Examples of Monte Carlo techniques applied for nuclear data uncertainty propagation

[a] Oscar Cabellos
oscar.cabellos@upm.es

[b] Luca Fiorito
luca.fiorito@oecd.org

a) INDUSTRIALES ETSII | UPM

b) NEA

5th Int. Workshop On Nuclear Data Evaluation for Reactor Applications (WONDER-2018), 8-12 October 2018

Abstract

The aim of this work is to review different Monte Carlo (MC) techniques used to propagate nuclear data uncertainties

1. Uncertainty Quantification (UQ) studies
   - Required in **safety calculations of large scale systems ~ PWR**
   - ND uncertainty propagation on the main design parameters
   - **Decomposition of uncertainty in: ^{235}U-^{238}U-^{239}Pu & XS-ν-PFNS**

2. Bayesian Monte Carlo approaches for data adjustment
   - Multivariate Normal Bayesian model relying on NUDUNA/SANDY codes
   - TMC + Bayesian MC Approach (BMC)
   - **Selection of Benchmarks**
     - **BMC apply for Criticality + Shielding/Transmission**

1. MC techniques to perform Uncertainty Quantification (UQ)

- Uncertainty Quantification (UQ) analysis in large scale systems

  e.g. the core design in a **3-loop PWR Westinghouse** unit

  - In this work, we use our **SEANAP** system developed and applied for 3-D **PWR core analysis** which has demonstrated a very good agreement with the broad sets of parameters and cycles analysed at the Spanish PWR units.

- Methodologies for UQ:

  - **Monte Carlo approaches** which uses random samples of nuclear data libraries and perform a separate reactor calculation for each random sample

  - **S/U method** is based on first order perturbation theory approaches, which makes use of available covariance files.

1.1 S/U to perform to UQ in reactor calculations

- **S/U method** is based on first order perturbation theory approaches, which makes use of available covariance files.
  - Sensitivity coefficients -> sandwich rule
  - Easy decomposition of uncertainty in isotopic partial cross-section components
  - Low CPU time
  - Different theories [1]:
    - Standard Perturbation Theory (SPT) - > keff uncertainties
    - Generalized Perturbation Theory (GPT) -> power distribution uncertainty
  - **S/U Weaknesses**
    1) low efficiency for a large number of response functions
    2) applicability for small uncertainties - > it is based on linear-approach
    3) severe limitations as consequence of the non-linearity of multi-physics calculations (neutronics, thermohydraulic, depletion, …) in reactor calculations

1.2 MC to perform UQ in reactor calculations

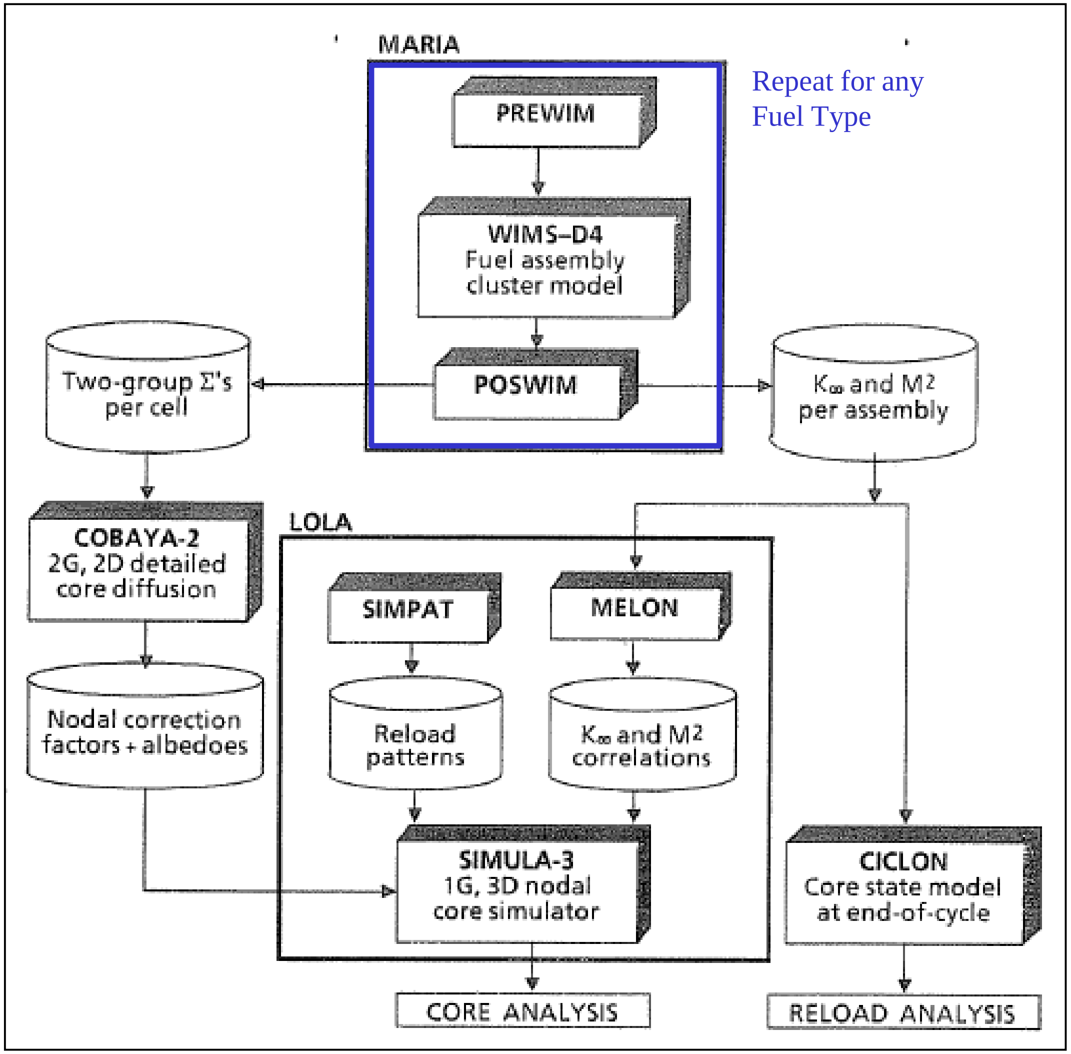
- **The Monte Carlo approaches** which uses random samples of nuclear data libraries and perform a separate reactor calculation for each random sample.
  - Large CPU time to perform enough sampling
    - The low execution times of SENAP code for a full scheme of PWR core cycle indicates that the parallelization of Monte Carlo sampling is reliable.
    - Nuclear data are sampled at the beginning of the simulation
    - Statistics of all SEANAP simulations yields the desired uncertainty quantification
    - SEANAP solves coupled multi-physics at different levels of approximation
  - Different approaches by their nuclear data uncertainty input
    - "**Total Monte Carlo**" (TMC) relies on model parameter covariances

      See our work: O. Cabellos et al., "Propagation of nuclear data uncertainties for PWR core analysis" (2014) Nuclear Engineering and Technology, 46 (3), pp. 299-312" [2]
    - **NUDUNA and SANDY** take as input the information provided by ND evaluations
    - **XSUSA** takes the form of covariance matrices in multigroups

1.3 UQ in reactor calculations: SEANAP-SANDY

❑ Scheme of the PWR Core Analysis SEANAP System

Ref.: *"Validation of PWR Core Analysis system SEANAP-86 with measurements in test and operation"*, C. Ahnert et al., M&C87



SEANAP is integrated by 4 subsystems:

1. **MARIA** system for assembly calculations
2. **COBAYA** system for a detailed (pin-by-pin) core calculations at reference conditions
3. **SIMULA** system for 3D 1 group corrected-nodal core simulation
4. **CICLON** system for fuel management analysis of reload cycles

CPU Time/cycle ~ 5-10 min / i7 870@2.93GHz

1.3 UQ in reactor calculations: SEANAP-SANDY

❑ Validation of SEANAP in PWR Core Analysis

Ref.: *"Upgraded SEANAP-PWR core simulator with JEFF-3.3: Impact of Nuclear Data Uncertainties for PWR cycle operation", O. Cabellos, JEFFDOC-1917, April 2018*

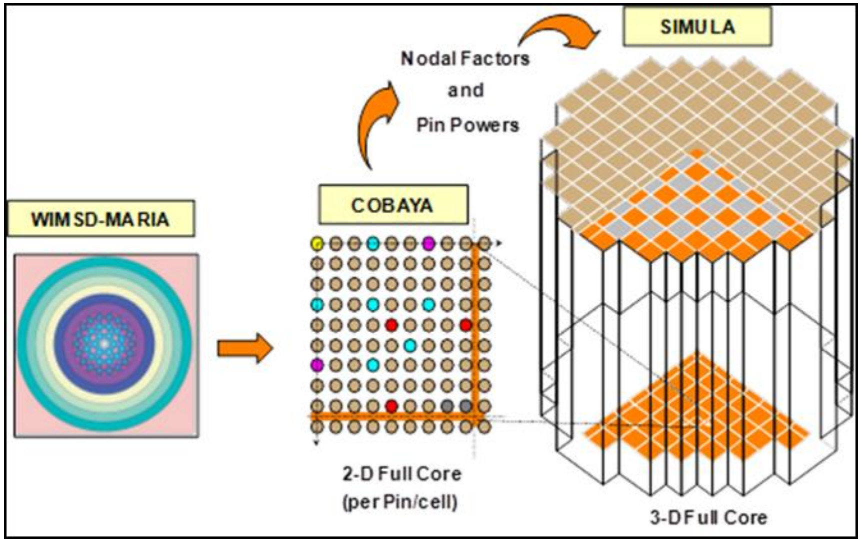


Fig. Scheme of SEANAP: WIMS-D5 (**JEFF-3.3**) + COBAYA + SIMULA

- SEANAP system has been developed and implemented as an **on-line simulator ~20 cycles of three PWRs (Vandellós-II, Ascó-I and Ascó-II)**

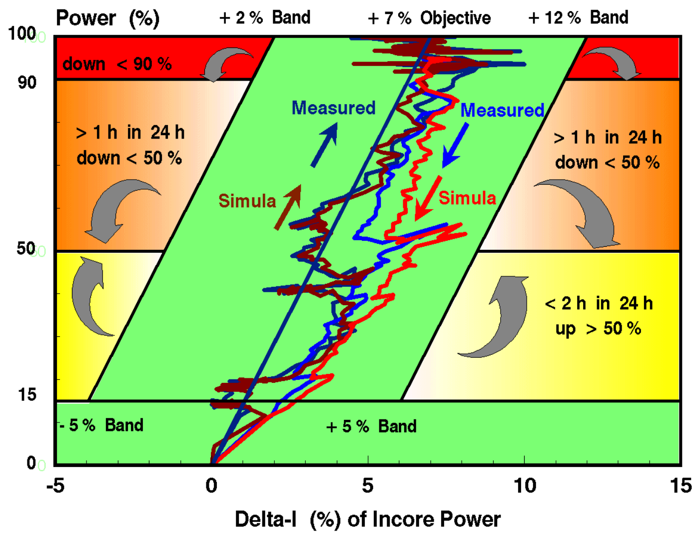
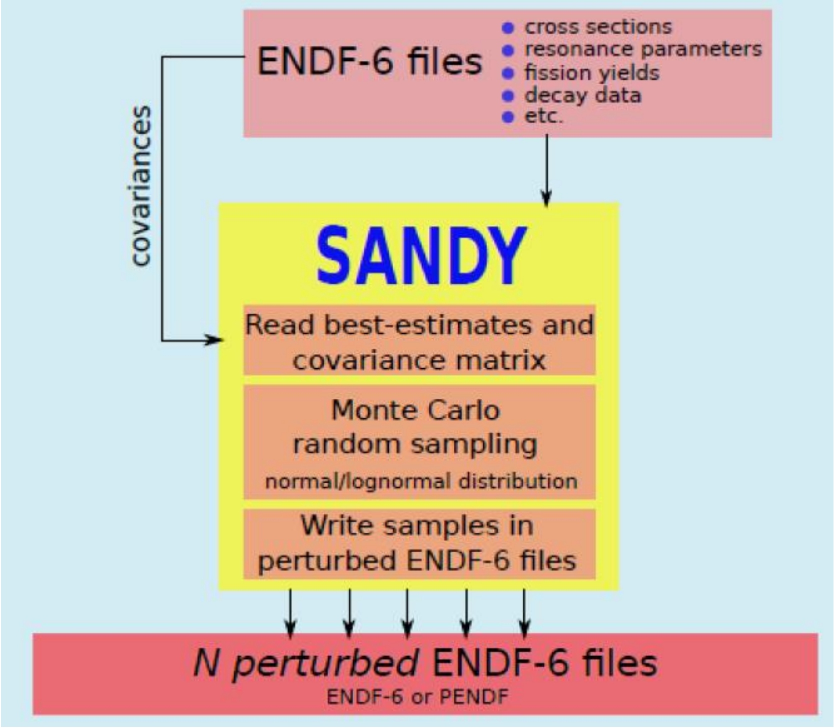


