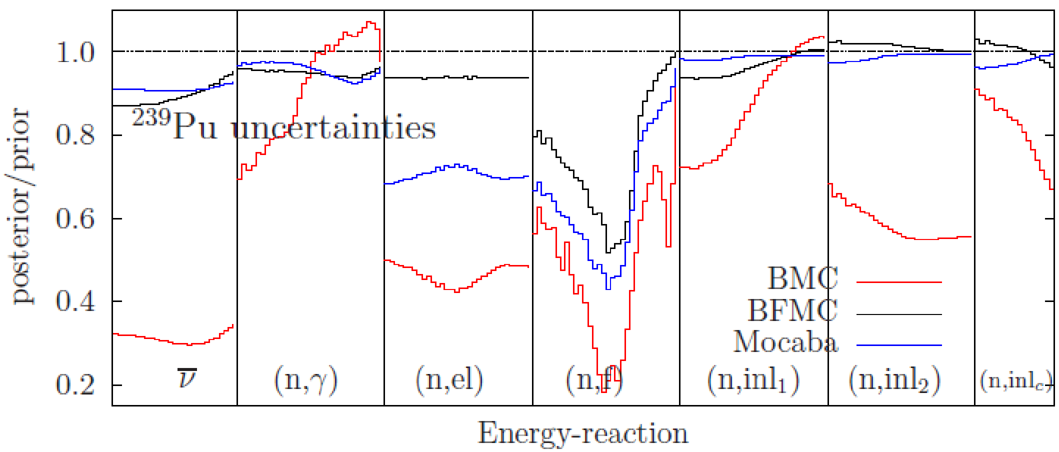


BMC/BFMC + 14 fast benchmarks

- Based on 14 fast benchmarks : ^{235}U- ^{238}U-^{239}Pu (EPJ Plus 133 (2018) 537)

