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On the combined use of differential and integral experiments in Bayesian optimization of nuclear data

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Outline

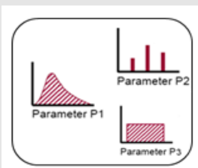
- Introduction
- Bayesian Optimization:
  - Incorporating differential data
  - Incorporating integral data
  - Global (combined) likelihood function
- Application of method: n+Pb208 in the fast region
- Conclusion

Introduction

Interactions between models and experiments in nuclear data adjustments

Goal: combine A and B

Input parameter distributions



$$\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix}$$

X → **LM: (TALYS)** → Y → **HM: (MCNP)** → Z

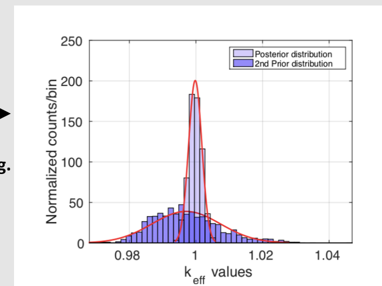
X = Input parameter vector

Y = LM output e.g. cross section vector

Z = HM output e.g. k_{eff}, β_{eff}

Differential Experimental data **(A)**

Integral Experimental data **(B)**



Feedback

LM → Lower level model (models implemented in TALYS)

HM → Higher level model (neutron transport models for e.g.)

Incorporating Differential Data (1/4)

Priors – model parameters

Contributions to the model covariance matrix (Ref. [*]):

M (mod) = M(par) + M(num) + M(def)

- M(par): Parameter Uncertainties
- M(num): Numerical implementation errors
- M(def): Model defects

Sensitivity analysis of model parameters:

- Let $p = (p_1, \dots p_l, \dots, p_L)$ → vector of adjustable parameters
- $\sigma = (\sigma_1, \dots, \sigma_i, \dots, \sigma_N)$ → a vector of N calculated cross sections
- Sensitivity for lth parameter and ith cross section:

$$S_{il} = \frac{(\sigma_i^{(1)} - \sigma_i^{(0)})}{(p_l^{(1)} - p_l^{(0)})} \frac{p_l^{(0)}}{\sigma_i^{(0)}}$$

Each parameter is perturbed within 10% of its nominal values using TASMAN-1.26

*H. Leeb et. al., Nuclear Data Sheets 109 (12) (2008) 2762–2767.

Table 1. Selected model parameters in the TALYS code

Parameter	Uncertainty(%)	Parameter	Uncertainty(%)
r_V^n	1.5	a_V^n	2.0
v_1^n	1.9	v_2^n	3.0
v_3^n	3.1	v_4^n	5.0
w_1^n	9.7	w_2^n	10.0
d_1^n	9.4	d_2^n	10.0
d_3^n	9.4	r_D^n	3.5
a_D^n	4.0	r_{SO}^n	9.7
a_{SO}^n	10.0	v_{so1}^n	5.0
v_{so2}^n	10.0	w_{so1}^n	20.0
w_{so2}^n	20.0	Γ_γ	5.0
$a(^{207}Pb)$	4.5	$a(^{206}Pb)$	6.5
$a(^{208}Pb)$	5.0	$a(^{205}Pb)$	6.5
σ^2	19.0	M_2	21.0
$g_\pi(^{207}Pb)$	6.5	$g_\nu(^{207}Pb)$	6.5

Prior uncertainties assigned to model parameters (were multiplied by a factor of 3)

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Incorporating Differential Data (2/4)

1st experimental constraint: differential experimental data

- Considered channels: (n,tot), (n,non-el), (n,inl), (n,2n), and (n,g)
- We use a reduced chi-square and assume that the experiments are uncorrelated:

Model calculations for channel *c*, random file *k* at energy *i*

Experimental data points for channel *c* at energy *i*

$$\chi^2_{c(k)} = \frac{1}{n_p} \sum_{i=1}^{n_p} \left(\frac{\sigma^i_{T(k)} - \sigma^i_E}{\Delta \sigma^i_E} \right)^2$$

Number of Experimental data for the experimental data set *p*

Experimental uncertainty at energy *i*

Chi-square per ND file (k):

$$\chi^2_{k(xs)} = \frac{1}{n_c} \sum_{c=1}^{N_c} \chi^2_{c(k)}$$

Similar to A.J. Koning, Bayesian Monte Carlo Method for Nuclear Data Evaluation, The European Physical Journal A 51 (12) (2015) 184.

