Monte Carlo integral adjustment of nuclear data libraries – experimental covariances and inconsistent data

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MC uncertainty reduction using integral data

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- Idea of using benchmarks for random-file calibration is not new.
  - Petten method for best estimates
- Here:
  - Multiple correlated benchmarks
  - Multiple isotopes within one benchmark
  - Addressing inconsistencies

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On the use of integral experiments for uncertainty reduction of reactor macroscopic parameters within the TMC methodology

CrossMark

E. Alhassan [a, *], H. Sjöstrand [a], P. Helgesson [a], M. Österlund [a], S. Pomp [a], A.J. Koning [a, b], D. Rochman [c]

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

CW 2017

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

Uncertainty reduction

Random nuclear data from the 1st step is used as the prior for the 2nd step.

Physical models parameters: TALYS based system (T6)

1st level of constraint: **Differential data**

A large set of acceptable ND libraries

Simulations: mcnp etc.

Applications: Criticality, burnup, Fuel cycle etc.

2nd level of constraint: **Integral benchmarks**

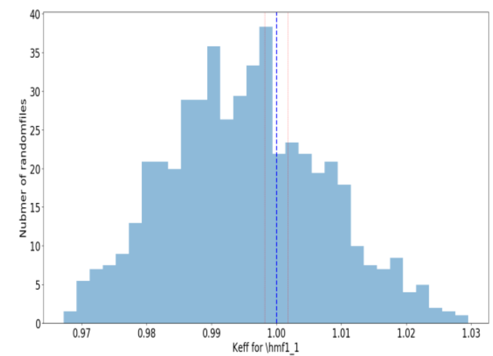
$$w_i = e^{-\frac{\chi_i^2}{2}}$$

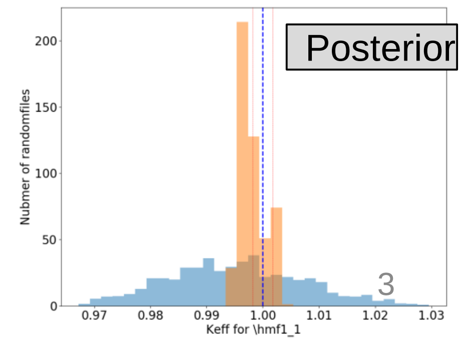
Assign weights to random files

Weighted random files

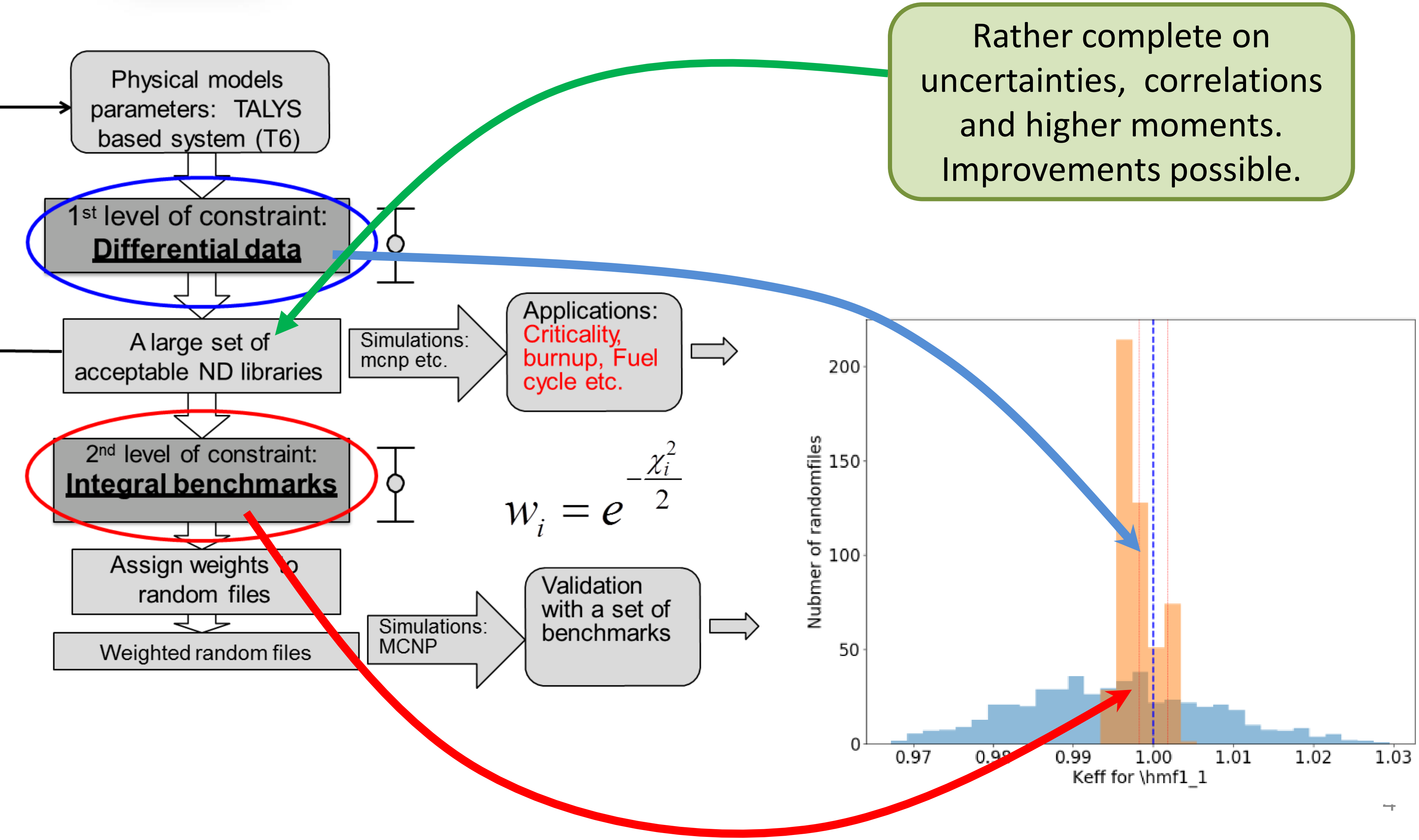
Simulations: MCNP

Prior k_{eff} distribution





The posterior is constrained by both the differential and integral data



Important to also include the calculation uncertainty

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- C/E $\neq 1$ can be due to σ_E, σ_{stat}, an error in the isotopes that we are calibrating, any of the other isotopes in the benchmark, or other errors not accounted for.

