Evaluation of Cross-Sections Uncertainties using Physical Constraints

$^{238}U$, $^{239}Pu$ and others…

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### CROSS SECTIONS “KNOWLEDGE”

<table>
<thead>
<tr>
<th>Experimentalist</th>
<th>Theoretician</th>
</tr>
</thead>
<tbody>
<tr>
<td>Knowledge of cross section</td>
<td>Knowledge of cross section</td>
</tr>
<tr>
<td>finest microscopic experiments and smartest integral experiments</td>
<td>knowledge of models parameters and/or nuclear reaction models (resonance parameters, optical models, fission barrier, average width, ...)</td>
</tr>
<tr>
<td>Calibration; Syst. Uncertainties ...</td>
<td>Systematics</td>
</tr>
</tbody>
</table>

Evaluation work is done “sometimes” independently between:
- Resolved resonance range / unresolved resonance range / continuum
- International Experts (that is what CIELO is all about right ??)

As a result, one may ended with several inconsistencies:
- mismatches and larger uncertainties at the boundaries for punctual cross section
- no cross correlation between high energy domain and resonance range.
- Good overall integral behavior with deviations among Evaluations (B. Morillon et al. JEFDO and P. Romain talk) →compensating effects

**Uncertainties must reflect the lack of knowledge, inconsistencies as well as advances**

**Add physical constraints to find the most physical values**
CONSTRANTS

- Physics:
  - Cross section is an observable
  - Isotopic lines (see CEA/DAM Romain talk)
  - General laws: “continuity” of cross sections, parameters

- Experiments
  - Vector of constraints: shapes and uncertainties
  - Different type of experiments
    - Transmission, Capture yields, Fission, Inelastic
    - Integral experiments but in a validation framework
  - Systematic uncertainties
  - Large domain experiments (decades) → several models
  - Integral experiment used during evaluation (Integral Data Assimilation)

- Nuclear Reaction Models
  - Vector of Uncertainties: parameters
  - Different models / different energy domain
  - Unconstrained models
  - Microscopic ingredients
  - Multi-model parameters
  - Model Defects

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CONSTRUCTS

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Nuclear Reaction Models
- Vector of Uncertainties: parameters
- Different models / different energy domain
- Unconstrained models
- Microscopic ingredients
- Multi-model parameters
- Model Defects
CIELO INITIATIVE
BIG THREE: WHAT SHOULD/COULD BE SHARED?

Ideal world

- Utopic view → Everything should be shared for Nuclear Physics advances

Real world

- Resolved and unresolved resonance range:
  - Various past SG ($^{238}$U, $^{239}$Pu, etc, …):
    - sharing among participant of resonance parameters, microscopic measurements, some integral experiments (“public”) + experimental knowledge
    - Test of advances on additional integral experiments (“proprietary”)
  - Covariances evaluation on the shared information could be performed and compared

- Continuum:
  - What about nuclear models?
    - Do we share Physics? Or Parameters (both?)
  - Microscopic and “public” integral experiments + experimental knowledge
  - “Confidential experiments”

For Uncertainty evaluation the shared part is crucial
CIELO should allow a step forward
CEA/CADARACHE STRATEGY FOR JEFF IN CIELO RELATED TO THE BIG THREE

Best Knowledge coming from
- Microscopic Measurements
- Nuclear Reaction Models

“Public” Integral Experiments
- Mini-Inca (ILL)
- ICSBEP
- ...

Breakthrough
- Covariances [0eV;20MeV]
- Evaluation methodologies
- Understanding of discrepancies
- Covariance methodologies
- Reduction of Uncertainties

Additional Integral Experiments
- Minerve
- PROFIL
- ...