Figure: Measured and Simulated Power vs Delta-I in return to Power after a Short Shutdown

1.3 UQ in reactor calculations: SEANAP-SANDY

SANDY

- SANDY: Numerical tool for nuclear data uncertainty quantification.
- Based on Monte Carlo sampling



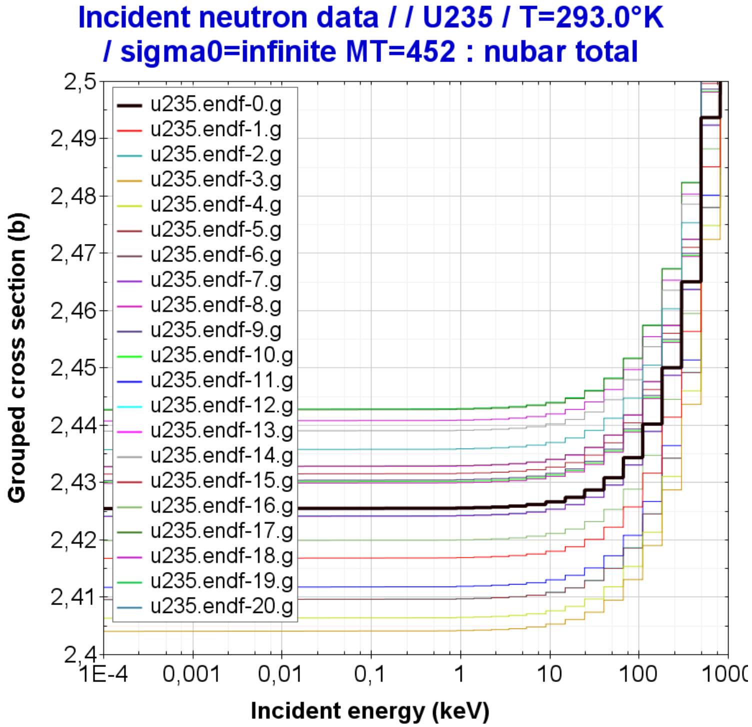


Figure: First 20 **JEFF-3.3** random files processed with NJOY/GROUPR in 69 energy groups at 293K with infinite dilution

1.4 Design and acceptance criteria for start-up and operation

Core parameter	Design criteria	Acceptance criteria
Critical boron concentration ARO	$\|(C_B)^M_{ARO}-(C_B)^C_{ARO}\|$ <50 ppm Boron	$\|(C_B)^M_{ARO}-(C_B)^C_{ARO}\|$ <100 ppm Boron
Isothermal temperature coefficient ARO at HZP	$\|(a^{ISO}{}_T)^M_{ARO}-(a^{ISO}{}_T)^C_{ARO}\|$ <3.6 pcm/ºC	$\|(a^{ISO}{}_T)^M_{ARO}-(a^{ISO}{}_T)^C_{ARO}\|$ <6.62 pcm/ºC
Moderator temperature coefficient ARO at HZP	$(a^{CTM})^{HZP}_{ARO}$ < 9 pcm/ºC	
Boron Worth Coefficient at HZP	$\| (aC_B)^M-(aC_B)^C \|$< 0.7 pcm/ppm	
Control banks worth for Reference Bank	$\| (I^{REF})^M-(I^{REF})^C \|$ <0.10x$(I^{REF})^C$	$\| (I^{REF})^M-(I^{REF})^C \|$ <0.15x$(I^{REF})^C$
Control Bank Worth value for other Banks using Rod Swap Technique	$\| (I^{CBW})^M-(I^{CBW})^C \|$ <0.15x$(I^{CBW})^C$ or 100 pcm	$\| (I^{CBW})^M-(I^{CBW})^C \|$ <0.30x$(I^{CBW})^C$ or 200 pcm
Total Control Bank Worth	1.10 x$(I^{TOT})^C$ > $(I^{TOT})^M$ >0.9x$(I^{TOT})^C$	$(I^{TOT})^M$ >0.9x $(I^{TOT})^C$
Axial Offset	$\| (AO)^M-(AO)^C \|$< 3%	
Max. Relative Assembly Power (P_A)	$\% \| (P_A)^M-(P_A)^C \|/(P_A)^C \begin{cases} < 10\% \text{ if } P \geq 90\% \\ < 15\% \text{ if } P<90\% \end{cases}$	

1.5 UQ for Core Measurements: Boron Concentration (ppm)

INDUSTRIALES ETSII | UPM

Core parameter	Design criteria	Acceptance criteria
Critical boron concentration ARO	$\lvert(C_B)^M_{ARO}-(C_B)^C_{ARO}\rvert$ <50 ppm Boron	$\lvert(C_B)^M_{ARO}-(C_B)^C_{ARO}\rvert$ <100 ppm Boron

	Burnup	Boron Meas.	WIMS-D4 + ND-1981		WIMSD5 + JEFF-3.3		Uncertainties in ppm (Boron Concentration) due to JEFF-3.3 covariance data						
Power (%)	(GWd/tHM)	(ppm)	C	C-M	C	C-M	P9-XS	P9-ν	P9-χ	U5-XS	U5-ν	U5-χ	U8-XS
50	0.015	1200	1150	-50	1165	-35	18	14	9	27	46	9	24
75	0.031	1113	1071	-42	1085	-28	18	15	9	27	46	10	24
100	0.134	985	1000	15	1011	26	19	15	9	27	46	10	25
100	1.340	870	897	27	896	26	22	16	9	25	47	10	24
100	2.487	779	806	27	797	18	24	17	9	24	45	10	24
100	2.842	755	778	23	768	13	25	19	9	24	43	10	24
100	3.591	688	714	26	701	13	27	19	9	24	43	10	24
100	4.441	604	645	41	629	25	28	20	9	23	41	10	24
100	5.549	504	544	40	526	22	30	21	9	22	40	10	24
100	6.692	412	439	27	420	8	32	22	9	22	39	10	23
100	7.716	319	340	21	321	2	34	23	9	21	38	10	23
100	8.823	227	239	12	219	-8	35	24	9	21	37	10	23
100	10.284	101	100	-1	79	-22	37	25	9	20	35	10	23
100	11.351	4					39	26	9	20	34	10	23

C= Calculated (ppm Boron)
M= Measured (ppm Boron)

1.5 UQ for Core Measurements: Axial Offset (%)

Core parameter	Design criteria	Acceptance criteria
Axial Offset	**| $(AO)^M$-$(AO)^C$ |< 3%**	

	Burnup	**Meas.**	WIMS-D4 + ND-1981		WIMSD5 + JEFF-3.3		**Uncertainties in A.O. % due to JEFF-3.3 covariance data**						
Power (%)	(GWd/tHM)	(in %)	C	C-M	C	C-M	**P9-XS**	**P9-ν**	**P9-χ**	**U5-XS**	**U5-ν**	**U5-χ**	**U8-XS**
50	0.015	7.7	5.6	-2.1	5.9	-1.8	**0.2**	0.1	0.1	**0.2**	0.3	0.1	**0.3**
75	0.031	3.8	3.7	-0.1	3.9	0.1	**0.3**	0.2	0.2	**0.3**	0.4	0.2	**0.4**
100	0.134	-0.7	0.7	1.3	0.8	1.5	**0.3**	0.2	0.2	**0.4**	0.5	0.2	**0.5**
100	1.340	-1.6	-1.2	0.4	-1.2	0.5	**0.2**	0.3	0.1	**0.2**	0.3	0.1	**0.3**
100	2.487	-2.4	-2.9	-0.5	-2.9	-0.6	**0.1**	0.2	0.1	**0.1**	0.2	0.1	**0.2**
100	2.842	-2.8	-3.0	-0.3	-3.1	-0.3	**0.1**	0.1	0.1	**0.1**	0.1	0.1	**0.1**
100	3.591	-3.8	-4.9	-1.1	-5	-1.2	**0.1**	0.1	0.1	**0.1**	0.1	0.1	**0.1**
100	4.441	-3.2	-3.8	-0.6	-3.9	-0.7	**0**	0.1	0	**0.1**	0.1	0	**0.1**
100	5.549	-3.9	-4.4	-0.5	-4.6	-0.6	**0**	0	0	**0**	0.1	0	**0**
100	6.692	-4.2	-4.4	-0.2	-4.5	-0.4	**0**	0	0	**0**	0	0	**0**
100	7.716	-4.7	-5.1	-0.4	-5.2	-0.5	**0**	0	0	**0**	0	0	**0**
100	8.823	-3.6	-2.8	0.8	-2.8	0.8	**0**	0	0	**0**	0	0	**0**
100	10.284	-3.5	-1.6	2.0	-1.5	2.0	**0**	0	0	**0**	0	0	**0**
100	11.351	-3.4	[illegible]	[illegible]	[illegible]	[illegible]	**0**	0	0	**0**	0	0	**0**

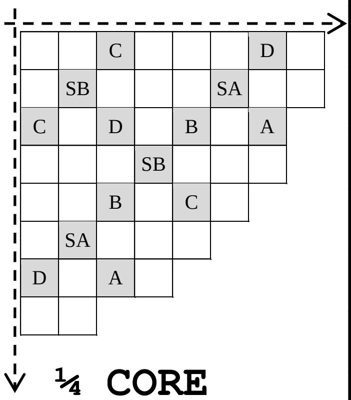
C= AO Calculated (%)
M= AO Measured (%)

1.5 UQ for Core Measurements: Control Bank Worth (ppm)

Core parameter	Design criteria	Acceptance criteria
Control banks worth for Reference Bank	$\mid (I^{REF})^{M}-(I^{REF})^{C} \mid <0.10x(I^{REF})^{C}$	$\mid (I^{REF})^{M}-(I^{REF})^{C} \mid <0.15x(I^{REF})^{C}$
Control Bank Worth value for other Banks using Rod Swap Technique	$\mid (I^{CBW})^{M}-(I^{CBW})^{C} \mid <0.15x(I^{CBW})^{C}$ or 100 pcm	$\mid (I^{CBW})^{M}-(I^{CBW})^{C} \mid <0.30x(I^{CBW})^{C}$ or 200 pcm

Control Bank Worth (ppm Boron)	WIMS-D4 + ND-1981	WIMSD5 + JEFF-3.3	Uncertainties in ppm Boron						
			Pu9-XS	Pu9-ν	Pu9-χ	U5-XS	U5-ν	U5-χ	U8-XS
D-IN (REF)	113	114	0.4	0.3	0.5	0.5	0.4	0.6	0.6
C-IN	90	87	1.5	1.3	0.8	0.8	1.3	0.8	1.0
B-IN	132	135	0.4	0.4	0.5	0.7	0.7	0.6	0.4
A-IN	81	90	2.3	1.8	0.5	1.9	3.4	0.6	1.2
SB-IN	91	86	1.9	1.6	1.0	1.2	2.1	1.1	1.6
SA-IN	112	120	1.7	1.4	0.4	1.5	2.5	0.4	0.8
D+C-IN	224	221	1.6	1.3	0.9	0.8	1.0	1.0	1.1
D+C+B-IN	399	400	2.3	1.9	1.3	1.1	1.3	1.5	1.5
D+C+B+A-IN	526	542	1.7	1.3	0.5	2.5	3.8	0.5	1.0
D+C+B+A+SB-IN	657	664	1.2	0.8	1.3	1.7	1.4	1.5	1.3
ARI	868	884	1.0	0.5	1.2	2.3	2.2	1.3	1.0

Fig. Location of control rod banks



2. Bayesian MC techniques to perform Data Adjustment

- ***"Integral benchmarks are used for data validation, but should be avoided for the adjustment of general-purpose libraries"***
  - Why ? This can lead to potential compensating effects due to both the impact of other isotopes included in the benchmark and defects in calculations attributed by complicated multi-physics.