$$\chi^2_{i,J} = \sum_B \frac{(C_{B,i} - E_B)^2}{\sigma^2_{B,J}}, i = randomfile, J = isotopes, B = benchmark$$

$$\sigma^2_{B,J} = \sigma^2_E + \sigma^2_{C,J} = \sigma^2_E + \sigma^2_{stat} + \sigma^2_{defects} + \sigma^2_{other} + \sum_{\substack{\text{overall p} \\ \text{where } p \neq J}} \sigma^2_{ND,p}$$

Method

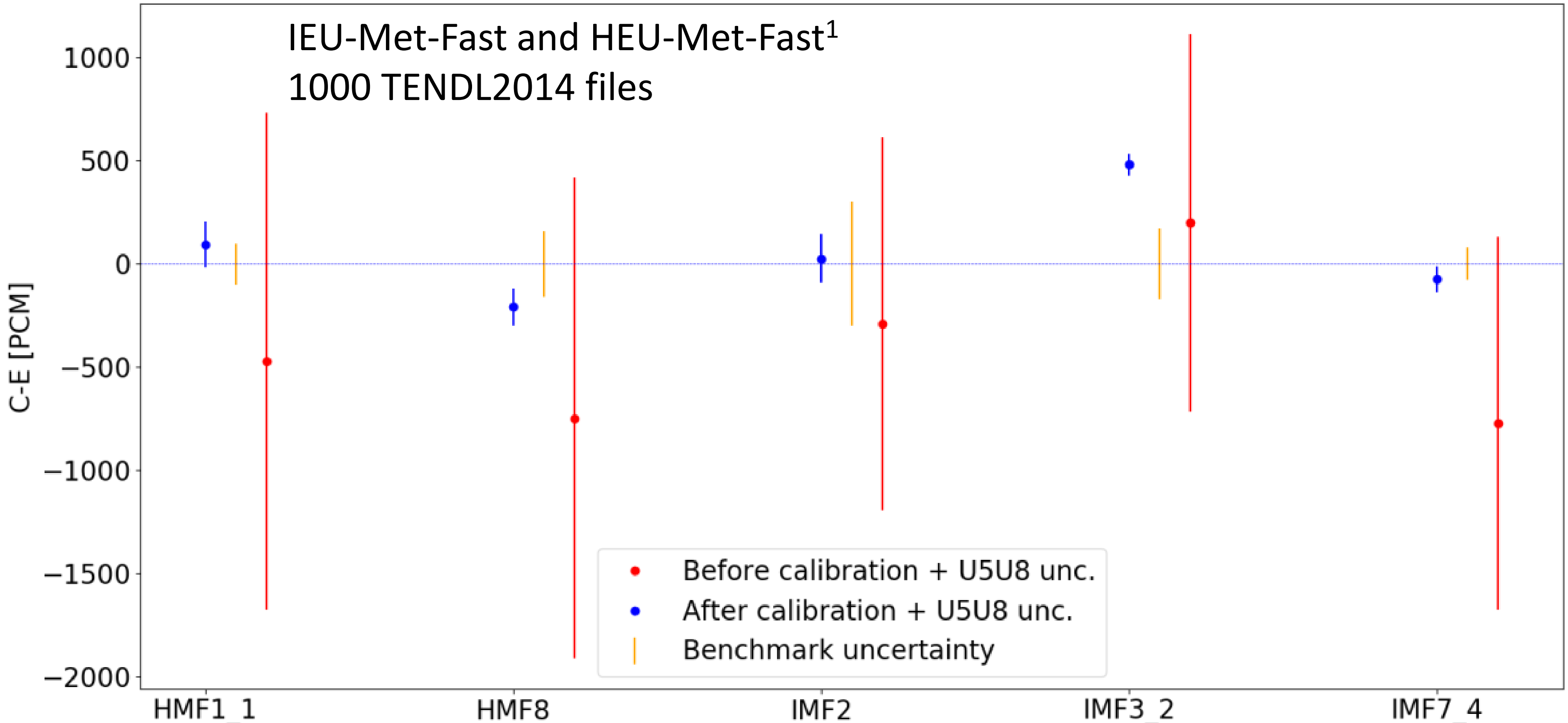
- Major isotopes are varied simultaneously.
- MCNP6 and TENDL2014
- Investigated for U8 and U5.
- $k_{eff,i}=f(U8_i,U5_i)$. i=randomfile number
- Intrinsically the uncertainty of the different isotopes are taking into account simultaneously