- Our main Goal: To find the combination of parameters that maximizes the likelihood function

Incorporating Differential Data (3/4)

Lets consider L parameters, p_j for model *M*, where j = 1,2, …, L

- We assume that all model parameters are of equal importance a priori (uniform distr.)

- **Let** $P^{prior}(M, p) \rightarrow$ **prior distribution of parameters p for model *M***
  $L(\sigma_E|M, p)]$ **→ likelihood function**
  σ_E **→ our training (differential experimental) data**

Our posterior can be given as:

$$P^{post}(M, p|\sigma_E) = L(\sigma_E|M, p) * P^{prior}(M, p)$$

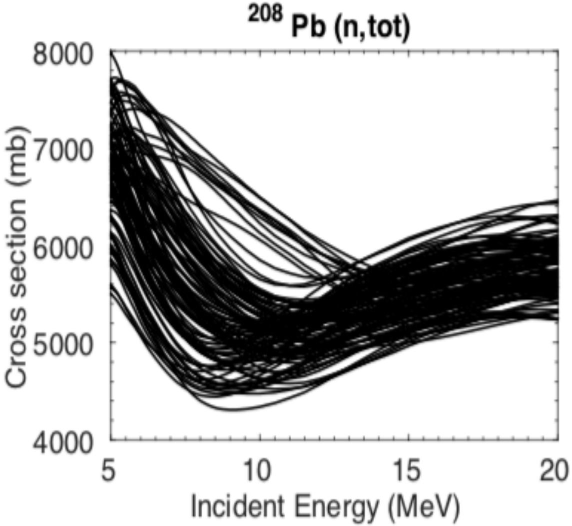
Using a uniform prior distribution of parameters → the posterior distribution is determined solely (or almost) by experimental data

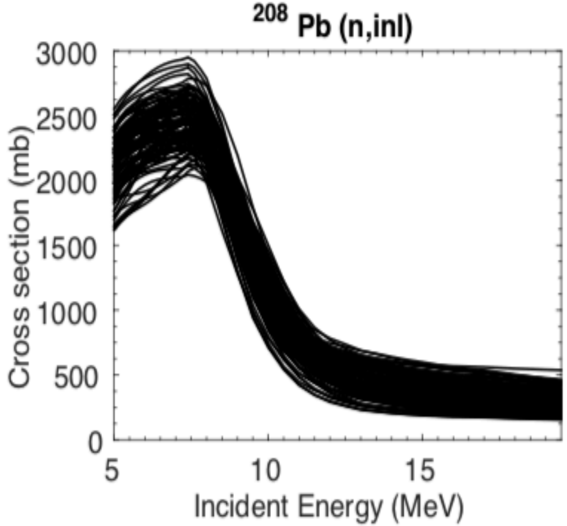
The likelihood function for each file (also known as BMC weights):

$$L(\sigma_E|M, p)] = exp(-\chi^2_{k(E)}/2)$$

Incorporating Differential Data (4/4)

Distributions of prior cross sections for the (n,tot) and (n,inl) channels of Pb208





Spread is due to model parameter variation

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Incorporating Integral Data (1/3)

2nd experimental constraint: integral experimental data

- The selected benchmark experimental data were obtained from the ICSBEP database.
- Chi-square is given by (since only one benchmark is used here):

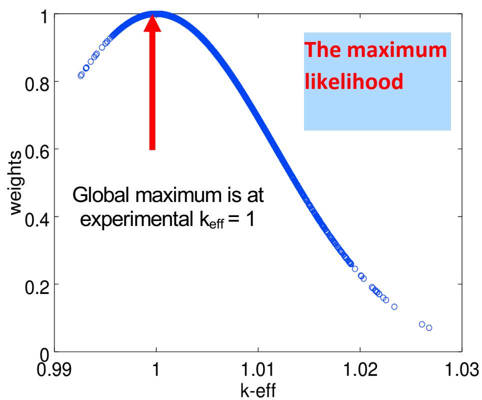
Calculated k_{eff} for random file k using MCNP

Experimental benchmark k_{eff}

$$\chi^2_{\mathrm{k(B,j)}} = \frac{(k^B_{\mathrm{eff,cal(k)}} - k^B_{\mathrm{eff,exp}})^2}{\sigma^2_{\mathrm{B,j}}}$$

Combined benchmark uncertainty

HMF57 case 1



- The chi square is used to compute a likelihood function (BMC weight):

$$\mathrm{L}\left(\boldsymbol{k}^{\boldsymbol{E}}_{\mathbf{eff}} \middle| \sigma_T\right) = \exp(-0.5 * \chi^2_{\mathrm{B(k,j)}})$$

Incorporating Integral Data (2/3)