- ***"However, it is known that such integral data have been used to perform tune or fine adjustment of specific nuclear data to improve the overall performance of an entire general-purpose library"***
  - Nuclear data adjustments should rely on high-fidelity experiments that can be used as simple (e.g. one single isotope), well-understood and so-called clean benchmarks
  - Consequently, these assumptions discharge other benchmarks (e.g. reactor calculations) for nuclear data adjustment into the evaluation procedure

- **In this work, experimental data is referred to integral information**
  - Criticality integral benchmarks (e.g. keff and spectral indices) in the ICSBEP
  - Shielding/transmission benchmarks (e.g. neutron leakage) in SINBAD/other databases
  - Delayed neutrons (e.g. beta), reactivity coefficients, etc…

2. Bayesian MC techniques to perform Data Adjustment

- Two distinct methods of nuclear data adjustment methodologies:
  - **Deterministic**
    - Generalized Linear Least Squares (GLLS)

$$[E - C'(\sigma')]^T V_E^{-1} [E - C'(\sigma')] + [\sigma' - \sigma_0]^T V_\sigma^{-1} [\sigma' - \sigma_0] = \chi^2_{min}$$

      Assumptions:
      - Experimental and nuclear data are normally distributed
      - Linear approximations between all observables
      - Model and experimental data are uncorrelated

  - **Stochastic/Monte Carlo methods**
    - Bayesian MC techniques -> direct application of Bayes' Theorem

$$(\sigma|E) \propto p_0(\sigma|\sigma_C, V_C) \times L(y_E, V_E|\sigma)$$

    - To avoid the need to linearize non-linear models
    - To handle model which are not necessarily normally distributed

2.1 GLLS

- **Generalized Linear Least Squares (GLLS)**
  - First-order Taylor series approximation

$$C(\sigma) \approx C(\sigma_0) + S(\sigma - \sigma_0)$$
$$V_C \approx S V_{\sigma_0} S^T$$

GLLS: "*This approach is a Bayesian approach in the sense that experimental data are used to adjust prior values. Although probability density functions are not considered explicitly*."

  - "A posteriori" mean and variance-covariance matrix

$$\sigma' = \sigma_0 + V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E\right]^{-1} [E - C(\sigma_0)]$$

$$V_{\sigma'} = V_{\sigma_0} - V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E\right]^{-1} S V_{\sigma_0}$$

$$C'(\sigma') \approx C(\sigma_0) + S(\sigma' - \sigma_0) = C(\sigma_0) + S V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E\right]^{-1} [E - C(\sigma_0)]$$

$$V_C' \approx S V_\sigma' S^T = S V_{\sigma_0} S^T - S V_{\sigma_0} S^T \left[S V_{\sigma_0} S^T + V_E\right]^{-1} S V_{\sigma_0} S^T$$

$$V_E' = V_E - V_E \left[S V_{\sigma_0} S^T + V_E\right]^{-1} V_E$$

$$V_{E-\sigma}' = V_E \left[S V_{\sigma_0} S^T + V_E\right]^{-1} S V_{\sigma_0}$$

2.2 Bayesian + MC Techniques

INDUSTRIALES ETSII | UPM

Bayesian MC techniques

- "Prior probability" $p_0(\sigma|\sigma_C, V_C)$ and "likelihood" $L(y_E, V_E|\sigma)$ are independent *pdf*s
- The principle of maximum entropy -> normal distributions
  - Note: "In case the normality assumption is not acceptable, σ may be mapped onto an approximately normally distributed vector by an invertible transformation" [10,16]
- Bayes' Theorem: "posterior" normal distribution: $p(\sigma|E) \sim N(\sigma', V_{\sigma'})$

Multivariate Normal Bayesian model	GLLS
$\sigma' = \sigma_C + M_{\sigma,C}\left[M_C + V_E\right]^{-1}[E - \bar{C}]$	$\sigma' = \sigma_0 + V_{\sigma_0} S^T\left[S V_{\sigma_0} S^T + V_E\right]^{-1}[E - C(\sigma_0)]$
$V_{\sigma'} = V_C - M_{\sigma,C}\left[M_C + V_E\right]^{-1} V_{\sigma,C}^T$	$V_{\sigma'} = V_{\sigma_0} - V_{\sigma_0} S^T\left[S V_{\sigma_0} S^T + V_E\right]^{-1} S V_{\sigma_0}$
$C'(\sigma') = \bar{C} + M_C\left[M_C + V_E\right]^{-1}[E - \bar{C}]$	$C'(\sigma') = C(\sigma_0) + S V_{\sigma_0} S^T\left[S V_{\sigma_0} S^T + V_E\right]^{-1}[E - C(\sigma_0)]$
$V_C' = M_C - M_C\left[M_C + V_E\right]^{-1} V_C$	$V_C' = S V_{\sigma_0} S^T - S V_{\sigma_0} S^T\left[S V_{\sigma_0} S^T + V_E\right]^{-1} S V_{\sigma_0} S^T$

… or MOCABA equations [10]

2.2 Bayesian + MC Techniques

- **Bayesian MC (BMC) techniques [3,4,5,6,7,8,9]**
  - Provide many samples of nuclear data files, for each sampled nuclear data file simulation is performed
  - **Methodologies for randomly sampled "σ"**
    - **NUDUNA and SANDY + Bayesian Approach**
      - Samples of ND files for "a priori" $p_0(\sigma|\sigma_C, V_C)$ evaluated files
      - Based on normal (or log-normal) distributions because no further information on the distribution of the nuclear data are provided in evaluated files [11,12]
    - **"Total Monte Carlo"(TMC) + Bayesian MC Approach [3,4,7,8]**
      - Sampling performed at the level of nuclear parameters in nuclear reaction codes (e.g. TALYS or EMPIRE)
      - $p_0(\sigma|\sigma_C, V_C)$ will NOT be normal !?. Then, lost of information about the prior function if it is approximated by a normal pdf

2.3 Bayesian + Monte Carlo: MOCABA

❑ NUDUNA and SANDY + Bayesian Approach

Multivariate Normal Bayesian model

$$\sigma' = \sigma_C + M_{\sigma,C}\left[M_C + V_E\right]^{-1}[E - \bar{C}]$$

$$V_{\sigma'} = V_C - M_{\sigma,C}\left[M_C + V_E\right]^{-1} V_{\sigma,C}^T$$

$$C'(\sigma') = \bar{C} + M_C\left[M_C + V_E\right]^{-1}[E - \bar{C}]$$

$$V_C' = M_C - M_C\left[M_C + V_E\right]^{-1} V_C$$

… or MOCABA equations

- NUDUNA/SANDY provides samples of nuclear data files

$$\overline{\sigma_i} = \frac{\sum_{k=1}^{N} \sigma_{i,k}}{N}$$

$$V_{\sigma_{ij}} = \frac{\sum_{k=1}^{N} \left(\sigma_{i,k} - \overline{\sigma_i}\right)^T \left(\sigma_{j,k} - \overline{\sigma_j}\right)}{N}$$

$$\overline{C_m} = \frac{\sum_{k=1}^{N} C_m(\sigma_k)}{N}$$

$$M_{C_{mn}} = \frac{\sum_{k=1}^{N} \left(C_m(\sigma_k) - \overline{C_m}\right)^T \left(C_n(\sigma_k) - \overline{C_n}\right)}{N}$$

$$M_{\sigma_i - C_m} = \frac{\sum_{k=1}^{N} \left(\sigma_{i,k} - \overline{\sigma_i}\right)^T \left(C_m(\sigma_k) - \overline{C_m}\right)}{N}$$

2.4 Bayesian Monte Carlo: BMC

TMC + Bayesian MC Approach (BMC)

- "The requirement of a well-defined prior pdf is a serious limitation of the previous approach if non-informative prior distributions are known [3,4]"
  - e.g. model parameters (x) which lead through a model transformation $\sigma=\mathcal{M}(x)$
- BMC approach will use TMC method to generate "a priori" random files which are not explicitly well-defined normal pdfs
- BMC incorporates integral "a priori" information through **likelihood factors**

… normality assumption in ω_k !?

$$L(y_E, V_E|\sigma) \sim e^{-\chi_k^2/2} \quad \text{with:} \quad \chi_k^2 = [E - C(\sigma_k)]^T V_E^{-1} [E - C(\sigma_k)]$$

- One can calculate a "weight" for any k-sample set: $\omega_k = e^{-\chi_k^2/2}$
- "A posteriori" moments:

$$\sigma_i' = \frac{\sum_{k=1}^{N} \omega_k \times \sigma_{i,k}}{\sum_{i=k}^{N} \omega_k} \qquad V'_{\sigma_{ij}} = \frac{\sum_{k=1}^{N} \omega_k \times \left(\sigma_{i,k} - \sigma_i'\right)^T \left(\sigma_{j,k} - \sigma_j'\right)}{\sum_{k=1}^{N} \omega_k}$$

2.4 Bayesian Monte Carlo: BMC

❑ TMC + Bayesian MC Approach (BMC)

- “A posteriori” moments:

$$\sigma_i' = \frac{\sum_{k=1}^{N} \omega_k \times \sigma_{i,k}}{\sum_{i=k}^{N} \omega_k} \qquad V'_{\sigma_{ij}} = \frac{\sum_{k=1}^{N} \omega_k \times \left(\sigma_{i,k} - \sigma_i'\right)^T \left(\sigma_{j,k} - \sigma_j'\right)}{\sum_{k=1}^{N} \omega_k}$$

$$C_m' = \frac{\sum_{k=1}^{N} \omega_k \times C_m(\sigma_k)}{\sum_{k=1}^{N} \omega_k} \qquad V'_{C_{mn}} = \frac{\sum_{k=1}^{N} \omega_k \times \left(C_m(\sigma_k) - C_m'\right)^T \left(C_n(\sigma_k) - C_n'\right)}{\sum_{k=1}^{N} \omega_k}$$

- Other “weights” definitions
  - Simpler definitions of ω_k values can lead to very low small weights
  - So-called BFMC method, renormalization of ω_k

$$\omega_k = e^{-\chi_k^2 / \chi_{min}^2} \qquad \omega_k = e^{-\left(\chi_k^2 / \chi_{min}^2\right)^2}$$

✓ lost of normality assumption!? ... still Bayesian? pre-requisite (not limitation) of any Bayesian to have a well-defined prior distribution and a well-defined likelihood function

2.5 Selection of Benchmarks

❑ Scope of nuclear data adjustment (DA)