$$w_i = e^{-\frac{\chi_i^2}{2}}$$

$$\chi_i^2 = (C-E)^T COV_{B,J}^{-1} (C-E)$$

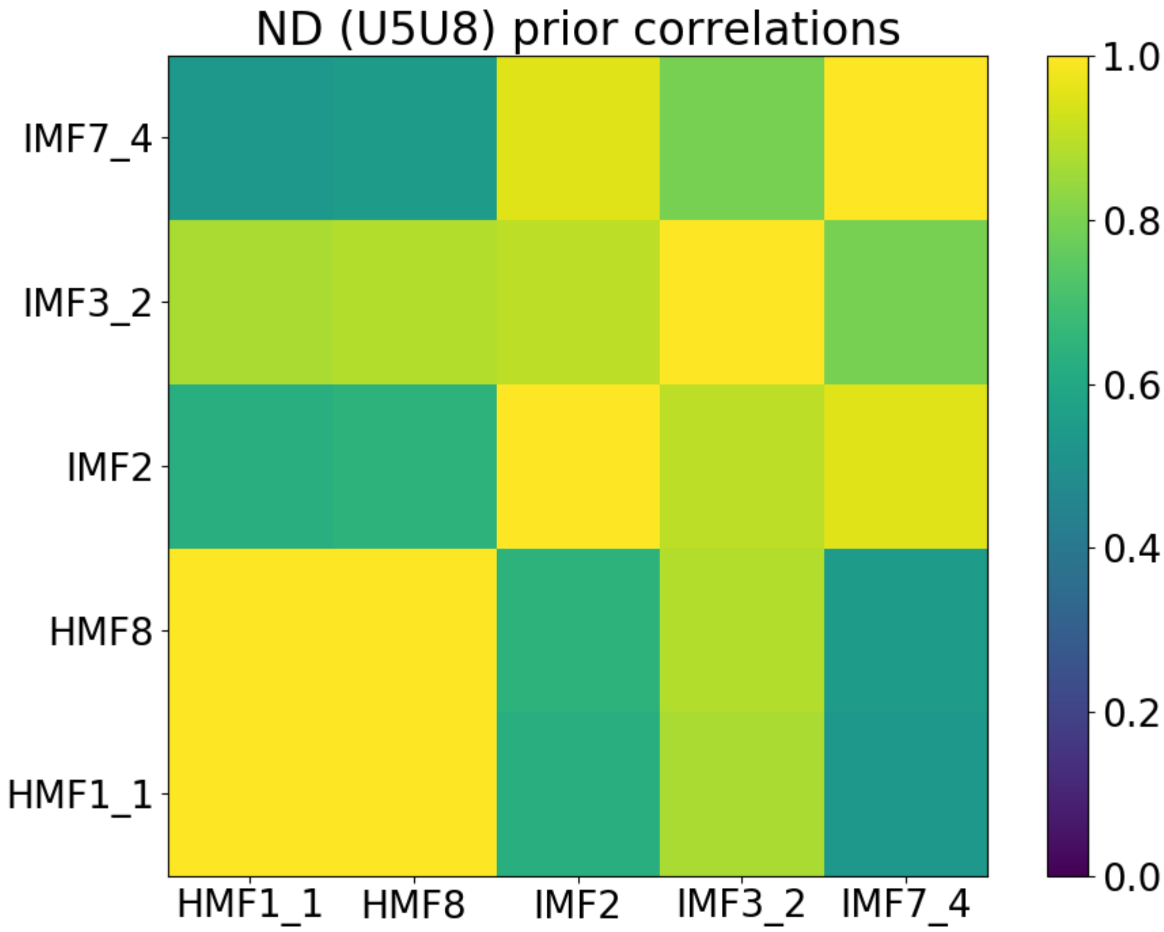
$$COV_{B,J} = COV_E + COV_{stat}$$

Before and after calibration



[1]Curtesy of Steven Van Der Marck

Difficult to fit the experimental data - prior correlations



Difficult to fit the experimental data - inconsistent data

- Model defects.
  - E.g., ND uncertainties not taking into account[1]
  - Models inability to reproduce the true ND
- Unaccounted experimental uncertainties or covariances.
- Underestimated statistical uncertainties.
- Isotopes not taken into account

$$\sigma_{B,J}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sigma_{defects}^2 + \sigma_{other}^2 + \sum_{\substack{\text{overall p} \\ \text{where } p \neq J}} \sigma_{ND,p}^2$$

[1]See, e.g., Gerald Rimpaults presentation: *Trends on major actinides from an Integral data assimilation.*

Marginalized Likelihood Optimization

- We add an extra uncertainty to each experiment.

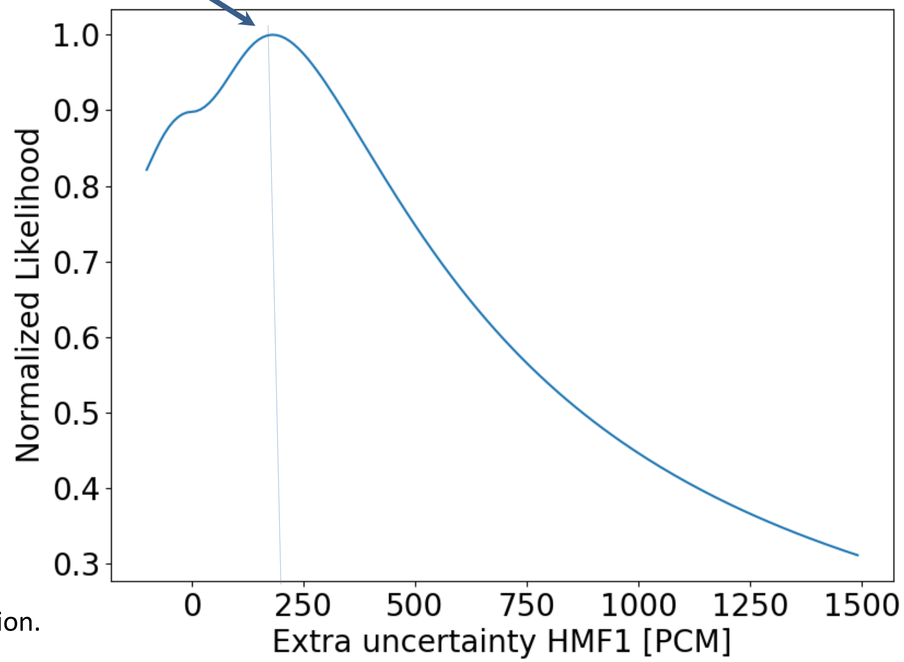
$$\sigma_{B,J}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sigma_{defects}^2 + \sigma_{other}^2 + \sum_{\substack{\text{overall p} \\ \text{where } p \neq J}} \sigma_{ND,p}^2$$

$$\sigma_{B,l,J}^2 = \sigma_E^2 + \sigma_{stat}^2 + \sigma_{extra,l}^2$$

- σ_{extra} found by maxzimizing[1] L:

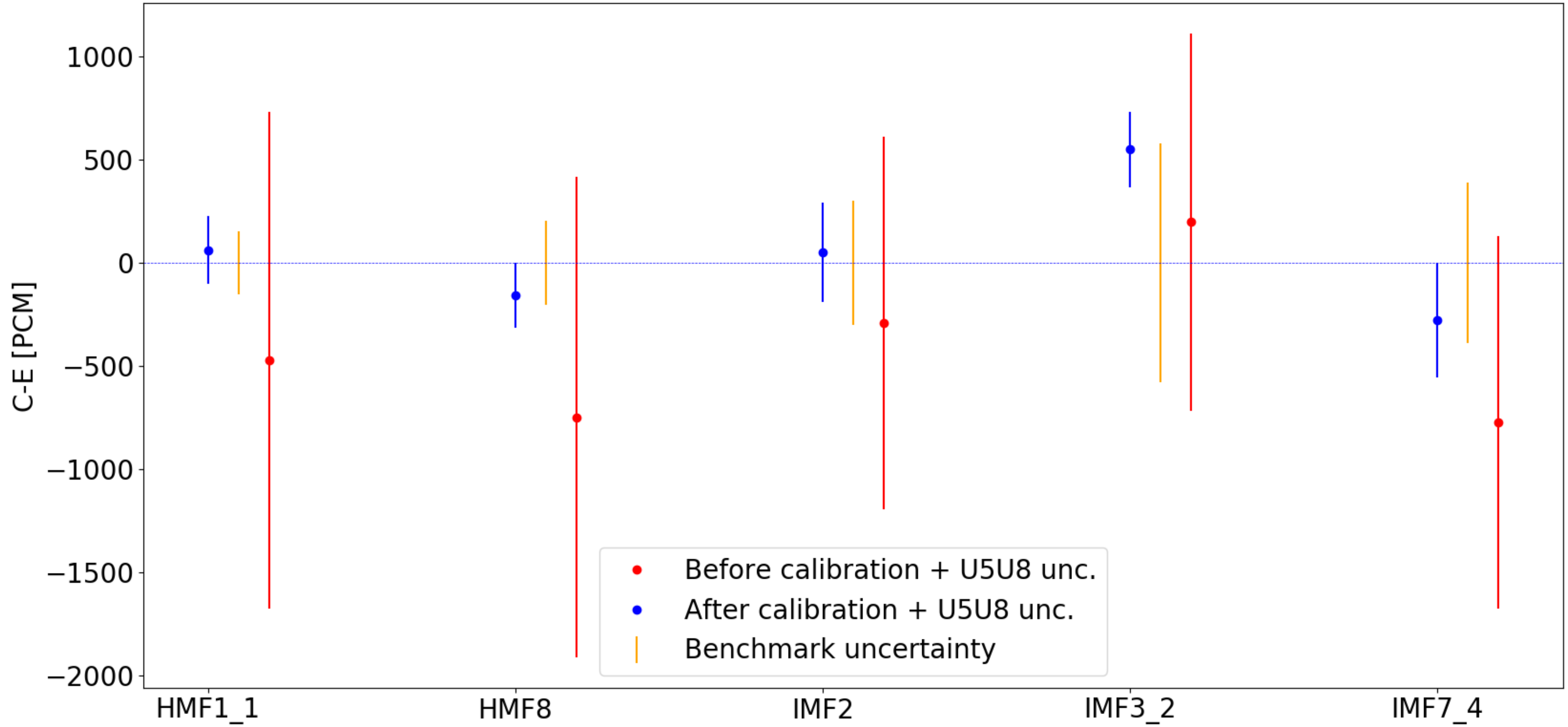
$$L = \frac{1}{\sqrt{2\pi n \left| \mathrm{cov}_{\exp,stat,extra} \right|}} \sum_i e^{-\frac{\chi_i}{2}}$$

