UPPSALA UNIVERSITET

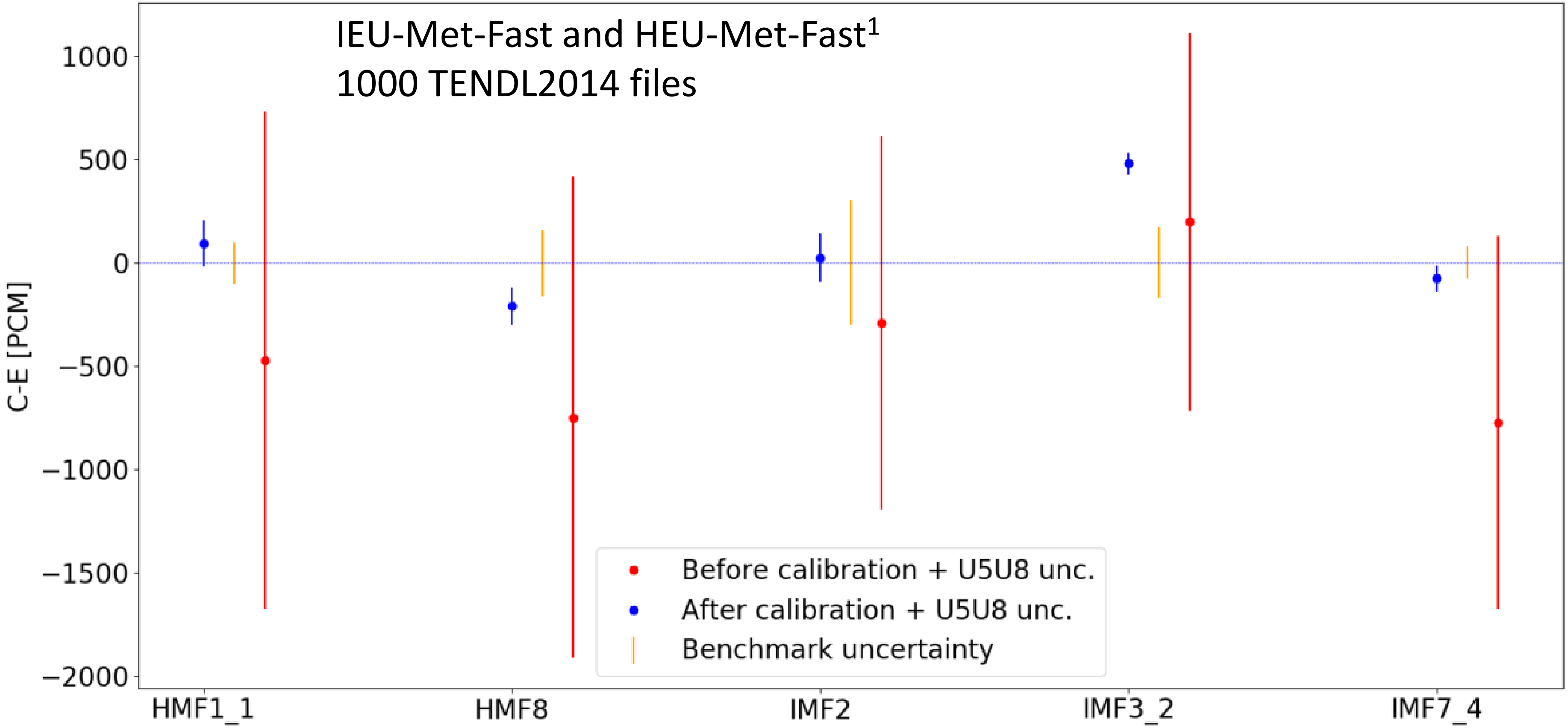
Treating inconsistent data in integral adjustment using Marginal Likelihood Optimization.

Henrik Sjöstrand[1,a], Georg Schnabel[a], Daniel Siefman[b]
Dimitri Rochman[c]

[a]Uppsala University, Sweden
[b]École polytechnique fédérale de Lausanne (EPFL), Switzerland
[c]Paul Scherrer Institute (PSI), Switzerland
[1]henrik.sjostrand@physics.uu.se

UPPSALA UNIVERSITET

Inconsistent data



[1]Curtesy of Steven Van Der Marck

Inconsistent data - causes

- Model defects
  - e.g., ND uncertainties or correlation not taking into account (lack of nuisance parameters).
  - models inability to reproduce the true ND.
- Unaccounted experimental uncertainties or correlations.
- Underestimated statistical uncertainties.
- Isotopes not taken into account.

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

Previous attempts to address inconsistent integral experiments

UPPSALA UNIVERSITET

Adjustment Margin (AM)

Reject

$$\frac{\Delta C}{C}+\frac{\Delta E}{E}-\left|\frac{C-E}{E}\right|=AM<0$$

$\Delta\chi^2$ filtering

$$\chi^2=(\mathrm{E}-\mathrm{C}(\sigma))^T(\mathrm{M_C}+\mathrm{M_E})^{-1}(\mathrm{E}-\mathrm{C}(\sigma))$$

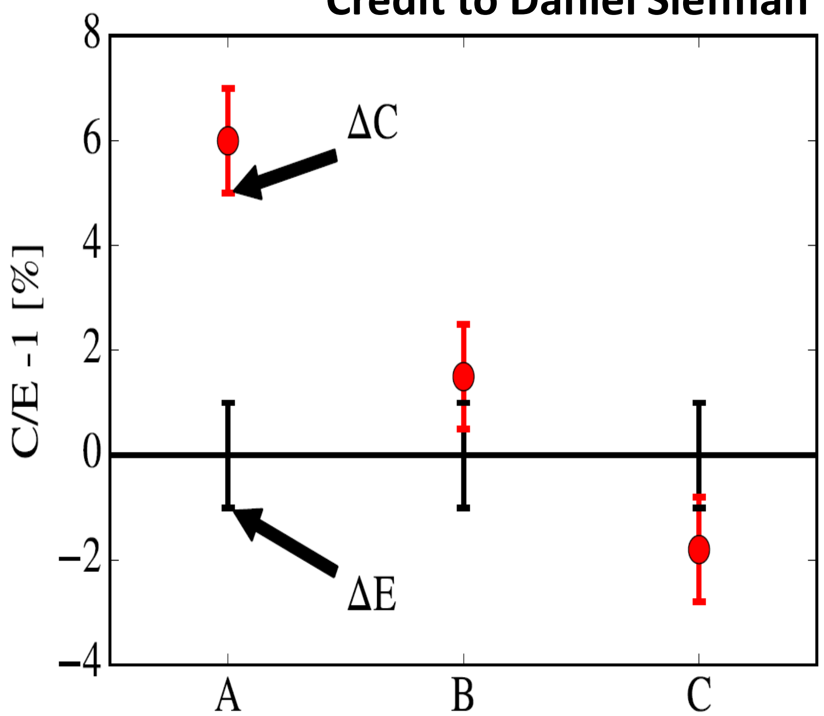
Includes correlations

$$\chi^2-\chi^2_{\neq i}=\Delta\chi^2>Th$$

$$Th=1.2\ (\text{Scale})$$

Reject

Credit to Daniel Siefman



Possible issues

AM

1) does not take into account correlations.

