DE LA RECHERCHE À L'INDUSTRIE

INFLUENCE OF SYSTEMATIC EXPERIMENTAL UNCERTAINTIES IN THE EVALUATION OF NUCLEAR DATA

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CEA/DEN/Cadarache

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OUTLINES

1 Reminders, context and objectives

2 Bayesian inference (Generalize least square and Monte-Carlo)

3 Systematic **Microscopic** Uncertainties:

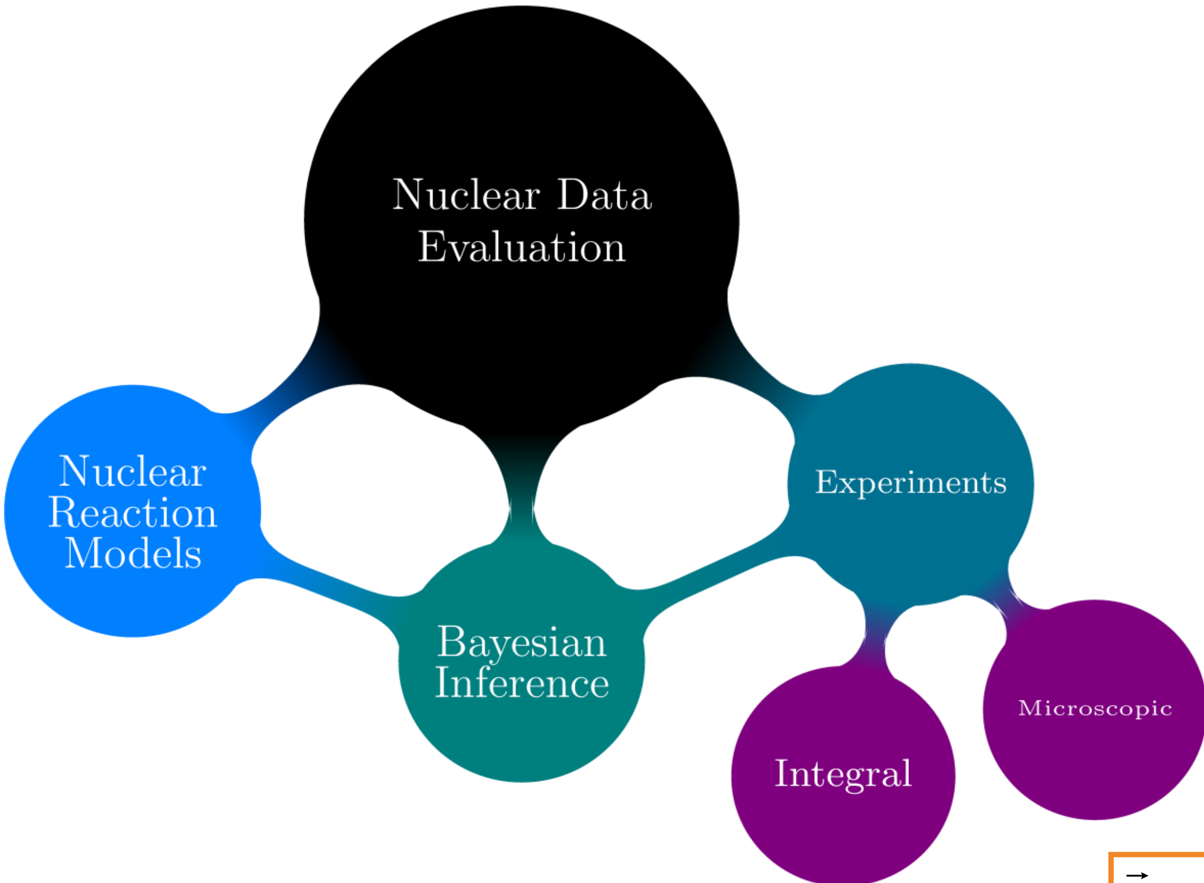
A. What ?
B. Marginalization
C. Covariances ^{239}Pu, an example

4 Integral Data Assimilation ans Syst. Uncertainties

A. What ?
B. Single experiment (JEZEBEL) → Covariances ^{239}Pu, an example
C. Several experiments : PU-SOL-THERM → Syst. Uncertainty
D. A positive aspect of Syst. Uncertainties

5 Conclusions and Perspectives

CROSS SECTIONS “KNOWLEDGE” EVALUATION IN THE RESONANCE RANGE AND HIGHER



Issues :

- Systematic experimental uncertainties
- Phenomenological Nuclear reaction model theories + Parameters
- Model defects (Epistemic Uncertainties)
- Integral experiment assimilation
- Common Physics from RRR to Continuum

$$\vec{t}\,(M, \vec{x}, \vec{\theta})$$

$$\vec{x} = \{\gamma_{a\lambda}, E_{\lambda}, a_c, R'\}$$

$$\vec{x} = \{\langle\Gamma_a\rangle, a_c, R^{\infty}, D_0, S_a\}$$

$$\vec{x} = \{\beta_2, a_c, d_c, V, W, ...\}$$

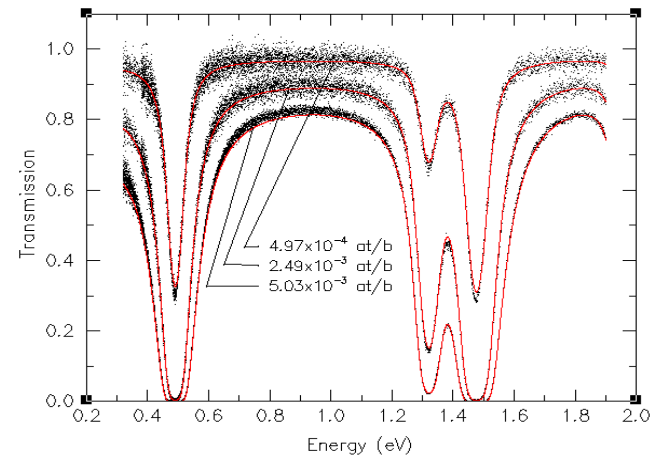
$$\vec{x} = \sigma_g^r, \chi_g, \upsilon ...$$

Microscopic and Integral experiments

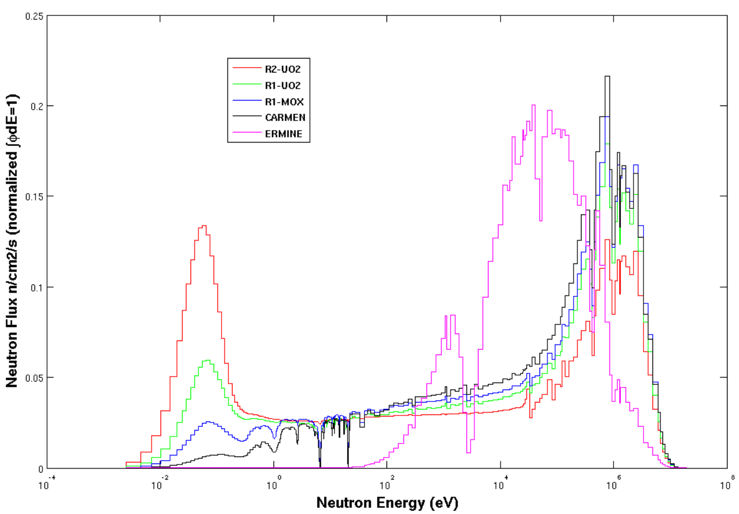
Microscopic experiments

- Fine resolution in energy
- All reactions: (n,γ), (n,f), (n,n'), (n,xn)…
- Outgoing particles (n, γ, α...) caracterized in terms of spectrum/multiplicity/angular distribution…
- ***Systematic uncertainties (normalization, background, detector efficiency…)***

Transmission measurements at JRC/Geel (GELINA)