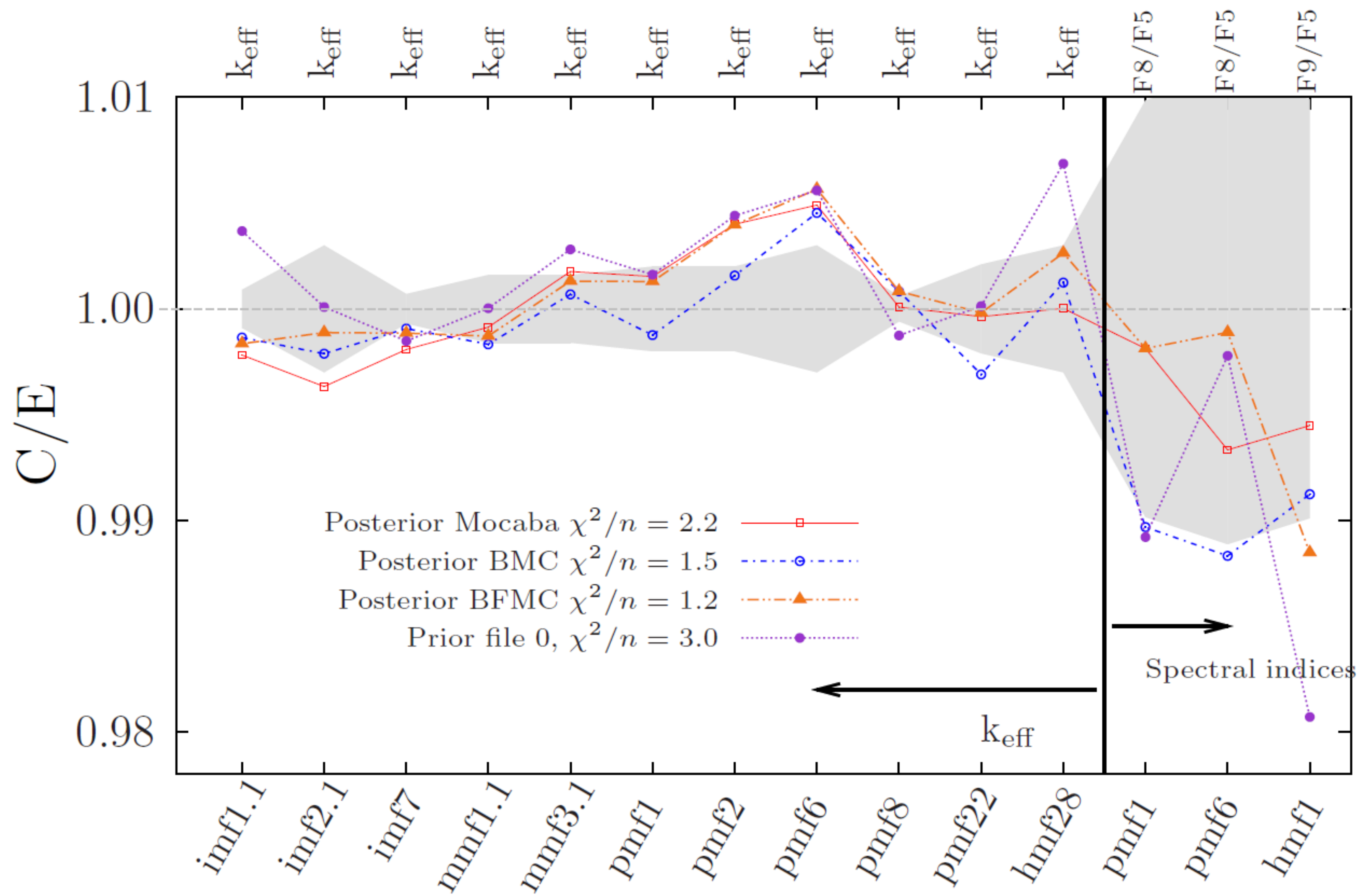






BMC/BFMC + 14 fast benchmarks

- Based on 14 fast benchmarks : ^{235}U-^{238}U-^{239}Pu (EPJ Plus 133 (2018) 537)



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BFMC with a PWR boron concentration

- System: realistic PWR cycle with measured boron concentration
- Random nuclear data: generated based on the ENDF/B-VII.1 library for all isotopes
- Simulation tool: (CASMO5 + SIMULATE5) x (a few thousands of random files)
- EPJ Plus 133 (2019) 453.

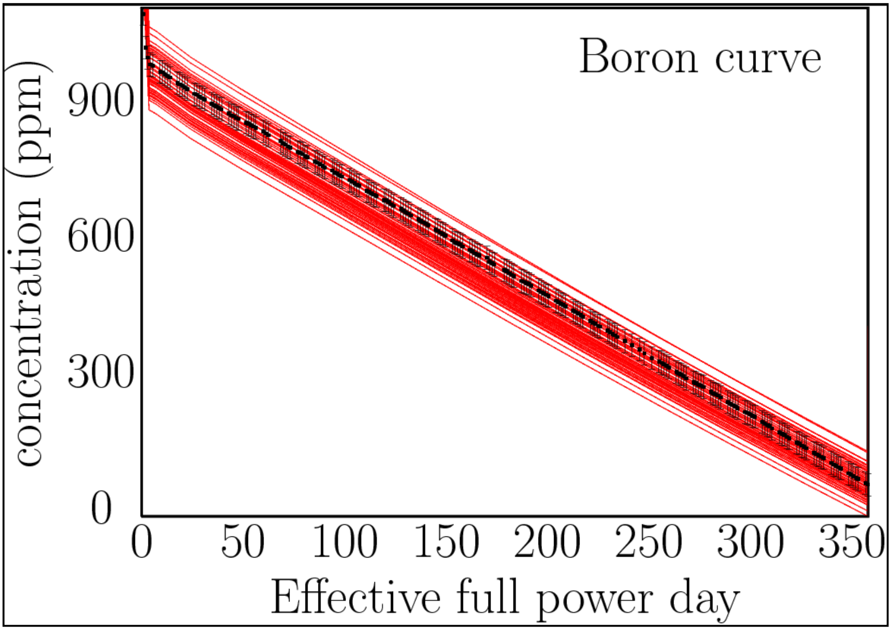
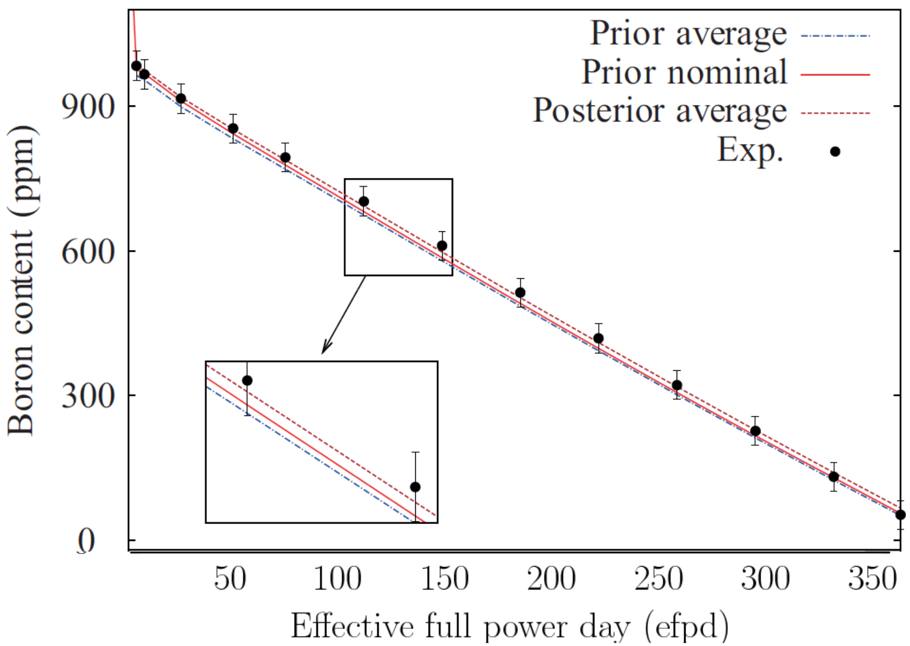