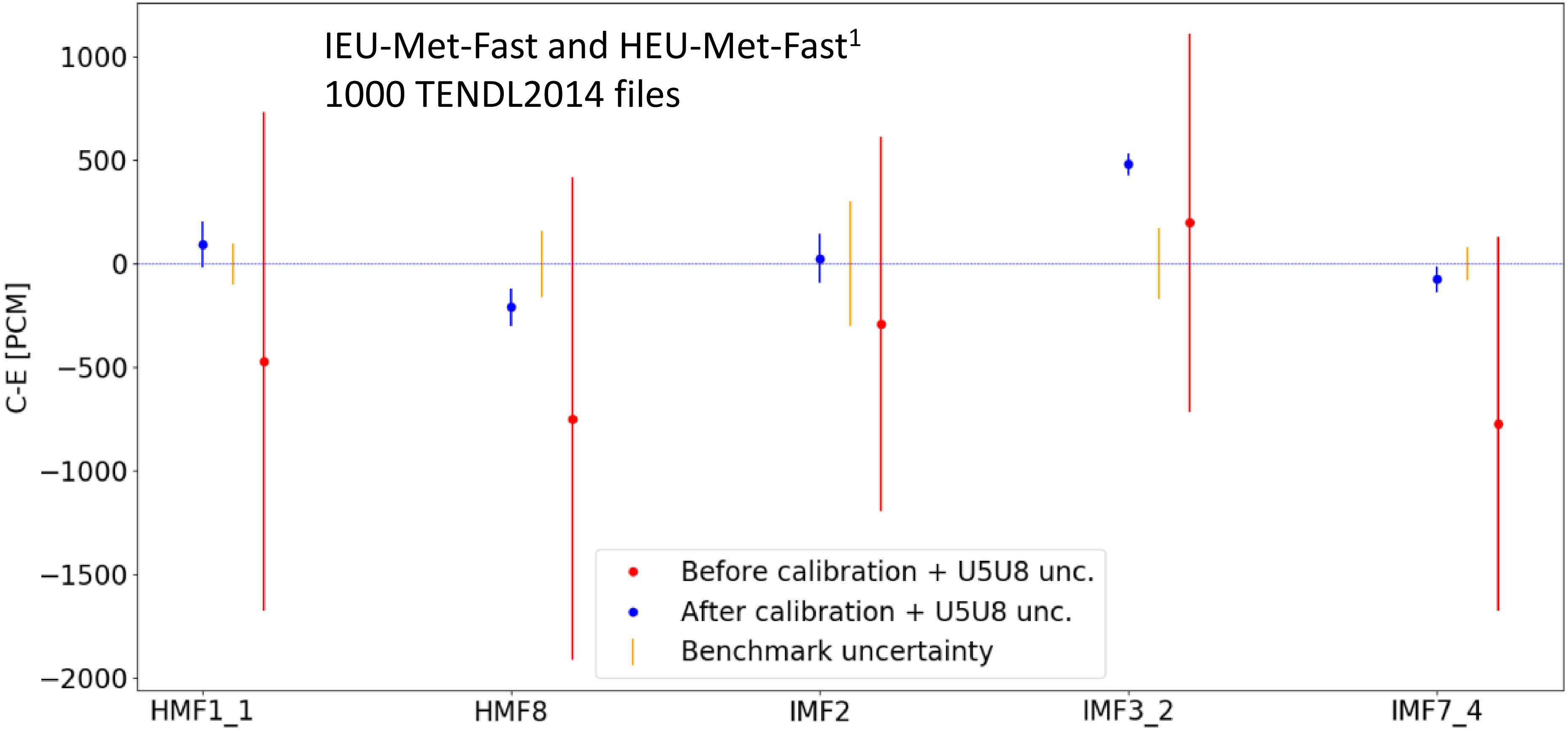
2) is binary.

$\Delta\chi^2$ **filtering**

1) is binary.

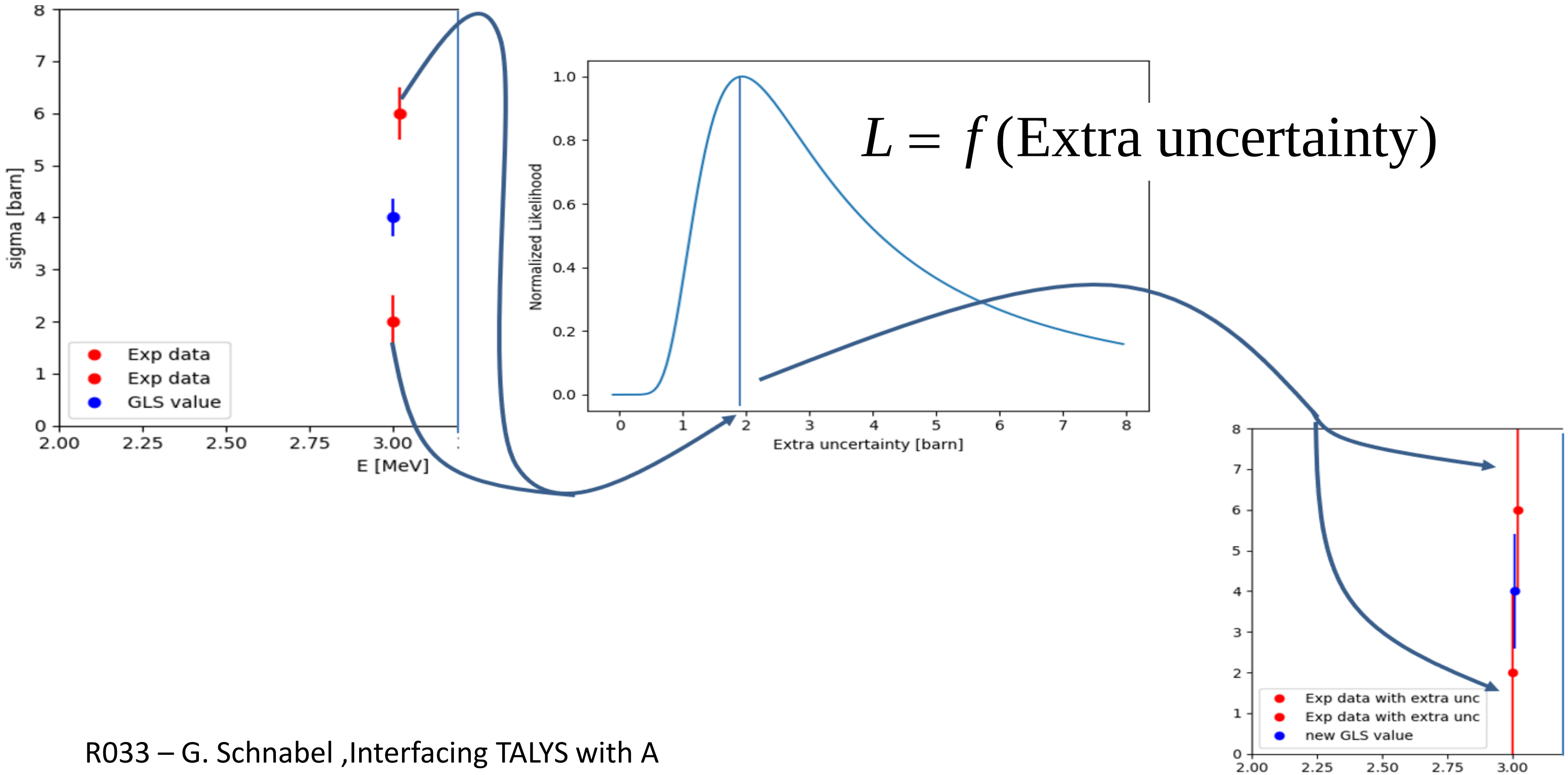
2) The choice of 1.2 is rather arbitrary? It should depend on the number of experiments. (Can be resolved)

Before and after calibration



AM would not reject any of the experiments.

Treating inconsistent data using Marginal Likelihood Optimization (MLO)



R033 – G. Schnabel ,Interfacing TALYS with A Bayesian Treatment of **Inconsistent Data** and Model Defects, ND2019

MLO for integral data and BMC

- We add an extra uncertainty to each experiment.