Neutron flux in MINERVE

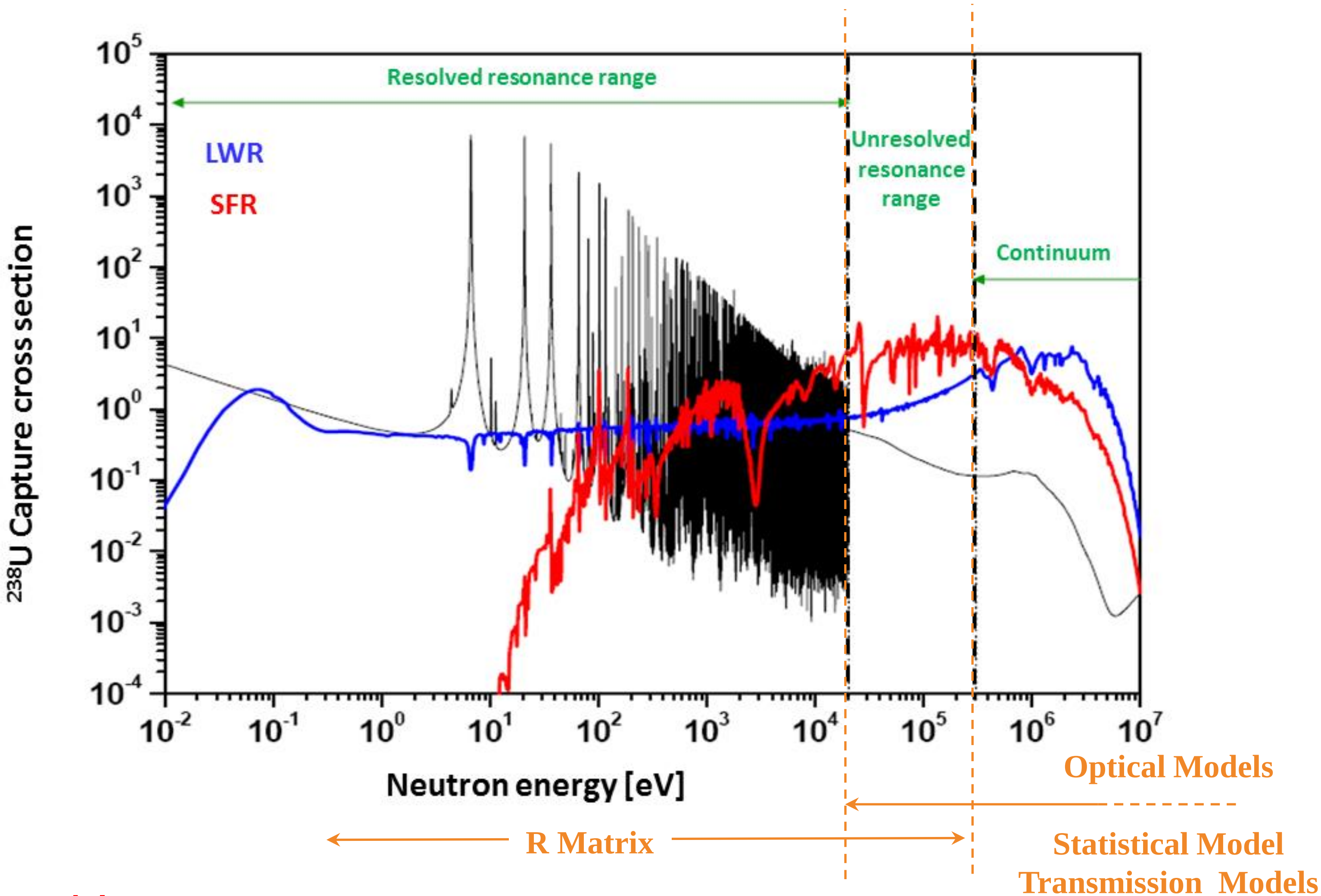


Oscillation measurements in Minerve

Integral experiments

- Integrated measurements in angle/energy/space
- Better overall precision) <3% (1s) for difficult regions
- Representativity w/t to Industrial concepts:
- keff, reactivity effects, flux/power distribution …
- ***Integral experiments correlations (systematic uncertainties)***
- ***Evaluation →Processing →Transport code → feedback ND***

CROSS SECTIONS "KNOWLEDGE"
EVALUATION IN THE RESONANCE RANGE AND HIGHER



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Nuclear reaction models

Experiments (microscopic/integral)

Bayesian inference technique

Evaluation of uncertainties (variances and correlations)

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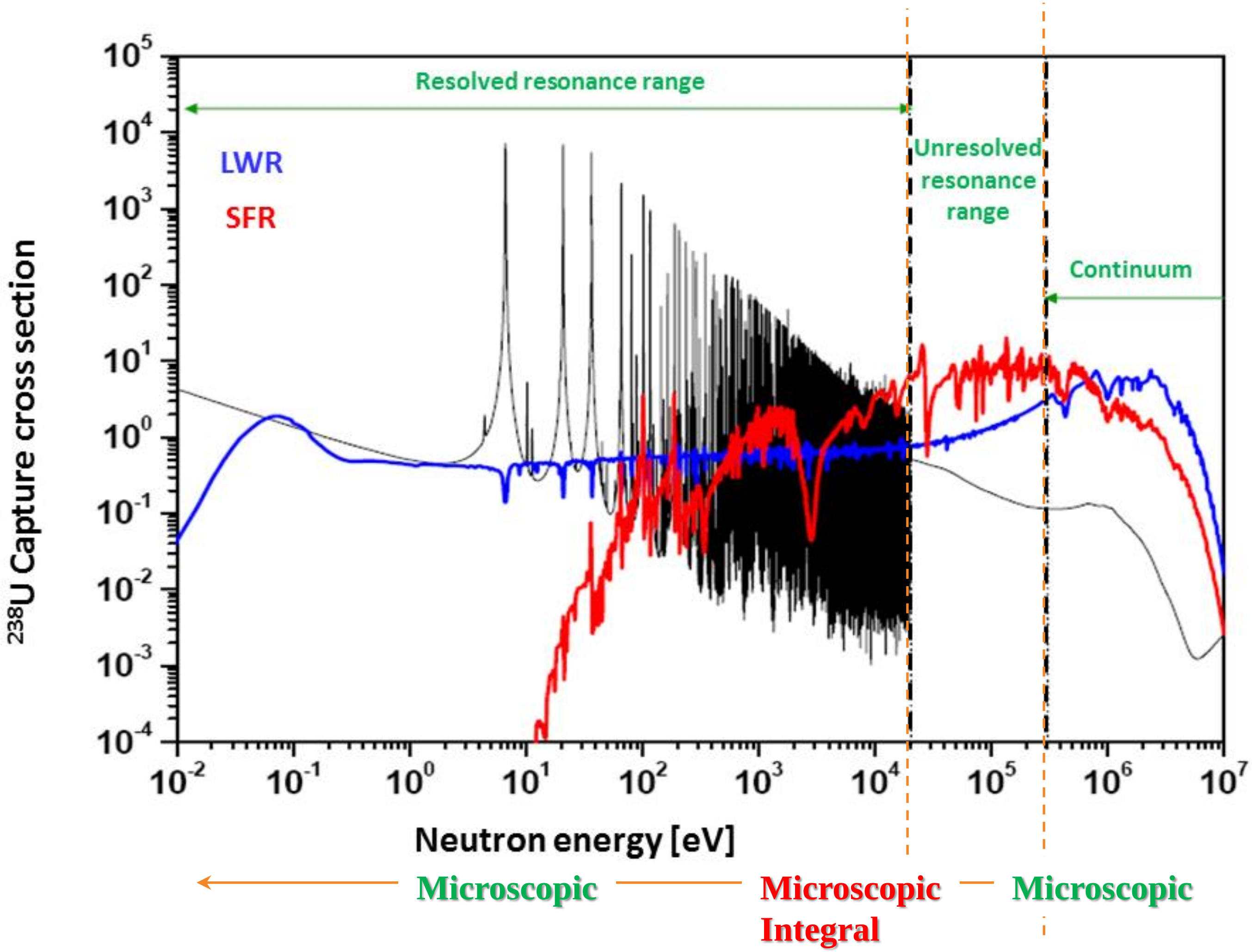
EVALUATION IN THE RESONANCE RANGE AND HIGHER