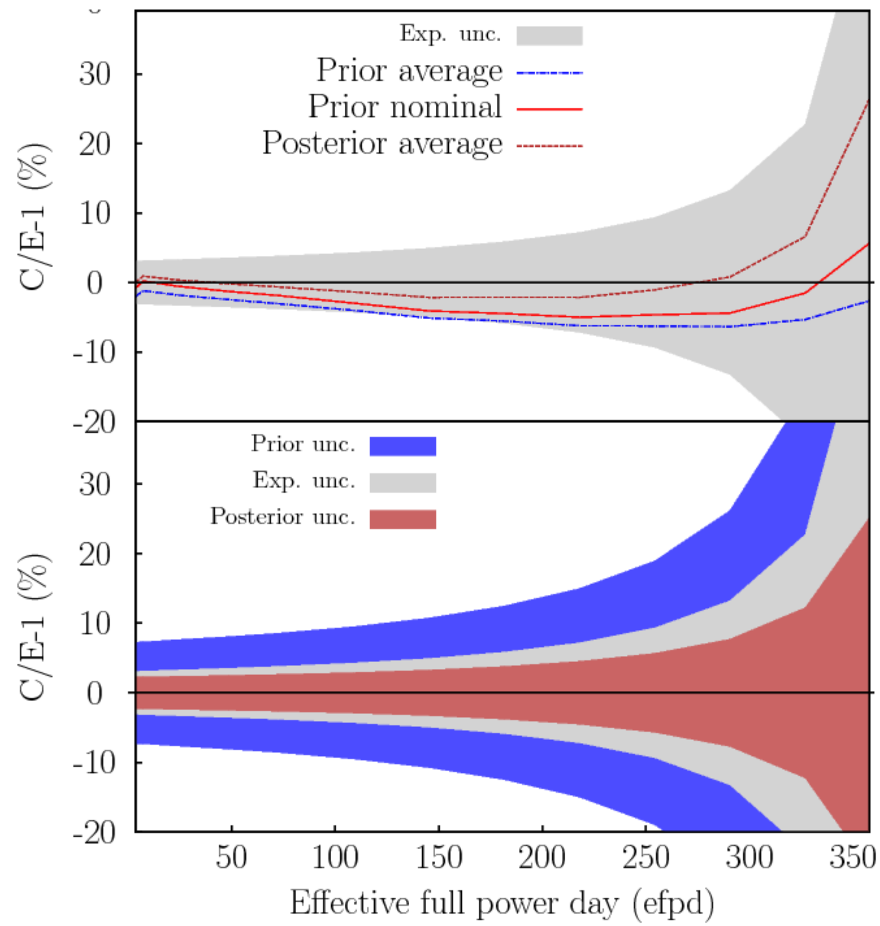
Table 2. Impact in percent of the variations of specific nuclear data at the middle of cycle (close to 150 efpd). The 5 reactions are $^{235}U_{\overline{\nu}_p}$, $^{235}U(n,f)$, $^{238}U(n,\gamma)$, $^{239}Pu(n,f)$ and $^{239}Pu_{\overline{\nu}_p}$.