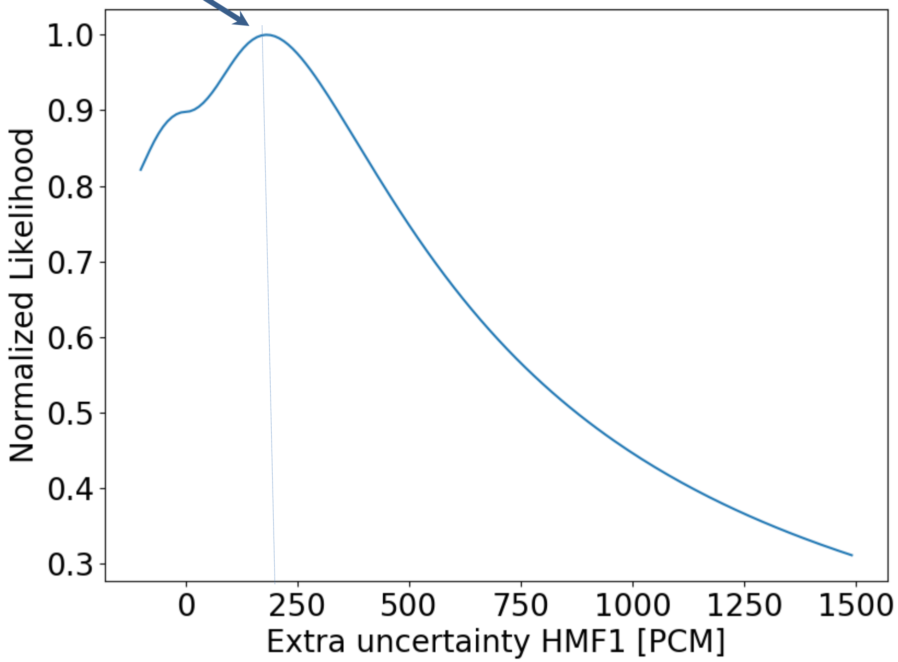
$$\sigma^2_{B,J} = \sigma^2_{rep} + \sigma^2_{stat} + \sigma^2_{defects} + \sigma^2_{other} + \sum_{\substack{\text{overall p} \\ \text{where } p \neq J}} \sigma^2_{ND,p}$$

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

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

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

n = number of experiments



[1] Here MC and integral information. Compare with

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

UPPSALA UNIVERSITET

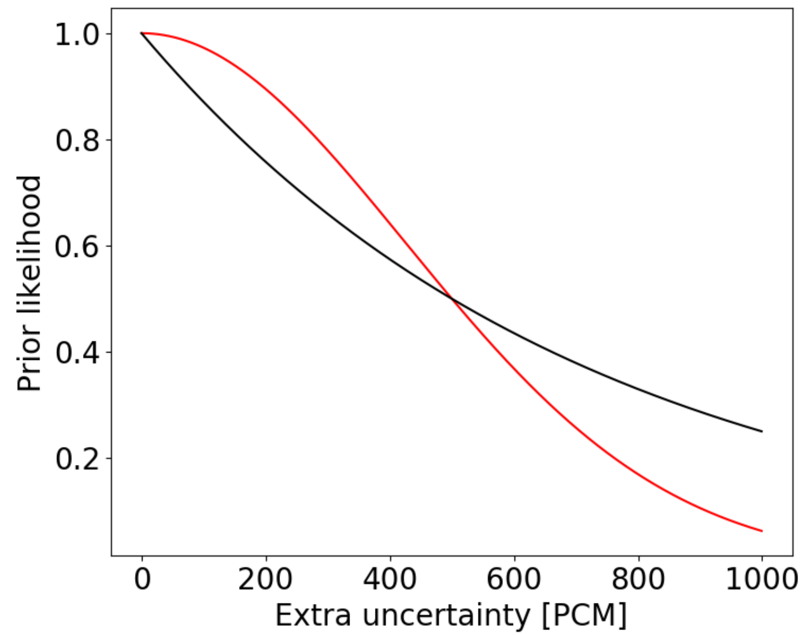
Adding a prior

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

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

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

To favor small extra uncertainties.
Includes more of expert judgement.



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

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

MLO for BMC / GLS

$$L_{\mathrm{BMC}} = \frac{1}{\sqrt{2\pi n \left| \mathrm{cov}_{rep} + \mathrm{cov}_{extra} \right|}} e^{-\beta \sum \sigma_{extra}^2} \sum_i e^{-\frac{\chi_i}{2}}$$

$$L_{\mathrm{GLS}} = \frac{1}{\sqrt{2\pi n \left| SA_0S^T + \mathrm{cov}_{rep} + \mathrm{cov}_{extra} \right|}} e^{-\beta \sum \sigma_{extra}^2} e^{-\frac{\chi^2}{2}}$$

$A_0 = \text{prior covariance}$

$n = number\ \text{of experiments}$

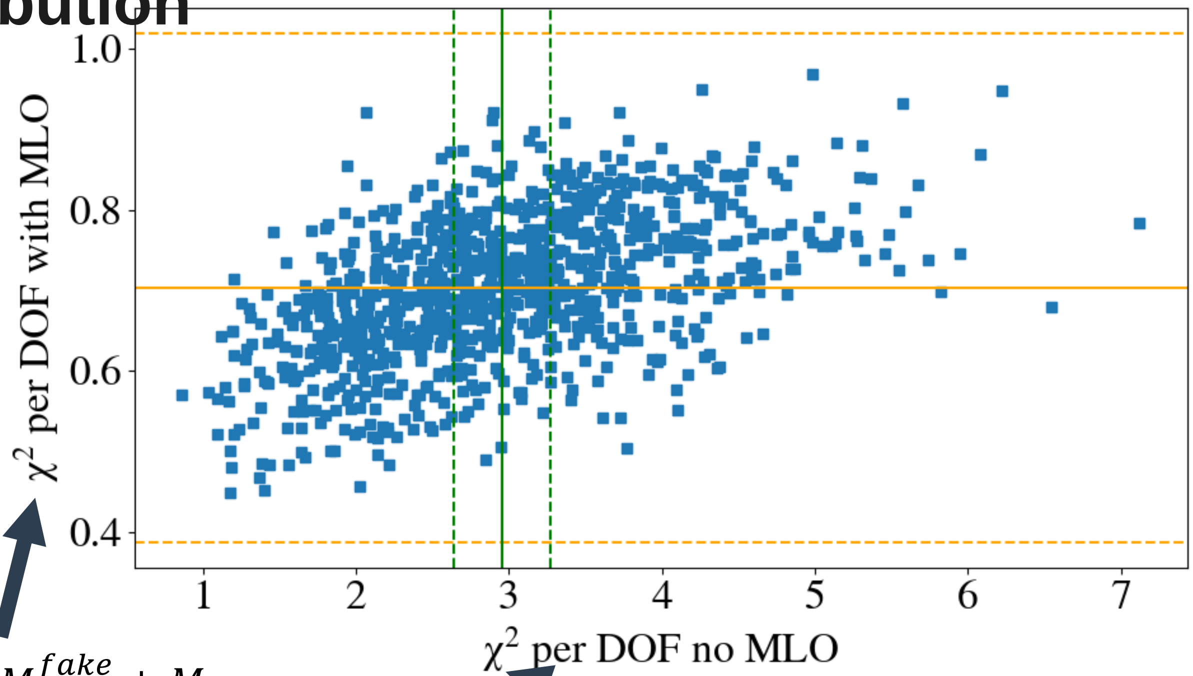
UPPSALA UNIVERSITET

Synthetic data study MLO - GLS

- Characterize MLO's performance,
  - GLS
  - No prior on the extra uncertainty
- Take hypothetical integral parameters (IPs)
- Have calculated values (C) and experimental (E), which have covariance matrices M_E and M_C
- Manipulate the reported uncertainty in M_E to see if MLO can account for it
  - Under-reported: $M_E^{fake} = M_E * 0.1$
- Give M_E^{fake} to MLO, and see if it reproduces M_E

