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Correlations in nuclear data from integral constraints

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Summary

- Motivations

- Methods
  - Bayesian Monte Carlo (BMC)
  - Generalized Non-linear Least Square (GNLS)
  - Back to a unique evaluated file

- Examples
  - A single benchmark (*e.g.* imf7, hmf1, pmf1…)
  - Many benchmarks together

All slides can be found here: https://tendl.web.psi.ch/bib_rochman/presentation.html

Motivations

1. Not all relevant correlations are included in the current evaluations, *e.g.*:

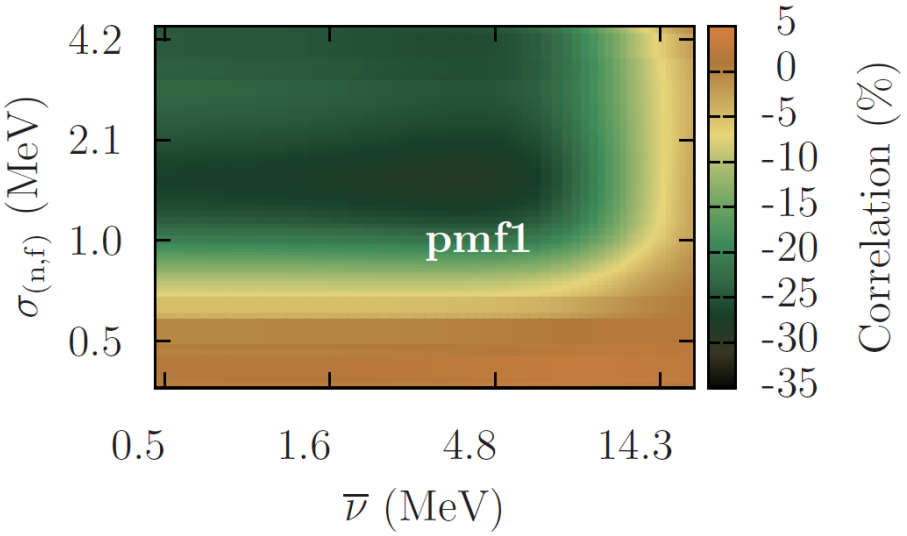


Fig. 3. Correlation matrix between ^{239}Pu ν and σ considering the fast pmf1 benchmark. The X- and Y-axis are in log scale.

2. Calculated uncertainties for benchmarks based on current evaluations are larger than ICSBEP evaluated uncertainties:

	Exp		Prior
		iso	average
	k_{eff} $\pm\Delta k$		$\overline{k}$ $\pm\Delta k$
hmf1	1.00000 ± 200	^{235}U	0.99551 ± 1130
hmf3	1.00000 ± 300	^{235}U	0.99414 ± 990
pmf1	1.00000 ± 200	^{239}Pu	1.00077 ± 780

Uncertainty reduction

- Solution: include selected integral information in the evaluation process

- 3 methods:
  - BMC: Bayesian Monte Carlo = TMC + weights on random files,
  - GLLS: Generalized Linear Least Square (not detailed here),
  - GNLS: Generalized Nonlinear Least Square = MOCABA + feedback to nuclear data (Monte Carlo version of the GLLS)

Method	GLLS	GNLS	BMC
Assumption	Linear+Normal	Normal	None
Drawback/Advantages	Fast, ignore nonlinearity	Not so fast, ignore linearity	Even slower, ignore linearity and non Normal inputs

Uncertainty reduction with BMC

- 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.

- Some BMC/BFMC references:
  - EPJ/A 51 (2015) 184, Nucl. Data Sheets 123 (2015) 201, EPJ/N 3, 14 (2017)