- Criticality Benchmarks
  - Nuclear data evaluations have used mainly criticality benchmarks to match C/E
  - However, **keff** is a global parameter that can be achieved trough many possible combinations of nuclear data - > inherent compensating effects in DA
- Other sources of integral data
  - Spectral index measurements
  - Delayed neutron fraction [14]
  - **Shielding/transmission leakage neutron spectra [14]**

▪ **Exercise:**	BMC with criticality and transmission benchmarks jointly!!
	5000 random files 235U/TENDL2014
	Calculations with MCNP6.1.1

3. Exercise: BMC – 235U, Criticality & Transmission Integral Benchmarks

❑ LLNL-235U pulsed sphere

Total χ^2=3.54

- U-235, 0.7 mfp, fwhm=2.0 ns, NE213-B bias=1.6, FP=945.54 cm, 26-deg

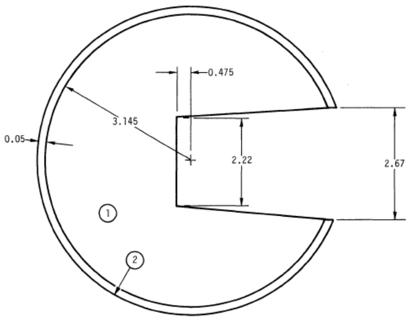
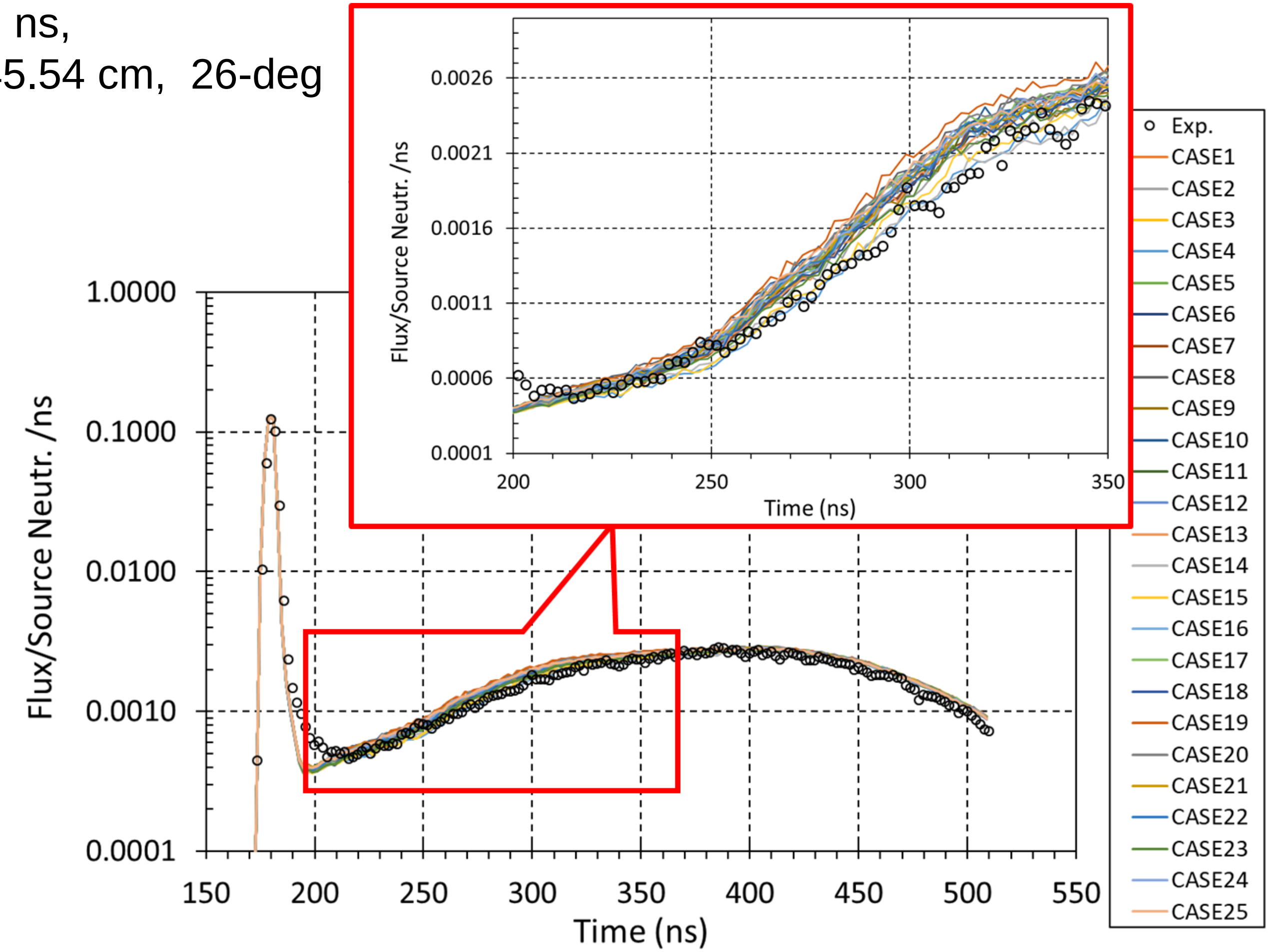
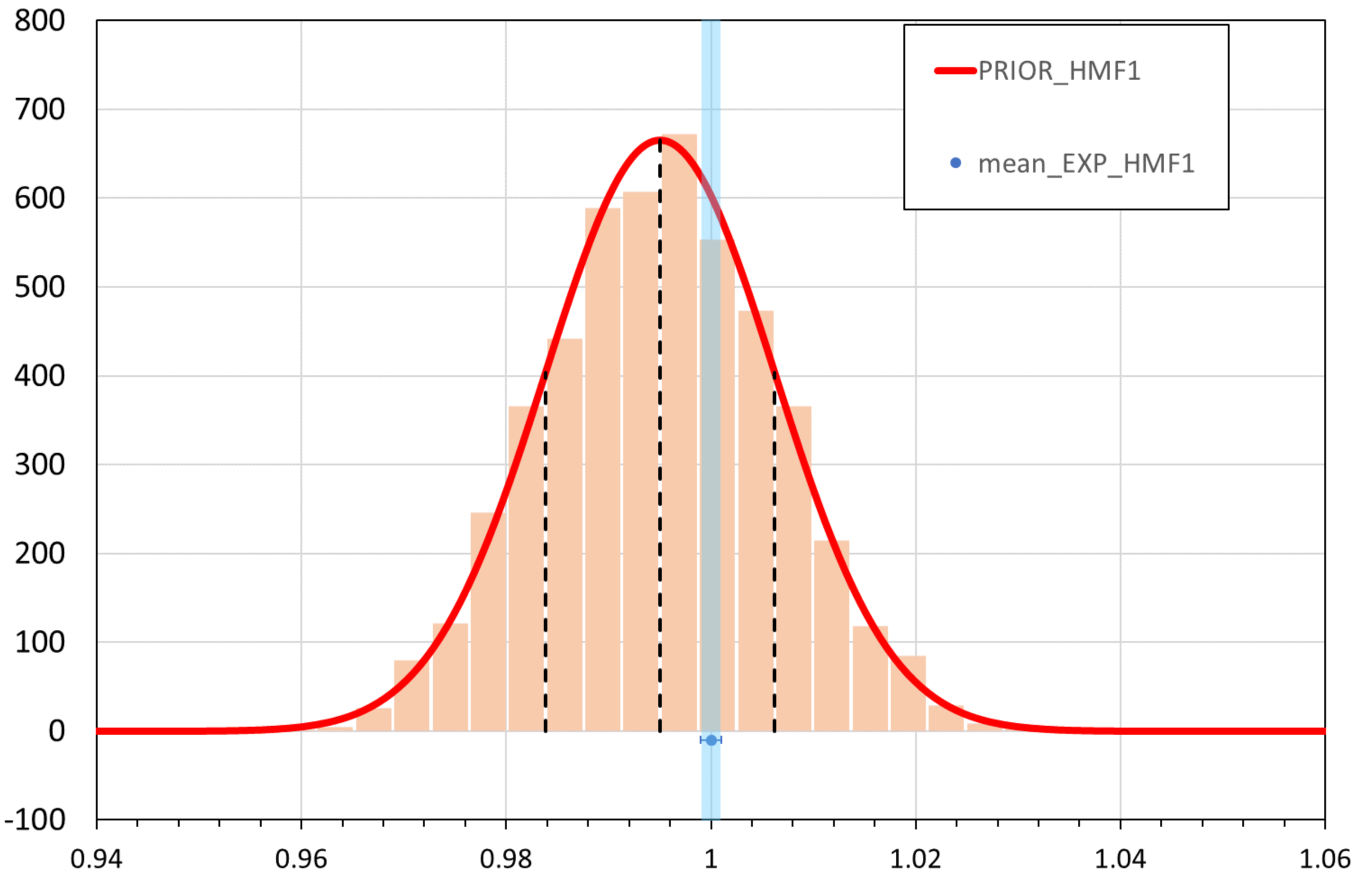


Fig. Dimensions of the small 235U solid spherical target , Report: LLNL UCID-17332



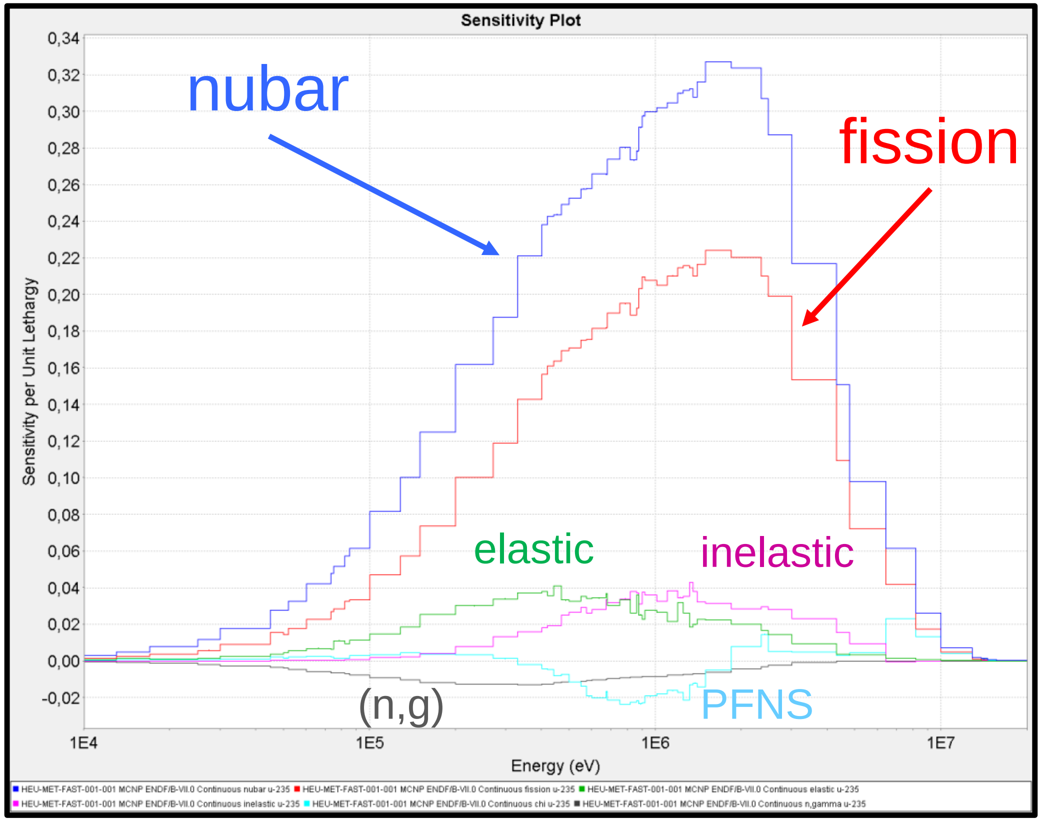
3. Exercise: BMC – 235U, Criticality & Transmission Integral Benchmarks