SG39

CIELO-SG40
Covariances Matrices evaluation on $^{238}\text{U}$ and $^{239}\text{Pu}$

Determination of Matrices
Bayesian inference (probability density):

\[
p(\tilde{x} | \bar{y}, U) = \frac{p(\tilde{x} | U) \cdot p(\bar{y} | \tilde{x}, U)}{\int d\tilde{x} \cdot p(\tilde{x} | U) \cdot p(\bar{y} | \tilde{x}, U)}
\]

**Formulation:**

\[
\text{posterior}[p(\tilde{x} | \bar{y}, U)] \propto \text{prior}[p(\tilde{x} | U)] \cdot \text{likelihood}[p(\bar{y} | \tilde{x}, U)]
\]

Estimation of the first two moments of the \textit{a posteriori} distribution
Marginalization philosophy

\[ \sigma = f(\vec{x}, \vec{\theta}) \]

Model parameters « nuisance » parameters

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

\[ \sigma = f(\vec{x}, \vec{\theta}) \quad \Rightarrow \quad \sigma = f(\vec{x}) + \text{Covariances} \]

Marginalization of the probability density:

\[ p(\vec{x}, \vec{\theta}|\vec{y}, U) \quad \Rightarrow \quad p_{\vec{\theta}}(\vec{x}|\vec{y}, U) = \int d\vec{\theta} \cdot p(\vec{x}, \vec{\theta}|\vec{y}, U) \]

Marginalization: estimation of the first two moments of the marginal probability density
Transmission Measurement

Comparison

\[ T_{th} = i(\bar{\sigma}(\bar{x}), \bar{\theta}) \]

\[ \approx \exp^{-n_\theta \sigma_i(\bar{x})} + B_{\theta} \]

\[ T_{exp} = N \frac{C_{in} - B_{in}}{C_{out} - B_{out}} \]

Data Assimilation

\( \bar{x} = \{\gamma_{a\lambda}, \theta_{\lambda}, a_c, R\} \)

\( \bar{x} = \{\Gamma_a, a_c, R^\infty, D_0, S_a\} \)

\( \bar{x} = \{\beta_2, a_c, d_c, V, W, \ldots\} \)

\( \bar{x} = \{\gamma_{a\lambda}, \theta_{\lambda}, a_c, R\} \)

\( \bar{x} = \{\Gamma_a, a_c, R^\infty, D_0, S_a\} \)

\( \bar{x} = \{\beta_2, a_c, d_c, V, W, \ldots\} \)
Resolved Resonance Range (SG34 and Jeff3.2)
- The RRR was divided in three energy ranges to account for the thermal cross section, the 1\textsuperscript{st} resonance around 0.3 eV and the resonance integral (E>0.5 eV)
- Final uncertainties dominated by normalization accuracy introduced in the Marginalization procedure (0.5-3\% for the fission cross section and 4-9\% for the capture cross section)
- A neutron width selection based on the truncated Porter-Thomas integral distribution was performed to produce a “manageable” large covariance matrix
Continuum Covariances (COMAC-V0.1)

- Construction of an a-priori based on JEFF-3.2 cross sections
- Systematic uncertainties on fission and capture XS, based on “International Evaluation of Neutron Cross Section Standards” by Carlson et al. (CRP Report)

- Improvements / On going work:
  - Use microscopic experiments
  - Add “public” integral nuclear data oriented experiment
  - Add CEA integral nuclear data oriented experiment
Resolved Resonance Range (Jeff3.2 and COMAC-V0.1)

- Proposed to Jeff3.2 (resonance parameters and cross sections)
- Based on Microscopic measurements + Systematic uncertainties taken into account
- Bayesian Framework + Marginalization for systematic exp. Uncertainties

- Improvements / On going work:
  - Add additional microscopic experiments (Ex : Macklin 88 Capture data)
  - Add “public” integral nuclear data oriented experiment
  - Add CEA integral nuclear data oriented experiment
Continuum Covariances (COMAC-V0.1)

- Construction of an a-priori based on Jeff3.1.1
- “Simulated“ systematic uncertainties taken into account