Uncertainty reduction with GNLS

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

- Step 2 - GNLS: Based on step 1,
  - Generate n=100 000 (or 1000) random files (TMC-way)
  - Calculate n times the benchmarks,
  - Then:

$$\vec{\mathbf{C}}' = \vec{\mathbf{C}} + \mathbb{M}_{\mathbf{c}}(\mathbb{M}_{\mathbf{c}} + \mathbb{M}_{\mathbf{e}})^{-1}(\vec{\mathbf{E}} - \vec{\mathbf{C}}) \quad (3)$$

$$\mathbb{M}_{\mathbf{c}}' = \mathbb{M}_{\mathbf{c}} - \mathbb{M}_{\mathbf{c}}(\mathbb{M}_{\mathbf{c}} + \mathbb{M}_{\mathbf{e}})^{-1}\mathbb{M}_{\mathbf{c}}^{\mathbf{T}} \quad (4)$$

$$\vec{\sigma}' = \vec{\sigma} + \mathbb{M}_{\sigma,\mathbf{c}}(\mathbb{M}_{\mathbf{c}} + \mathbb{M}_{\mathbf{e}})^{-1}(\vec{\mathbf{E}} - \vec{\mathbf{C}}) \quad (5)$$

$$\mathbb{M}_{\sigma}' = \mathbb{M}_{\sigma}(\mathbb{M}_{\mathbf{c}} + \mathbb{M}_{\mathbf{e}})^{-1}\mathbb{M}_{\sigma,\mathbf{c}}^{\mathbf{T}} \quad (6)$$

  - C: calculated integral quantity (*e.g.* k_{eff}) from
  - $M_{c,e}$: covariance in calculated (measured) k_{eff}
  - M_{σ}: cross section covariance
- Original references: ANE 77(2015) 514, JNST 51 (2014) 590

Uncertainty reduction (final step)

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

- Step 2 - BMC or GNLS

- Step 3 - Back to a unique file:
  - From the n random files and their posterior (weights in BMC, σ' in GNLS), update the nominal evaluated file,
  - And update the covariance file,
  - Finally, benchmark the posterior nominal evaluated file for checking.

Example with imf7 (bigten) - BMC

- Based on 10 000 random files for $^{235,238}U$

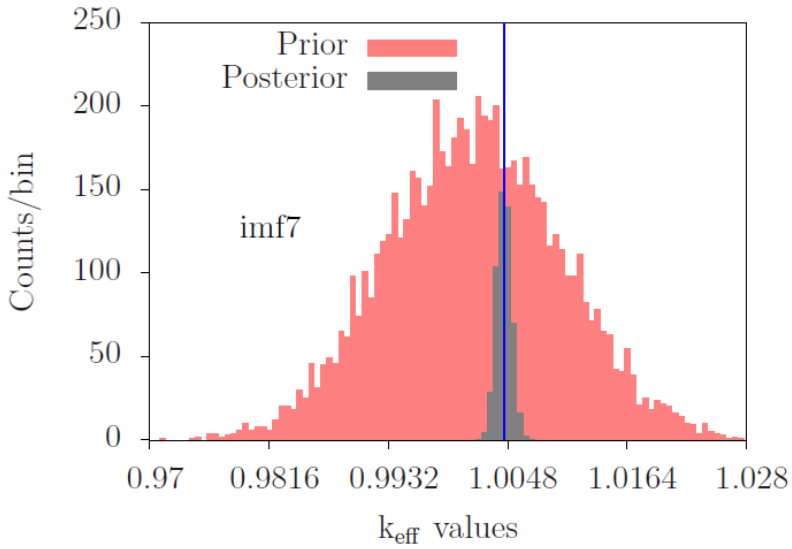


Fig. 12. Prior and posterior distributions of k_{eff} for imf7 benchmark. The blue line indicates the experimental value.