- The combined benchmark uncertainty: Taking calculation uncertainties into account in adjustments

- For single benchmarks, we compute a combined benchmark uncertainty is given as:

$$\boldsymbol{\sigma}^2_{B,j} = \boldsymbol{\sigma}^2_{E} + \boldsymbol{\sigma}^2_{C,j}$$

Where;

$$\boldsymbol{\sigma}^2_{C,j} = \sum_{\substack{over\ all\ p \\ where\ p\neq j}} \boldsymbol{\sigma}^2_{ND,p} + \boldsymbol{\sigma}^2_{calc.bias} + \boldsymbol{\sigma}^2_{geo.mod.} + \boldsymbol{\sigma}^2_{stat} + \text{others}$$

NOTE: In this work, we only consider the uncertainties due to nuclear data

- For multiple benchmarks, we can combine the covariances:

$$C_B = C_E + \sum_{\substack{over\ all\ p \\ where\ p\neq j}} C_{ND}$$

Ref. Alhassan et. al., Progress in Nuclear Energy, 88, pp. 43-52 (2016)

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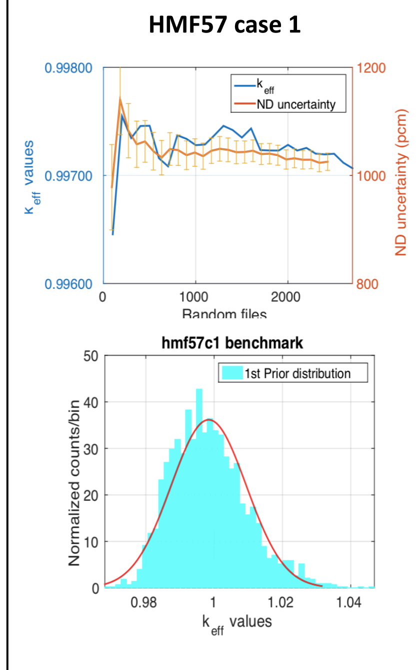
Incorporating Integral Data (3/3)

Prior and posterior distributions

Computed using only the experimental benchmark evaluated uncertainties

Posterior uncertainties computed using the combined benchmark uncertainties

Benchmark category	Evaluated Benchmark k_{eff}	Prior mean ± ND Uncertainty [pcm]	Posterior mean ± ND Uncertainty (1) [pcm]	Posterior mean ± ND Uncertainty (2) [pcm]
PMF035 case 1	1.0000	1.0028±547	1.001±157	1.0022±493
HMF027 case 1	1.0000	1.0055±506	1.0011±210	1.0045 ± 444
HMF057 case 1	1.0000	0.99851±1104	0.99986±199	0.99841±783
HMF057 case 2	1.0000	1.0057±879	1.002±228	1.0031±660
HMF057 case 3	1.0000	1.0272±1202	1.0029±350	1.0144±671
HMF057 case 4	1.0000	0.99471±817	0.99875±366	0.99598±694
HMF057 case 5	1.0000	1.0322±1287	1.0013±151	1.0163±663
HMF064 case 1	0.9996	1.0051±1244	0.99963±81	1.0012±783
HMF064 case 2	0.9996	1.0051±1244	0.99963±81	1.0012±783
HMF064 case 3	0.9996	1.0051±1244	0.99963±81	1.0012±783
LCT010 case 1	1.0000	1.0048±426	1.0009±197	1.0026±317
LCT010 case 20	1.0000	1.0023±451	1.0011±156	1.0022±227



Nuclear data uncertainties due to the variation of Pb-208 nuclear data was varied

Global (combined) likelihood function

Choosing the best file:

- If we assume that differential and integral benchmarks are uncorrelated:

$$L\left(\sigma_E, k^B_{\text{eff,exp}} \middle| \sigma_T, p; k^B_{\text{eff,cal}}\right) = L(\sigma_E|M,p)\,L\left(k^B_{\text{eff,exp}} \middle| k^B_{\text{eff,cal}}, \sigma_T\right)$$

- → Combined weight $w_{T,k} = w_{E(k)} \cdot w_{B(k,j)}$

where $L(\sigma_E|M,p)$ → likelihood function − differential data

$L\left(k^B_{\text{eff,exp}} \middle| k^B_{\text{eff,cal}}, \sigma_T\right)$ → likelihood function – integral data

σ_T → vector of TALYS calculated cross sections

Our combined posterior can now be given as:

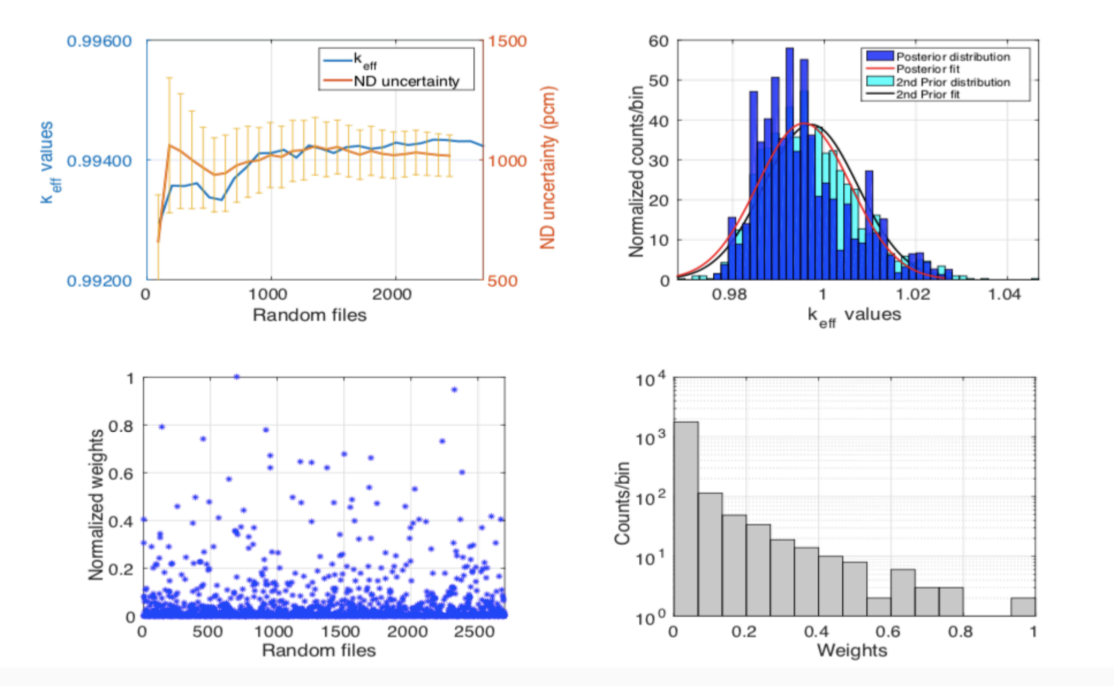
$$P^{post}_{comb}\left(k^B_{\text{eff,cal}} \middle| \sigma_E, k^B_{\text{eff,exp}}\right) = L\left(\sigma_E, k^B_{\text{eff,exp}} \middle| \sigma_T, p; k^B_{\text{eff,cal}}\right) * P^{prior}\left(k^B_{\text{eff,cal}} \middle| \sigma_T\right)$$

The parameter set which maximizes the likelihood function is selected:

$$BF = \arg\max_p \left[L\left(\sigma_E, k^B_{\text{eff,exp}} \middle| \sigma_T, p; k^B_{\text{eff,cal}}\right)\right]$$

Results: Prior and posterior distributions

- The weights presented here were computed using only differential data
- k_{eff} → hmf57 case 1 benchmark with MCNP code (Pb208 varied)



Results: Differential validation (1/2)

For differential validation, we compare reduced chi squares computed for different libraries and this work

Libraries	(n,tot)	(n,non-el)	(n,inl)	(n,2n)	(n,γ)	Avg χ^2
ENDF/B-VIII.0	4.50	0.29	19.34	2.34	1.13	5.52
JEFF-3.3	3.16	0.16	23.03	3.82	0.37	6.11
JENDL-4.0	3.16	0.09	25.04	3.82	0.37	6.57
TENDL-2017	3.54	0.16	3.81	8.97	8.95	5.08
CENDL-3.1	4.55	1.17	23.48	1.61	2.38	6.64
Nominal (prior) file	4.78	0.16	17.52	2.10	8.30	6.57
This work (1st update) (unweighted channels)	5.34	0.02	10.51	4.60	3.62	4.82
This work (1st update) (weighted channels)	3.26	0.18	6.70	3.83	69.11	16.61
This work (2nd update) (unweighted channels)	8.02	6.40	5.52	39.45	70.66	26.01
This work (global likelihood)	10.57	4.22	7.94	0.88	0.83	4.89