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Nuclear reaction models

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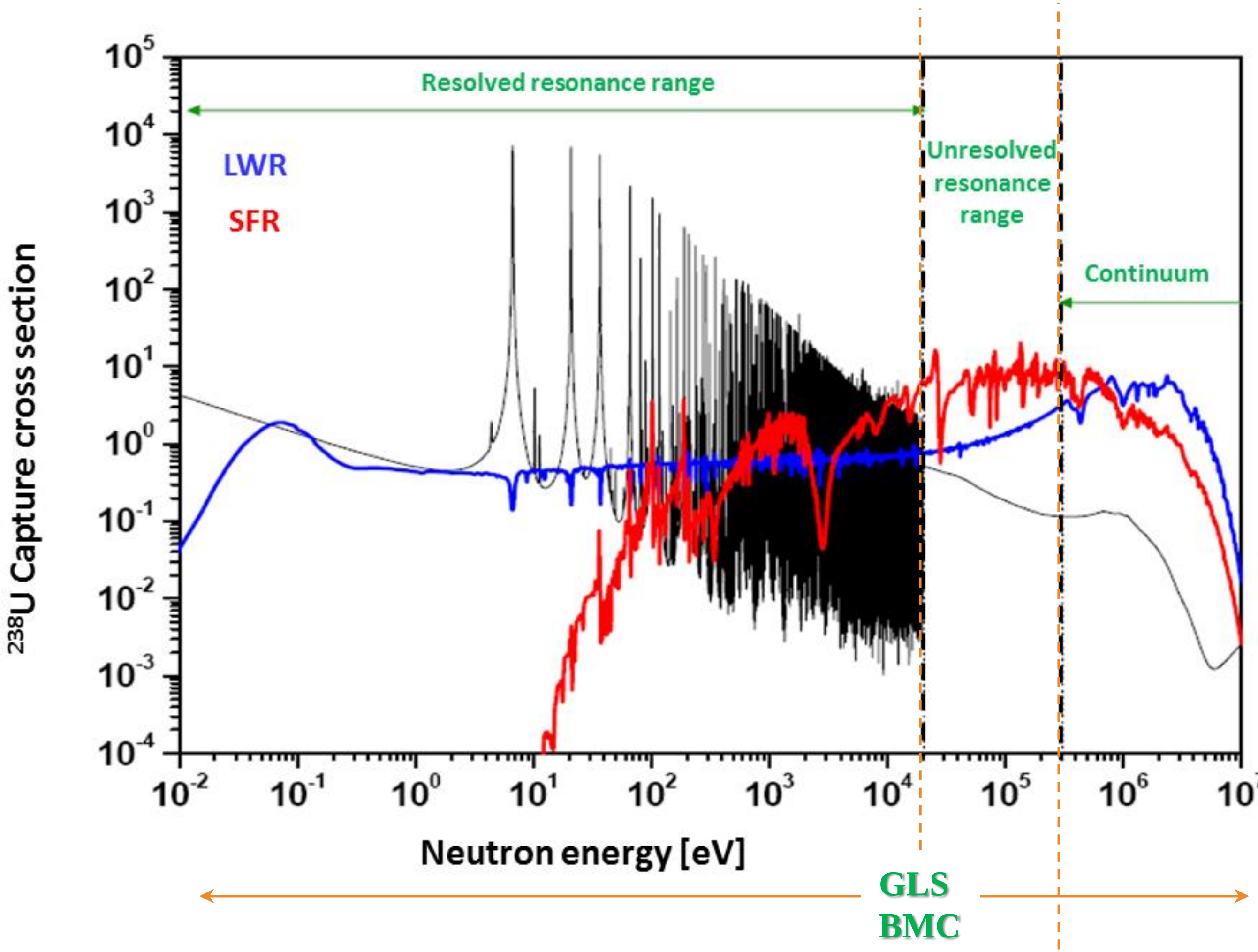

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Nuclear reaction models
Experiments (microscopic/integral)
Bayesian inference technique
Evaluation of uncertainties (variances and correlations)

Bayesian inference (probability density):

Model

$$p(\vec{x}\,|\,M,\vec{y},U) = \frac{p(\vec{x}\,|\,M,U)\cdot p(\vec{y}\,|\,M,\vec{x},U)}{\int d\vec{x}\cdot p(\vec{x}\,|\,M,U)\cdot p(\vec{y}\,|\,M,\vec{x},U)}$$

Model parameters

New measurements

a priori information

Formulation:

$$posterior[p(\vec{x}|\vec{y},U)] \propto prior[p(\vec{x}|U)] \cdot likelihood[p(\vec{y}|\vec{x},U)]$$

Estimation of the first two moments of the *a posteriori* distribution

EVALUATIONS AND UNCERTAINTIES
GENERAL MATHEMATICAL FRAMEWORK

Bayesian inference (probability density):

Maximum Entropy Principle

Laplace approximation
(Sammy,Refit,Conrad, SOK…)

Monte-Carlo
(BMC, Forward-Backward…)

Estimation of a cost function
(Generalized Chi-square)

$$\chi^2_{GSL} = \left(\vec{x}-\vec{x}_m\right)^T M_x^{-1}\left(\vec{x}-\vec{x}_m\right) + \left(\vec{y}-\vec{t}(\vec{x})\right)^T M_y^{-1}\left(\vec{y}-\vec{t}(\vec{x})\right)$$

- Estimate 1st two moments of $p(\vec{x}|M,\vec{y},U)$
- with Monte-Carlo
- Sample of $p(\vec{x}\,|\,M,U)$ → $\vec{x}_k$
- For each $\vec{x}_k$ → associate a weight
- For ex. →Likelihood $\mathcal{L}_k[p(\vec{y}|M,\vec{x}_k,U)]$

COVARIANCES EVALUATION STRATEGY

Basic Nuclear Physics (1)
- ❑ Microscopic Experiments
- ❑ Nuclear Reaction Models

Integral Experiments (2)
- ❑ Mini-Inca (ILL),
- ❑ MINERVE, ICSBEP,
- ❑ PROFIL

Basic Nuclear Data and Covariances
Cross Sections / Spectra / Multiplicities/…

Mock-up Experiments (3)
- ❑ MASURCA
- ❑ EOLE

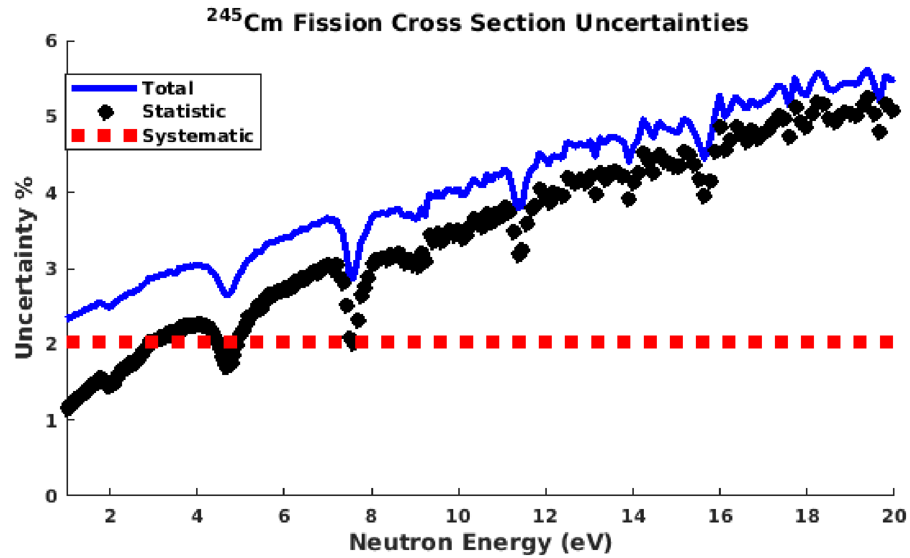
Reactor Experiments
- ❑ PWR Power Plants
- ❑ SPX,PX,…

Experimental Validation
Transposition to Reactors

MICROSCOPIC EXPERIMENT SYSTEMATIC UNCERTAINTIES

Counting rates: statistical uncertainties

The more you count, the lower is the uncertainty
Uncorrelated bins



Normalization, efficiency, ….