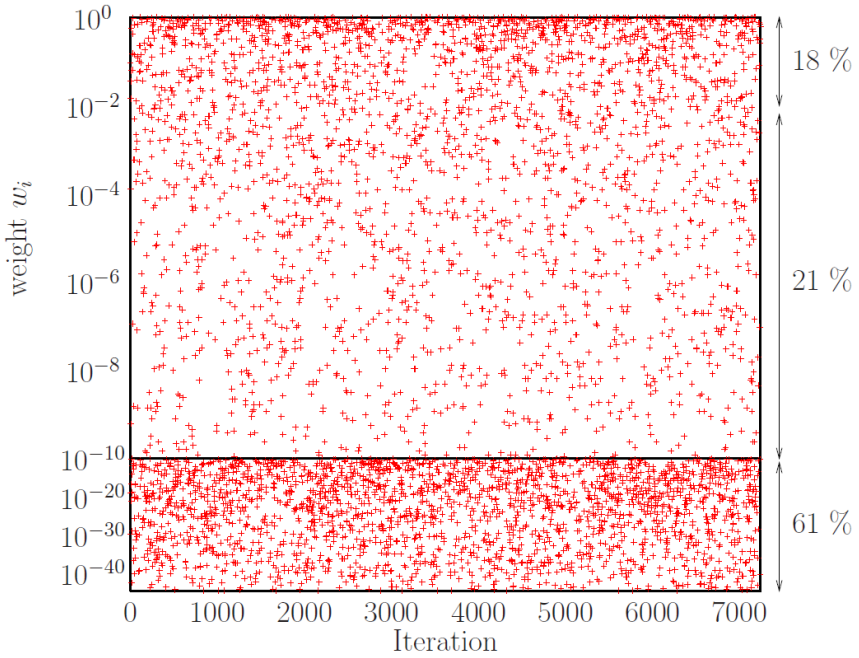


Fig. 1. Calculated weights w_i for the 7000 random cases considered in this work. The number on the right are the percent of weights within the space defined by the arrows.