Under-estimated E Uncertainty

- - Chi2 plotted with sample mean, std from chi2 distribution



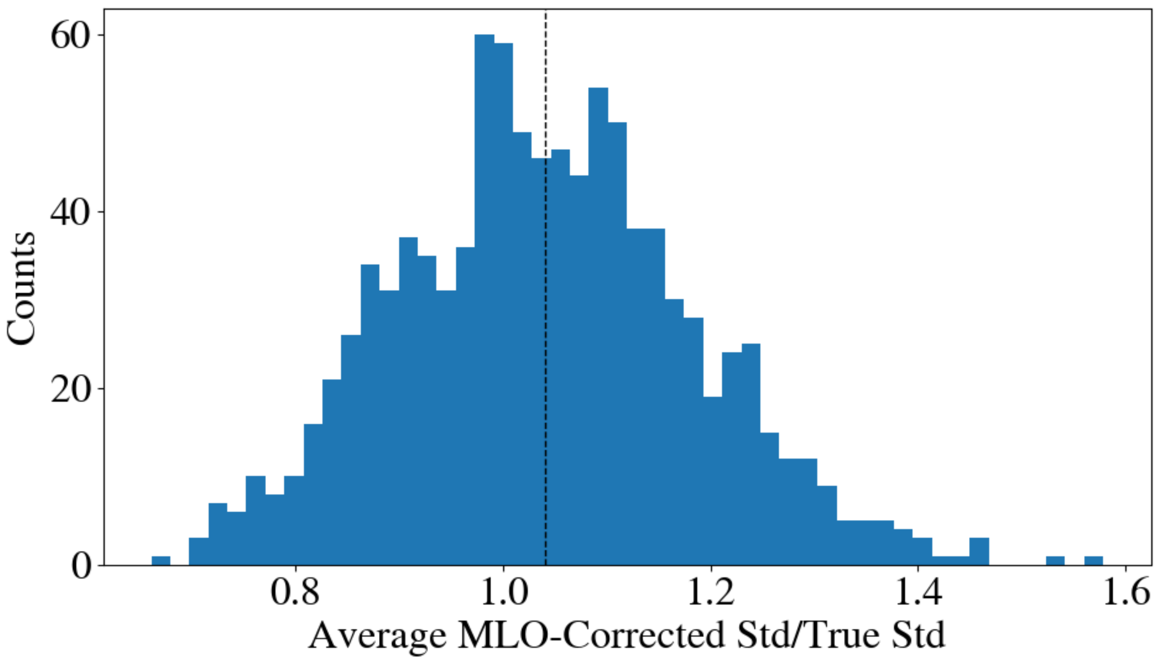
$(C-E)^T\left(M_E^{fake}+M_C\right.$

$(C-E)^T\left(M_E^{fake}+M_C\right)^{-1}(C-E)$

Under-estimated E Uncertainty

$$\frac{\sqrt{\delta_{Efake}^2 + \delta_C^2 + \delta_{MLO}^2}}{\sqrt{\delta_E^2 + \delta_C^2}}$$