Uncertainty Propagation of COMAC-V0 matrices on a SFR

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Fission</th>
<th>Capture</th>
<th>Elastic</th>
<th>Inelastic</th>
<th>Nxn</th>
<th>Nu</th>
<th>Total</th>
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<tr>
<td>B-10</td>
<td>—</td>
<td>11</td>
<td>—</td>
<td>—</td>
<td>—</td>
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<td>C-0</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>0</td>
<td>—</td>
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<tr>
<td>O-16</td>
<td>—</td>
<td>34</td>
<td>29</td>
<td>2</td>
<td>—</td>
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<td>—</td>
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<td>Na-23</td>
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<td>8</td>
<td>50</td>
<td>32</td>
<td>—</td>
<td>60</td>
<td>—</td>
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<td>Cr-52</td>
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<td>31</td>
<td>16</td>
<td>—</td>
<td>35</td>
<td>—</td>
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<td>Fe-56</td>
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<td>97</td>
<td>79</td>
<td>45</td>
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<td>Ni-58</td>
<td>—</td>
<td>19</td>
<td>7</td>
<td>24</td>
<td>—</td>
<td>24</td>
<td>—</td>
</tr>
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<td>U-235</td>
<td>4</td>
<td>18</td>
<td>1</td>
<td>1</td>
<td>6</td>
<td>19</td>
<td>—</td>
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<tr>
<td>U-238</td>
<td>367</td>
<td>533</td>
<td>/75</td>
<td>452</td>
<td>/42</td>
<td>784</td>
<td>—</td>
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<tr>
<td>Pu-238</td>
<td>35</td>
<td>67</td>
<td>1</td>
<td>3</td>
<td>59</td>
<td>94</td>
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<td>24</td>
<td>106</td>
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<td>52</td>
<td>65</td>
<td>124</td>
<td>—</td>
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<tr>
<td>Pu-241</td>
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<td>91</td>
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<td>5</td>
<td>1</td>
<td>28</td>
<td>112</td>
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<td>2</td>
<td>7</td>
<td>12</td>
<td>41</td>
<td>—</td>
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<tr>
<td>Am-241</td>
<td>3</td>
<td>27</td>
<td>0</td>
<td>1</td>
<td>3</td>
<td>27</td>
<td>—</td>
</tr>
<tr>
<td>TOTAL</td>
<td>1062</td>
<td>599</td>
<td>72</td>
<td>460</td>
<td>/42</td>
<td>142</td>
<td>1312</td>
</tr>
</tbody>
</table>

Improvements / On going work:
- Add additional microscopic experiments + “Stick” to Jeff3.2 evaluation
- Add “public” integral nuclear data oriented experiment
- Add CEA integral nuclear data oriented experiment
COVARIANCE MATRICES
CHALLENGES FOR CIELO

- RRR/URR/OM Full treatment + Influential Model Parameters
- Define “wrapping” benchmark for Covariance estimation in RRR/Continuum and RRR+Continuum
- Importance of cross-correlations between reactions / energy ranges for reactor applications
- Inelastic XS for $^{238}$U (new microscopic/integral experiment and new evaluation)
- $^{239}$Pu Capture (low and high energy range and capture to fission ratio),
- $^{235}$U Capture (intermediate energy range)
- Angular distributions, PFNS, nu-bar, O, Fe, $S_{\alpha\beta}$
- New microscopic/integral experiments even on well-known isotopes (Normalization and background issues, URR, angular distributions,…)
- More microscopic ingredient (less “free” parameters)
Additional Covariances Matrices evaluation methodologies used/to be used on $^{238}\text{U}$ and $^{239}\text{Pu}$ Determination of Matrices
Nuisance parameters are necessary during comparisons with experiments (data reduction, normalization,...) but not for the final evaluation.