Example with imf7 (bigten) - BMC

- Updated cross sections

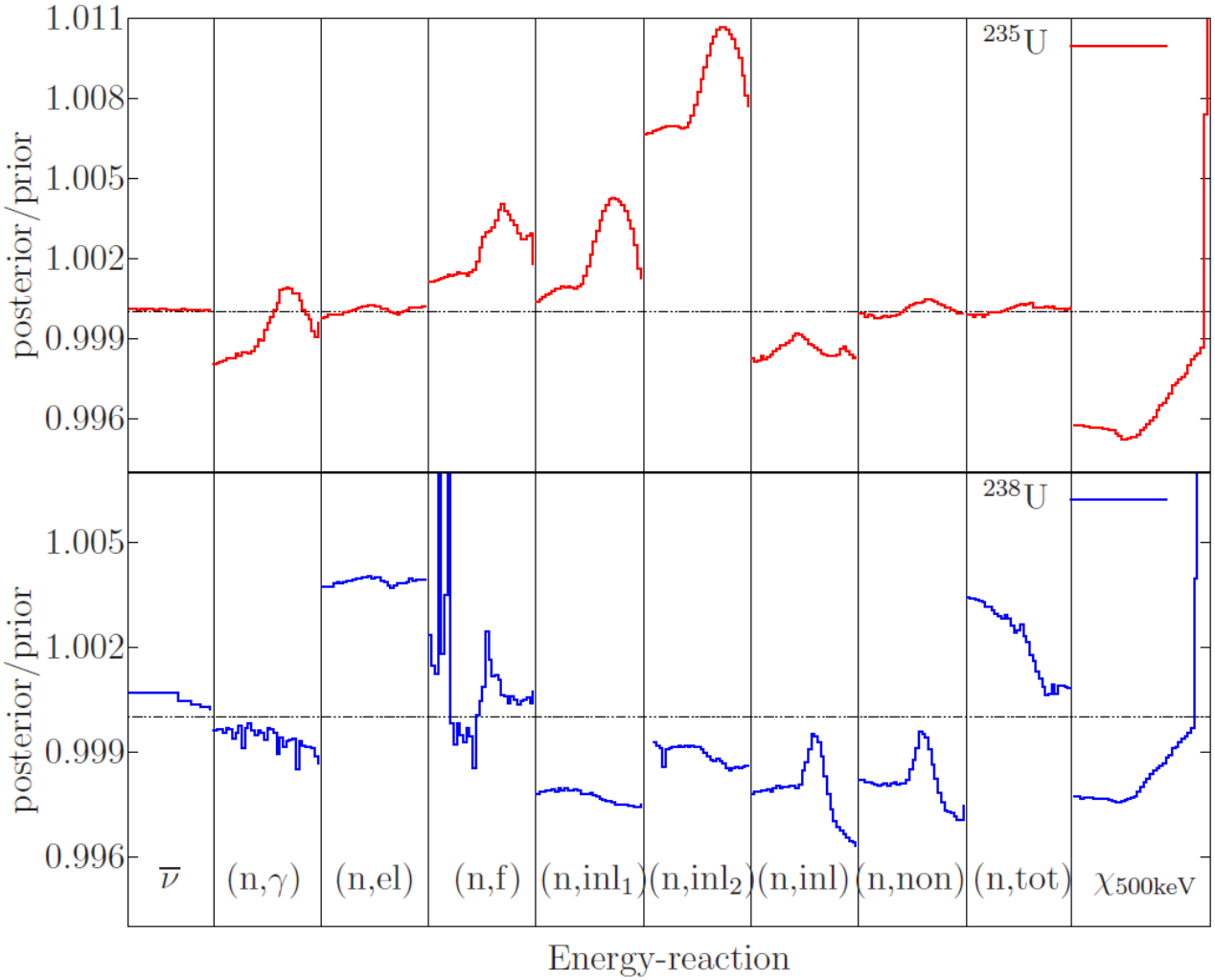


Fig. 9. Ratio of cross sections (and $\overline{\nu}$ and χ) for the post-adjusted (*a posteriori*) over the prior. The cross sections, $\overline{\nu}$ and χ are presented from 100 keV to 6 MeV on a logarithmic scale.

Example with imf7 (bigten) - BMC

- Updated cross section uncertainties

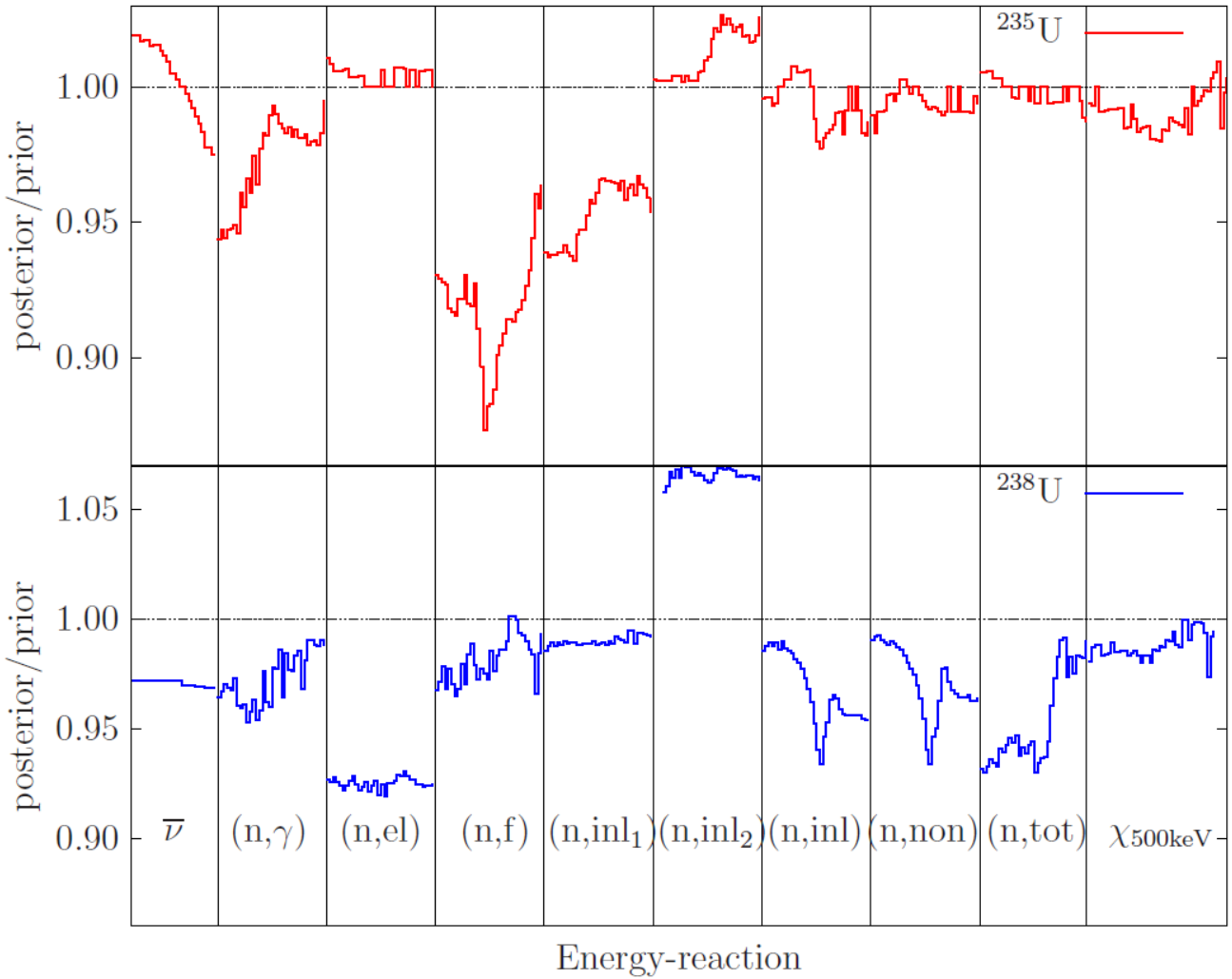
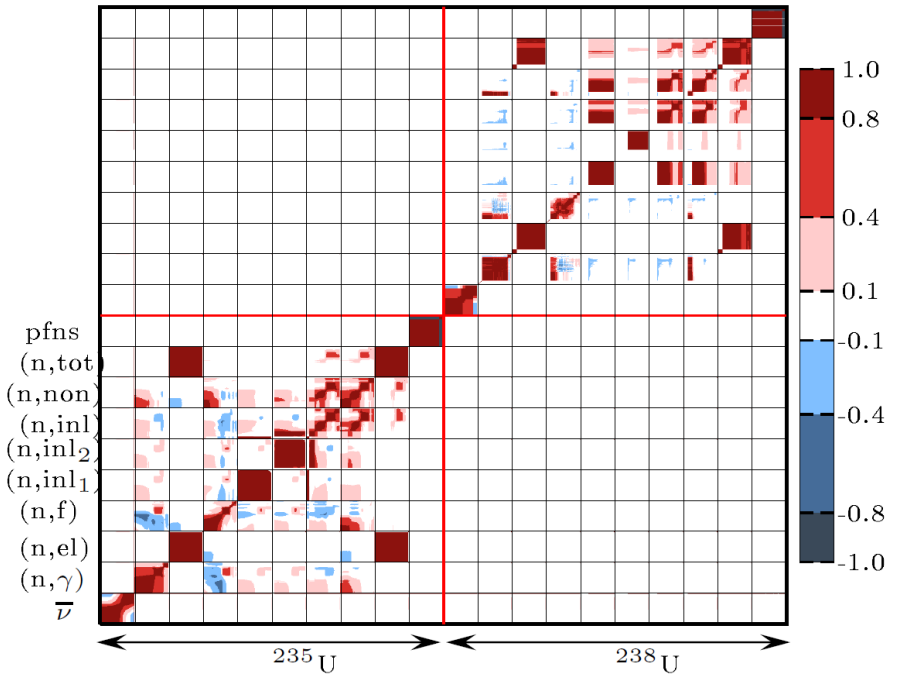