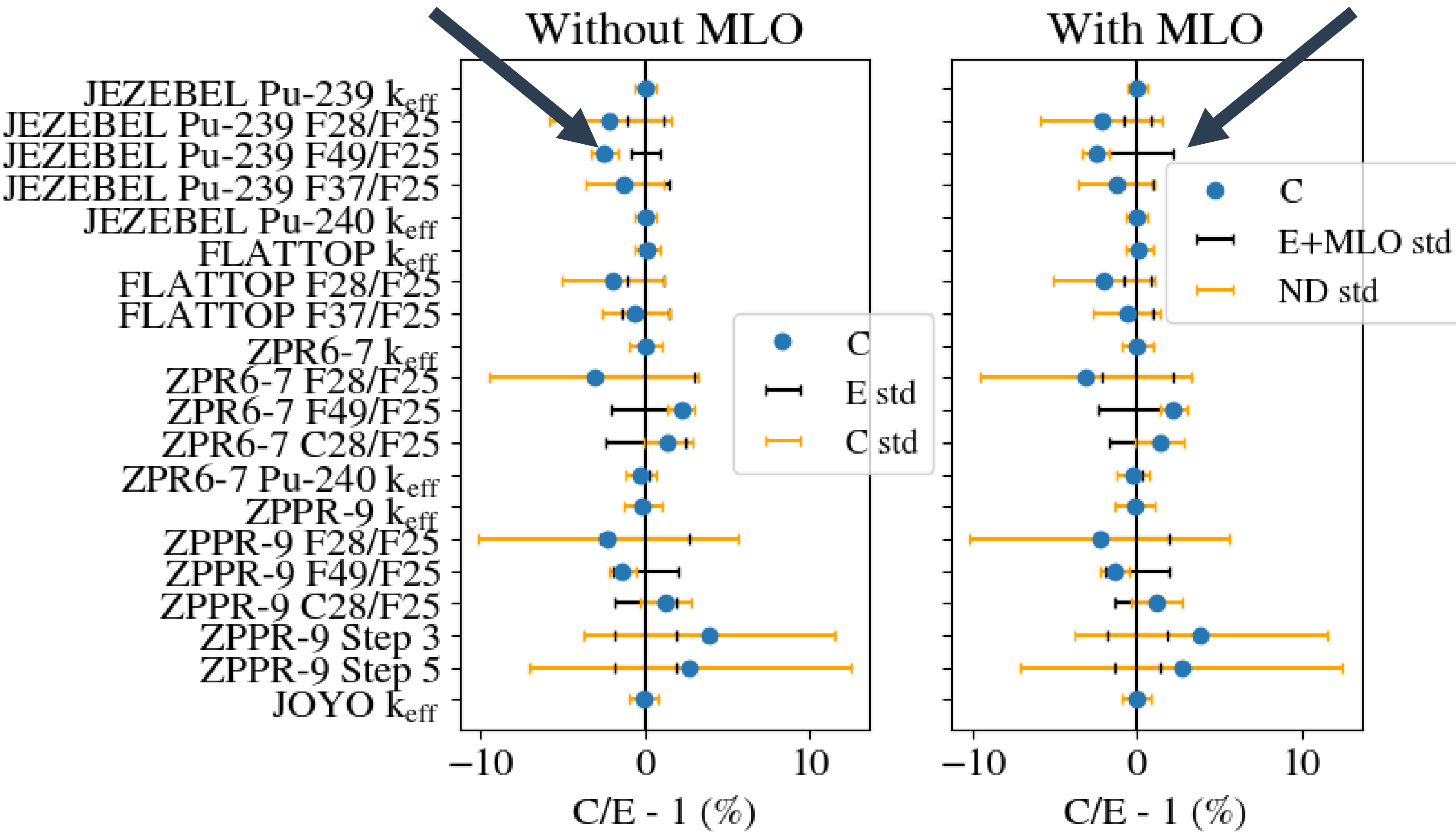
- Averaged across all IPs



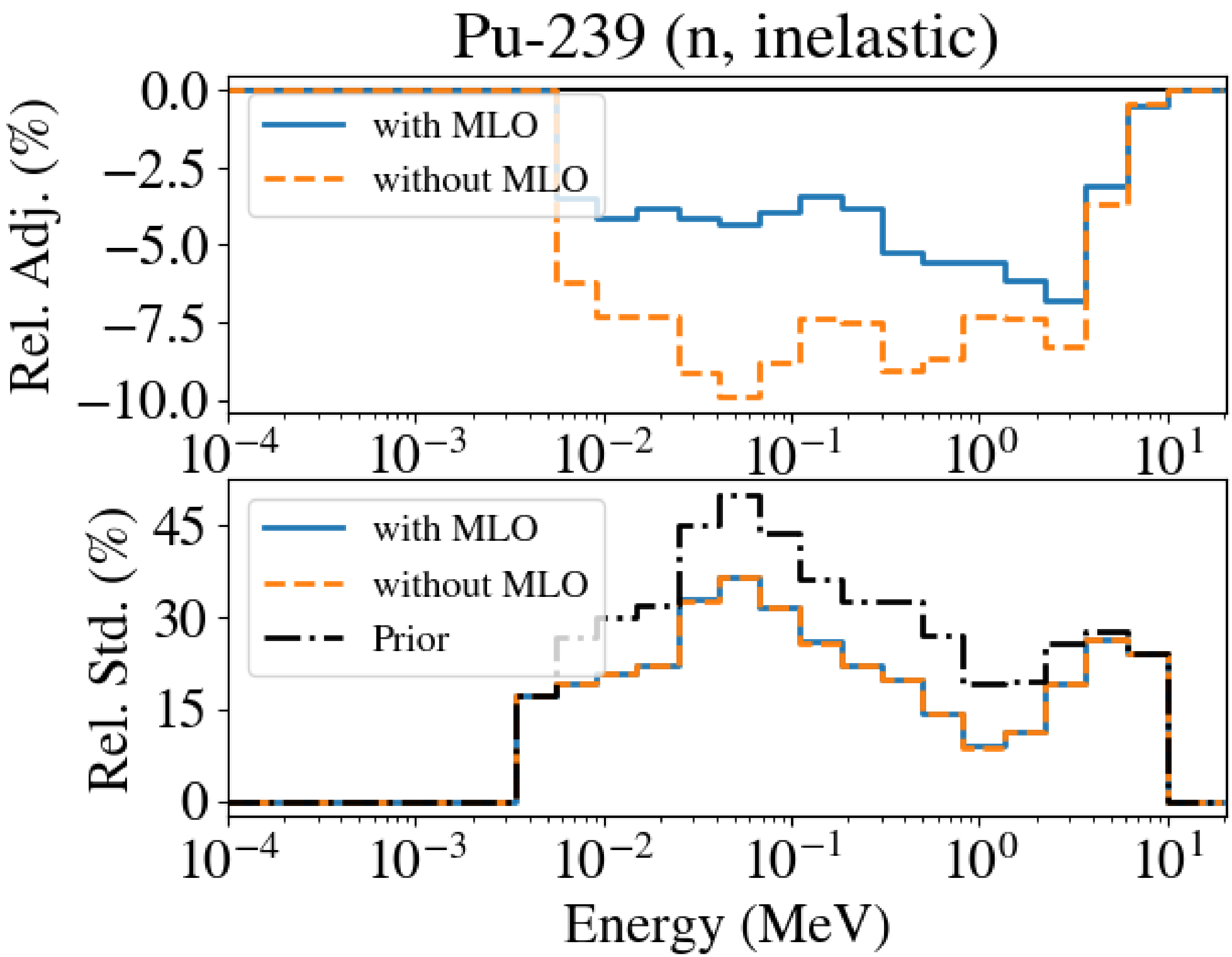
MLO Applied to SG33 Benchmark

- Apply MLO to controlled set of benchmarks using GLS version of the formula
    - No prior on extra uncertainty and no experimental correlations between the IP.
- Conceptually easy case: one inconsistent IP
- Perhaps not ideal case:
    - Prior chi2 is already too small, likely overconistent, (data already tuned to these experiments?)
- Using MLO here to only identify inconsistent IP
- 33 group ENDF/B-VII.0 and COMMARA- 2.0.
- B-10, O-16, Na-23, Fe-56, Cr-52, Ni-58, U-235/238, Pu-239/240/241