❑ HMF1 – Godiva Benchmark



3. Exercise: BMC – 235U, Criticality & Transmission Integral Benchmarks

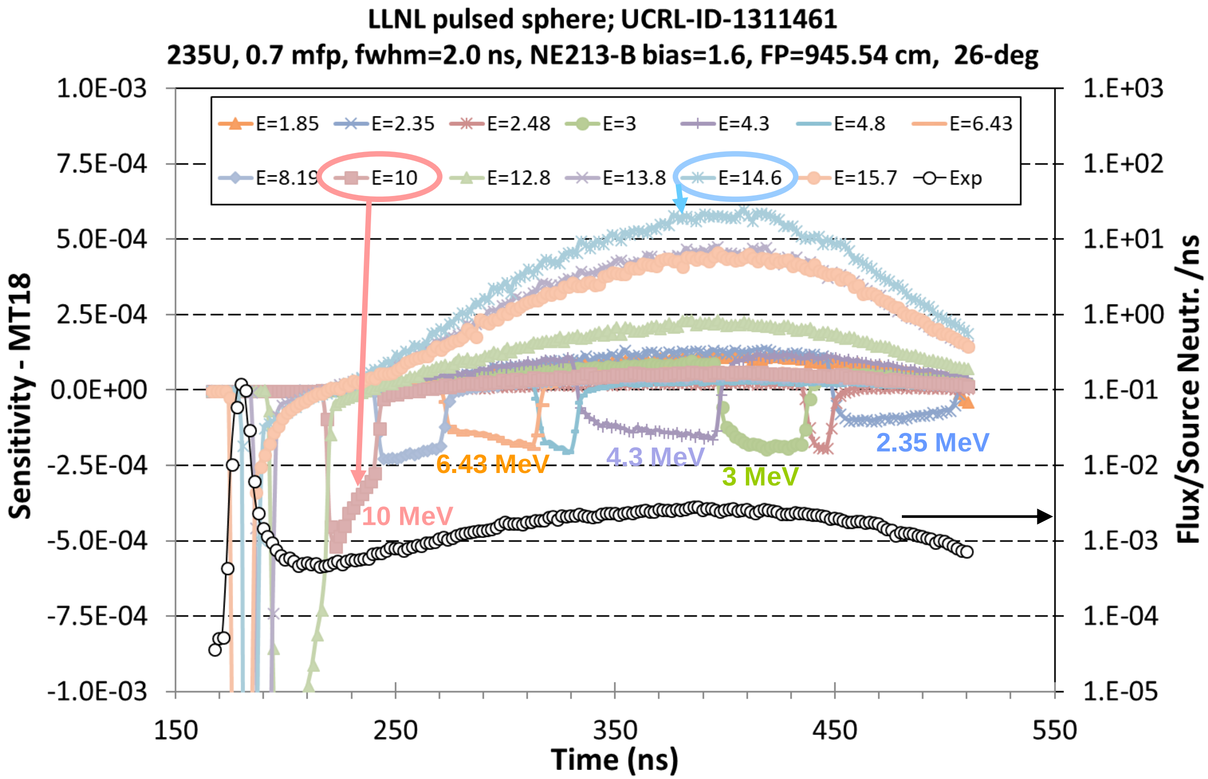
- Sensitivity Analysis
  - HMF1(**DICE database**)
    - Large values for **nubar** and **fission**
    - Elastic and inelastic 10 times lower than fission/nubar
    - En < 5 MeV



3. Exercise: BMC – 235U, Criticality & Transmission Integral Benchmarks

Note: Sensitivities predicted with MCSEN code [15]

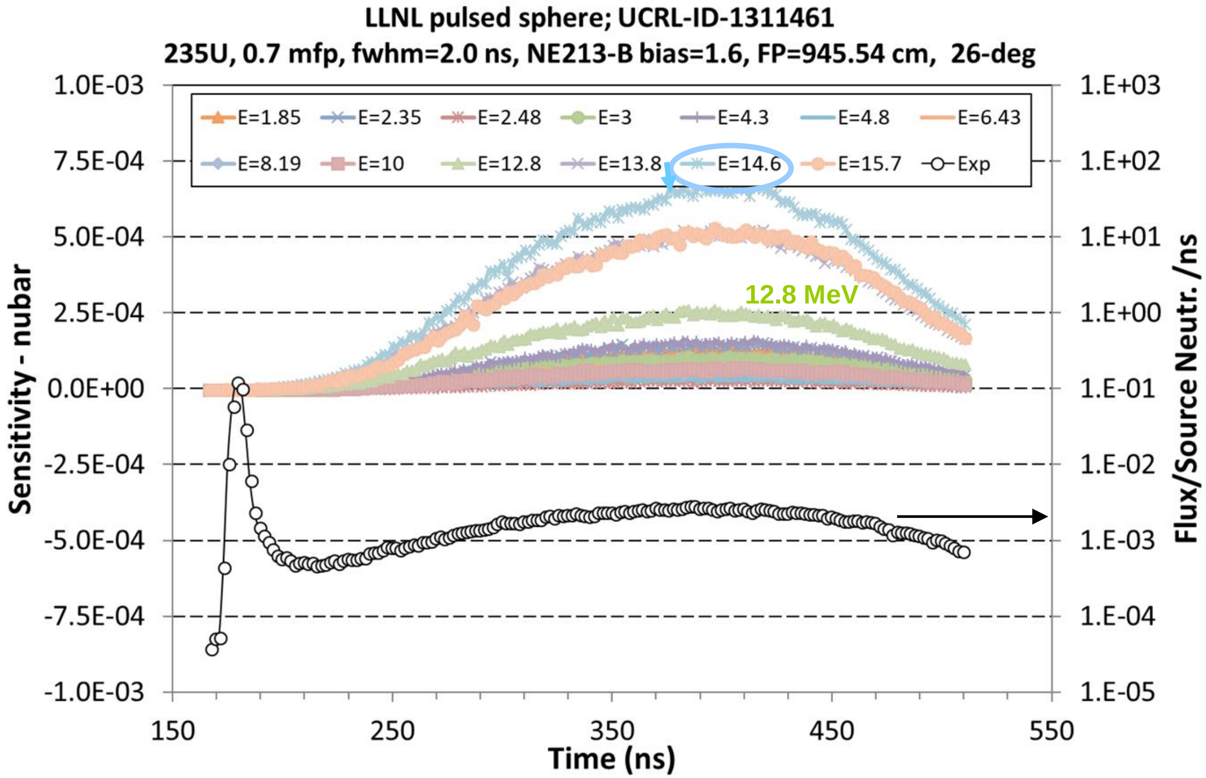
- Sensitivity Analysis : "LLNL- 235U" pulsed sphere
  - **Fission** mainly around 14 MeV, other terms with lower values



3. Exercise: BMC – 235U, Criticality & Transmission Integral Benchmarks

Note: Sensitivities predicted with MCSEN code [15]

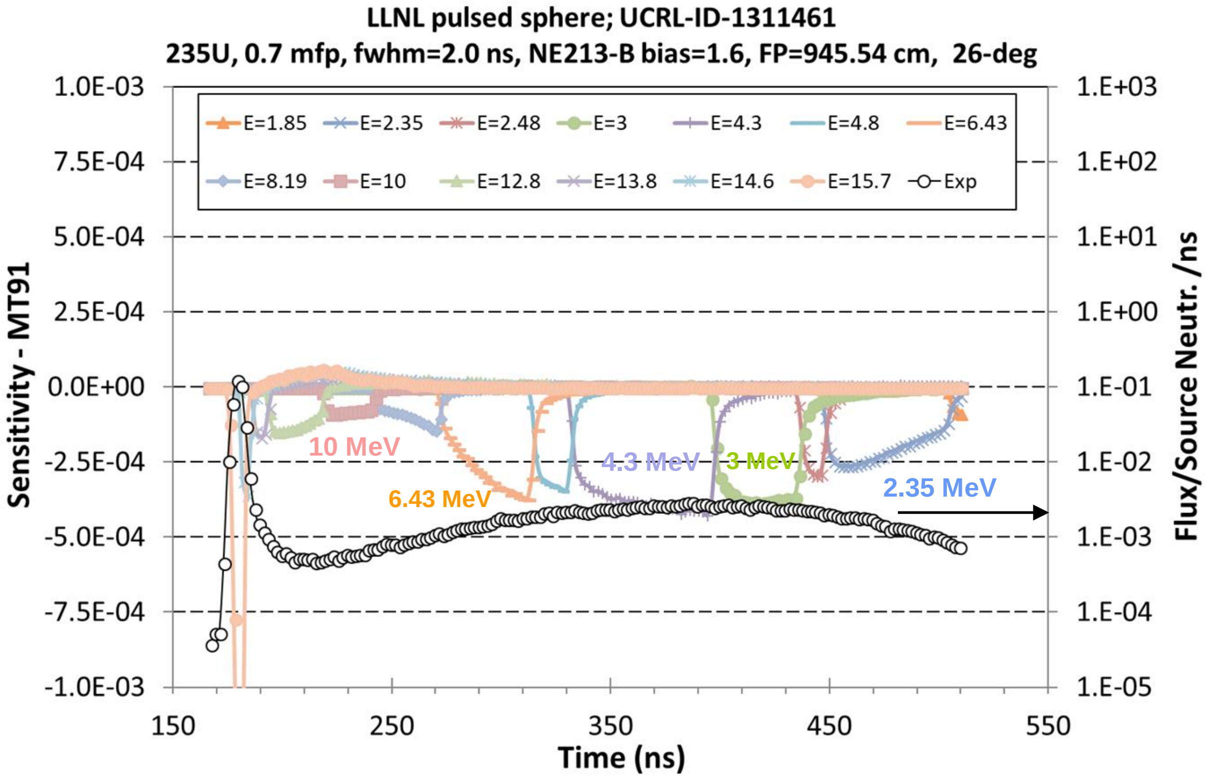
- Sensitivity Analysis : “LLNL- 235U” pulsed sphere
  - **Nu-bar** mainly 14 MeV



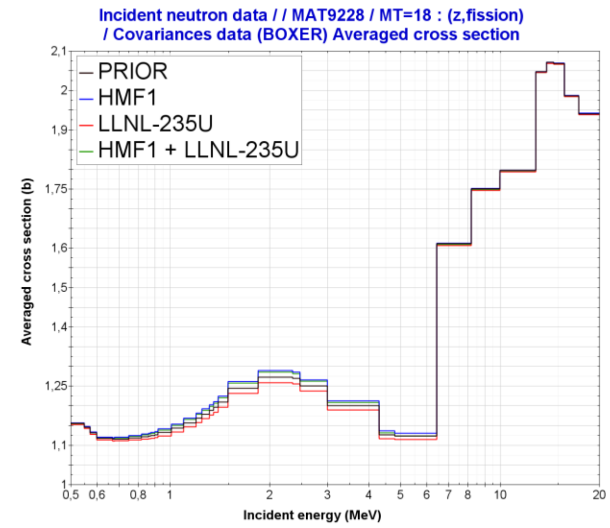
3. Exercise: BMC – 235U, Criticality & Transmission Integral Benchmarks