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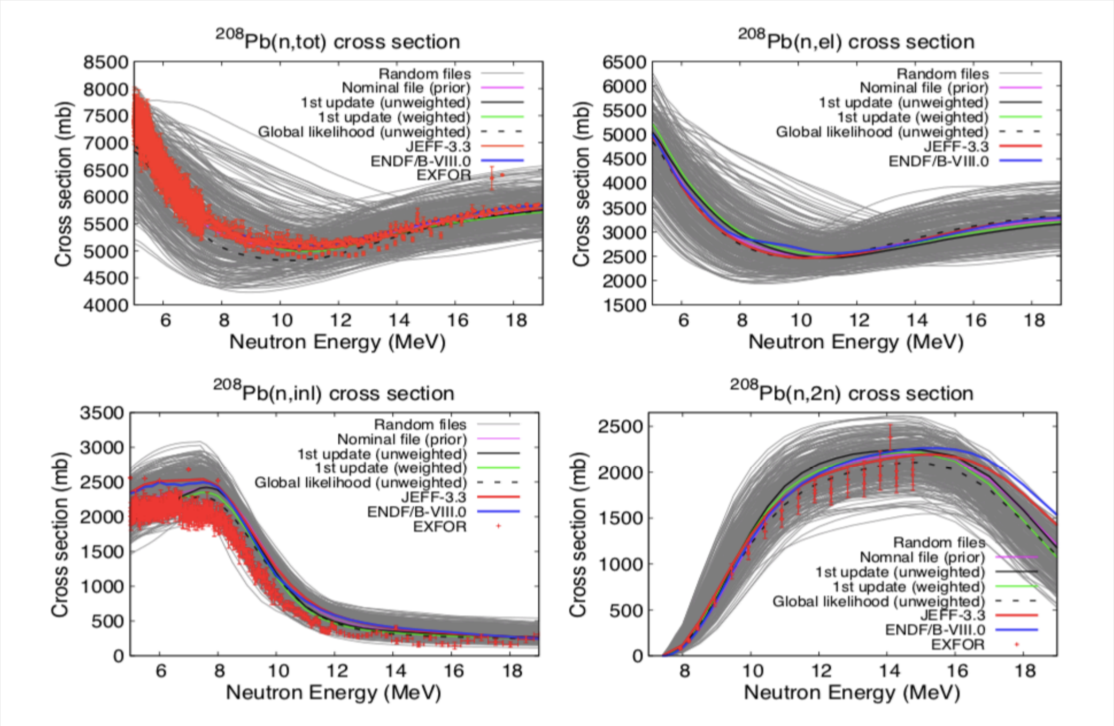
Results: Differential validation (2/2)

Graphical comparison with differential experimental data for selected channels



Results: Integral validation

- Ratios of calculated to experimental values (C/E) for selected benchmark

Benchmarks	Exp. benchmark k_{eff} $\pm$ uncertainty [pcm]	1st update (unweighted channels)	1st update (weighted channels)	2nd update (hmf57c1)	Global likelihood (EXFOR + hmf57c1)	ENDF/B-VII.0
hmf57c1	1.0000±200	1.01285	0.99629	1.00002	1.00042	0.98959
hmf57c2	1.0000±230	1.01633	1.00439	1.00851	1.00201	0.99888
hmf57c3	1.0000±320	1.04167	1.02459	1.03023	1.02918	1.01726
hmf57c4	1.0000±400	1.00462	0.99293	0.99793	0.99565	0.98784
hmf57c5	1.0000±190	1.04884	1.02934	1.03580	1.03437	1.02188
hmf57c6	1.0000±290	1.02047	1.00322	1.00909	1.00769	0.99713
hmf27c1	1.0000±250	1.01150	1.00363	1.00676	1.00558	1.00182
pmf35c1	1.0000±160	1.00891	1.00015	1.00635	1.00290	0.99856
hmf64c1	0.9996±80	1.02110	1.00237	1.00936	1.00263	0.99455
hmf64c2	0.9996±100	1.02852	1.00532	1.01265	1.01058	0.99613

- 1st update → Results obtained using only differential data
- 2nd update → Results obtained using only integral benchmark (hmf57 case 1 in this case)
- Global likelihood → Results using both differential and integral (hmf57c1) experiments
- Weighted → cases were weights equal to the average channel cross section are assigned to each channel

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Conclusion

- A method for the combined use of differential and integral experiments for nuclear data adjustments within a Bayesian framework is presented.
- The method has been applied for the adjustment of p+Pb208 in the fast energy region.
- The study shows that, there is a potential for the improvement of nuclear data evaluations through the (explicit) combination of experimental information from both differential and integral benchmarks in Monte Carlo adjustments procedures.
- Combining differential experiments and multiple benchmarks for Monte Carlo adjustments in the fast region, is planned for future work

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Wir schaffen Wissen – heute für morgen

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