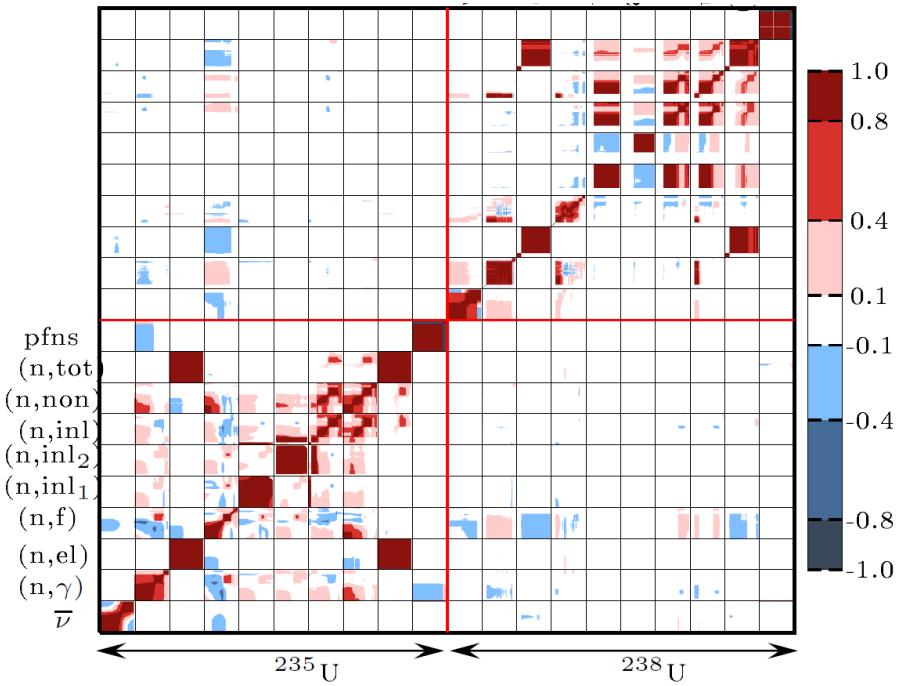
Fig. 10. Same as Fig. 9 but for the uncertainties.