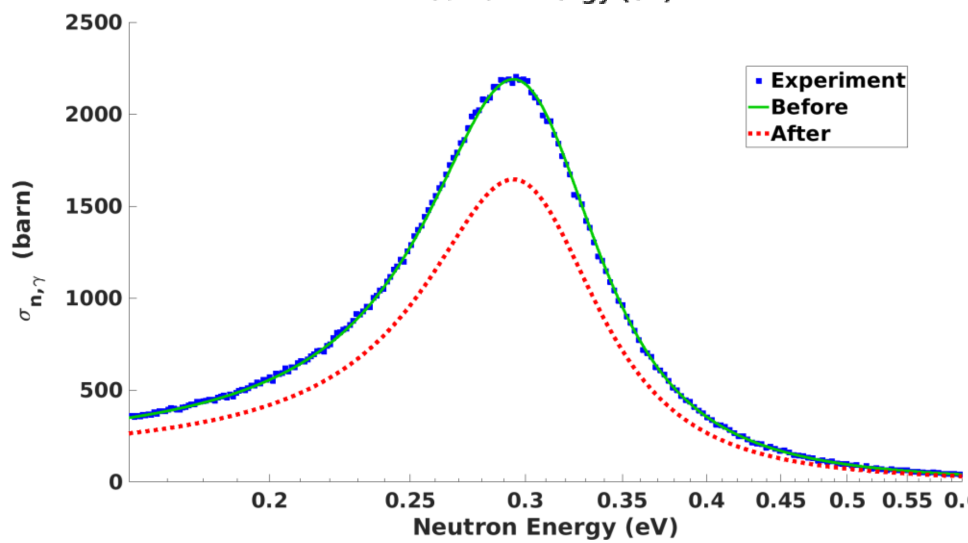
Asymptotic uncertainties → Constants
Long range correlations

Bayesian Inference issues : ex ^{239}Pu

- Analysis of capture (Gwin 73) ; Syst. Unc.~ **3%**
- « Classical» (GLS/BMC) for fission and radiative widths

- Obviously bad result (see Fig.)
- Due to the likelyhood pdf **and** experimental covariance

$$\chi^2_{GSL} = \left(\vec{x} - \vec{x}_m\right)^T M_x^{-1}\left(\vec{x} - \vec{x}_m\right)$$
$$+\left(\vec{y} - \vec{t}(\vec{x})\right)^T M_y^{-1}\left(\vec{y} - \vec{t}(\vec{x})\right)$$



Solution: Marginalisation of pdf's

Marginalization philosophy

$$t(\sigma(\vec{x}),\vec{\theta}) \Leftrightarrow \vec{y}$$

Model parameters

« **nuisance**» parameters

Nuisance parameters are **necessary** during comparisons with experiments (data reduction, normalization,…), but not for the final evaluation

$$t(\sigma(\vec{x}),\vec{\theta}) \Rightarrow \sigma = f(\vec{x})$$ + **Covariances**

Marginalization of the probability density:

$$p(\vec{x},\vec{\theta}\,|\,M,\vec{y},U) \Rightarrow p_{\vec{\theta}}(\vec{x}\,|\,M,\vec{y},U) = \int d\vec{\theta}\cdot p(\vec{x},\vec{\theta}\,|\,M,\vec{y},U)$$

Marginalization :

estimation of at least the first two moments of the marginal probability density

SYSTEMATIC EXPERIMENTAL UNCERTAINTIES MARGINALIZATION

- Analytical method* : Full covariance kept:

$$G_x M_x^{Marg} {G_x}^T = GMG^T \quad \text{with} \quad G = \begin{pmatrix} G_x \\ G_\theta \end{pmatrix} \text{ and } M = \begin{pmatrix} M_x & M_{x,\theta} \\ M_{\theta,x} & M_\theta \end{pmatrix}$$

- Hybrid Monte-Carlo/GLS**:

1. Sampling of nuisances parameters following its pdf : $\vec{\theta}_k$
2. For each realization k, do a GLS → $\vec{x}_k + M_k$
3. Use total variance – covariance theorem on the K-Statistic

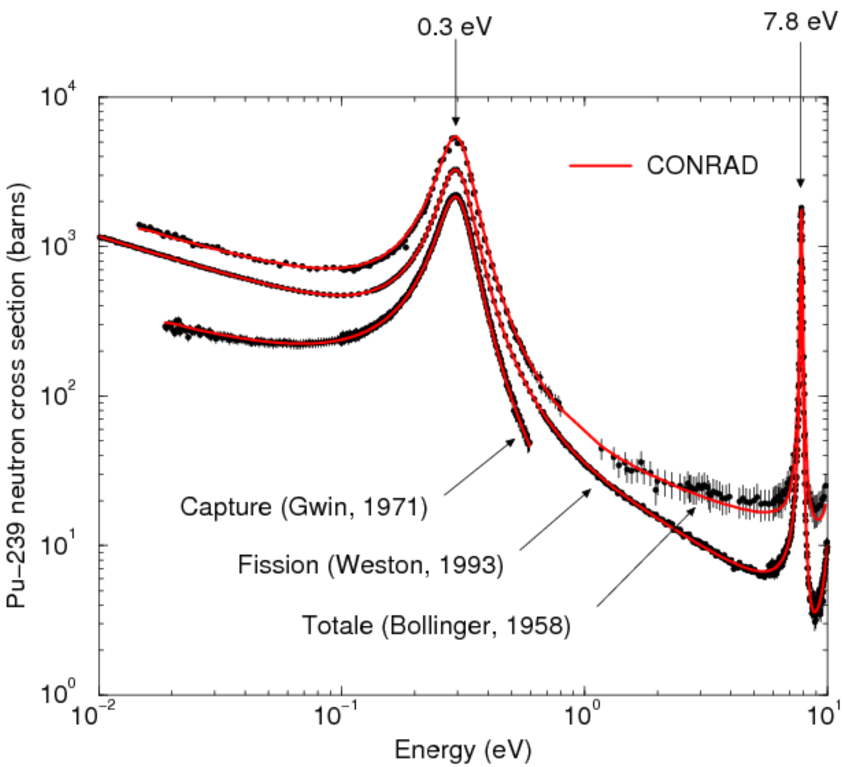
- Full Monte-Carlo*** : double Monte Carlo integration (BMC)

$$p_\theta\left(\vec{x}|\vec{y},U\right) = p\left(\vec{x}|U\right) \int \frac{p\left(\vec{\theta}|U\right) \cdot p\left(\vec{y}|\vec{\theta},\vec{x},U\right)}{\int p\left(\vec{x}|U\right) \cdot p\left(\vec{y}|\vec{\theta},\vec{x},U\right) dx} d\vec{\theta}$$

* B. Habert et al., Nuc. Sci. Eng., **166**, 276 (**2010**) + PhD Thesis
** C. De Saint Jean et al., Nuc. Sci. Eng., **161**, 363 (**2009**).
*** E. Privas PhD thesis + C. De Saint Jean et al., EPJ Web (ND2016)

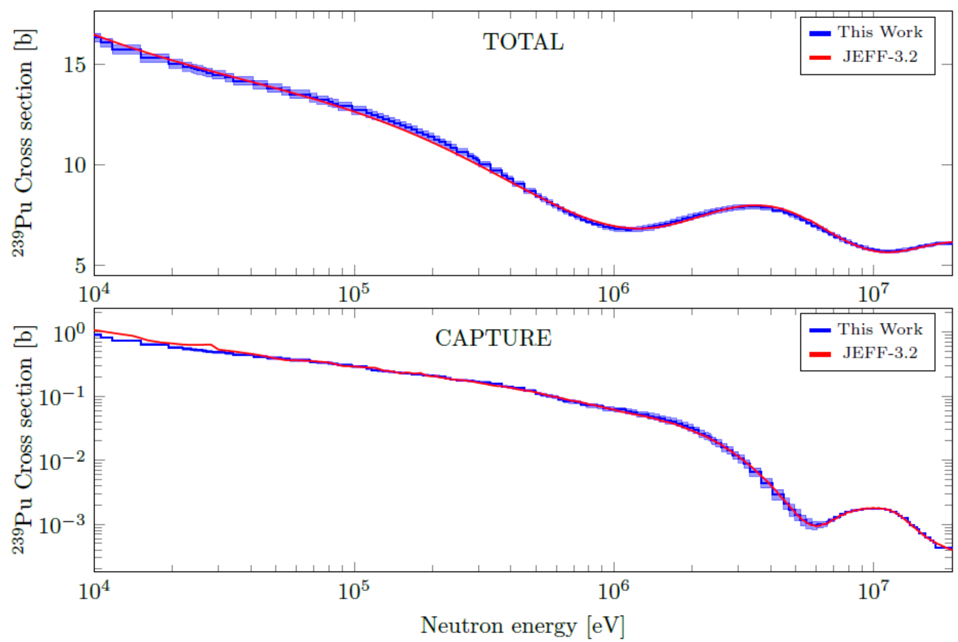
Example : Pu239

Resolved Resonance Range



- Analysis of main EXFOR experiments (E<2500 eV) with R-Matrix code CONRAD.
- Marginalization of Exp. systematic uncertainties (normalization, background, …)