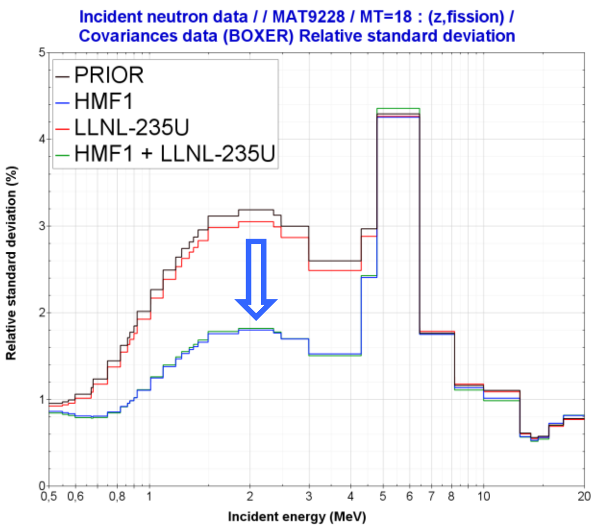
Note: Sensitivities predicted with MCSEN code [15]

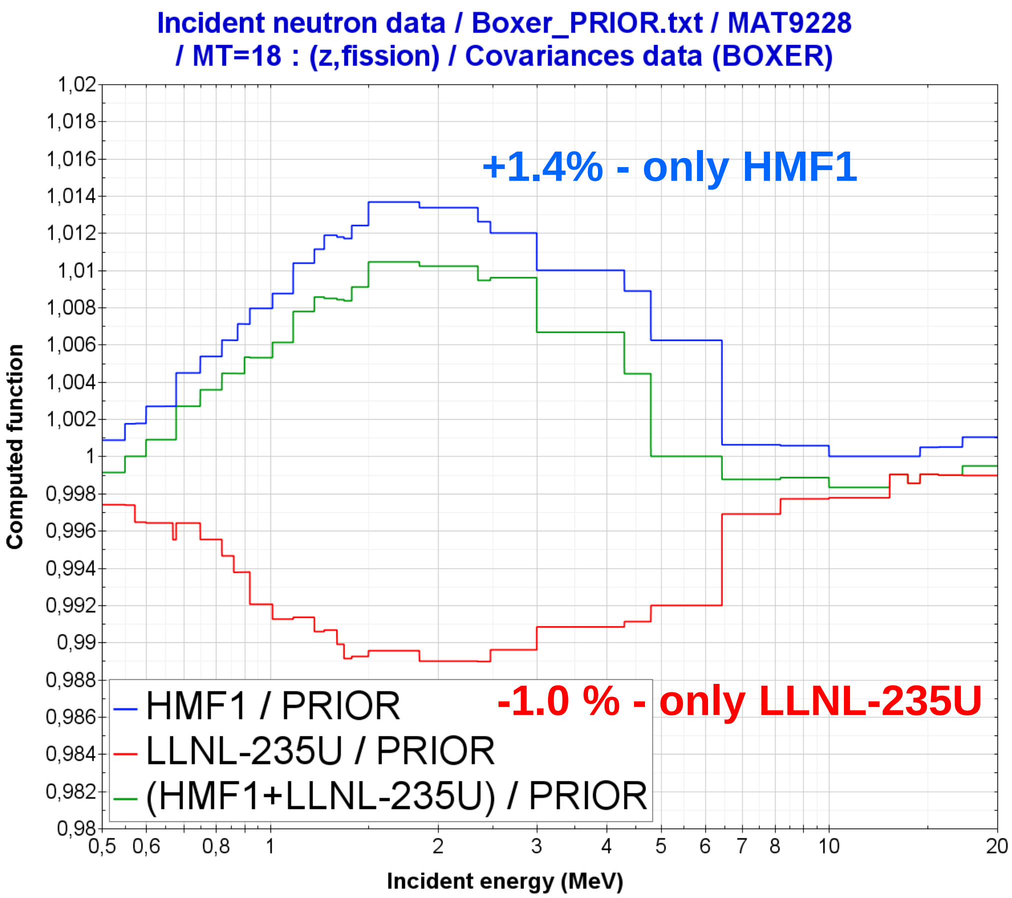
- Sensitivity Analysis : “LLNL- 235U” pulsed sphere
  - **MT91**, between 1.8-14 MeV



BMC ND Adjustment – MT18 (fission)

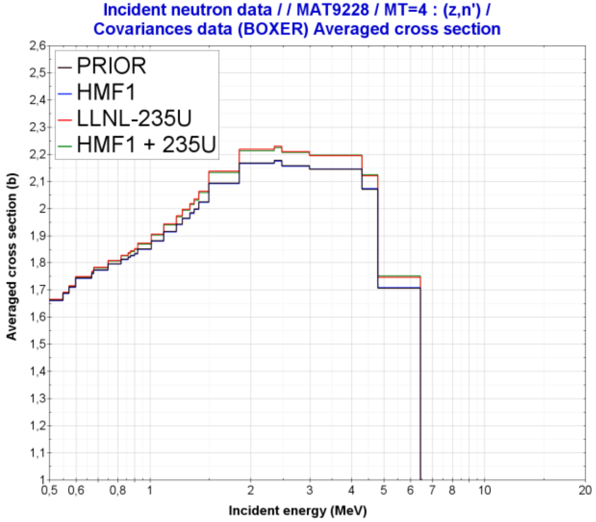


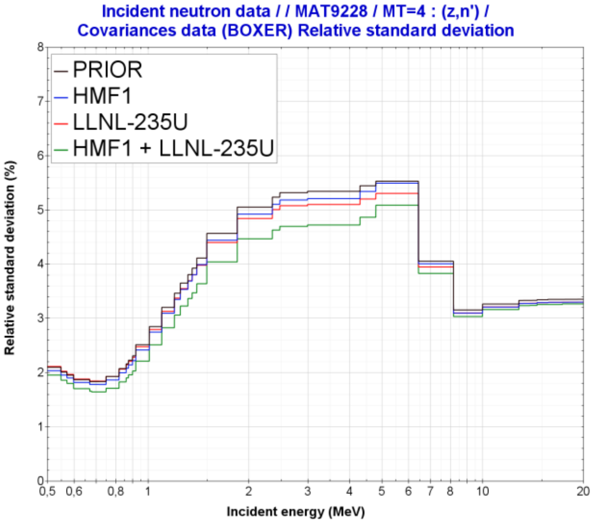


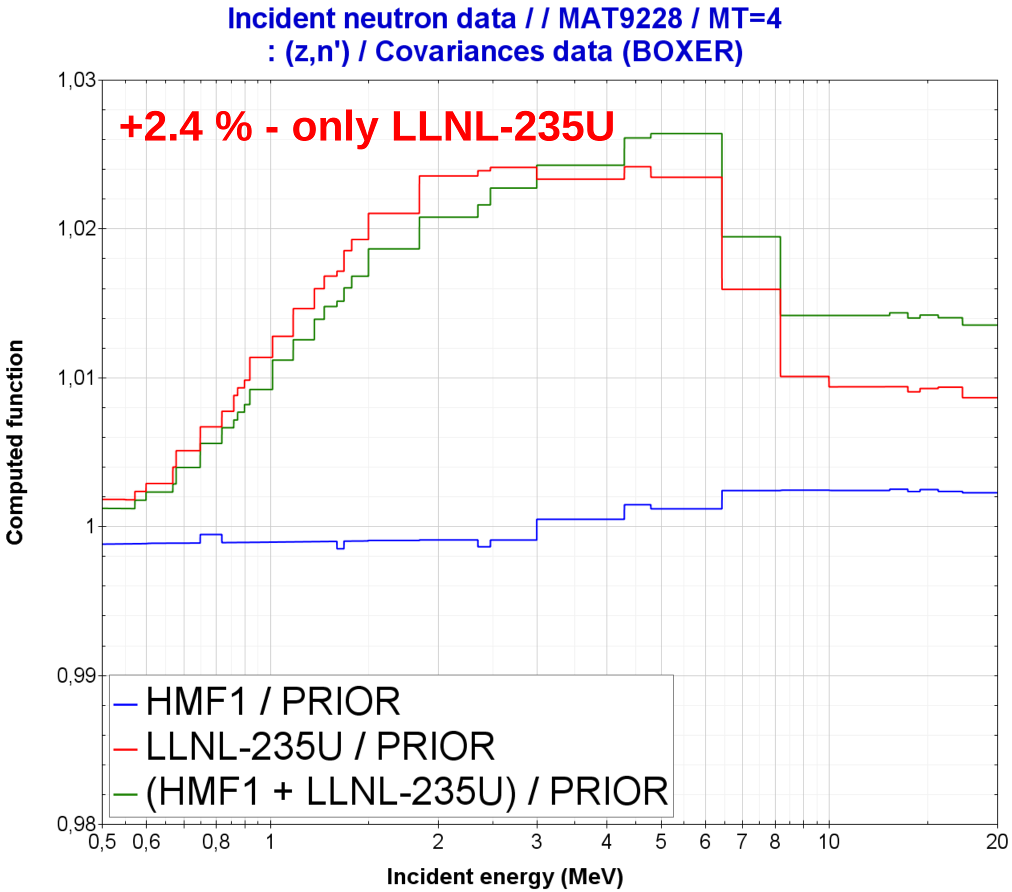


- High sensitivity in criticality for HMF1 (and LLNL-235U)
  - large MT18 “motive force”… cause of the cross-section alteration
- Strong reduction of uncertainty: ~1.5%

BMC ND Adjustment – MT4 (inelastic)





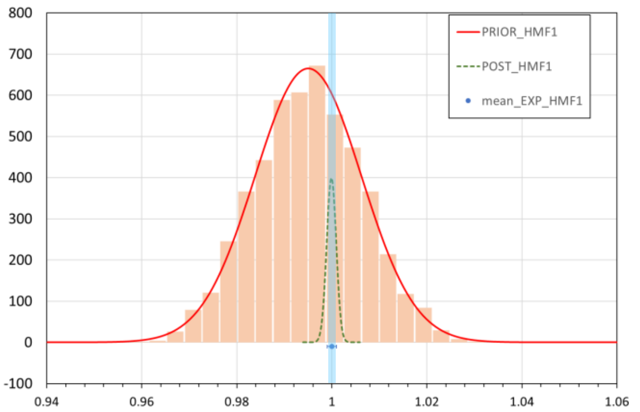


- High sensitivity in LLNL-235U : +2.4%
  - large MT4 “motive force”… cause of the cross-section alteration
- Reduction of uncertainty: ~0.6%

3. Conclusion

❑ Bayesian MC adjustment for "HMF1- Godiva" Benchmark

	Constraints	HMF1	
		keff (MEAN)	Dkeff (STD)
PRIOR....		0.99504	0.01119
POST....	Only HMF1	0.99992	0.00100
POST....	Only LLNL-235U	0.99146	0.01069
POST....	Both HMF1 +LLNL-235U	0.99985	0.00099



❑ Bayesian MC adjustment for "LLNL-235U" Benchmark

	Constraints	Total CHI^2 LLNL- 235U/0.7mfp Benchmark
PRIOR....		3.52
POST....	Only HMF1	3.69
POST....	Only LLNL-235U	3.13
POST....	Both HMF1 +LLNL-235U	3.37

3. Conclusion

The aim of this work is to review different Monte Carlo (MC) techniques used to propagate nuclear data uncertainties

1. Uncertainty Quantification (UQ) studies
   - Required in safety calculations of large scale systems ~ PWR
   - ND uncertainty propagation on the main design parameters
   - Decomposition of uncertainty in: ^{235}U-^{238}U-^{239}Pu & XS-ν-PFNS
     - **Assessing nuclear data/uncertainty trends** ✓
     - **Determining contributors & uncertainty targets for a safety operation**
2. Bayesian Monte Carlo approaches for data adjustment
   - Multivariate Normal Bayesian model relying on NUDUNA/SANDY codes
   - TMC + Bayesian MC Approach (BMC)
   - Selection of Benchmarks.
   - Exercise:
     - **BMC applied for Criticality + Shielding/Transmission** ✓
     - **Importance of additional sensitivity analysis (…"motive force" [13] !?)**

References

[1] A. Santamarina, P. Blaise, N. Dos Santos, C. Vaglio, C. De Saint-Jean, Nuclear Data Uncertainty Propagation on Power Maps in Large LWR Cores, PHYSOR 2014 – The Role of Reactor Physics Toward a Sustainable Future. Kyoto, Japan, September 28 – October 3, 2014

[2] O. Cabellos, E. Castro, C. Ahnert, C. Holgado, Propagation of Nuclear Data Uncertainties for PWR Core Analysis, Nuclear Engineering and Technology, 46 No.3 (2014)

[3] D.L. Smith, A Unified Monte Carlo Approach to Fast Neutron Cross Section Data Evaluation, Proceedings of the 8th International Topical Meeting on Nuclear Applications and Utilization of Accelerators, Pocatello, July 29 - August 2, 2007, p. 736.