Example with imf7 (bigten) - BMC

- Updated correlations



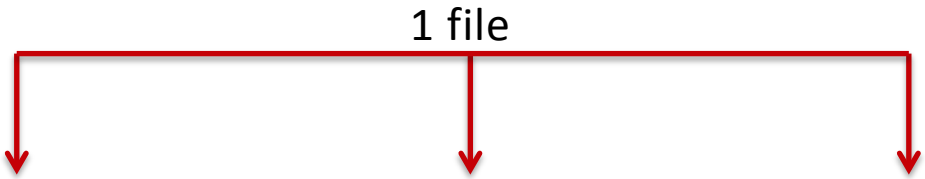
Prior



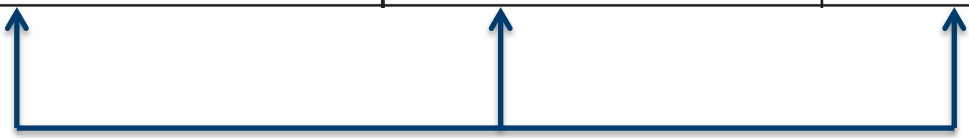
Posterior

Example with imf7 (bigten) – BMC and GNLS

- Back to a single file



	Exp		Prior		Posterior BMC		Posterior GNLS	
		iso	average	run 0	average	run 0	updated	run 0
	$k_{eff} \pm \Delta k$		$\overline{k} \pm \Delta k$	k_{eff}	$\overline{k} \pm \Delta k$	k_{eff}	$k \pm \Delta k$	k_{eff}
imf7	1.00450 ± 70	^{235,238}U	1.00158 ± 850	1.00297	1.00449 ± 70	1.00344	1.00449 ± 70	1.00402



