DE LA RECHERCHE À L'INDUSTRIE

cea

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

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

σ−χ−ν correlations in the fast region via integral information

Cross-observables correlations

Eur. Phys. J. N **3**, 14 (2017)

EPJ Nuclear Sci. Technol. **3**, 14 (2017)

DOI: 10.1051/epjn/2017009

EPJ Nuclear Sciences & Technologies

Available online at:
http://www.epj-n.org

REGULAR ARTICLE OPEN ACCESS

Correlation $\bar{\nu}_p - \sigma - \chi$ in the fast neutron range via integral information

Dimitri Rochman[1], Eric Bauge[2,*], Alexander Vasiliev[1], and Hakim Ferroukhi[1]

[1] Laboratory for Reactor Physics Systems Behaviour, Paul Scherrer Institut, Villigen, Switzerland
[2] CEA, DAM, DIF, 91297 Arpajon cedex, France

Received: 18 January 2017 / Received in final form: 20 March 2017 / Accepted: 20 March 2017

Abstract. This paper presents a Bayesian approach based on integral experiments to create correlations which do not appear with differential data. Some quantities such as the fission cross section (σ), neutron multiplicity ($\bar{\nu}_p$), neutron spectra (χ), etc. are usually neither modeled together nor measured in coincidence, thus there is no correlation matrices in evaluated nuclear data libraries. One can nevertheless use the information from integral experiments such as fast criticality-safety benchmarks to correlate such quantities for possible inclusion in nuclear data libraries. A simple Bayesian set of equations is presented with random nuclear data, similarly to the usual methods applied with differential data. An example for ^{239}Pu is proposed.

$\sigma-\chi-\nu$ correlations in the fast region via integral information

Cross-observables correlations ?

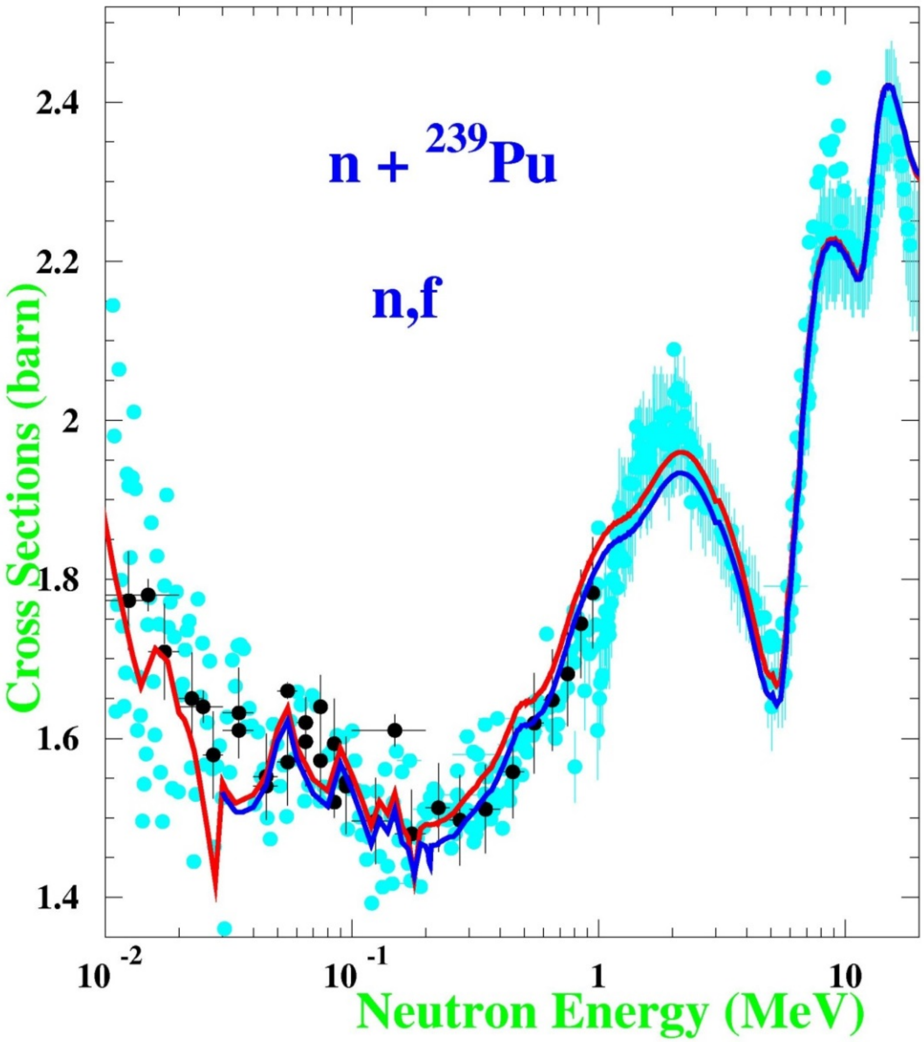
σ : cross sections (integrated $\sigma(E)$, simply differential $d\sigma/dE$, $d\sigma/d\Omega$, doubly differential $d^2s/d\Omega dE$, for all reaction channels).

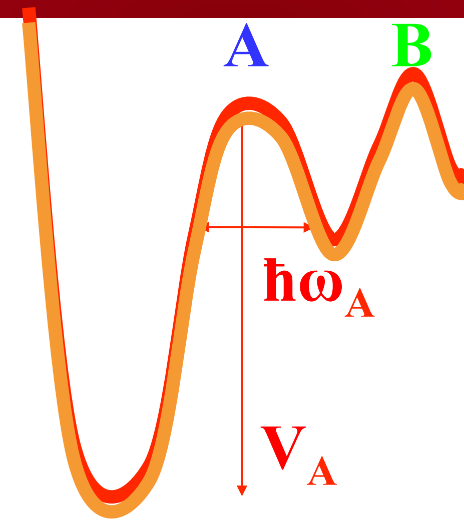
χ : prompt fission neutron spectra (PFNS normalized to 1).

ν : (nubar) average number of prompt fission neutrons

σ–χ–ν correlations in the fast region via integral information

Integral constraints ?





-20 keV on V_A
≈ 0.34%

➔1000 pcm on K_{eff} !!!

+ Integral experiments produce strong constraints on model parameters and the resulting nuclear data

In real life (ND evaluator's perspective)

One model for cross sections, with parameters adjusted on differential measurements (a few % for fission, a few 10% for capture, inelastic,)

One model for PFNS, with parameters adjusted on differential measurements (<E> within a few %).

One model for nubar, with parameters adjusted on differential measurements (nubar within 2 %)

Integral experiments measured within 0.2-0.3 %

To reach the "good" integral performance, evaluators select the "good" $\sigma-\chi-\nu$ set.

➔ $\sigma-\chi-\nu$ are strongly correlated, but that correlation is never quantified.

Quantification of $\sigma-\chi-\nu$ correlations

At PSI using the T6 system used to produce the TENDL library.

Total Monte-Carlo (TMC) approach: model (TALYS, TAFIS,…) parameter sampling such as differential data is accounted for (σ, χ and ν).