n = number of parameters



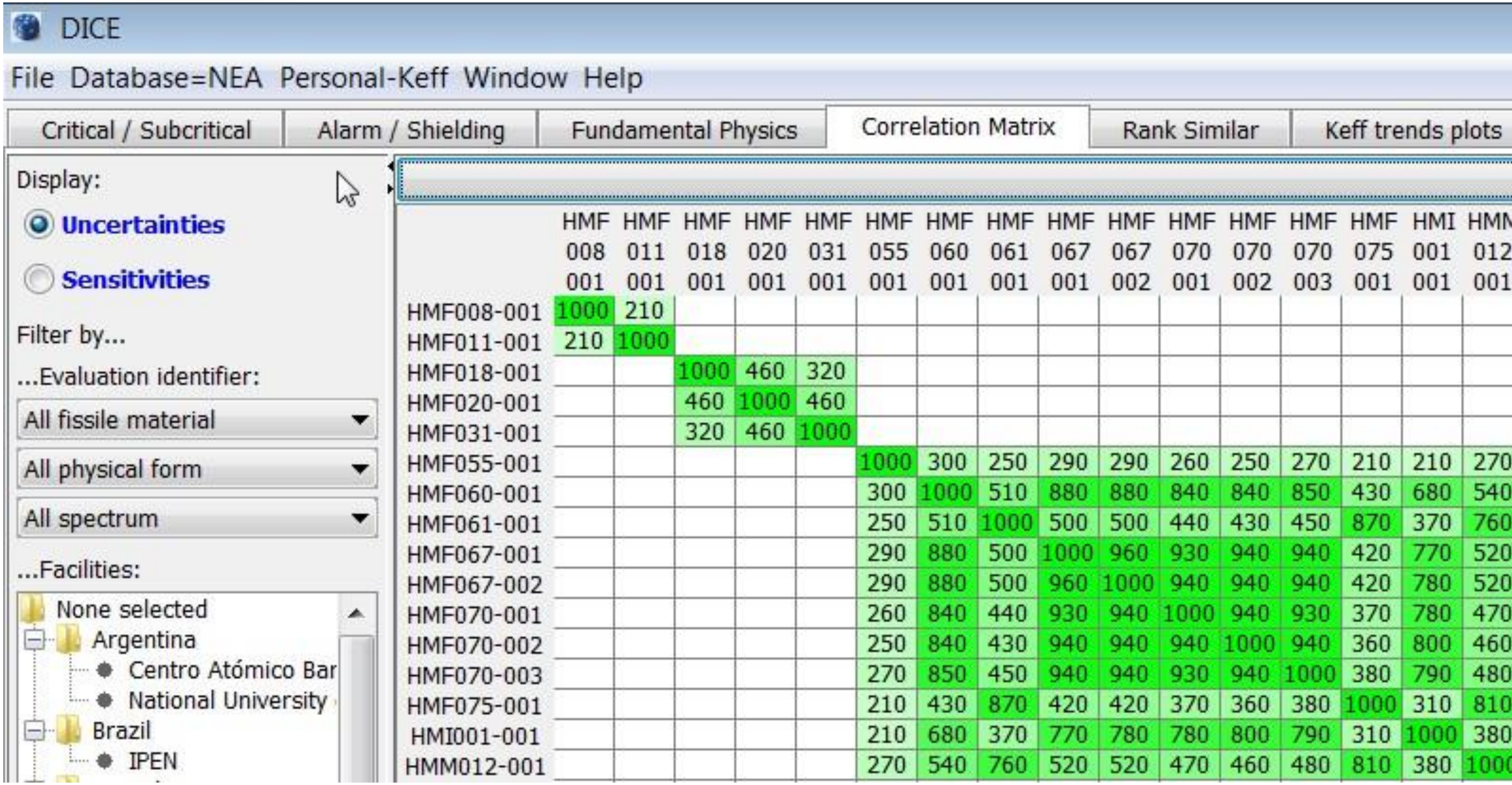
[1] Here MC and integral information. Compare with G.Schnabel's presentation.
[1]G.Schnabel, *Fitting and analysis technique for inconsitent data*,MC2017

Results



Benchmark uncertainties [PCM]	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4
No ML: Reported uncertainties	100	160	300	170	80
Uptated uncertainties	153	204	300	580	390