Marginalization philosophy:

\[ \sigma = f(\vec{x}, \theta) \]

Nuisance parameters « model parameters »

Marginalization philosophy:

\[ \sigma = f(\vec{x}, \theta) \]

Marginalization of the probability density:

\[ p(\vec{x}, \theta | \vec{y}, U) \rightarrow p_{\theta}(\vec{x} | \vec{y}, U) = \int d\theta \cdot p(\vec{x}, \theta | \vec{y}, U) \]

Marginalization:

estimation of the first two moments of the marginal probability density
Unified model on an energy domain

\[[E_L, E_R] + Boundary \at \ E_C: \]
\[
\tilde{t} = \tilde{t}_L(x_\mu) \text{ if } E_L \geq E \geq E_c \\
\tilde{t} = \tilde{t}_R(x_\mu) \text{ if } E_R \leq E \leq E_c
\]

“Simulated” experimental Data:
- Based on theoretical points (red)
- 3% statistical uncertainties
- No/0.5/1/3% systematic uncertainties

Didactic example: Sodium inelastic cross sections
- Energy Range studied [1.9 – 2.1 MeV]; Boundary at 2 MeV.
- Below 2 MeV: Resolved resonance range (Jeff3.2Beta)
- Above 2 MeV: Jeff3.2Beta (Optical Potential + Partial models)

Considered parameters:
- Resonance Range
  - Neutron and inelastic Width ($\Gamma_n, \Gamma_n'$)
- Optical Model
  - Reduced Scattering Radius ($r_0$)
  - Diffusiveness ($a_0$)

<table>
<thead>
<tr>
<th>$E$(MeV)</th>
<th>$J^\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.9215</td>
<td>3^-</td>
</tr>
<tr>
<td>1.9625</td>
<td>2^+</td>
</tr>
<tr>
<td>1.9723</td>
<td>1^+</td>
</tr>
</tbody>
</table>
IMPOSING CONSTRAINTS ON SEVERAL MODELS
SYST. EXP.; UNCERTAINTIES; $^{23}$Na EXAMPLE

Statistical Uncertainty 3%
No Systematic Uncertainty
IMPOSING CONSTRAINTS ON SEVERAL MODELS
SYST. EXP.; UNCERTAINTIES; $^{23}$NA EXAMPLE

Statistical Uncertainty 3%
Normalization Uncertainty 0.5%
Statistical Uncertainty 3%
Normalization Uncertainty 1%
IMPOSING CONSTRAINTS ON SEVERAL MODELS
SYST. EXP.; UNCERTAINTIES; ²³NA EXAMPLE

Statistical Uncertainty 3%
Normalization Uncertainty 3%
Correlations obtained on parameters as well (3% normalization case)

<table>
<thead>
<tr>
<th></th>
<th>$\Gamma^3_n$</th>
<th>$\Gamma^3_{n'}$</th>
<th>$\Gamma^2_n$</th>
<th>$\Gamma^2_{n'}$</th>
<th>$\Gamma^1_n$</th>
<th>$\Gamma^1_{n'}$</th>
<th>$R_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma^3_n$</td>
<td>1</td>
<td>0.83</td>
<td>0.74</td>
<td>-0.11</td>
<td>0.41</td>
<td>0.83</td>
<td></td>
</tr>
<tr>
<td>$\Gamma^3_{n'}$</td>
<td>1</td>
<td>-0.37</td>
<td>0.89</td>
<td>0.03</td>
<td>0.56</td>
<td>0.98</td>
<td></td>
</tr>
<tr>
<td>$\Gamma^2_n$</td>
<td>1</td>
<td>-0.36</td>
<td>-0.05</td>
<td>-0.32</td>
<td>-0.38</td>
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<td></td>
</tr>
<tr>
<td>$\Gamma^2_{n'}$</td>
<td>1</td>
<td>-0.09</td>
<td>0.42</td>
<td>0.90</td>
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<tr>
<td>$\Gamma^1_n$</td>
<td>1</td>
<td>-0.37</td>
<td>0.03</td>
<td>0.58</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Gamma^1_{n'}$</td>
<td>1</td>
<td>0.58</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$R_0$</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Parameters driving the cross section "level" end up correlated

Correlation created between two different models: $\Gamma_n$, $\Gamma_{n'}$ and $R_0$
We impose constraints on several models using Lagrange multipliers. The equation for the penalty function is given by:

\[
\chi^2_{GSL} = (\bar{x} - \bar{x}_m)^T M_x^{-1} (\bar{x} - \bar{x}_m) + (\bar{y} - \bar{t}(\bar{x}))^T M_y^{-1} (\bar{y} - \bar{t}(\bar{x}))
\]