10000 ENDF6 formatted files, with different combinations of σ, χ and ν and MCNP calculations for 9 fast spectrum ^{239}Pu configurations.
Bayesian-like weighting of samples according to χ^2 between exp. and calc.

i : sample index

$$Q_i = \left(\frac{\mathrm{k_{eff,i}} - \mathrm{k_{exp}}}{\Delta \mathrm{k}}\right)^2$$

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

Good agreement = high weight
Bas agreement = low weight

$$\begin{cases} \omega = \sum_i^n w_i \\ \omega_{\sigma_\alpha} = \sum_i^n w_i \cdot \sigma_{\alpha,i}/\omega \end{cases}$$

$$\begin{cases} \mathrm{var}_{\sigma_\alpha} = \sum_i^n \left[(\sigma_{\alpha,i} - \omega_{\sigma_\alpha})^2 \cdot w_i\right]/\omega \\ \mathrm{var}_{\sigma_\beta} = \sum_i^n \left[(\sigma_{\beta,i} - \omega_{\sigma_\beta})^2 \cdot w_i\right]/\omega \\ \mathrm{cov}_{\sigma_\alpha \sigma_\beta} = \sum_i^n \left[(\sigma_{\alpha,i} - \omega_{\sigma_\alpha}) \cdot (\sigma_{\beta,i} - \omega_{\sigma_\beta}) \cdot w_i\right]/\omega \end{cases}$$

$$\rho(\sigma_\alpha, \sigma_\beta) = \frac{\mathrm{cov}_{\sigma_\alpha \sigma_\beta}}{\sqrt{\mathrm{var}_{\sigma_\alpha} \cdot \mathrm{var}_{\sigma_\beta}}}$$

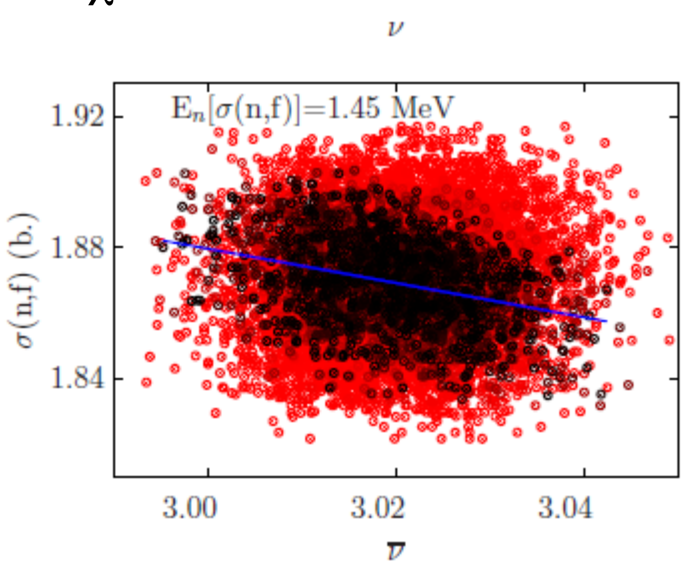
Quantification of σ–χ–ν correlations

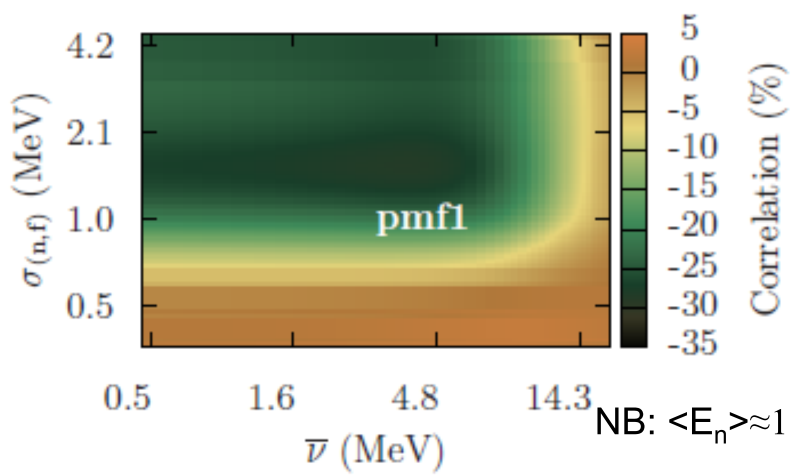
At PSI using the T6 system used to produce the TENDL library.

Total Monte-Carlo (TMC) approach: model (TALYS, TAFIS,…) parameter sampling such as differential data is accounted for (σ, χ and ν).

10000 ENDF6 formatted files, with different combinations of σ, χ and ν and MCNP calculations for 9 fast spectrum ^{239}Pu configurations.
Bayesian-like weighting of samples according to χ^2 between exp. and calc.

➔ σ–χ–ν correlations

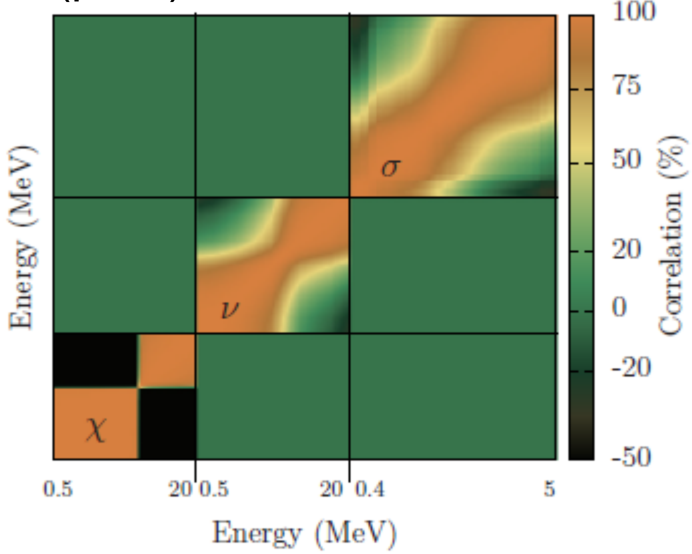




NB: $\langle E_n \rangle \approx 1.4$ MeV

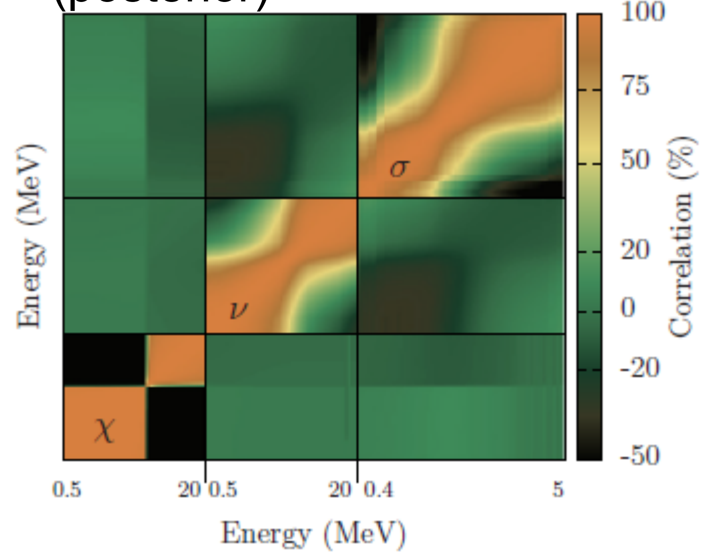
Results

Without σ–χ–ν correlation (prior)