Benchmark exp. errors are correlated

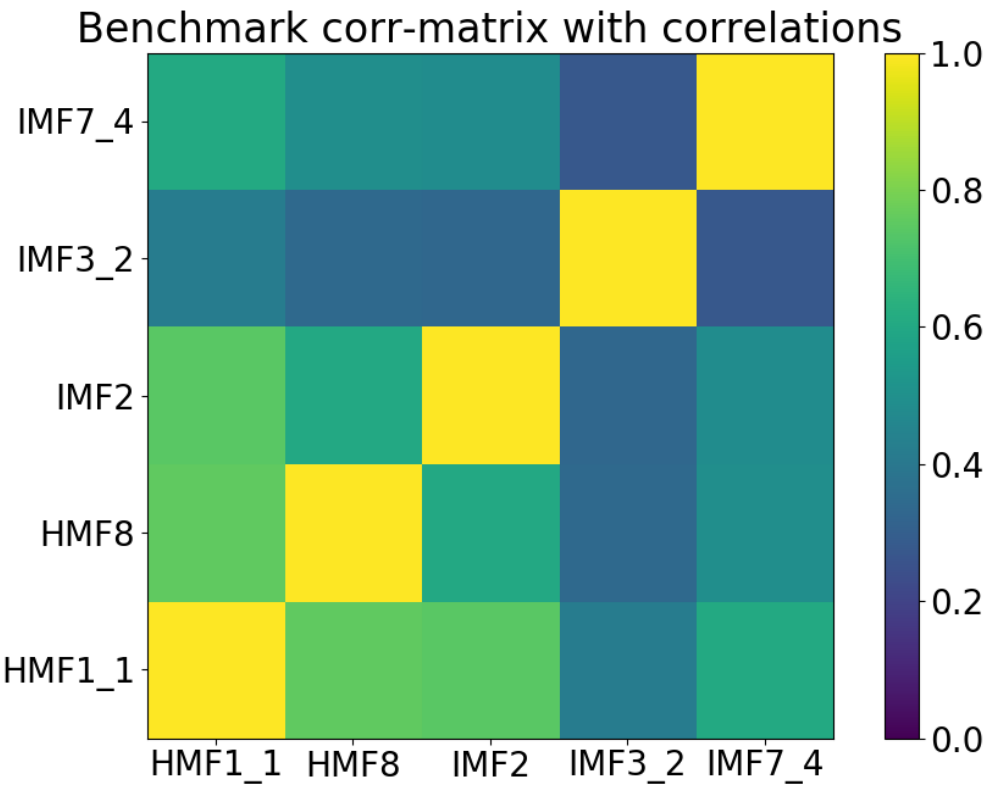


	HMF 008 001	HMF 011 001	HMF 018 001	HMF 020 001	HMF 031 001	HMF 055 001	HMF 060 001	HMF 061 001	HMF 067 001	HMF 067 002	HMF 070 001	HMF 070 002	HMF 070 003	HMF 075 001	HMI 001 001	HMM 012 001
HMF008-001	1000	210														
HMF011-001	210	1000														
HMF018-001			1000	460	320											
HMF020-001			460	1000	460											
HMF031-001			320	460	1000											
HMF055-001						1000	300	250	290	290	260	250	270	210	210	270
HMF060-001						300	1000	510	880	880	840	840	850	430	680	540
HMF061-001						250	510	1000	500	500	440	430	450	870	370	760
HMF067-001						290	880	500	1000	960	930	940	940	420	770	520
HMF067-002						290	880	500	960	1000	940	940	940	420	780	520
HMF070-001						260	840	440	930	940	1000	940	930	370	780	470
HMF070-002						250	840	430	940	940	940	1000	940	360	800	460
HMF070-003						270	850	450	940	940	930	940	1000	380	790	480
HMF075-001						210	430	870	420	420	370	360	380	1000	310	810
HMI001-001						210	680	370	770	780	780	800	790	310	1000	380
HMM012-001						270	540	760	520	520	470	460	480	810	380	1000

Database for the International Criticality Safety Benchmark Evaluation Project (DICE), https://www.oecd-nea.org/science/wpncs/icsbep/dice.html

Adding a correlation term

- Correlations: σ_E, σ_{defect}, $\sigma_{other\_isotopes}$
- A fully correlated uncertainty to all experiments is added.



$$\sigma^2_{B,l,J} = \sigma^2_E + \sigma^2_{stat} + \sigma^2_{extra,l} + \sigma^2_{extra\_all}$$

$$L = \frac{1}{\sqrt{2\pi n \left| \mathrm{cov}_{\exp,stat,extra} \right|}} \sum_i e^{-\frac{\chi_i}{2}}$$

$$\max(L) \rightarrow \sigma^2_{extra,l} + \sigma^2_{extra\_all}$$

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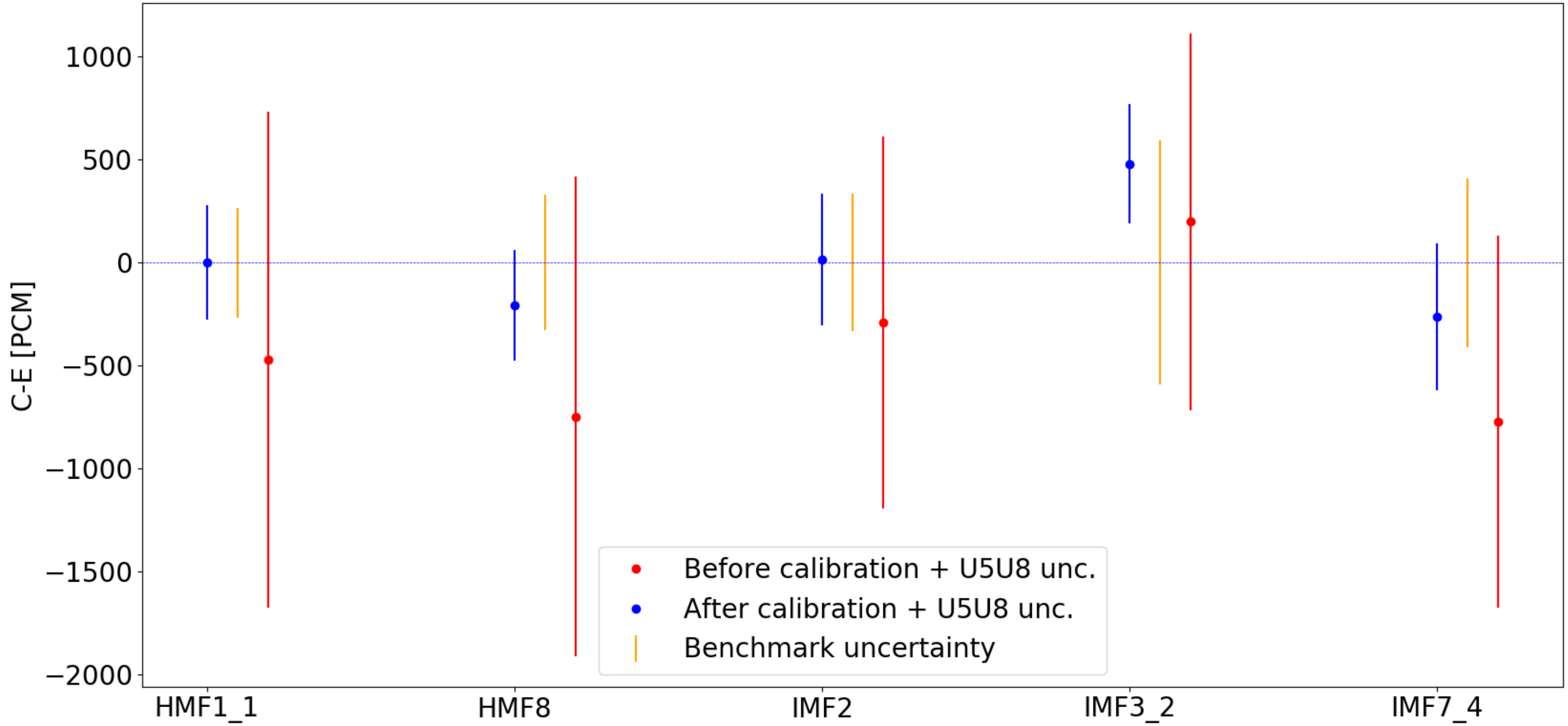
Results – with correlation