Data	All	light	minor actinides	5 reactions considered here
Impact (%)	12	1.2	1.9	11

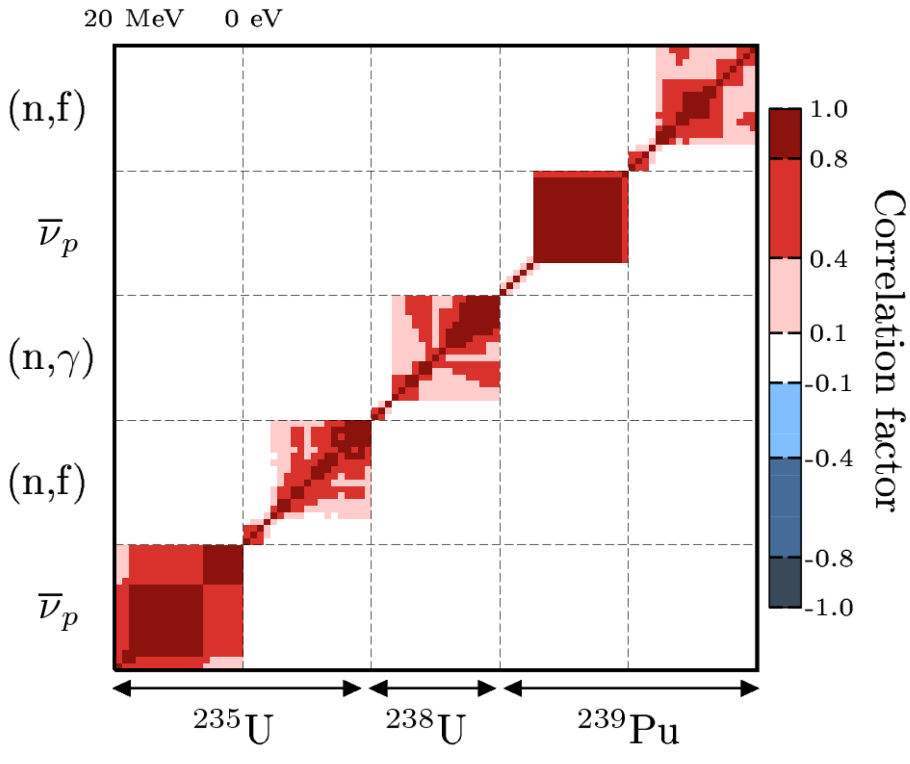
BFMC with a PWR boron concentration

- Impact on the boron concentration

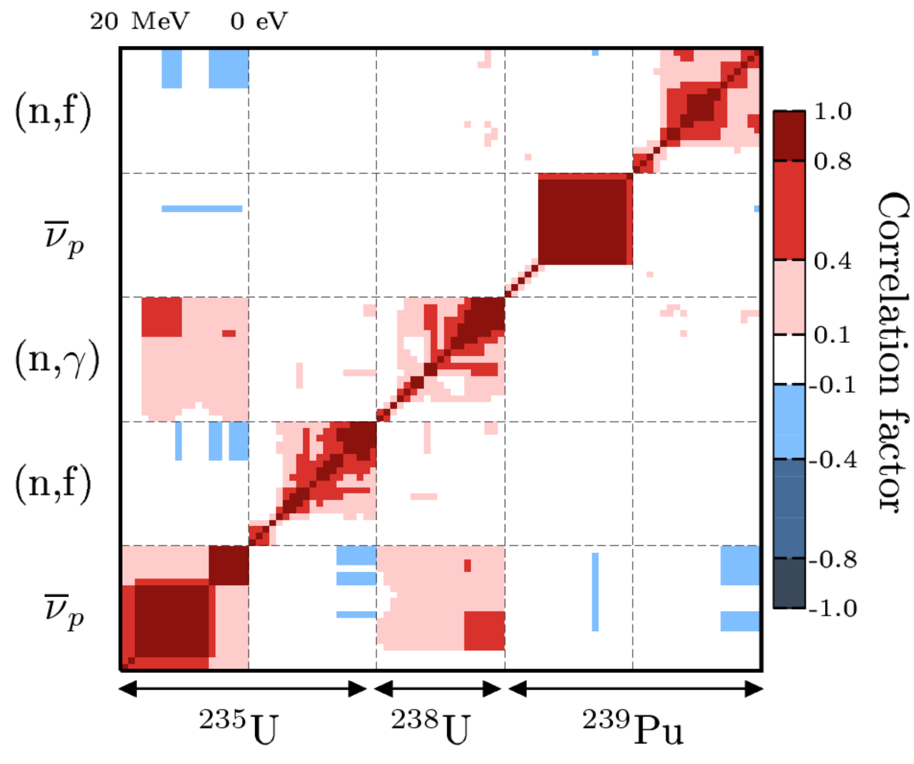




PWR boron concentration : Correlation matrices

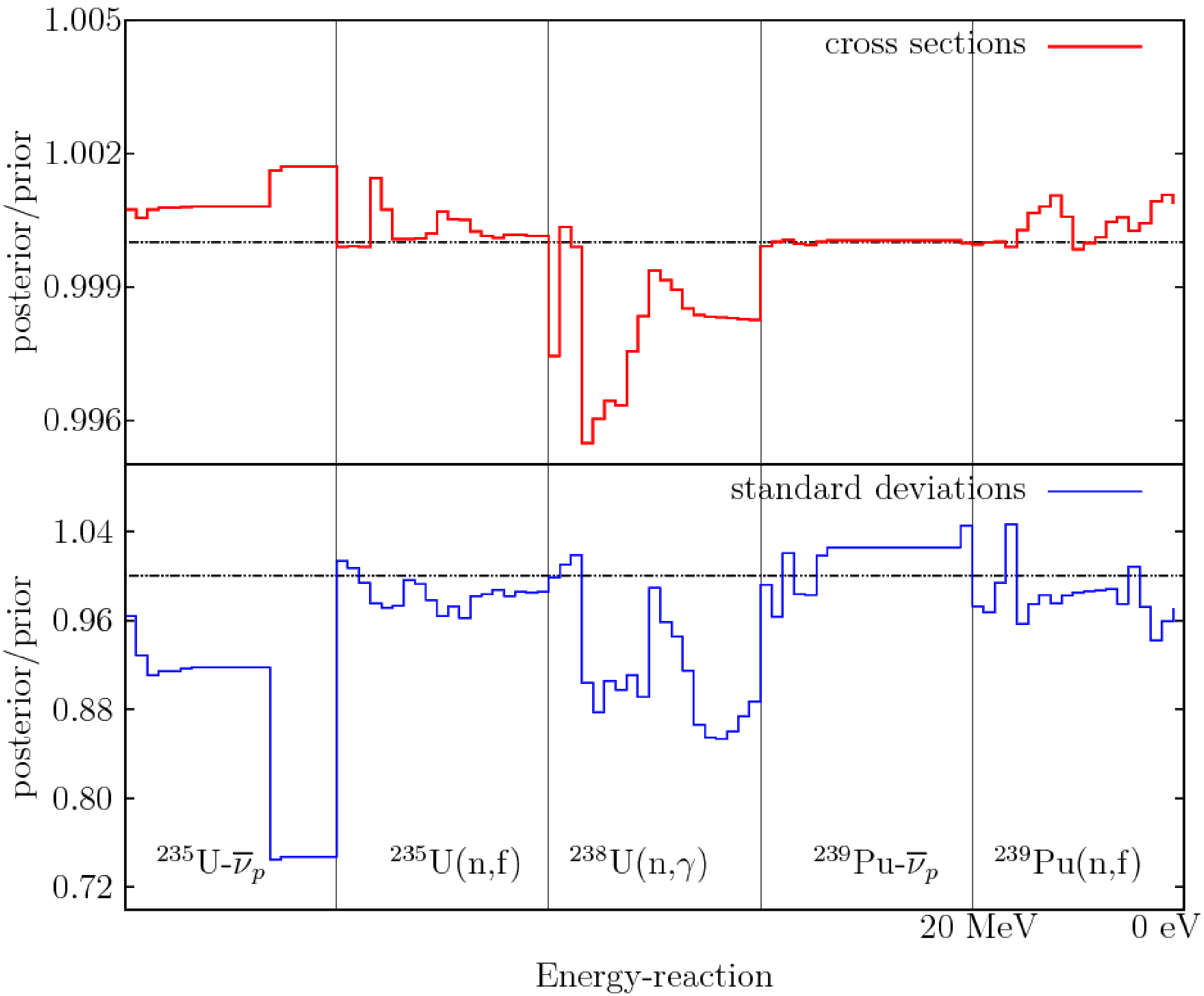


Prior



Posterior

PWR boron concentration : Posterior cross sections and uncertainties



Conclusions

- Cross-correlations found between isotopes from EXFOR or from integral data in the fast and thermal ranges
- The same can be found using EXFOR with the standards, or any relative measurements
- Decrease of the uncertainties for posterior quantities
- A suggestion: use integral data during the evaluation process,
- Outcome: more correlations, smaller uncertainties and less biases

Wir schaffen Wissen – heute für morgen