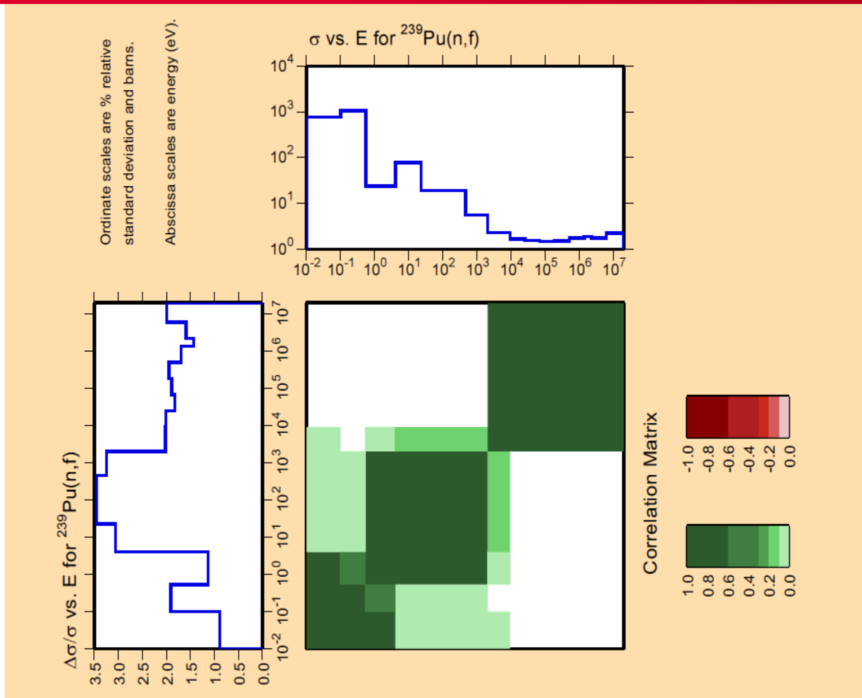
Unresolved Resonance Range and Continuum

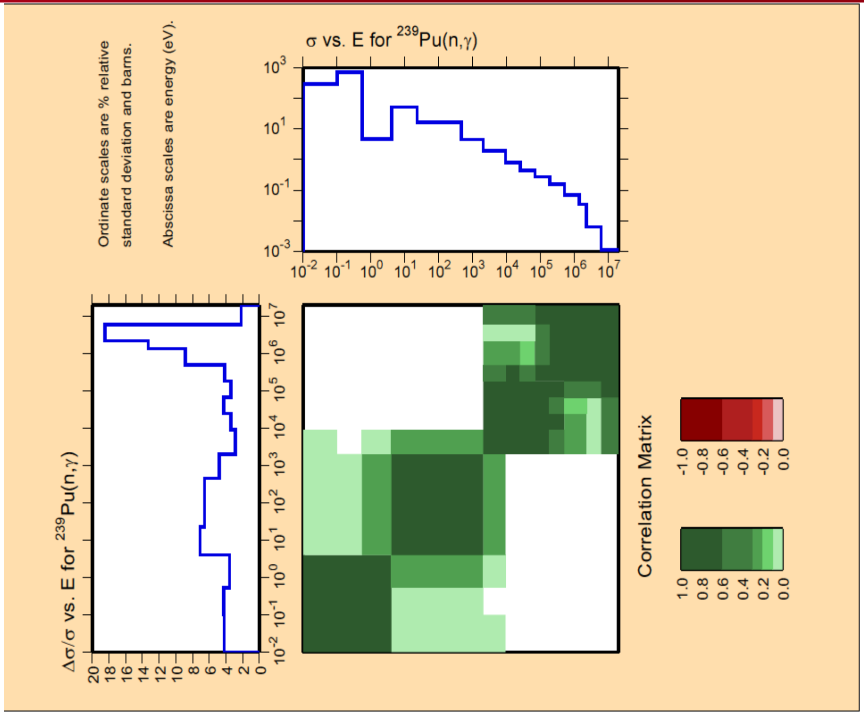


- Fit of JEFF3.2 with CONRAD → in house models
- Marginalization of Exp. systematic uncertainties (normalization, background, …)

* G. Noguere, P. Archier et C. De Saint Jean : JEFFDOCs (04/15 ; 11/15 ; 04/16)

Example : Pu239





- **High impact of Exp. Systematic Uncertainties**
  - Long range correlations (~0.8-1)
  - High uncertainties ~0.5-10 % (Thermal Capture; Fission in Fast range)
  - ~1000 pcm on MISTRAL2 (EOLE Reactor) and ASTRID (FR prototype)
- **Energy domain treated separatly**
  - Beware of potential impact for Fast Reactor (URR)

Additional Experimental information needed

* G. Noguere, P. Archier et C. De Saint Jean : JEFFDOCs (04/15 ; 11/15 ; 04/16)

Systematic Uncertainties for Integral Experiments

- Systematics Uncertainties ** (see WPEC/SG33-SG39):
  - Fuel composition uncertainties
  - Detector efficiencies and calibrations
  - …

- One experiment analyzed

It will increase the initial uncertainty

- Several experiments

It will increase the initial uncertainty

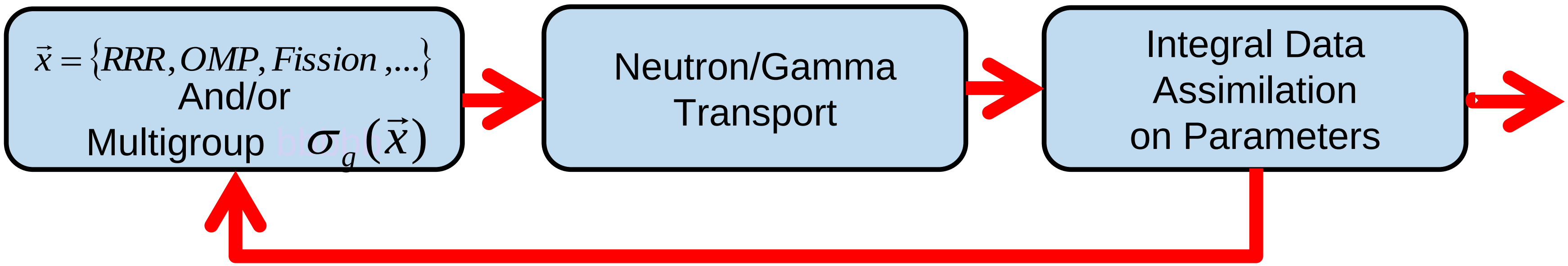
It will give a correlation coefficient between the experiments

What are the effect on Integral Data Assimilation or Nuclear Data Validation ?

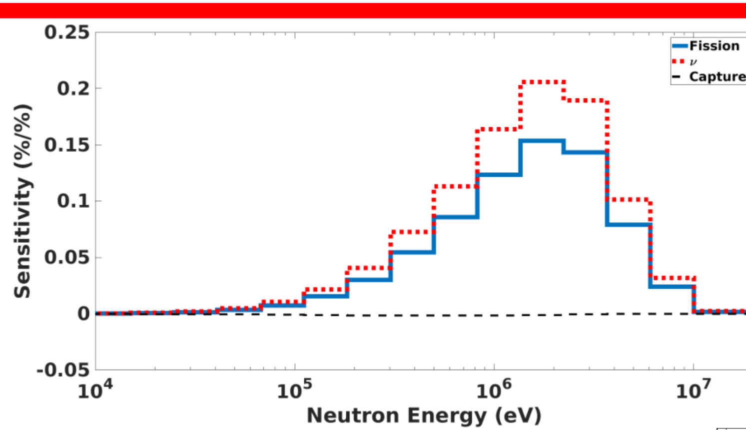
Integral Data Assimilation and Fast energy range : ^{239}Pu

Data assimilation of JEZEBEL*

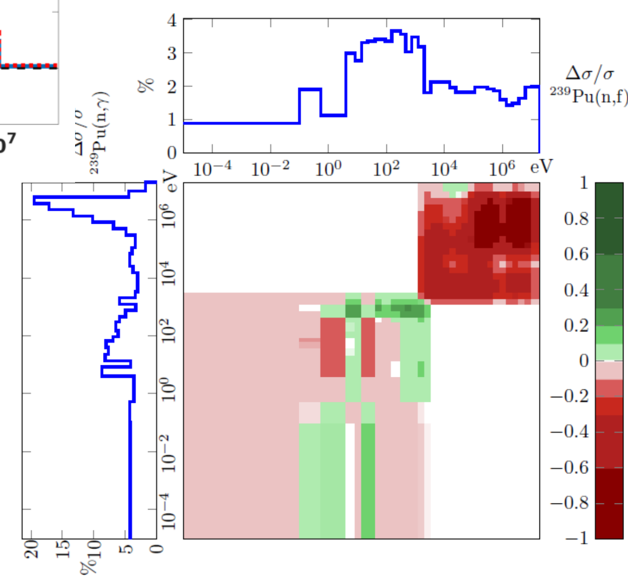
Limited nuclear data adjustement (σ) but with two schemes



JEZEBEL is an indirect measurement of $\chi + \nu\sigma_f$
Here : Focus on XS
δE~200-250 pcm !!!