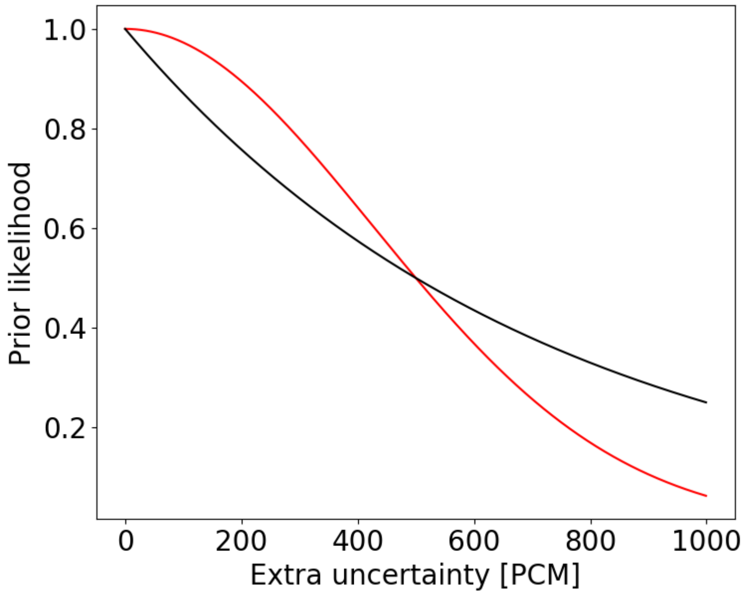
Benchmark uncertainties [PCM]	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Fully correlated
No ML: Reported uncertainties	100	160	300	170	80	0
Uptated uncertainties	153	204	300	580	390	0
With correlation	267	329	333	591	409	257

Adding a prior

$$prior(\sigma_{extra}) = e^{-\beta\sigma_{extra}^2} \text{ or,}$$

$$prior(\sigma_{extra}) = e^{-\beta\sigma_{extra}}$$

$$L = \frac{1}{\sqrt{2\pi n \left|\mathrm{cov}_{\exp,stat,extra}\right|}} e^{-\beta\sum\sigma_{extra}^2} \sum_i e^{-\frac{\chi_i}{2}}$$



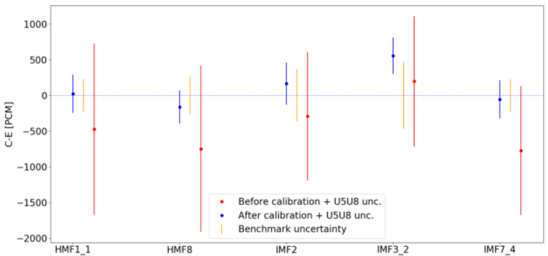
β is chosen **by expert judgement** or in a data-driven approach[1].