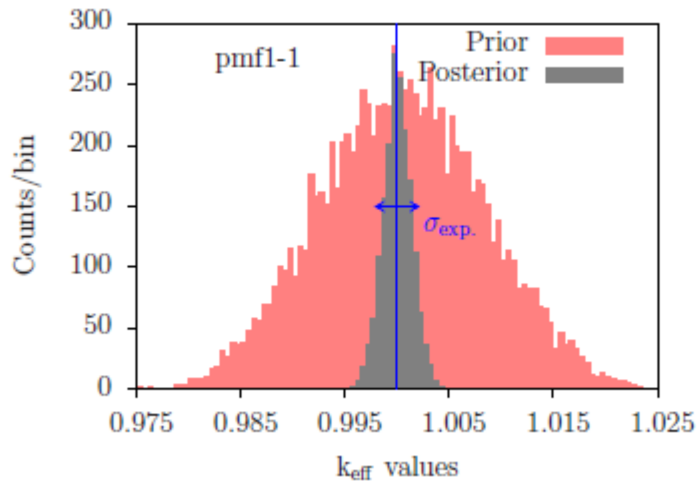


Correlations resulting from model response to parameter variations

With σ–χ–ν correlation (posterior)



Correlations resulting from model response to parameter variations
+ 9 PMF configurations integral constraints



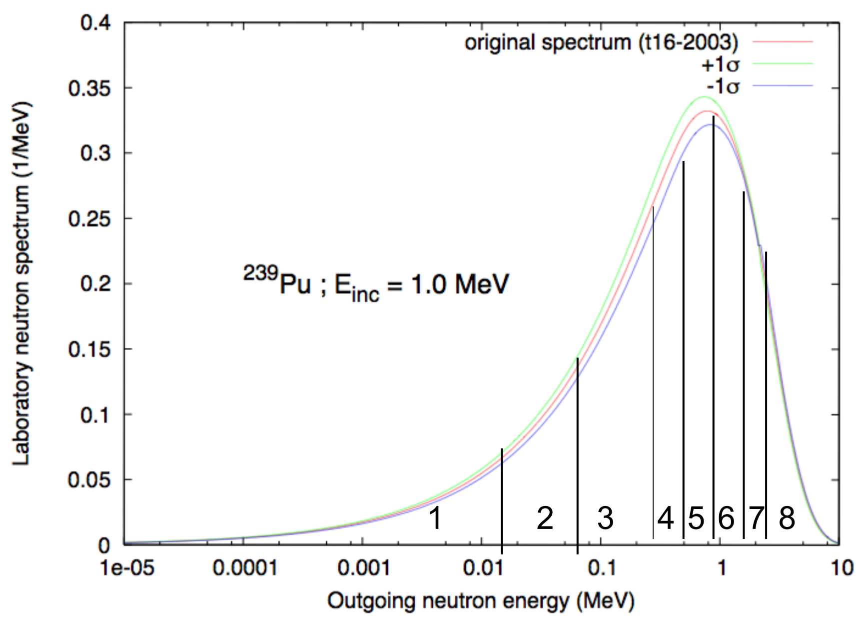
Such correlations allow for variance reduction of calculated K^{eff} !

Easy (1 slide) prompt neutronics with point geometry

$$\Phi_i^{t+1} = \sum_j \nu_{ji} \Phi_j \Sigma_j^f - \Phi_i \Sigma_i^c - \Phi_i \Sigma_i^{inel} + \sum_{j \neq i} \Phi_j \Sigma_j^{inel \to i}$$

Source term = $\Phi \cdot \nu_i \cdot \chi_{ij} \cdot \sigma_i$

with $\nu_{ij} = \nu_i \chi_{ij}$



$K_{eff} \approx \Phi^{t+1} / \Phi^t$

$\Phi^{t+1} > \Phi^t$ Runaway reaction

$\Phi^{t+1} = \Phi^t$ Stable reaction

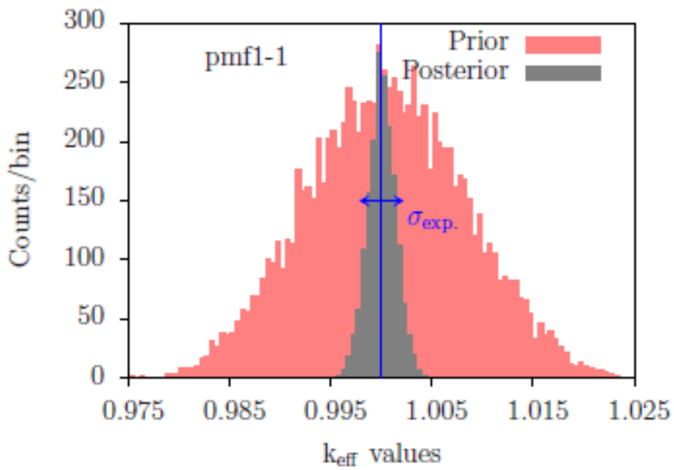
$\Phi^{t+1} < \Phi^t$ Reaction stops

Typically measured with 0.2-0.3% precision (200-300 pcm)

Results

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.

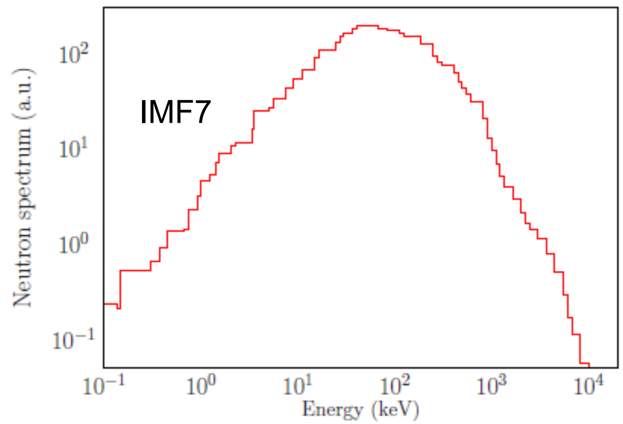
Benchmark	Prior		Posterior		$C/E-1$ Prior (%)	$C/E-1$ Posterior (%)
	$\bar{k}$	$\pm\Delta k$	$\bar{k}$	$\pm\Delta k$		
pmf1	1.00082	±782	0.99999	±133	0.08	0.00
pmf2	1.00171	±705	1.00023	±143	0.17	0.02
pmf3-1	1.00240	±725	1.00016	±207	0.24	0.02
pmf5-1	1.00056	±782	1.00002	±93	0.06	0.02
pmf6-1	1.00156	±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



Such correlations allow for variance reduction of calculated K^{eff} !

Cross-isotopes correlations

Some benchmarks exhibit strong sensitivity to several isotopes.
Example: IMF7 « Big Ten » a highly enriched U core surrounded by a massive reflector made of depleted U.



It is sensitive to both ^{235}U and ^{238}U data.
Its exp. Keff value (1.00450 (70 pcm)) **cannot** be reproduced by mixing different libraries.