Need of a coherent (Microscopic) prior (previous analysis)

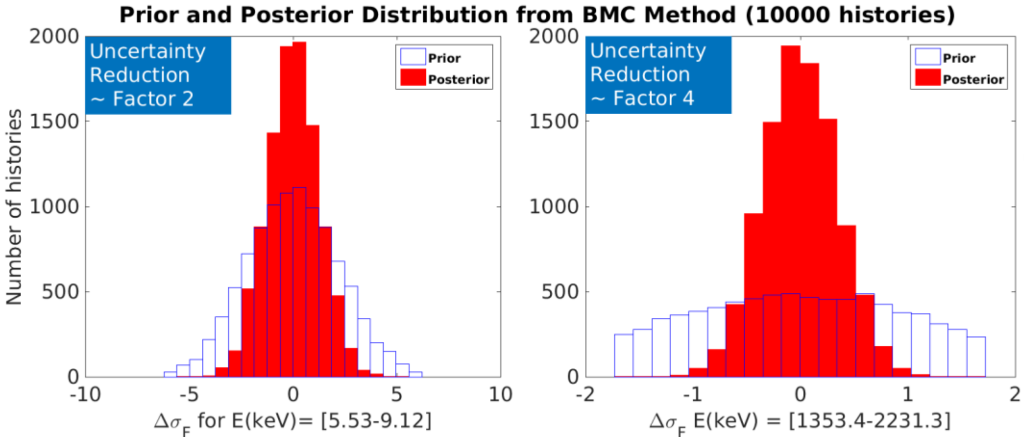


* C. De Saint Jean et al, Nuclear Data Sheet **123** (2015), 178-184

Integral Data Assimilation and Fast energy range : ^{239}Pu

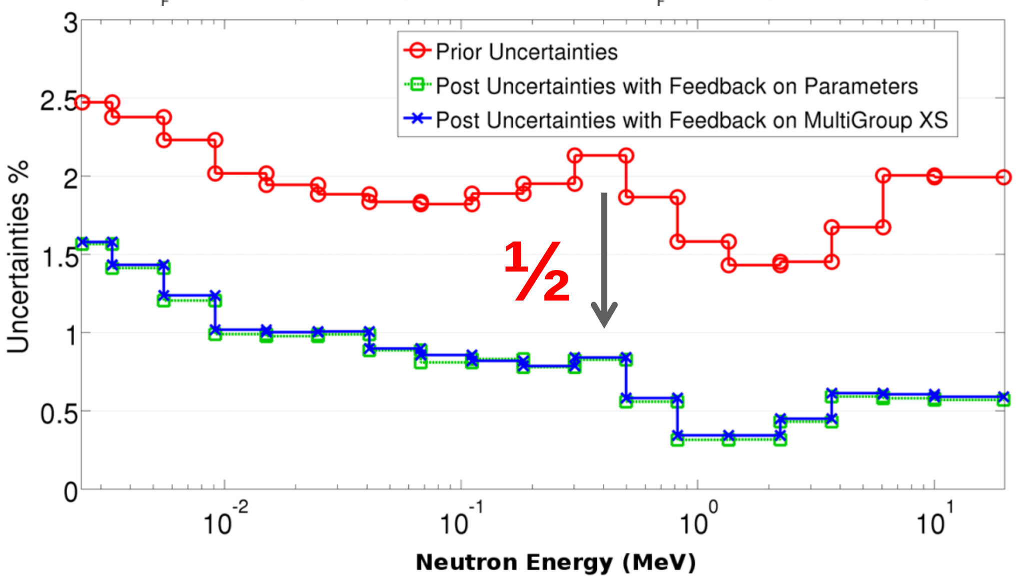
Data assimilation of JEZEBEL*

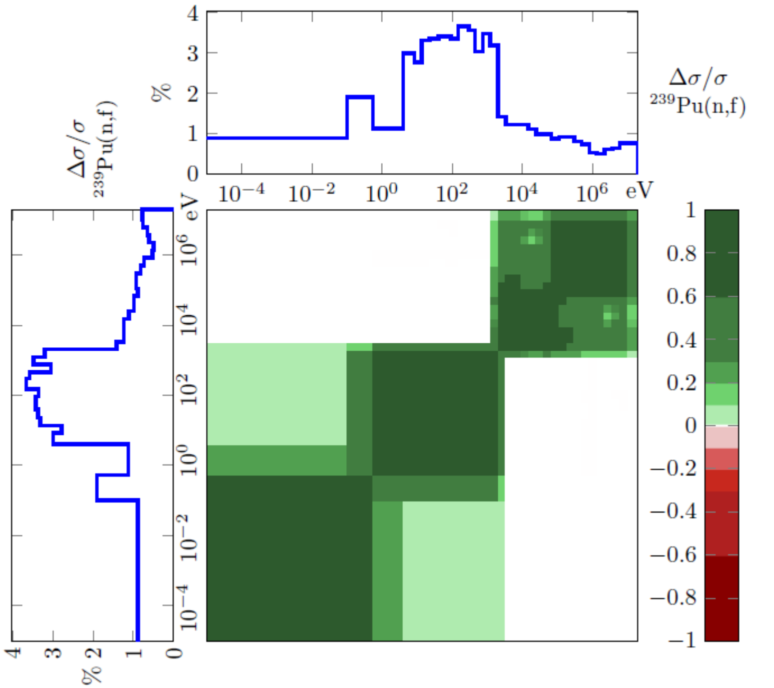
Limited nuclear data adjustement (σ) but with two schemes



Bayesian Monte-Carlo ~ GLS
Results: coherent for both methods

With a coherent (Microscopic) prior
Results: coherent for both schemes



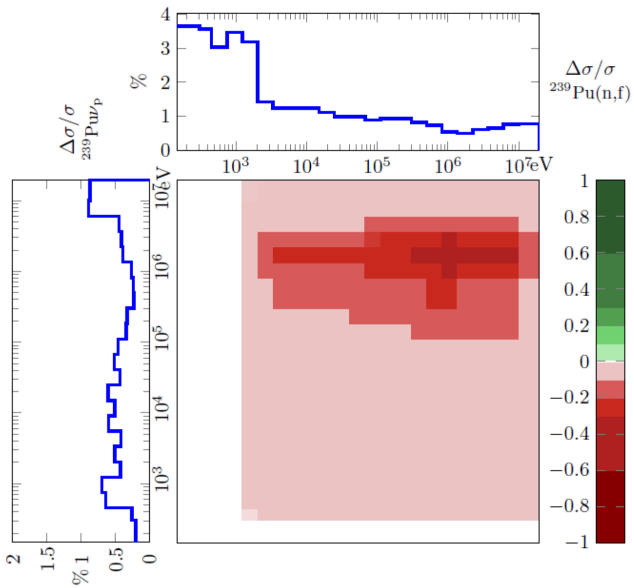


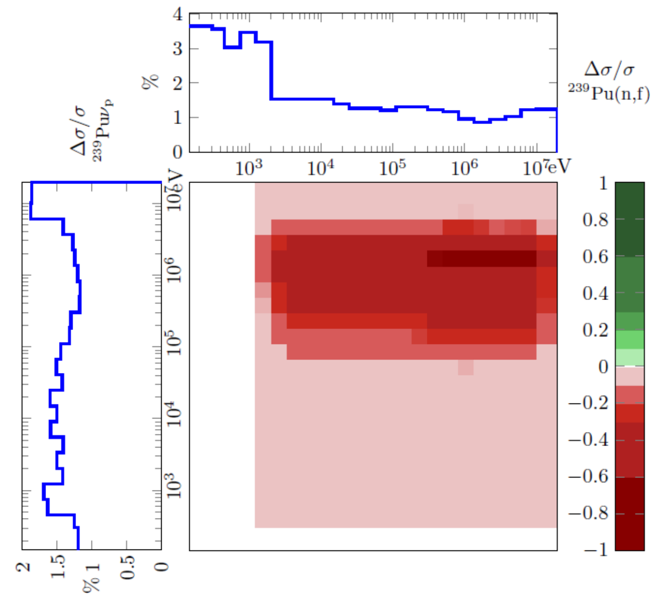
* C. De Saint Jean et al, EPJ Web, ND2016 (2017)