[1]G.Schnabel, *Fitting and analysis technique for inconsitent data*,MC2017

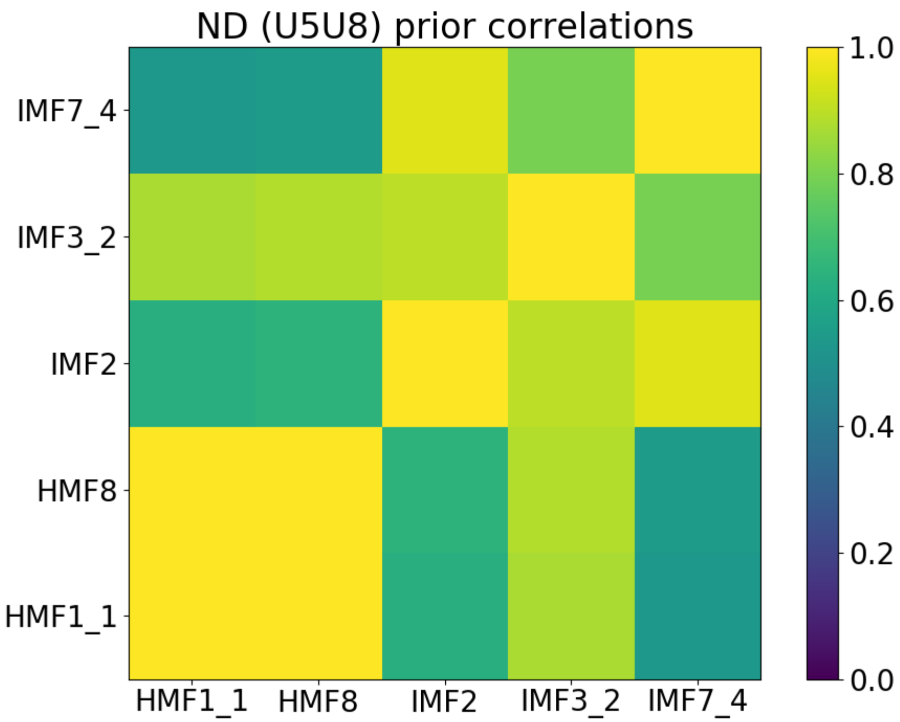
Results with an added prior

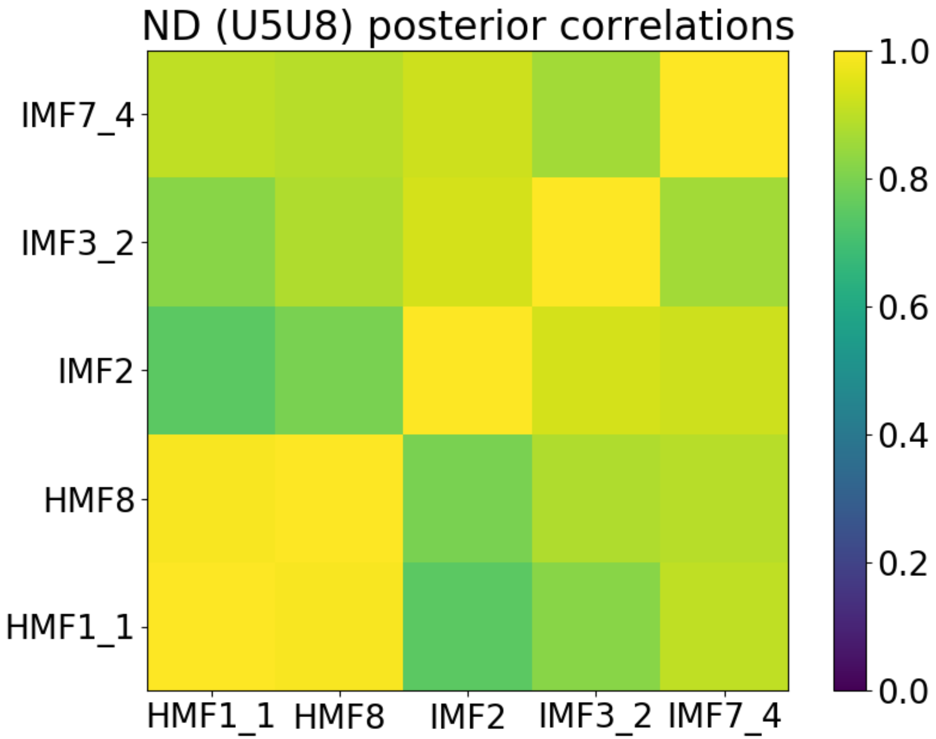
Benchmark uncertainties [PCM]	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Fully correlated
No ML: Reported uncertainties	100	160	300	170	80	0
Uptated uncertainties	153	204	300	580	390	0
With correlation	267	329	333	591	409	257
With prior	232	263	366	468	228	209

Posterior	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Chi2	p_value
No ML	69	28	103	52	34	2,1	6%
Uptated uncertainties	139	131	234	183	273	0,38	86%
With correlation	264	254	313	290	351	0,4	84%
With Prior	253	214	288	256	265	0,58	72%



Posterior correlations

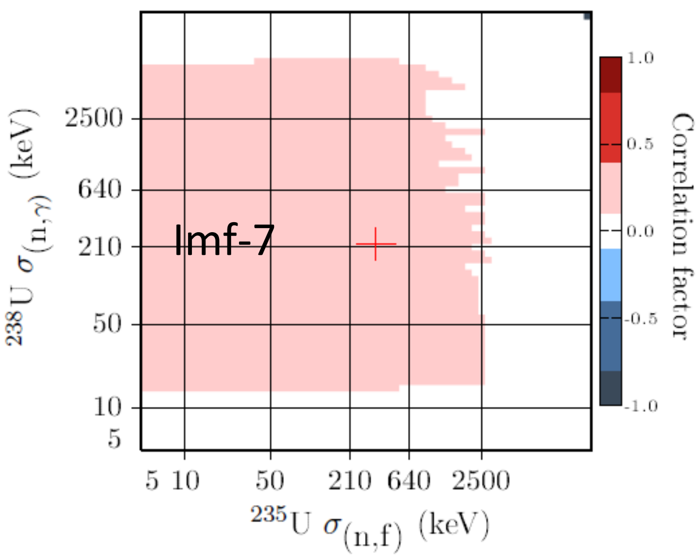




How is the uncertainty reduced?

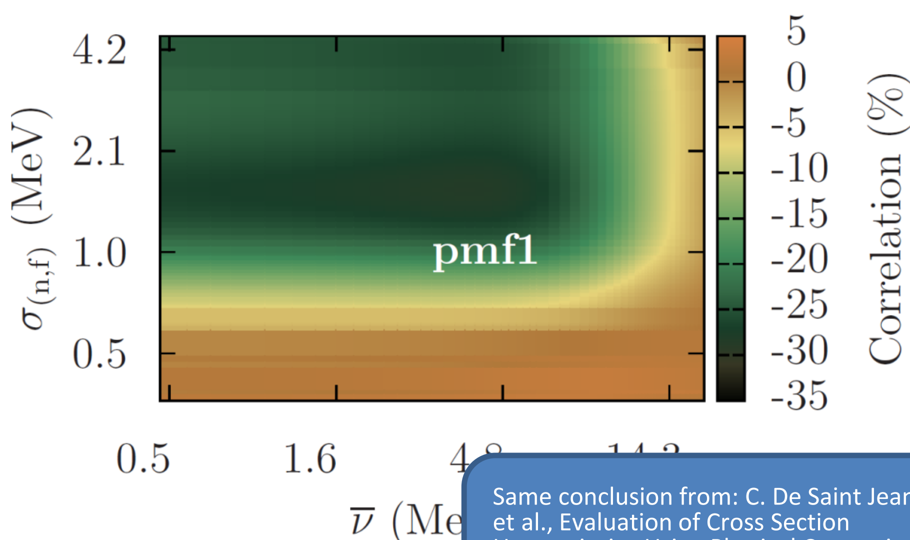
E.Bauge."*Correlations in nuclear data from integral constraints: cross-observables and cross-isotopes* ", *CW2017:*

- Using integral data introduce correlations: between isotopes and between different parts of the ND file.
- The integral weighing only slightly change the best estimate <1% and std dev < 10%



D. Rochman: Nuclear data correlation between different isotopes via integral information

D. Rochman et al., EPJ Nuclear Sci. Technol. 3, 14 (2017)

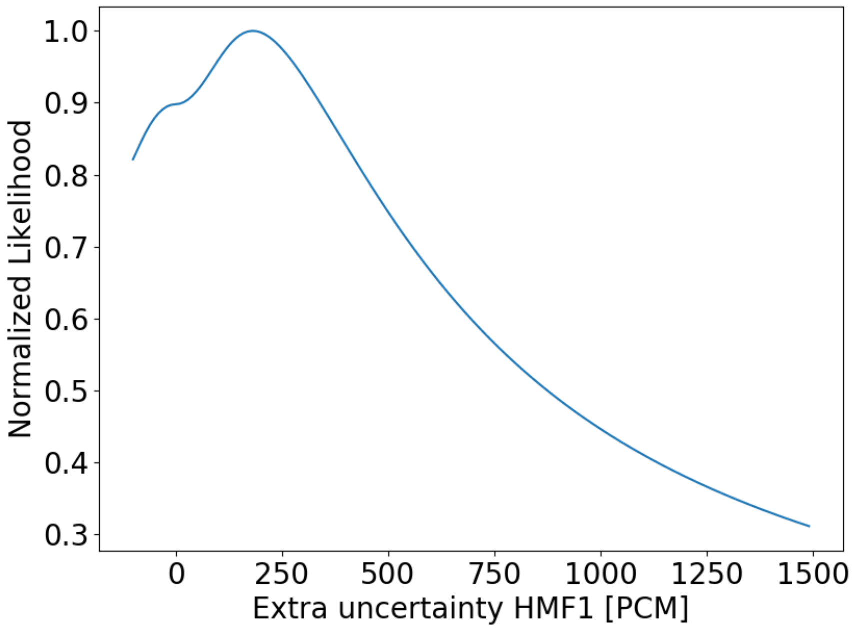


Same conclusion from: C. De Saint Jean et al., Evaluation of Cross Section Uncertainties Using Physical Constraints: Focus on Integral Experiments, Nuclear Data Sheets,Volume 123, Pages 178-184