$\downarrow$ ^{238}U \ ^{235}U $\longrightarrow$	JEFF-3.3	ENDF/B-VII.1
JEFF-3.3	1.00522	1.01315
ENDF/B-VII.1	0.99617	1.00478

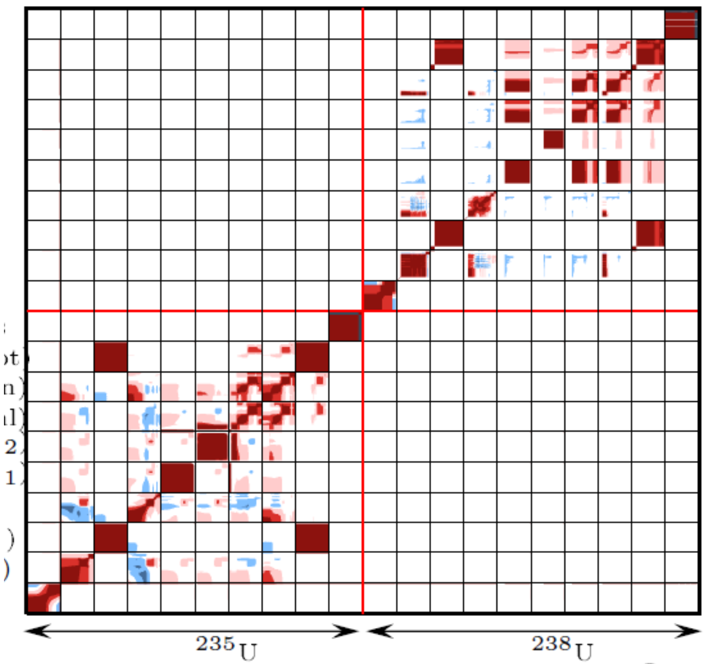
Therefore : ^{235}U and ^{238}U data are effectively correlated in evaluated libraries

The same Bayesian weighting technique can be used to quantify those correlations

Cross isotopes correlations

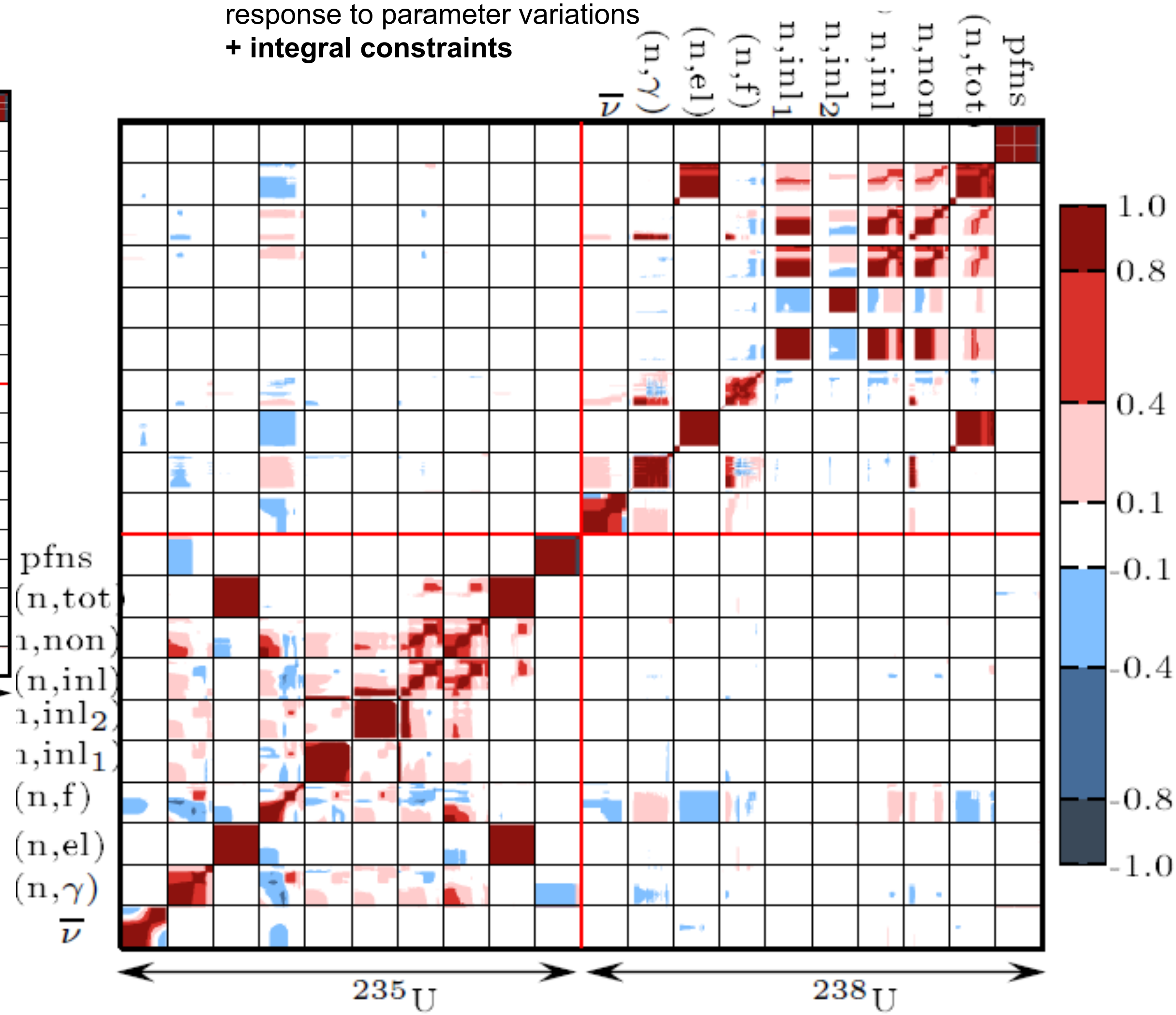
Unweighted (prior)

Correlations resulting from model response to parameter variations



With IMF7-derived weights (posterior)

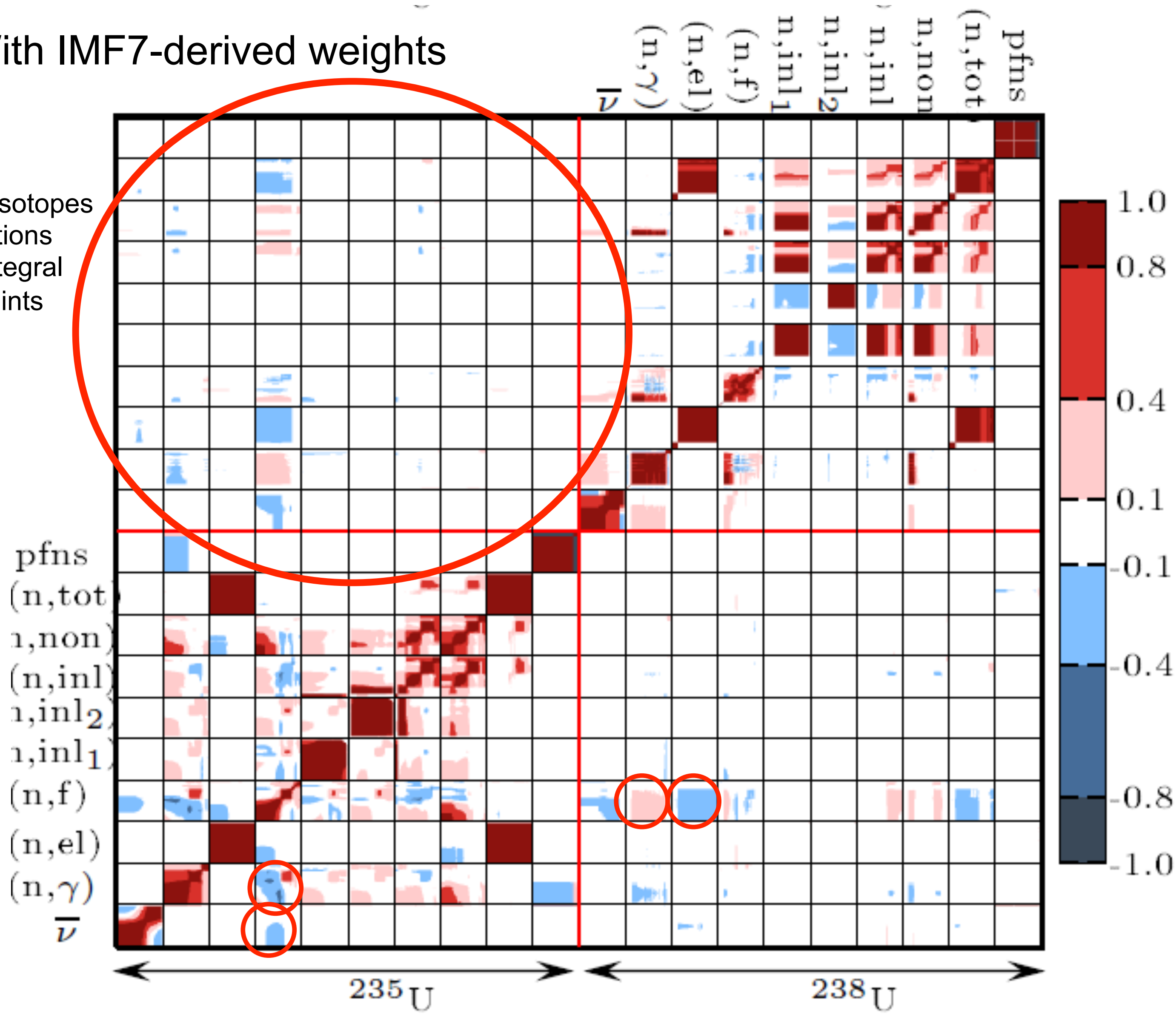
Correlations resulting from model response to parameter variations
+ integral constraints