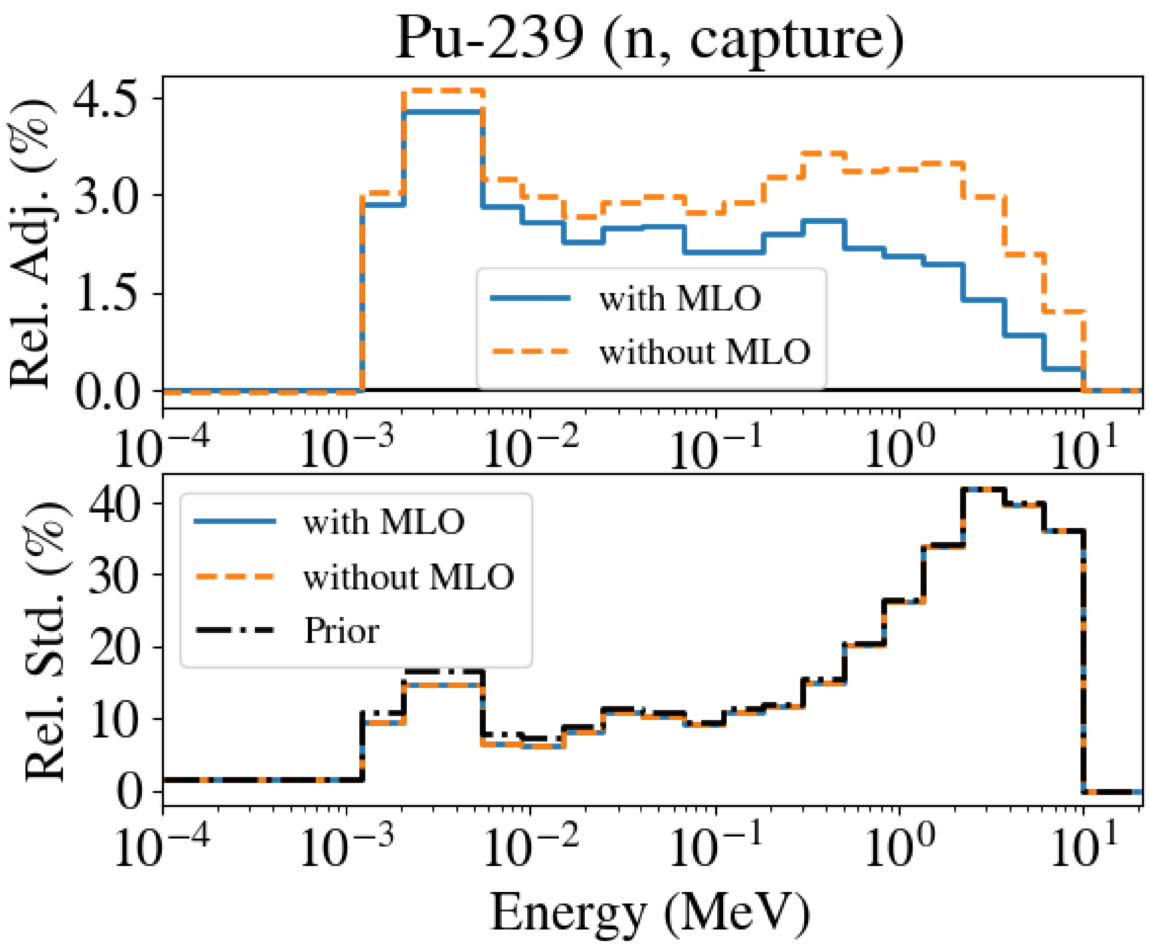
MLO Effects on SG33 Benchmark



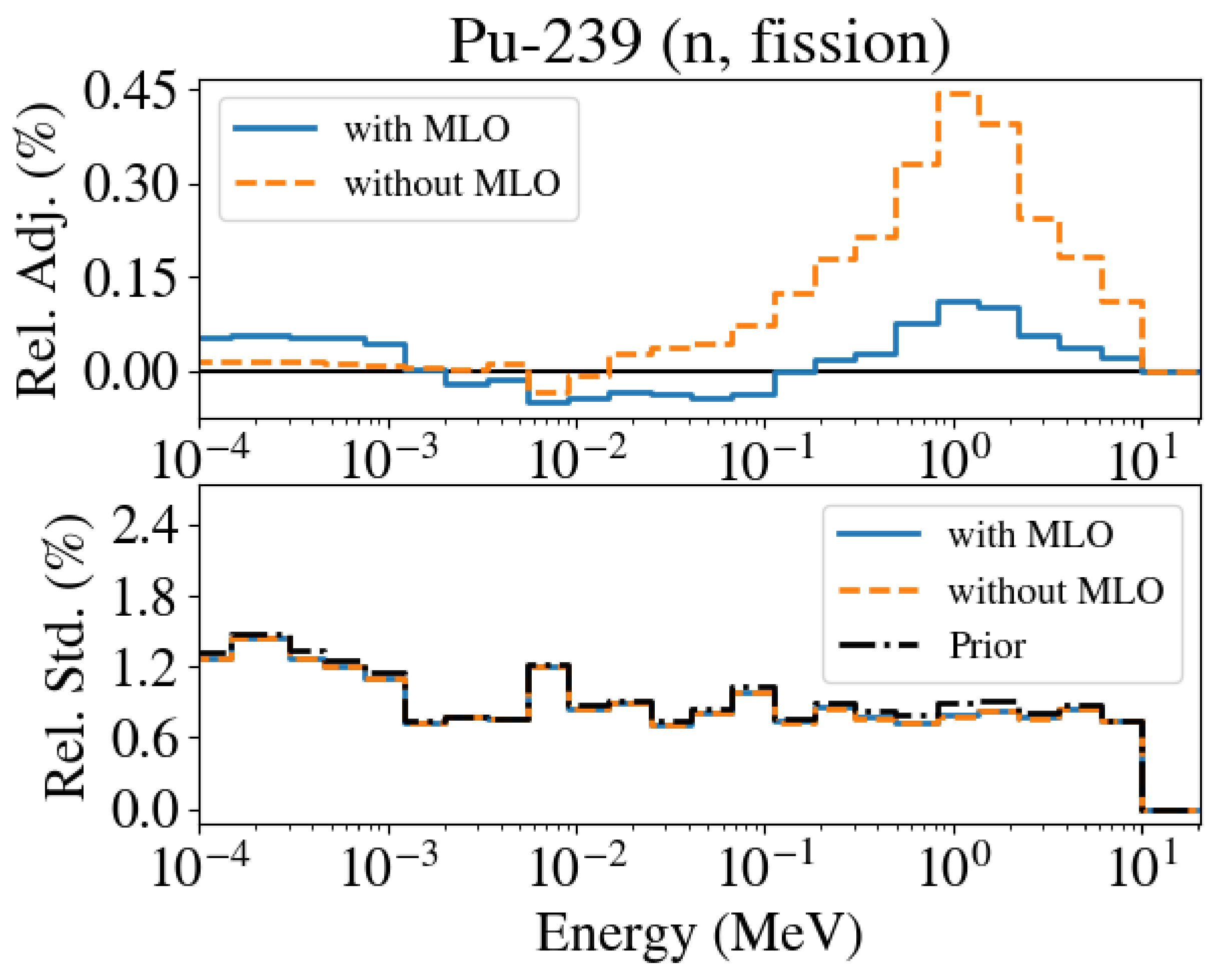
Posterior Nuclear Data Adjustments



Posterior Nuclear Data Adjustments

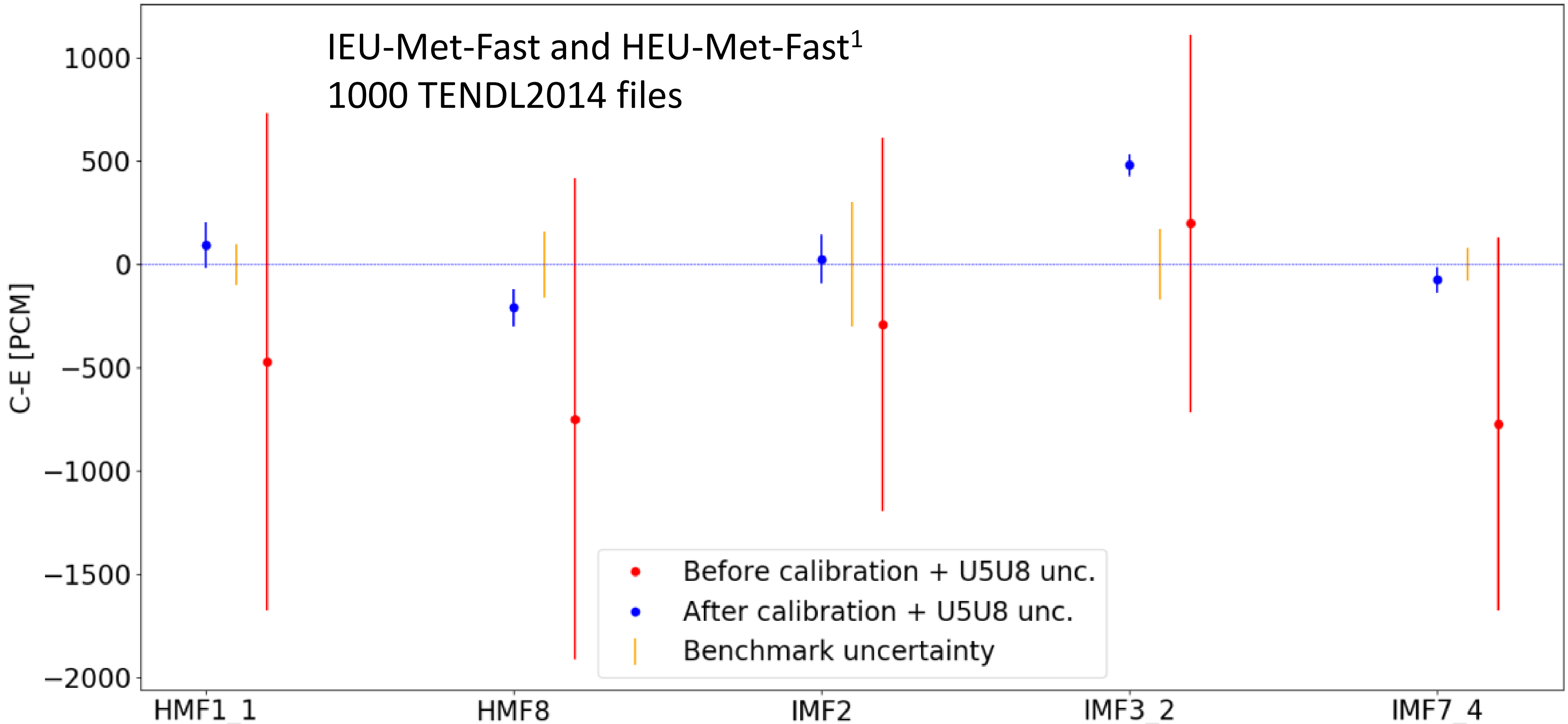


Posterior Nuclear Data Adjustments



Correlations were also changed.

BMC case



IEU-Met-Fast and HEU-Met-Fast[1]
1000 TENDL2014 files
1000
500
0
−500
−1000
−1500
−2000
C-E [PCM]
HMF1_1
HMF8
IMF2
IMF3_2
IMF7_4
Before calibration + U5U8 unc.
After calibration + U5U8 unc.
Benchmark uncertainty

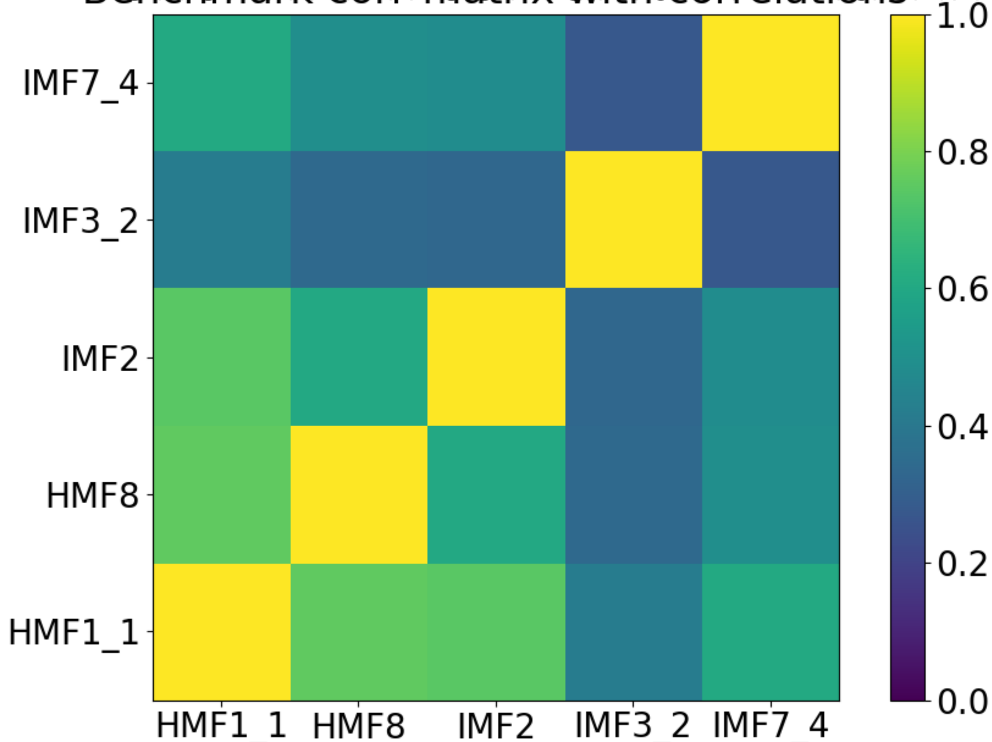
Benchmark errors are correlated: Adding a correlation term