Conclusion

- MC - Marginalized Likelihood maximization to account for discrepant integral data.
- Results still constrained by differential data and the model.
  - improvements necessary (G. Schnabel's presentation)

- Include calculation uncertainties
  - e.g., multiple isotopes (and observables not accounted for).
- The correlation between the benchmarks are important.
- Outlook: sampling of L[1] + validation / transposition.



[1]G.Schnabel, *Fitting and analysis technique for inconsitent data*,MC2017

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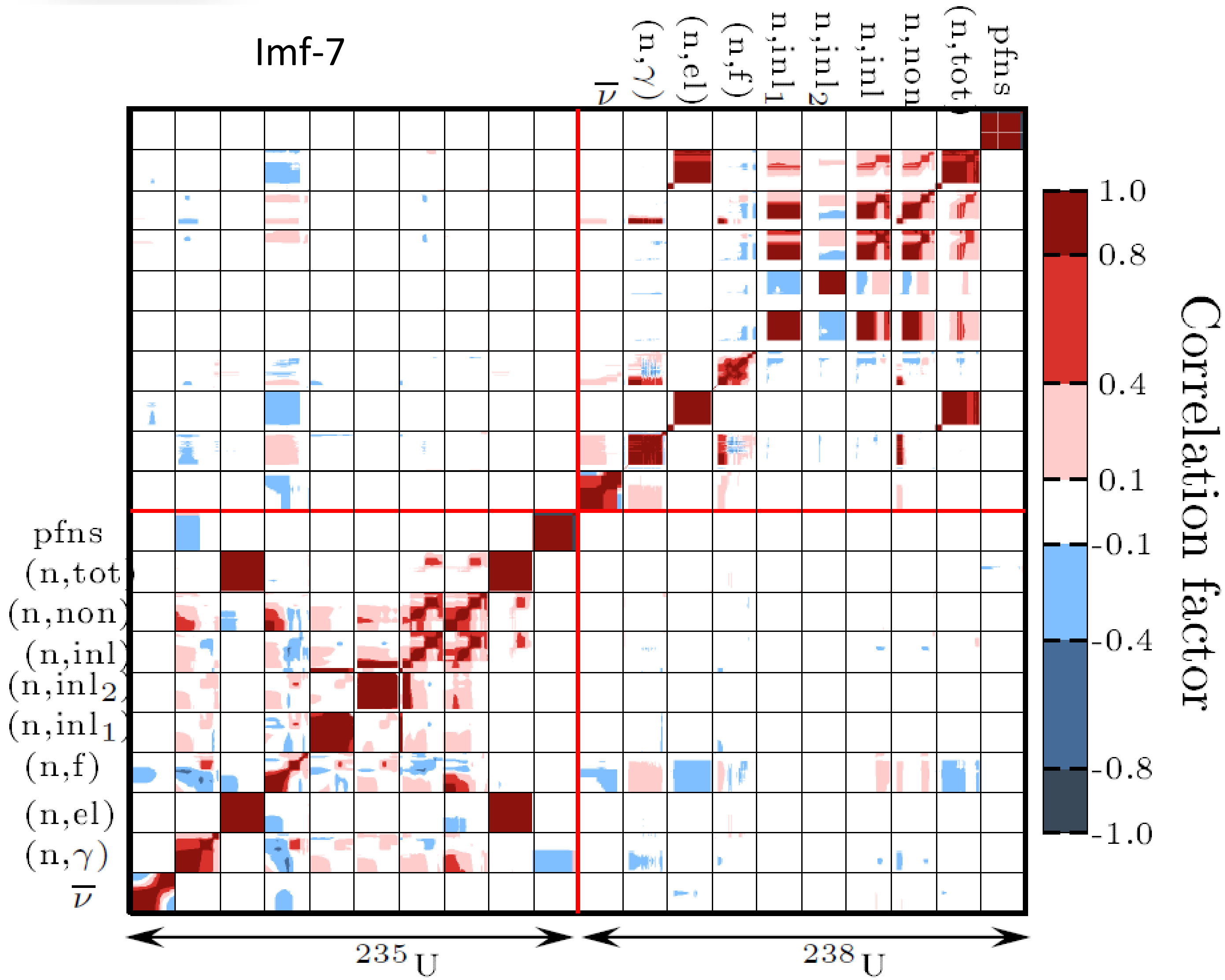
THANK YOU FOR YOUR ATTENTION!

References

1. Alhassan, E., et al. On the use of integral experiments for uncertainty reduction of reactor macroscopic parameters within the TMC methodology, Progress in Nuclear Energy, 88, pp. 43-52. (2016)
2. D. Rochman, et al. Nuclear data correlation between different isotopes via integral information , EPJ Nuclear Sci. Technol. 4, 7 (2018)
3. D. Rochman et al., EPJ Nuclear Sci. Technol. 3, 14 (2017)
4. C. De Saint Jean et al., Evaluation of Cross Section Uncertainties Using Physical Constraints: Focus on Integral Experiments, Nuclear Data Sheets,Volume 123, Pages 178-184
5. G.Schnabel, *Fitting and analysis technique for inconsistent data*,MC2017

Cross-isotope correlations

Imf-7



D. Rochman: Nuclear data correlation between different isotopes via integral information

$$\log\_L = c - 0.5 \cdot \left|cov_{exp} + cov_{extra}\right| + \ln\left(\sum e^{-\frac{\chi}{2}}\right)$$

Posterior	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Chi2 priori(exp)	Chi2_post(exp)	Chi2_prior(tot)	Chi2_post(tot)	p_value-post
No ML	69	28	103	52	34	28	2,3	1,81	2,1	6%
Uptated uncertainties	139	131	234	183	273	6,42	0,46	0,68	0,38	86%
With correlation	264	254	313	290	351	1,66	0,48	0,74	0,4	84%
With Prior	253	214	288	256	265	3,7	0,68	1,06	0,58	72%