Cross isotopes correlations

With IMF7-derived weights

Cross-isotopes correlations from integral constraints

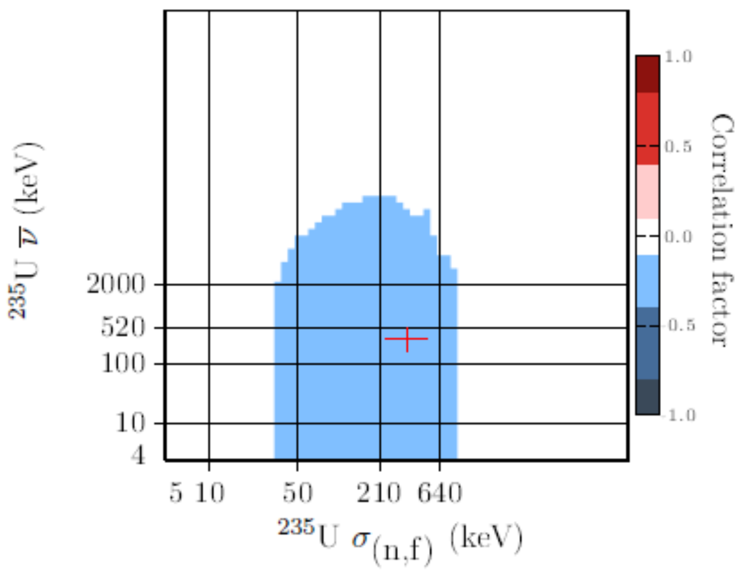


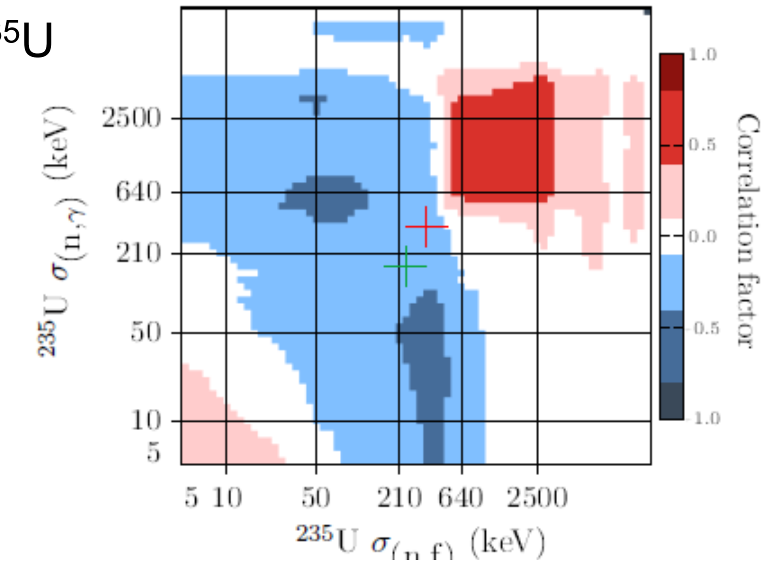
Cross-observables correlations from integral constraints