[4] A.J. Koning, Bayesian Monte Carlo Method for Nuclear Data Evaluation, Nuclear Data Sheets 123 (2015) 207–213

[5] C. de Saint Jean, P. Archier, E. Privas and G. Noguere, On the use of Bayesian Monte-Carlo in evaluation of nuclear data, EPJ Web of Conferences 146 (2017) 02007.

[6] C. De Saint Jean, P. Archier, E. Privas, G. Noguere, B. Habert, P. Tamagno, Evaluation of Neutron-induced Cross Sections and their Related Covariances with Physical Constraints, Nuclear Data Sheets 148 (2018) 383–419

[7] D. Rochman, E. Bauge, A. Vasiliev, H. Ferroukhi and G. Perret, Nuclear data correlation between different isotopes via integral information, European Physics Journal N 4 (2018) 7.

[8] D.Rochman, Monte Carlo nuclear data adjustment via integral information, EPJ. To be published (2018)

[9] D.J. Siefman, M. Hursin, P. Grimmy, A. Pautz, Case Study of Data Assimilation Methods with the LWR-Proteus Phase II Experimental Campaign, Conference: M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & EngineeringAt: Jeju, South Korea (2017)

[10] A. Hoefer, O. Buss, M. Hennebach, M. Schmid and D. Porsch, MOCABA: A general Monte Carlo-Bayes procedure for improved predictions of integral functions of nuclear data, Annals of Nuclear Energy 77 (2015) 514.

[11] C.J. Díez, O. Buss, A. Hoefer, D. Porsch, O. Cabellos, Comparison of nuclear data uncertainty propagation methodologies for PWR burn-up simulations, Annals of Nuclear Energy 77 (2015) 101–114

[12] E. Castro, C. Ahnert, O. Buss, N. García-Herranz, A. Hoefer, D. Porsch, Improving PWR core simulations by Monte Carlo uncertainty analysis and Bayesian inference, Annals of Nuclear Energy 95 (2016) 148–156

[13] K. Yokoyama, M. Ishikawa, Use and Impact of Covariance Data in the Japanese Latest Adjusted Library ADJ2010 Based on JENDL-4.0, Nuclear Data Sheets 123 (2015) 97–103

[14] I. Kodeli, L. Plevnik, Nuclear data adjustment exercise combining information from shielding, critical and kinetics benchmark experiments ASPIS-Iron 88, Popsy and SNEAK-7A/7B, Progress in Nuclear Energy 106 (2018) 215–230

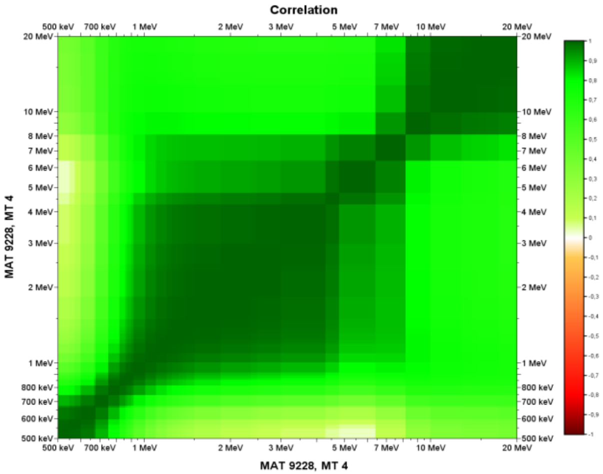
[15] R.L. Perel, J.J. Wagschal, Y. Yeivin, Monte Carlo Calculation of Point-Detector Sensitivities to Material Parameters, Nuclear Science and Engineering, 124 (1), 197–209 (1996)

[16] A. Hoefer, private communication

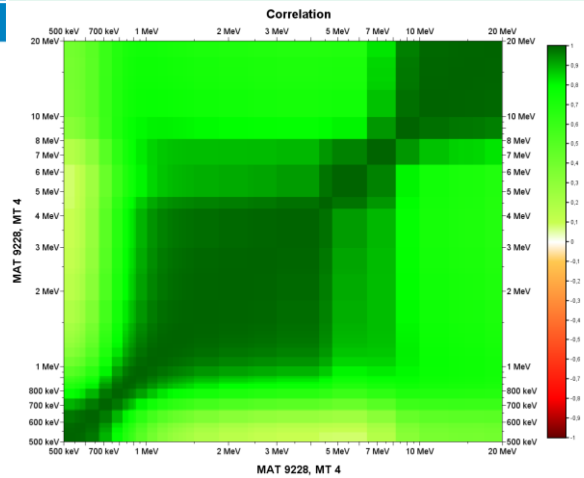
MT4

Extra slides …

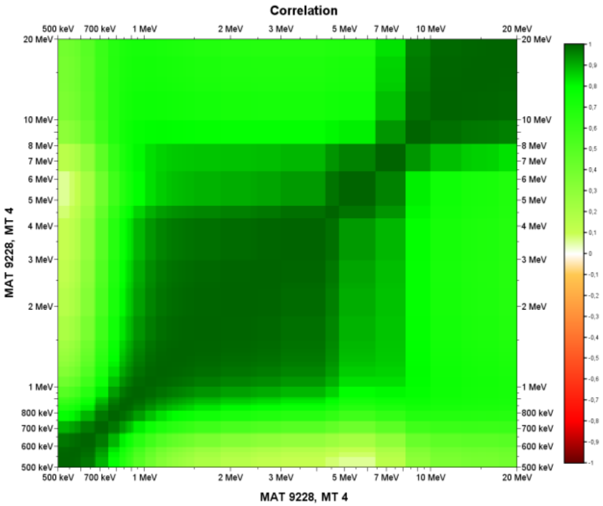
PRIOR



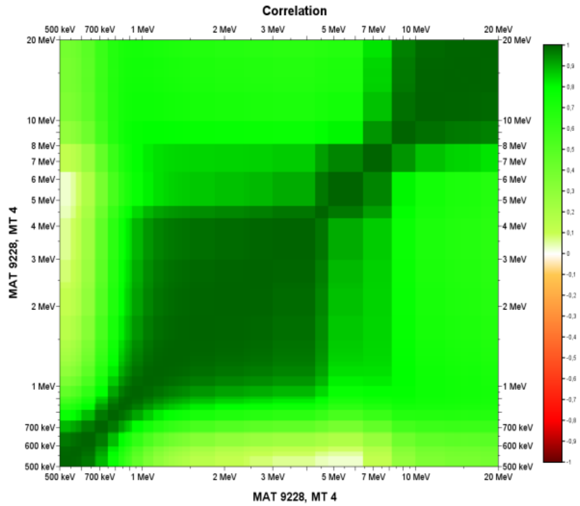
HMF1



LLNL-235U



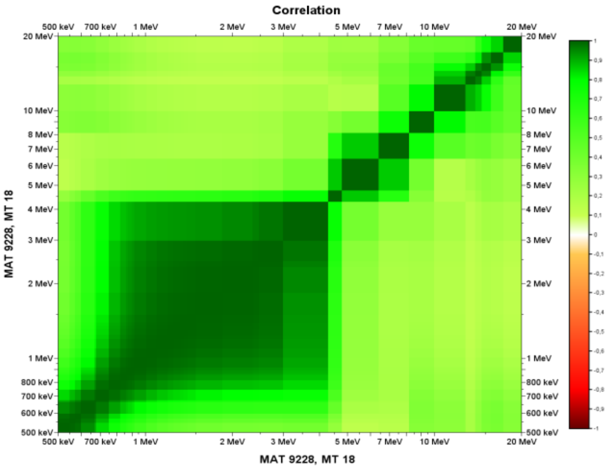
HMF1 + LLNL-235U

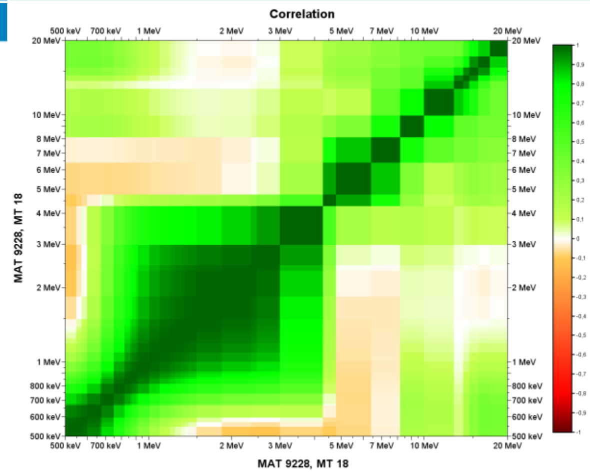


MT18

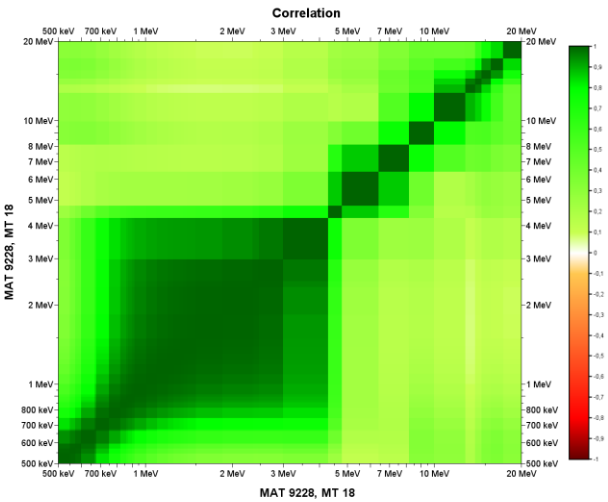
Extra slides …

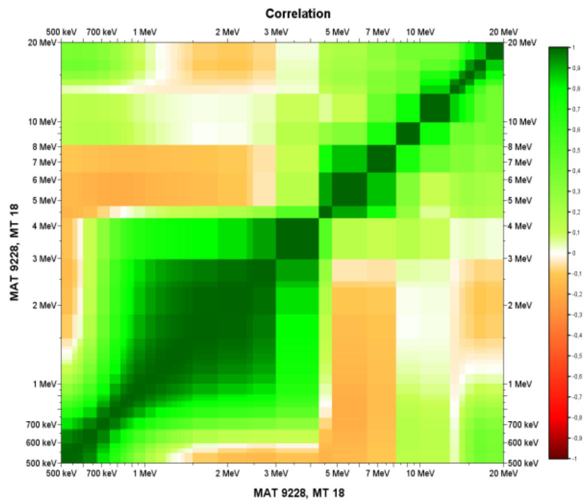
PRIOR	HMF1





LLNL-235U	HMF1 + LLNL-235U

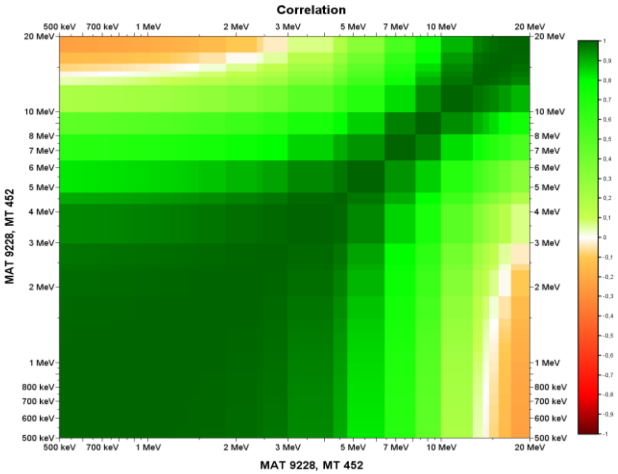




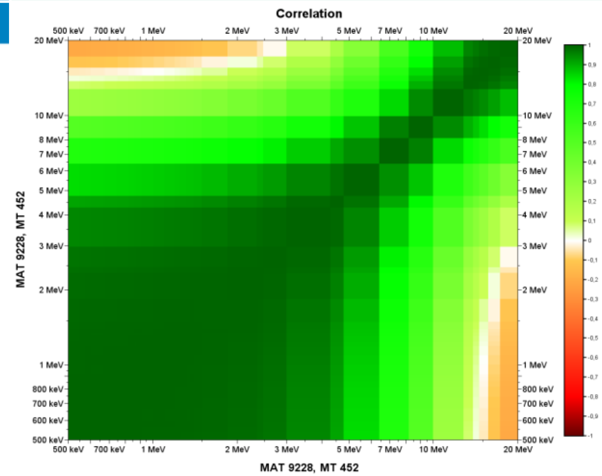
MT452

Extra slides ...