Example with different benchmarks

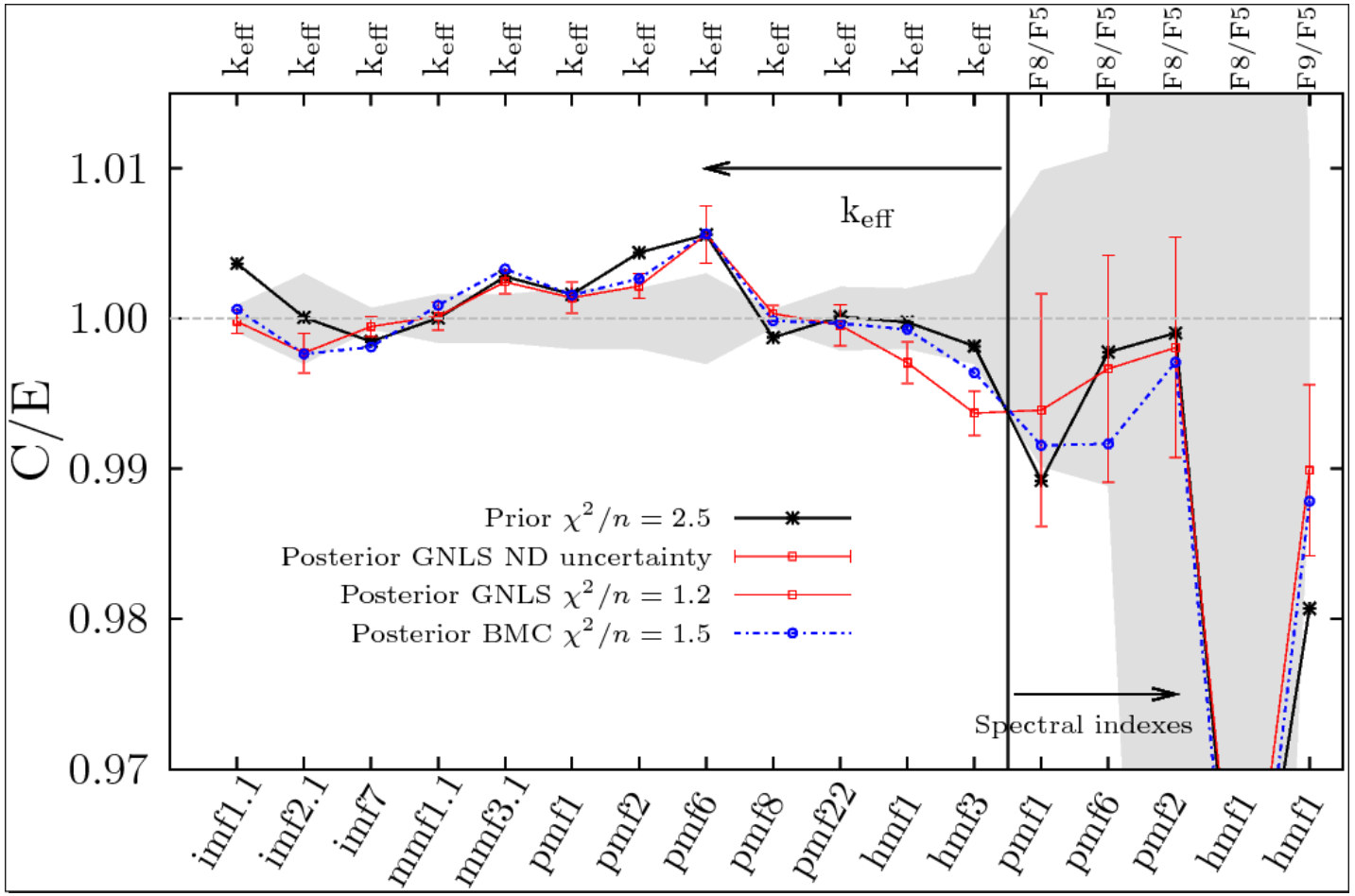
- Many benchmarks, independent calculations

	Exp	Prior			Posterior BMC		Posterior GNLS	
		iso	average	run 0	average	run 0	updated	run 0
	$k_{eff} \pm \Delta k$		$\overline{k} \pm \Delta k$	k_{eff}	$\overline{k} \pm \Delta k$	k_{eff}	$k \pm \Delta k$	k_{eff}
hmf1	1.00000 ± 200	^{235}U	0.99551 ± 1130	0.99976	1.00005 ± 195	0.99979	0.99999 ± 197	1.00008
pmf1	1.00000 ± 200	^{239}Pu	1.00077 ± 780	1.00162	1.00011 ± 195	1.00017	1.00010 ± 195	1.00000
imf7	1.00450 ± 70	$^{235,238}U$	1.00158 ± 850	1.00297	1.00449 ± 70	1.00344	1.00449 ± 70	1.00402
mmf3	0.99930 ± 160	all 3	1.00047 ± 640	1.00210	0.99945 ± 155	0.99917	0.99946 ± 155	0.99942

Example with different benchmarks

- Many benchmarks, all together: 17 quantities (12 k_{eff}, 5 spectral indexes)