Cross-isotopes and cross-observables correlations, zoom in…

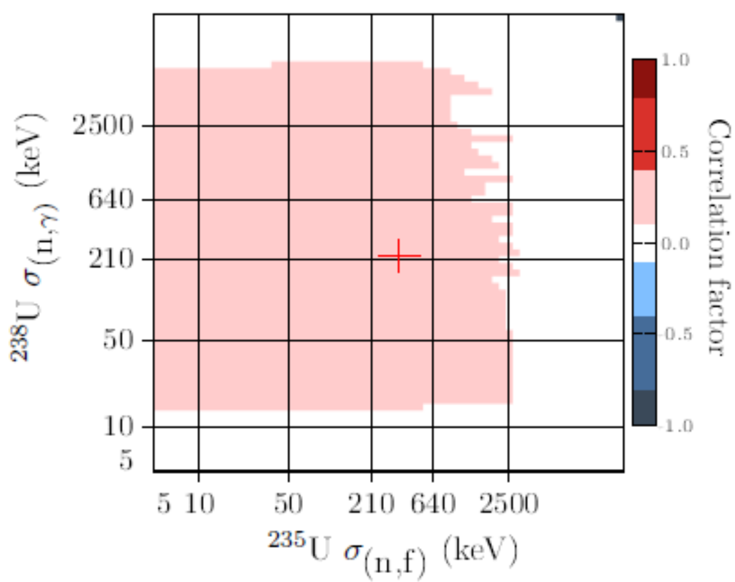
With IMF7-derived weights

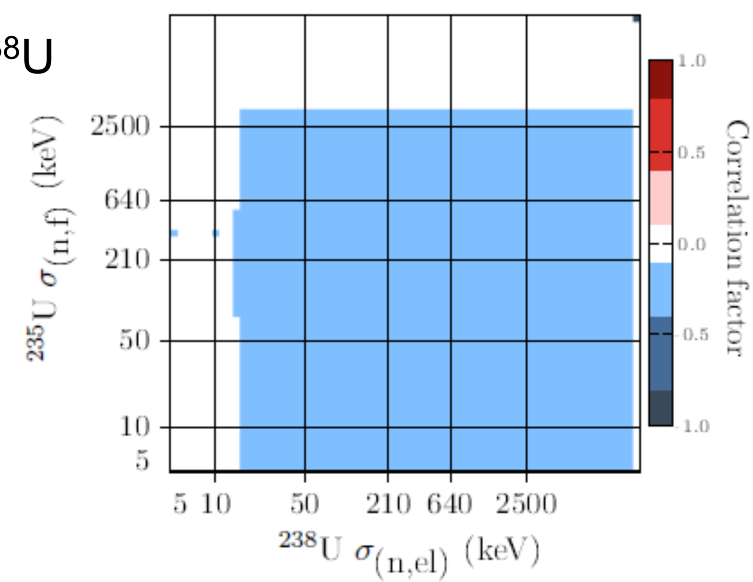
$^{235}U/^{235}U$





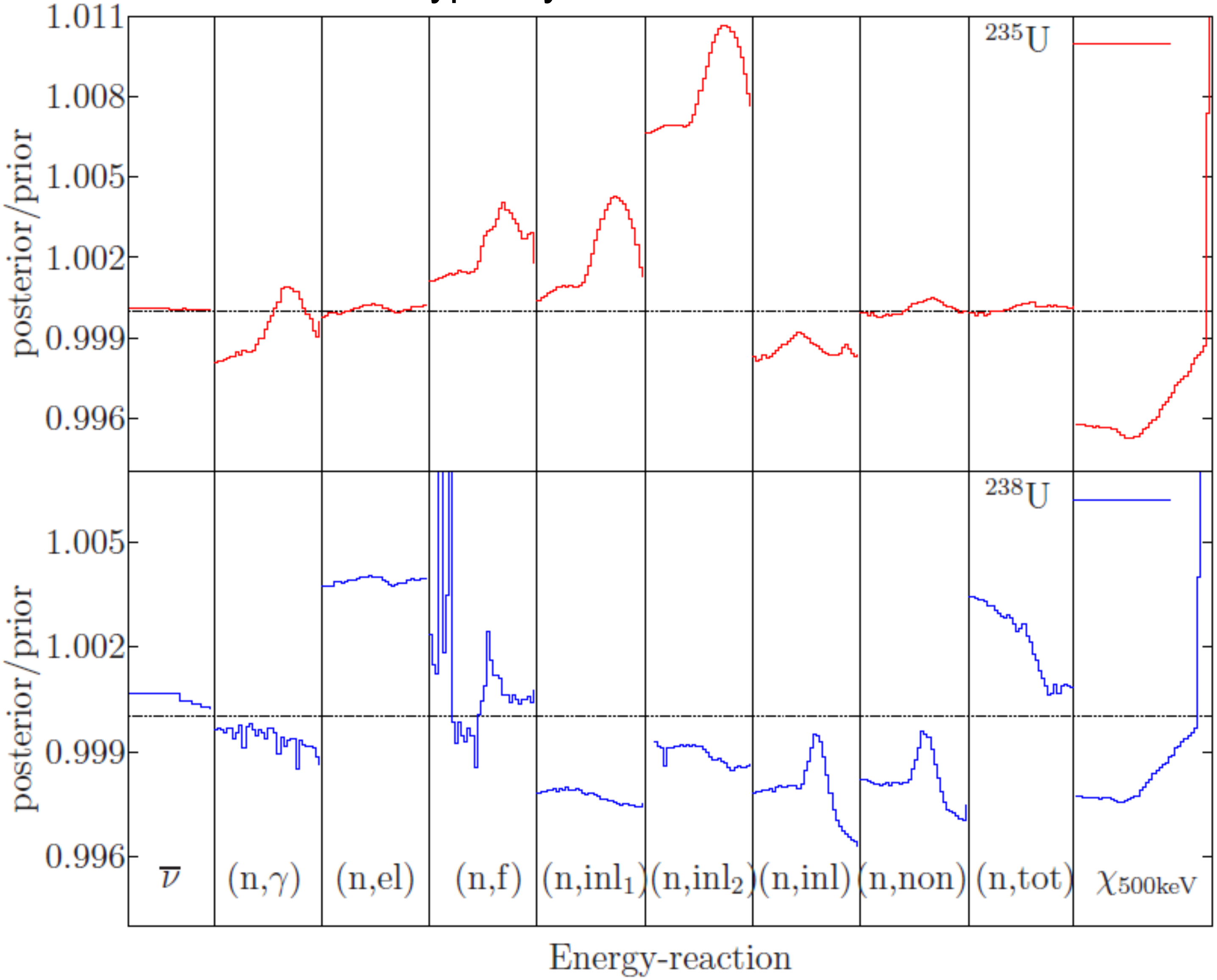
$^{235}U/^{238}U$





The Bayesian weights slightly change the central values

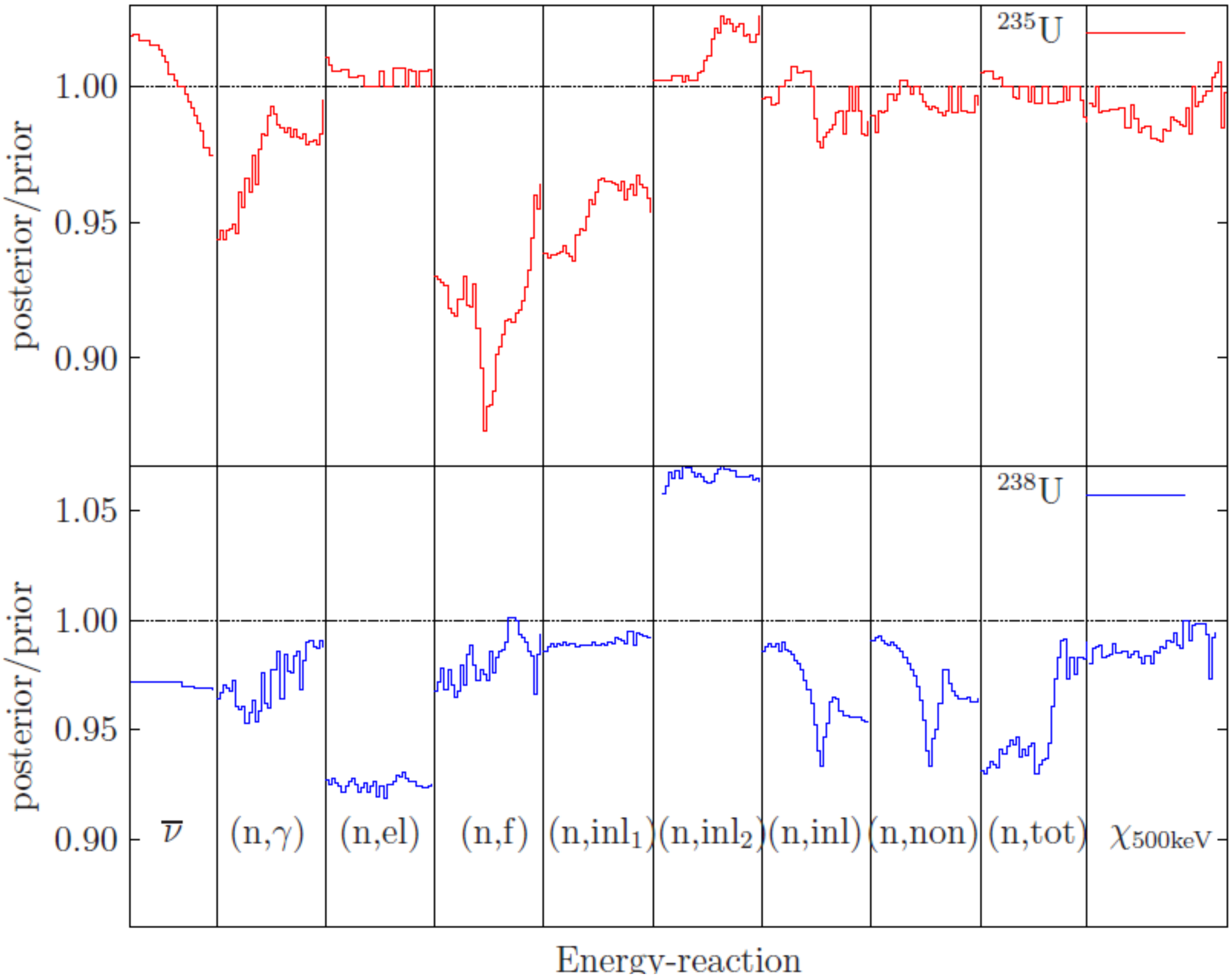
Typically less than 1%



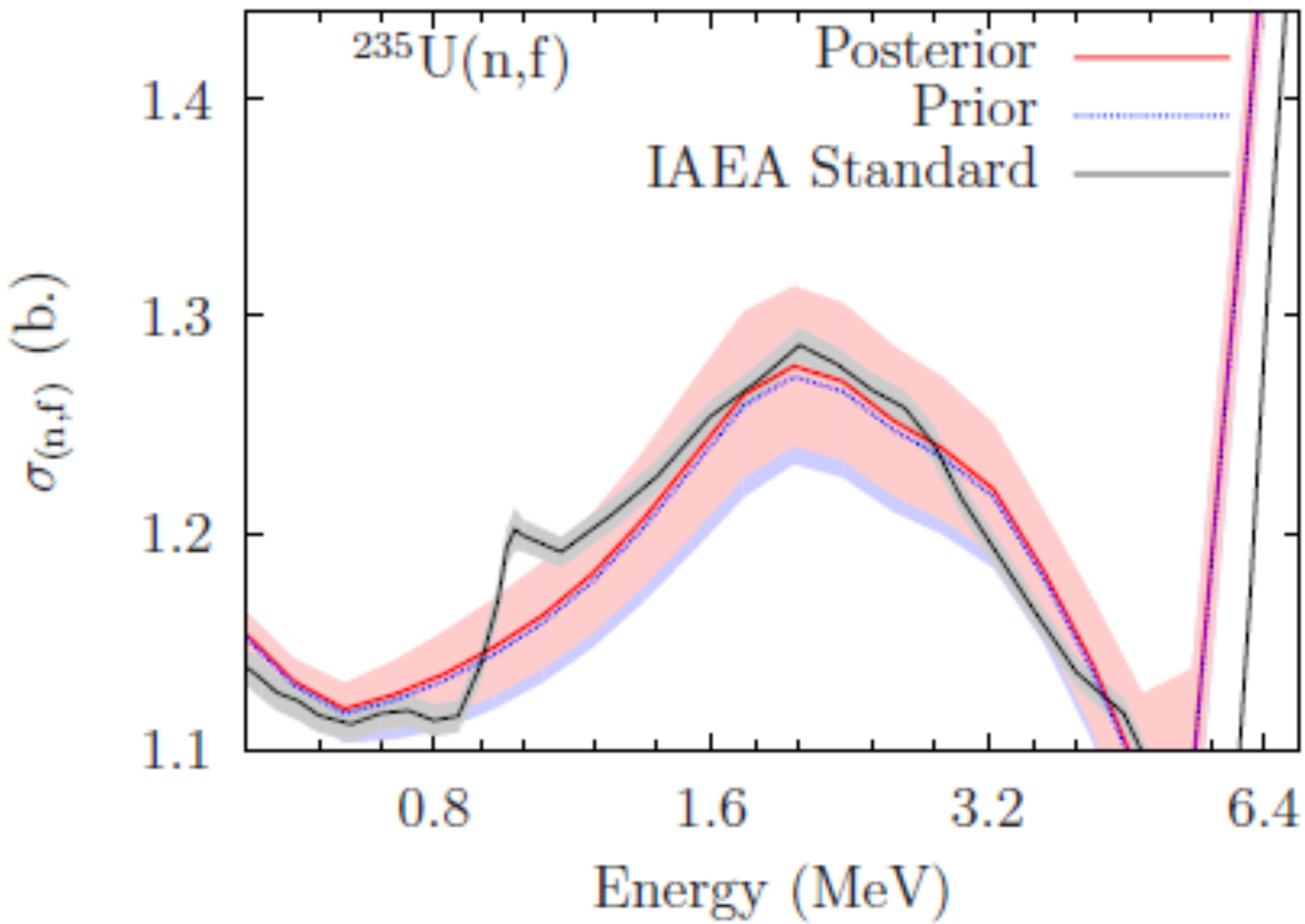
A

The Bayesian weights slightly change the std dev

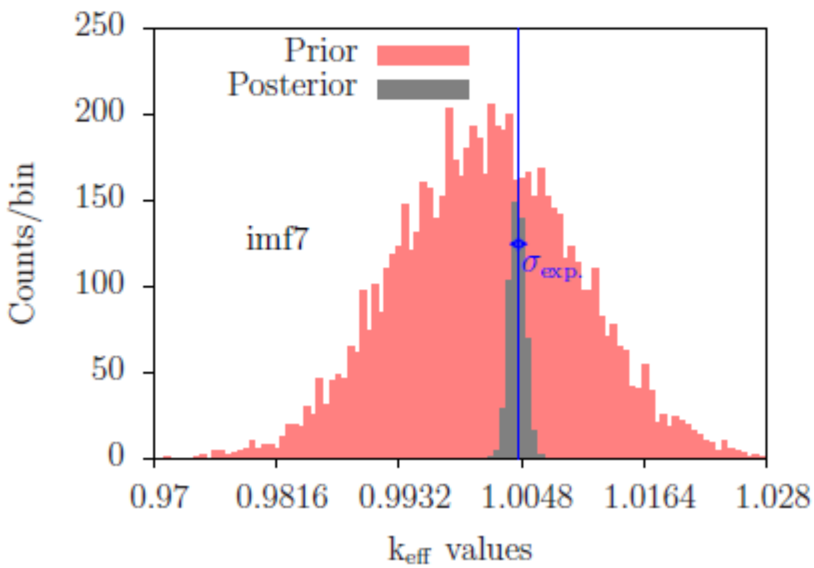
Mostly reduced by a few % up to ~10%



Differential data



Posterior Keff distribution in agreement with exp.



The IMF7-derived weights do not degrade the agreement of other benchmarks, they even slightly improve the central value and calculated uncertainties !

Benchmark	Used in Bayesian update	Exp		Prior		Posterior		Prior C/E-1 (%)	Posterior C/E-1 (%)
		k_{eff}	$\pm\Delta k$	$\bar{k}$	$\pm\Delta k$	$\bar{k}$	$\pm\Delta k$		
imf7	yes	1.00450	± 70	1.00156	± 2240	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

Summary

- A first attempt at the rigorous quantification of the $\sigma-\chi-\nu$ correlations existing in all the present evaluated nuclear data files

- These correlation allow nuclear data files to reach target integral performance. (Evaluators have known that for a long time, but never advertised it).

- A first demonstration is limited to a few PMFs (Eur. Phys. J. N **3**, 14 (2017))

- Cross isotopes correlations (IMF7: BIGTEN known to strongly depend on both ^{235}U and ^{238}U) can be quantified (submitted to EPJ N).