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

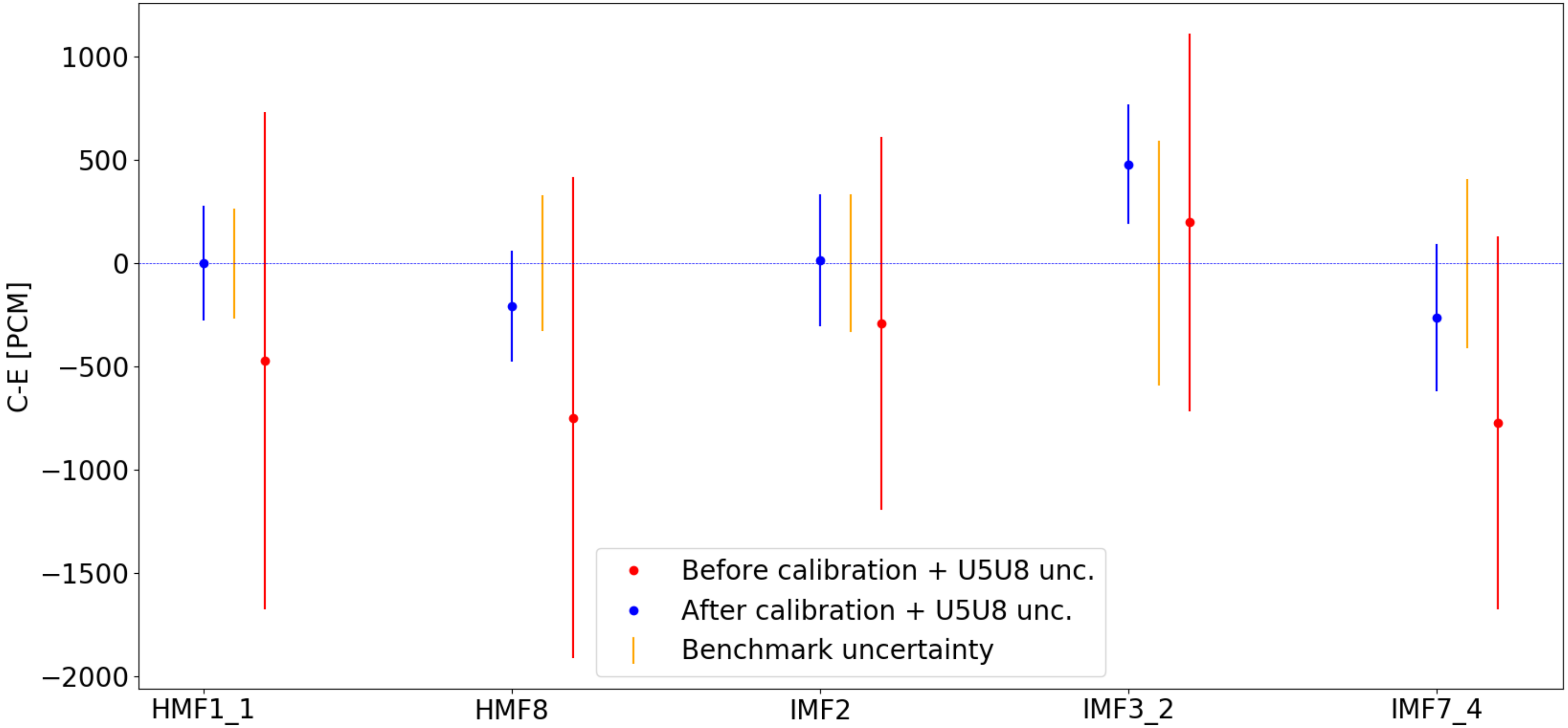
$$\sigma_{B,l}^2 = \sigma_{E,l}^2 + \sigma_{stat,l}^2 + \sigma_{extra,l}^2 + \sigma_{extra\_all}^2$$

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

Benchmark correlation-matrix



Results – with correlation

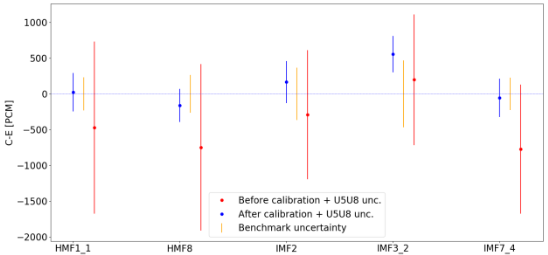


Benchmark uncertainties [PCM]	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Fully correlated
No ML: Reported uncertainties	100	160	300	170	80	0
Uptated uncertainties	153	204	300	580	390	0
With correlation	267	329	333	591	409	257