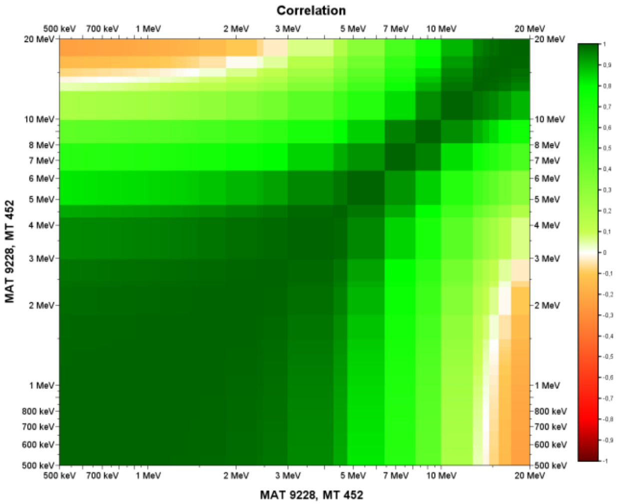
PRIOR



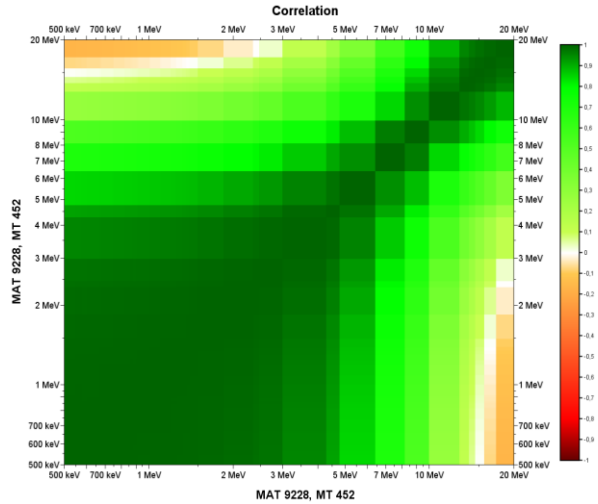
HMF1



LLNL-235U



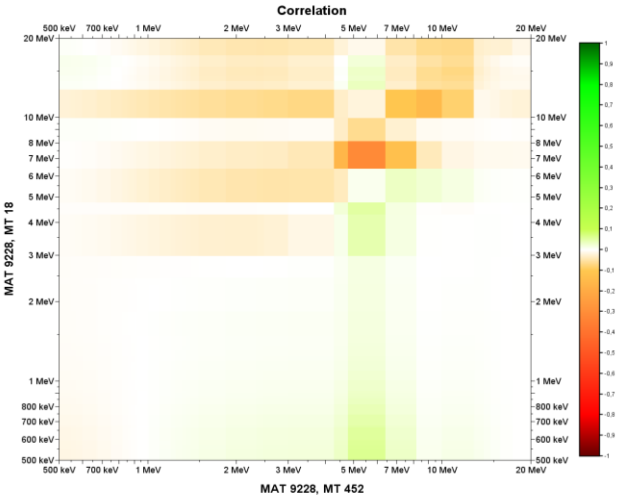
HMF1 + LLNL-235U



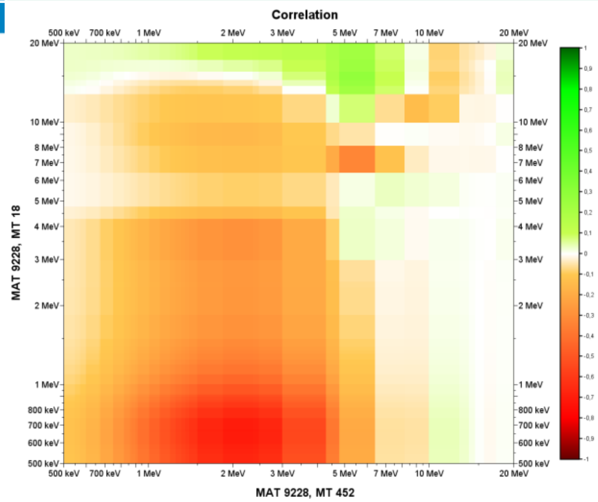
MT18 –MT452

Extra slides ...

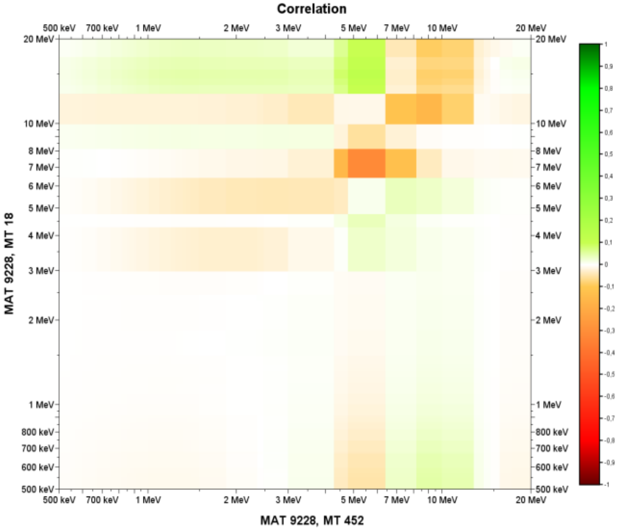
PRIOR



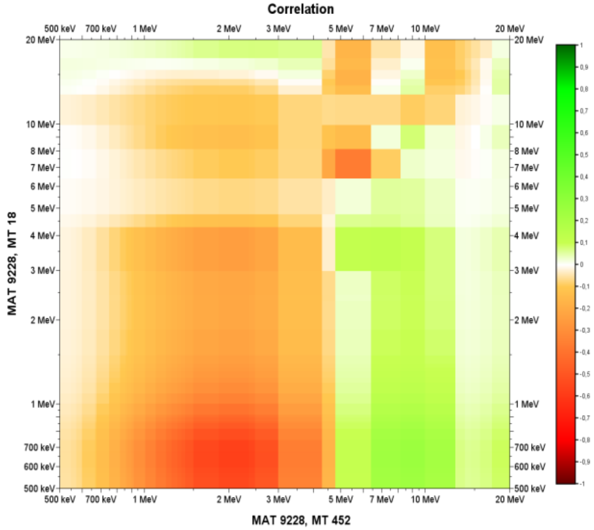
HMF1



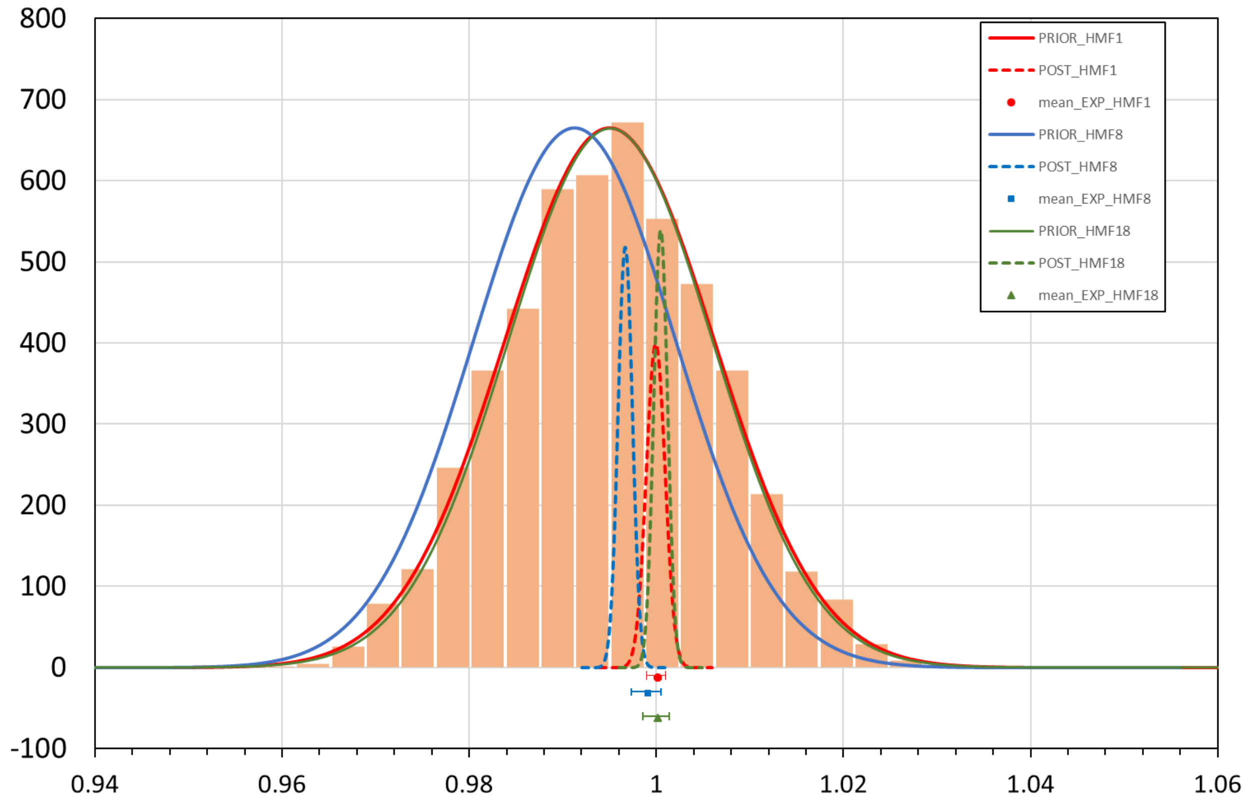
LLNL-235U



HMF1 + LLNL-235U



Extra slides ...



		HMF1		HMF8		HMF18	
#	Bayesian MC	keff (MEAN)	Δkeff (STD)	keff (MEAN)	Δkeff (STD)	keff (MEAN)	Δkeff (STD)
PRIOR....		0.99504	0.01119	0.99125	0.01080	0.99510	0.01090
POST....	HMF1	0.99992	0.00100	0.99595	0.00104	0.99984	0.00100
POST....	HMF1_HMF8_HMF18	0.99985	0.00099	0.99572	0.00103	0.99971	0.00100
POST....	LLNL-235U	0.99146	0.01069	0.98765	0.01029	0.99155	0.01041
POST....	HMF1 +LLNL-235U	0.99985	0.00099	0.99572	0.00103	0.99971	0.00100