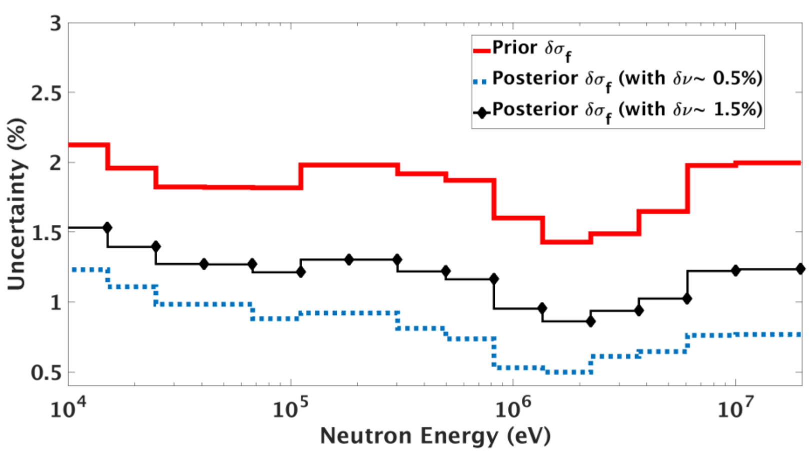
Integral Data Assimilation and Fast energy range : ^{239}Pu

Data assimilation of JEZEBEL

Full nuclear data adjustement (σ, χ, ν)*







Results are very sensitive to priors
Even for this “clean” case, cross correlations are introduced between **(σ, χ, ν)**
→ENDF issue ; GND ?
Uncertainty reduction ~ δE
250 pcm is low : Unrealistic ? Syst. Unc.?

* C. De Saint Jean et al, Nuclear Data Sheet **123** (2015), 178-184

Systematic Uncertainties for Integral Experiments
Example of Pu-Sol-Therm serie

First Integral Experiment : PU-SOL-THERM-001-1

WATER-REFLECTED 11.5-INCH DIAMETER SPHERES OF PLUTONIUM NITRATE SOLUTIONS

Fissile concentration (g/L) 73
(H1)/(Pu240,Pu242,Pu241,Pu239,Pu238) 370.1757
(H1)/(Pu241,Pu239) 352.9084
Vecteur isotopique :

238Pu	239Pu	240Pu	241Pu	242Pu
0.01%	95.01%	4.67%	0.31%	0.01%

Keff = 1.0000 ± 0.0050 E/C-1 (T4) = - 133 pcm

Second Integral Experiment : PU-SOL-THERM-002-1

WATER-REFLECTED 12-INCH DIAMETER SPHERES OF PLUTONIUM NITRATE SOLUTIONS

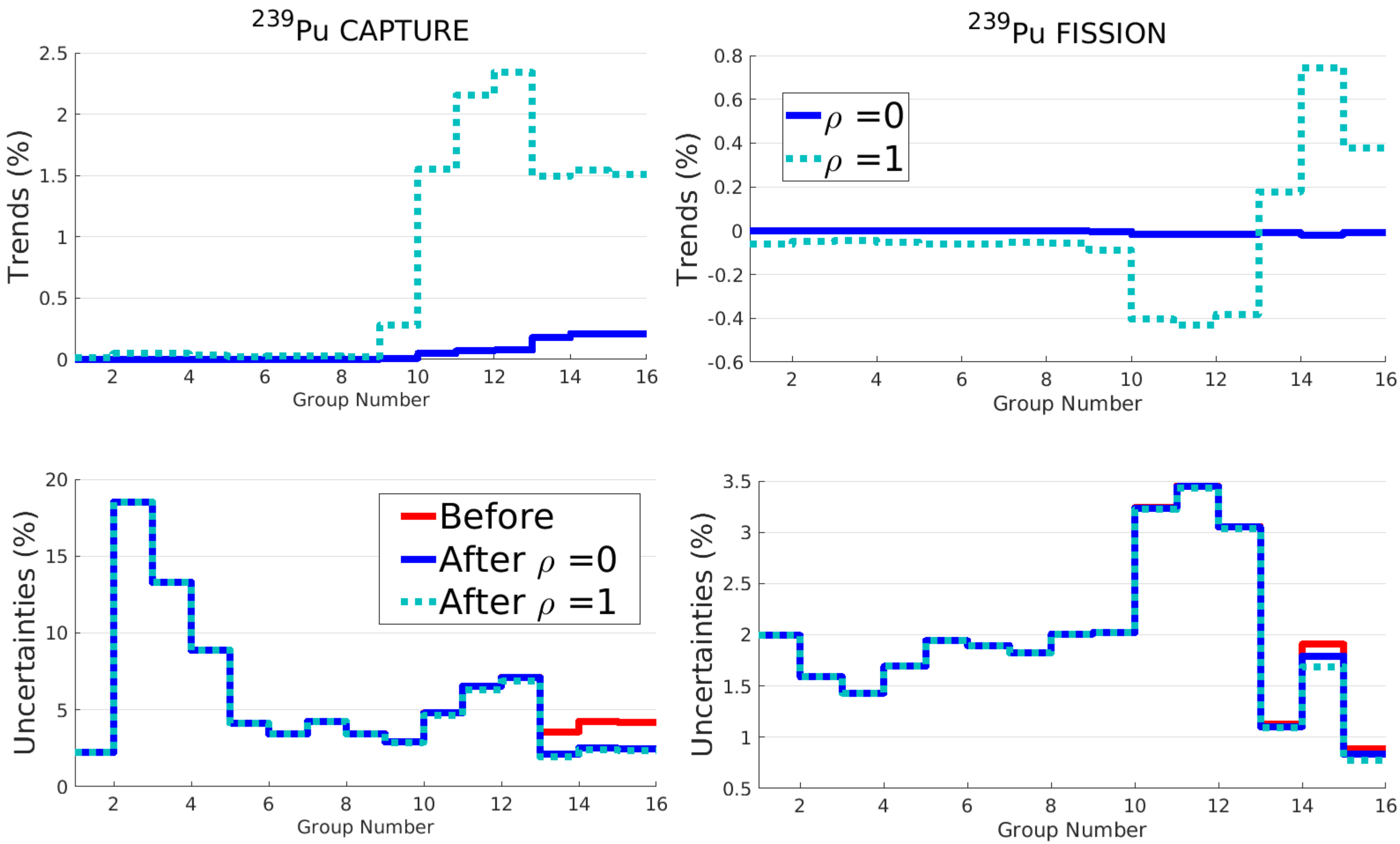
Fissile concentration (g/L) 49.84
(H1)/(Pu240,Pu239) 524.2683
(H1)/(Pu239) 507.9775
Vecteurs isotopiques :

239Pu	240Pu
96.88%	3.12%

Keff = 1.0000 ± 0.0047 E/C-1 (T4) = - 12 pcm

Integral Data Assimilation of Both PST on Pu Nuclear Data
With a correlation coefficient : ρ = 0 or 1

Systematic Uncertainties for Integral Experiments
Example of Pu-Sol-Therm serie



Identical uncertainty reduction on ^{239}Pu capture cross section
Very different trends between ρ = 0 or 1

Systematic Uncertainties for Integral Experiments
A positive use possible !