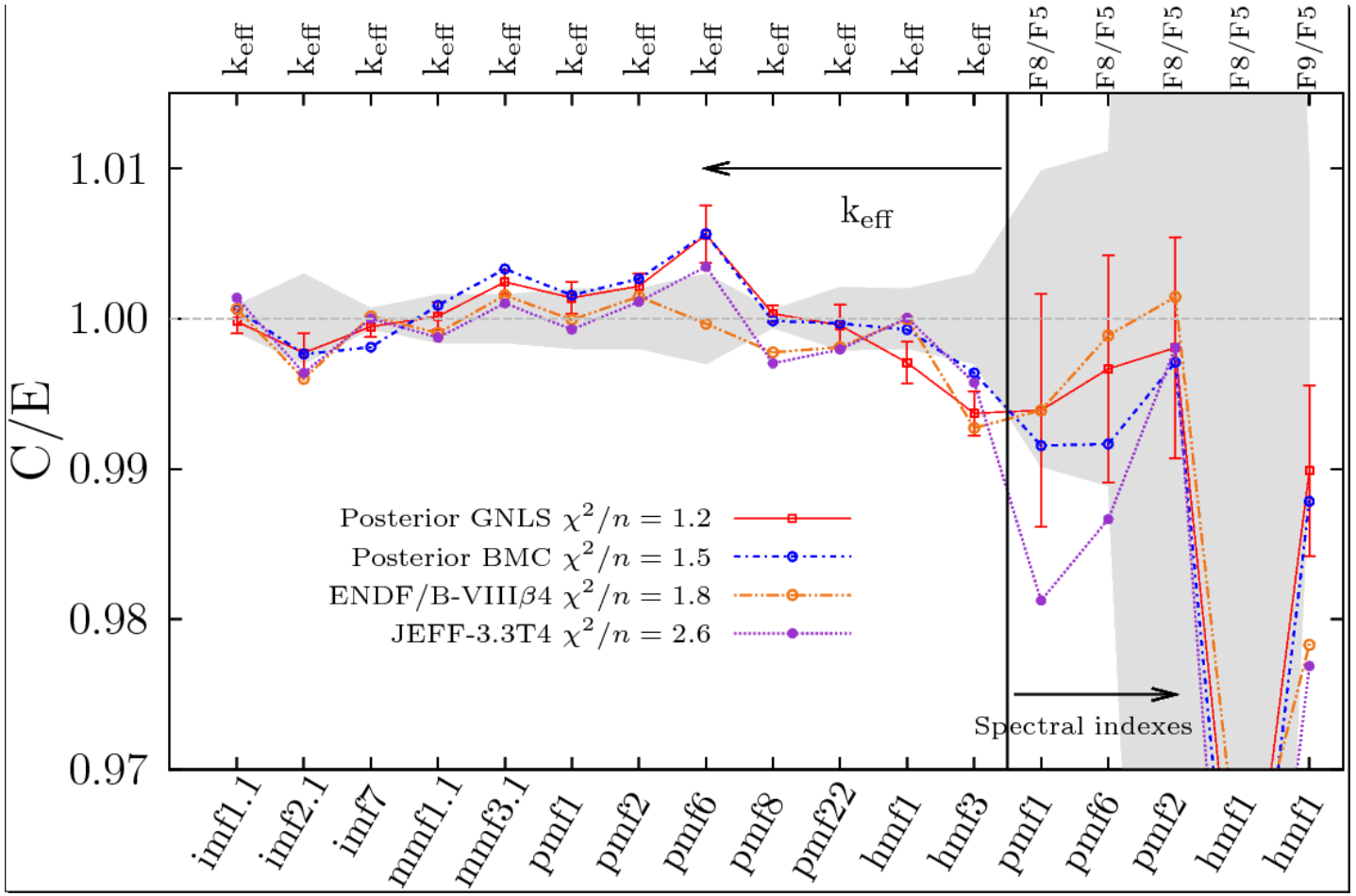
	Exp	Prior		Posterior BMC		Posterior GNLS	
	C $\pm\Delta$C	average $\overline{C}$ $\pm\Delta$C	run 0 C	average $\overline{C}$ $\pm\Delta$C	run 0 C	updated C $\pm\Delta$C	run 0 C
χ^2/n		3.2	2.5	1.2	1.5	0.9	1.2



Example with different benchmarks

- Many benchmarks, all together: 17 quantities (12 k_{eff}, 5 spectral indexes)

	Exp	Prior		Posterior BMC		Posterior GNLS	
	C $\pm\Delta$C	average $\overline{C}$ $\pm\Delta$C	run 0 C	average $\overline{C}$ $\pm\Delta$C	run 0 C	updated C $\pm\Delta$C	run 0 C
χ^2/n		3.2	2.5	1.2	1.5	0.9	1.2



Conclusion

- By considering integral benchmarks, correlations between isotopes appear,
- By considering integral benchmarks, cross section uncertainties decrease,
- Better agreement between experimental and calculated uncertainties,
- Also allows to include EXFOR data for natural and oxide samples,
- Two Monte Carlo methods are used, showing global improvements,
- Such approach makes clear and mathematical sound the adjustment procedure,
- Still, to be improved:
  - Better physics (for TALYS),
  - Consider benchmark experimental covariances,
  - More isotopes should be considered (such as ^{241}Pu, ^{16}O)

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Wir schaffen Wissen – heute für morgen