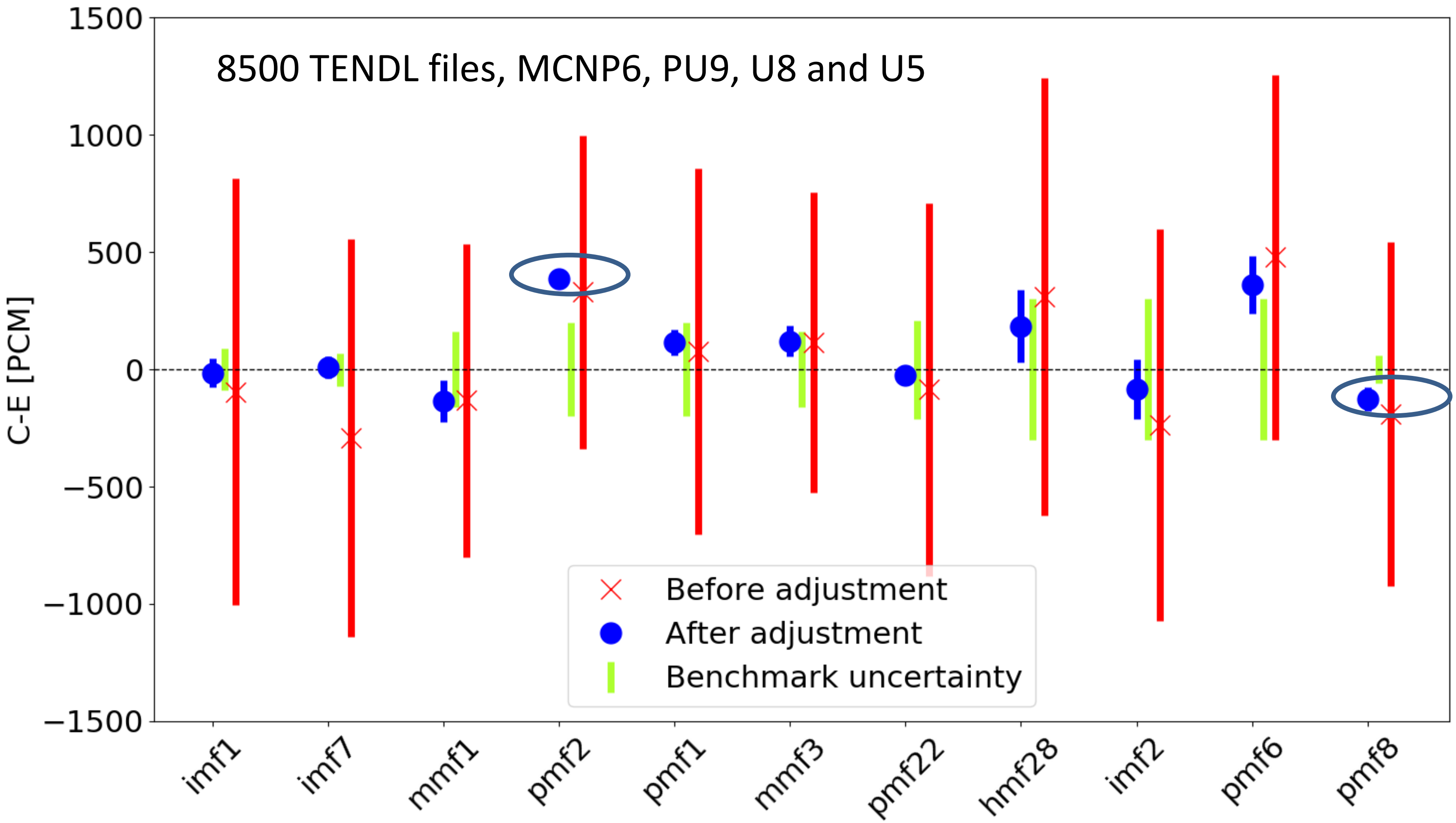
Results with an added prior

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

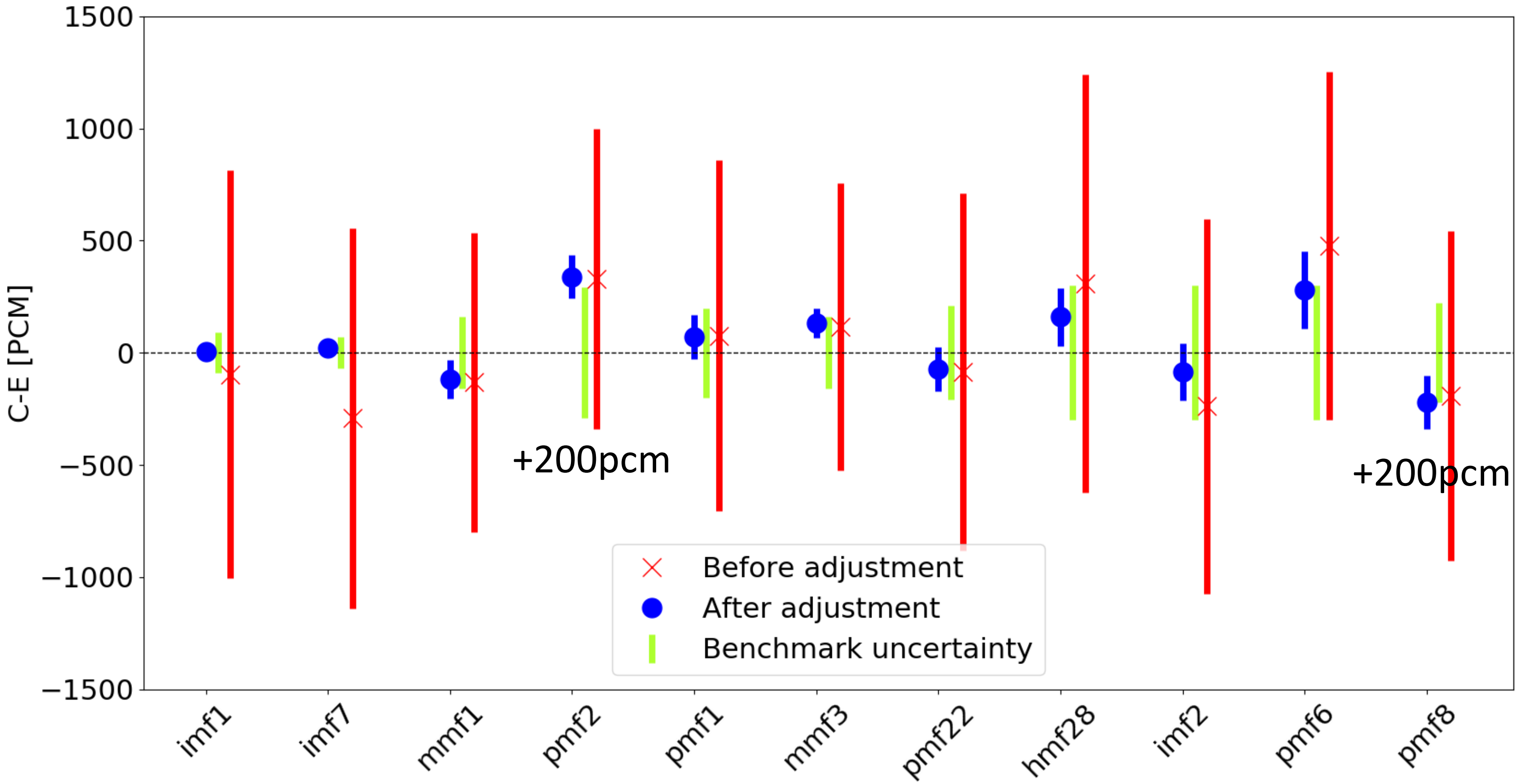
Posterior	HMF1_1	HMF8	IMF2	IMF3_2	IMF7_4	Chi2	p_value
No ML	69	28	103	52	34	2,1	6%
Uptated uncertainties	139	131	234	183	273	0,38	86%
With correlation	264	254	313	290	351	0,4	84%
With Prior	253	214	288	256	265	0,58	72%



A larger data set / BMC – No MLO



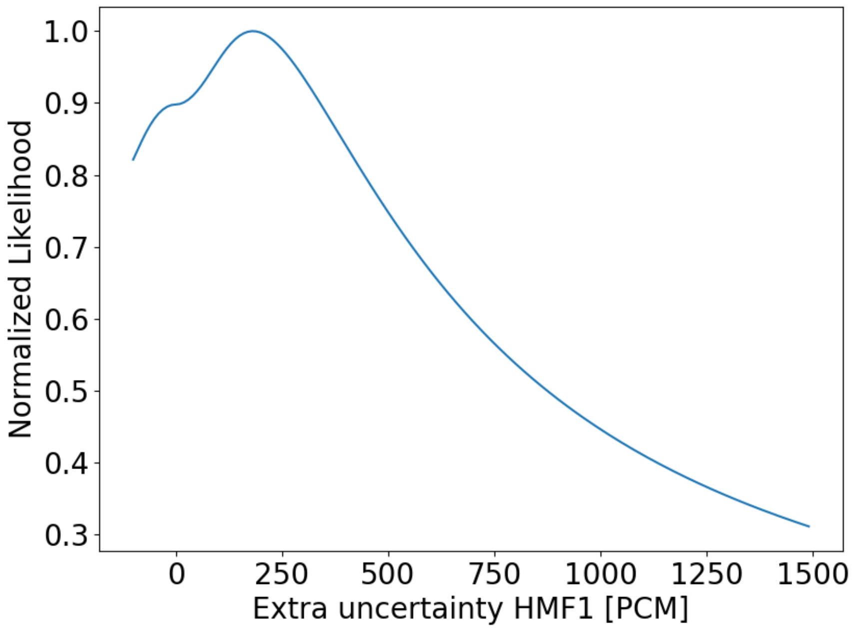
With MLO



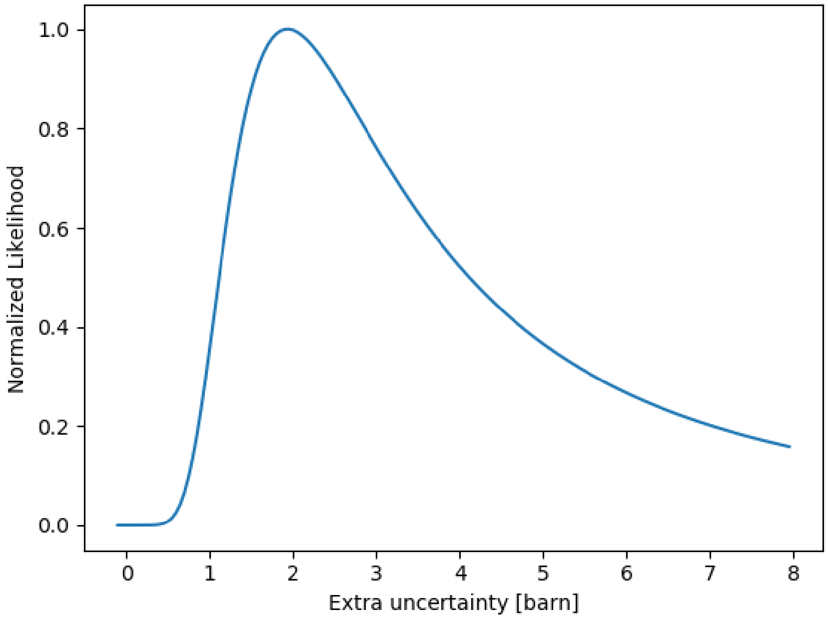
If allowed, the **MLO reduces the uncertainties** for most of the experiments, indicating that some tuning to these experiments have already been done.

Conclusion

- We need to find and treat unrecognized systematic uncertainties (USU).
- Marginal Likelihood Optimization (MLO) can be an effective tool for this.
- Treating USU reduces the risk of overfitting to the integral data.
  - MLO is our preferred method
    - Includes correlations
    - Can introduce correlations
    - Transparent
    - Not binary
    - Statistical well-founded
    - Can be combined with expert judgment.
    - Works with both GLS and BMC adjustment.



Next step: include the full likelihood functions.



- All values of the likelihood functions are possible, hence should be taken into account.
  - affects the best-estimate and normally increase the uncertainty → decrease the adjustment.
- Can be achieved by, e.g., sampling.
- Performed for differential data (reported in SG 44)

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
6. G. Schnabel ,Interfacing TALYS with A Bayesian Treatment of **Inconsistent Data** and Model Defects, ND2019