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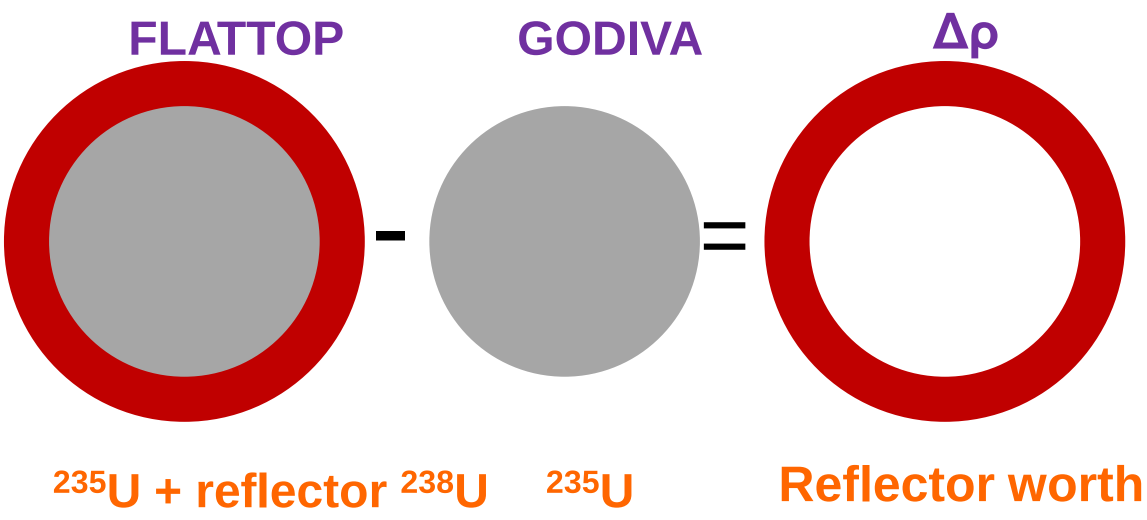
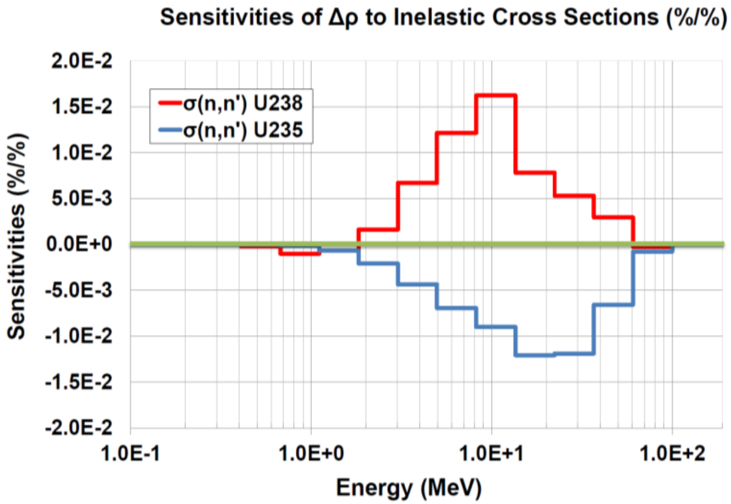




@E. Privas et al.

Contains fuel with equivalent caracteristics

- New interpretation of standard Integral Experiments*

Contains fuel with common Syst. Uncertainties

- Conceive integral experiments with Syst. Uncertainty
→can permit to reach different Nuclear Data

*D. Bernard et al., Nuclear Data Sheet 118 (2014), 118-121

Systematic Uncertainties for Integral Experiments Validation ; Figure of merit ;

Reduced χ^2

@ O. Cabellos, jefdoc-1843

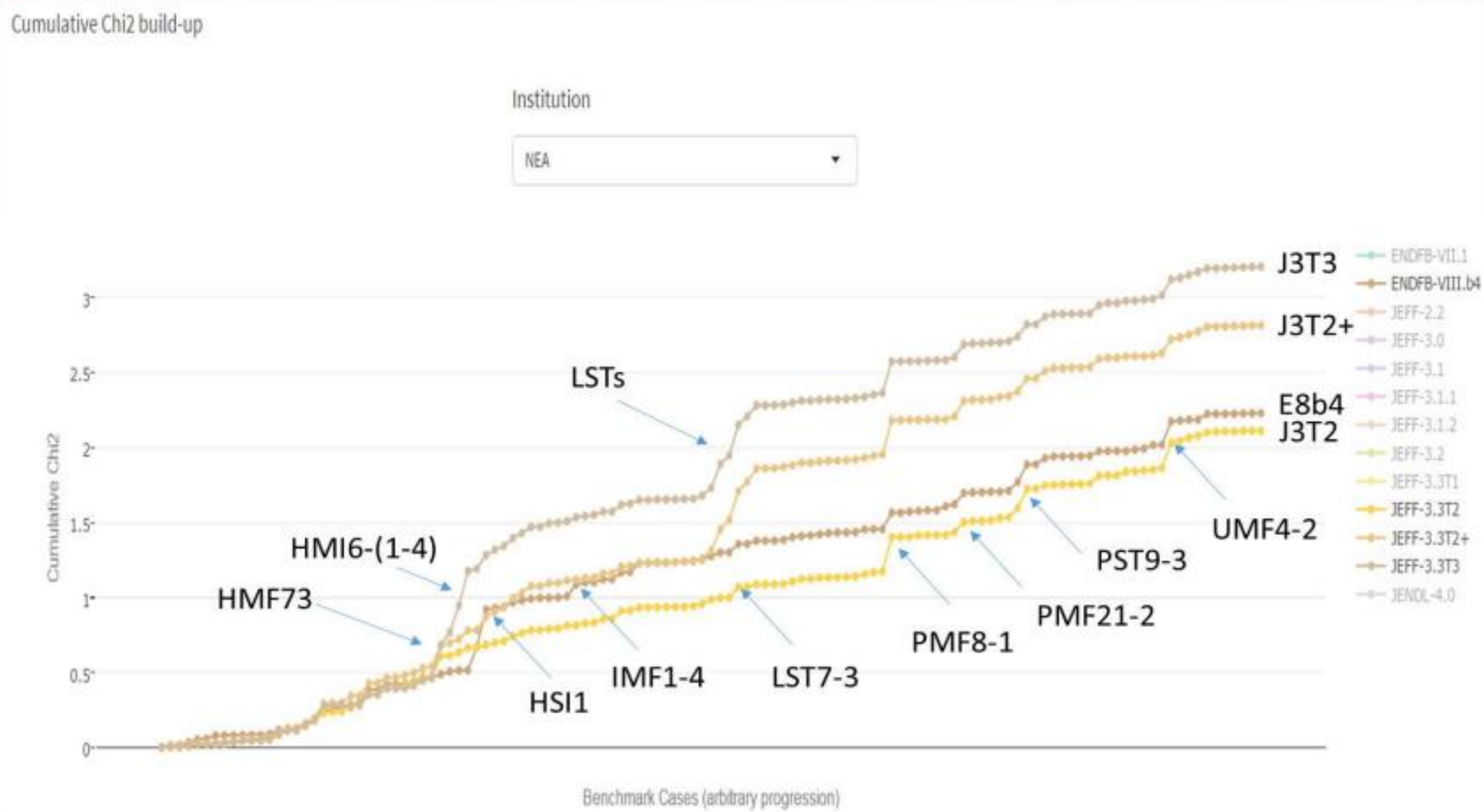
	NEA						JEFF-3.3T3
	ENDF/B-VII.1	ENDF/B-VIIIb4	JEFF-3.1.1	JEFF-3.2	JEFF-3.3.T2	JEFF-3.3T2+	
PU	4.2 (29)	2.2 (29)	2.9 (29)	3.6 (29)	2.8 (29)	2.4 (29)	2.4 (29)
HEU	6.1 (42)	4.1 (42)	5.3 (42)	11.8 (42)	2.2 (42)	3.5 (42)	3.9 (42)
IEU	5.0 (12)	1.9 (12)	11.3 (12)	4.9 (12)	2.7 (12)	2.1 (12)	2.2 (12)
LEU	0.9 (13)	1.4 (13)	1.4 (13)	0.9 (13)	1.8 (13)	3.7 (13)	4.0 (13)
U233	1.7 (18)	2.1 (18)	9.5 (18)	1.2 (18)	1.7 (18)	1.9 (18)	1.7 (18)
MIX	0.7 (8)	1.0 (8)	1.2 (8)	0.9 (8)	0.9 (8)	1.0 (8)	0.8 (8)
SPEC (C/E)	0.99249 (1)	0.99338 (1)	0.98719 (1)	0.98847 (1)	0.99142 (1)	0.99145 (1)	0.99118 (1)
Total	3.7 (123)	2.22 (123)	6.5 (123)	5.6 (123)	2.02 (123)	2.9 (123)	3.1 (123)

Reduced value will be impacted by correlations
Conclusions on the quality of the Library could be changed

Systematic Uncertainties for Integral Experiments Validation ; Figure of merit ;

Cumulative χ^2

@ O. Cabellos, jefdoc-1843



Very usefull to identify outliers

What happens when correlations exists ?

Conclusions

- Evaluation of systematic uncertainties is of prime interest for Nuclear Data evaluators
- Microscopic Experiments:
  - Still high Syst. Uncertainties on Fission (Continuum), Capture of Fissile isotopes
  - Mainly related to normalization, background, detectors efficiency, …
  - Create Evaluated Nuclear Data with long range (and high) correlations
- Integral Experiments:
  - A proper look on Syst. Uncert. for Integral Experiments is paramount

  →Go back to pre-ICSBEP (Experimental reports ?)

  → If no information →be careful in the choice (ρ = 0 or 1)

  - Syst. Uncert. will change adjustments results (trends or uncertainty reduction) →SG46
  - Could be positive !!

  →Look at integral experiments such as godiva/flattop

  → Innovative Integral Experiments to be studied