- The posterior (weighted) distributions are not inconsistent with the best differential experiments.

- Adjusting for one integral exp. seems to improve agreement with other integral expt. (including with different neutronic spectra).

- Do we learn anything about the fission process ? NO !

- The ENDF6 format does not allow for storage or processing of such correlations

Perspectives

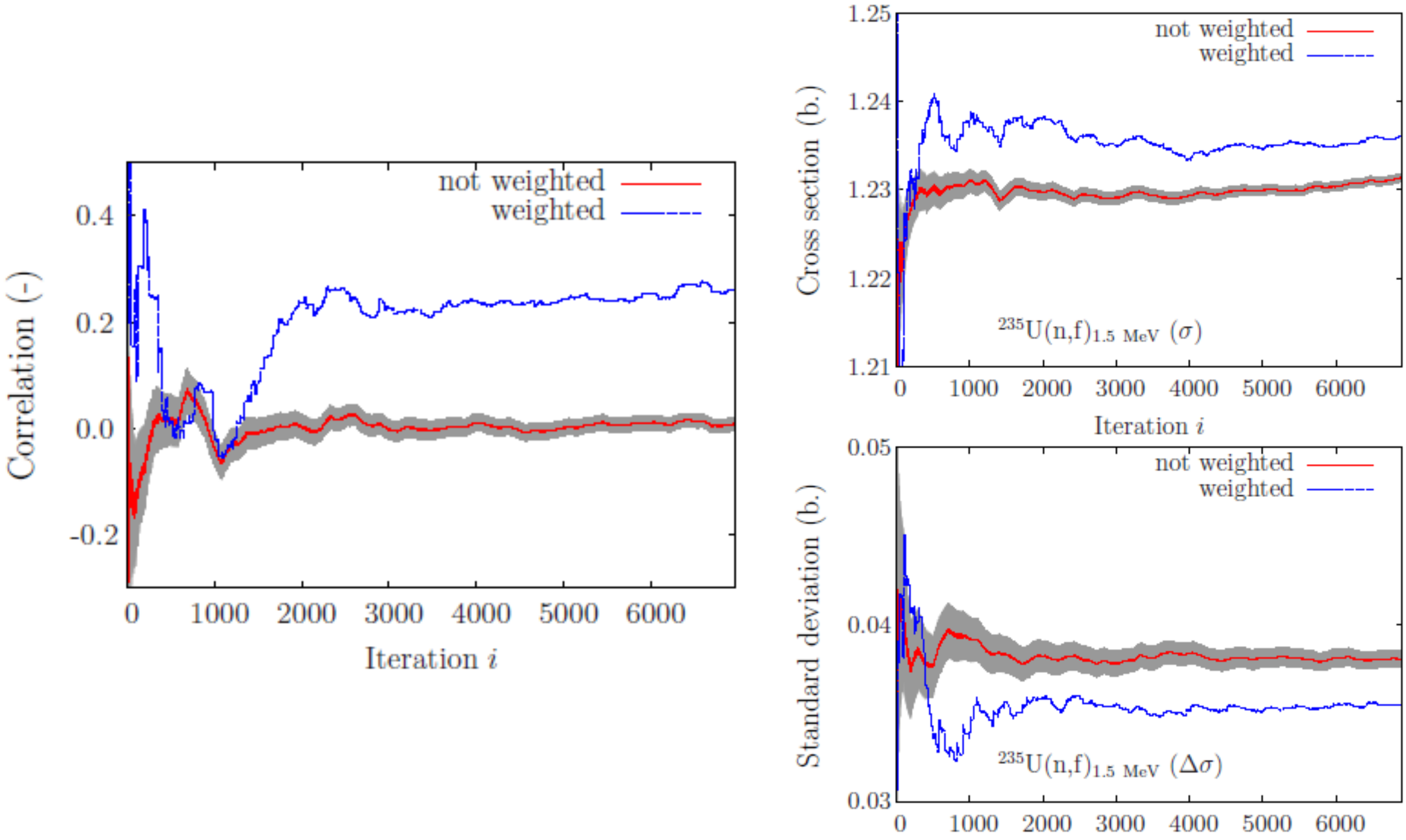
- New GND format will allow to store and process such correlations.
- New WPEC subgroup 44 starting on best practices for uncertainties evaluations
- Mix several integral constraints in the weights (ex HMF1 +IMT7 +LCT6 +…)
- Also add differential weights (EXFOR + AIEA Std)
- Extension to wider spectral constraints (thermal,…), other isotopes (^{235}U, ^{238}U), other observables (spectral indices), all reaction channels is underway.
- Use better models (the models used for TENDL are quite simple)

Commissariat à l’énergie atomique et aux énergies alternatives
Centre de Saclay | 91191 Gif-sur-Yvette Cedex
T. +33 (0)1 XX XX XX XX | F. +33 (0)1 XX XX XX XX

Direction
Département
Service

Etablissement public à caractère industriel et commercial | RCS Paris B 775 685 019

Convergence of the sampling process ?



IMF7 details

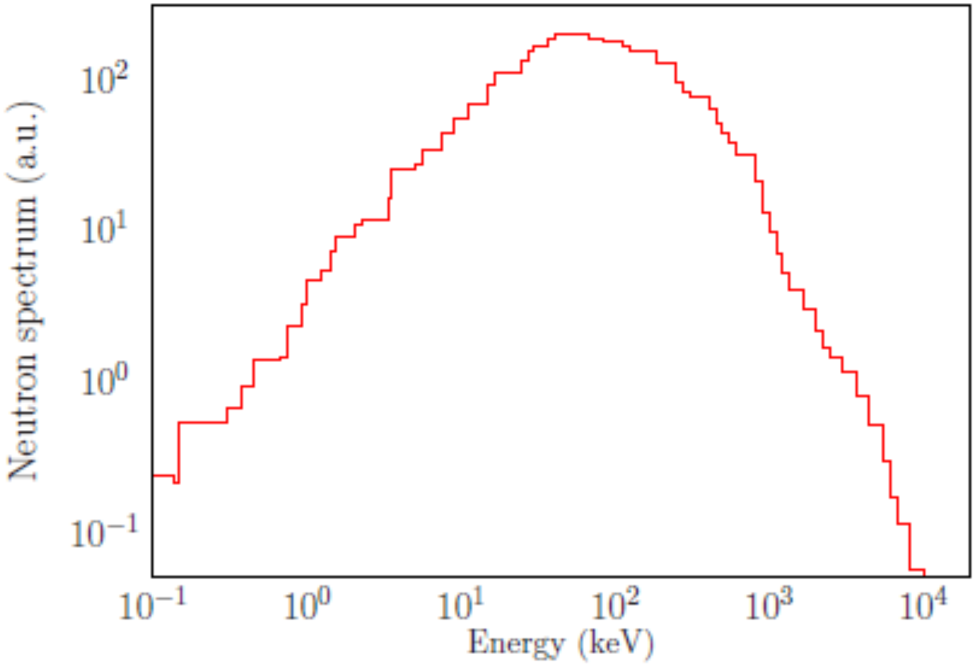


Table 1. Average neutron energy in keV causing fission or capture in the two main zones of the imf7 benchmark.

^{235}U				^{238}U			
core		Blanket		core		Blanket	
(n,f)	(n,γ)	(n,f)	(n,γ)	(n,f)	(n,γ)	(n,f)	(n,γ)
507	227	285	162	3070	281	3060	182