We further consider the case of GLS with constraints:

\[
\chi^2_{GLS+C} = (\bar{x} - \bar{x}_m)^T M_x^{-1} (\bar{x} - \bar{x}_m) + (\bar{y} - \bar{t})^T M_y^{-1} (\bar{y} - \bar{t}) + 2C^T(\bar{x}) \cdot \lambda
\]

This leads to the linearization:

\[
\begin{pmatrix}
A(\tilde{x}) & ST_c(\tilde{x}) \\
S_c(\tilde{x}) & 0
\end{pmatrix}
\begin{pmatrix}
x \\
\lambda
\end{pmatrix} =
\begin{pmatrix}
A(\tilde{x})\tilde{x} - St^T(\tilde{x})M_y^{-1}(y(\tilde{x}) - t) \\
S_c(\tilde{x})\tilde{x} - C(\tilde{x})
\end{pmatrix}
\]

with

\[
A(x) = M_x^{-1} + St^T(x)M_y^{-1}St(x)
\]
Unified model on an energy domain

\([E_L, E_R] + \text{Boundary at } E_C: \]
\[ t = t_L(x_\mu) \text{ if } E_L \geq E \geq E_C \]
\[ t = t_R(x_\mu) \text{ if } E_R \leq E \leq E_C \]

Constraint on Cross sections at \( E_C \)

\[ C(x) = \langle \sigma^R_t \rangle_{E_C} - \langle \sigma^L_t \rangle_{E_C} = 0 \]

“Real” experimental Data:
- Based on C.A.Uttley et al., 1966
- 1% statistical uncertainties
- No systematic uncertainties

Didactic example: Uranium Total cross section
- Energy Range studied [25 – 750 keV]; Boundary at 150 keV.
- Below 150 keV: Average R matrix
- Above 150 keV: Average R matrix or Optical Potential

Considered parameters:
- \textit{Unresolved Resonance Range}:
  - Effective Radius, Strength, Distant level
  - \( R', S_{l=0,1}, R^\infty_{l=0,1} \)

Optical Model:
- Reduced Scattering Radius (\( r_0 \))
- Diffusiveness (\( a_0 \))

Two cases studied:
1. URR/URR: Toy model → act as if they were 2 ≠ models
2. URR/Continuum: “Realistic application”
IMPOSING CONSTRAINTS ON SEVERAL MODELS
LAGRANGE MULTIPLIERS; $^{238}$U EXAMPLE

Toy Model URR/URR

Correlation without constraint

Energy (eV)

Energy (eV)
$\rho \leq \pm 0.9$
Realistic Application URR/OM

Parameters used:
- Strength function (l=0,1) ; Distant level (l=0,1) ; Effective Radius
- Reduce radius ; Diffusiveness

Diagram showing energy (in eV) vs. cross-section with different lines representing experiment, before (prior), after classical GLS, and after GLS with constraint.
Realistic Model URR/OM

Correlation After Classical GLS
Realistic Model URR/OM

\[ \rho \leq \pm 0.5 \]
Promising methods (Lagrange multipliers + Syst. Uncertainties on several models)

Correlations between energy ranges appear in cross section covariances: no more block diagonal matrices → could enhance final uncertainties on applications ...

Syst. Uncertainty
- Tends to ensure cross section continuity...if no gap in experiment in energies
- 1st attempt with normalization → Generalize to other experimental parameters creating systematic uncertainties (backround, resolution parameters., isotopic concentration)

Lagrange multipliers → 1st constraint chosen is continuity between two models calculated cross sections; Other ideas are underway on nuclear model parameters, average cross sections, ...

Both method are not straightforward → choice of parameters to be included very important

Difficulty arises if:
- Parameters are not well chosen
- Boundary is not well chosen: too high or too low making one model outside its scope
- There are Model defects

Use of this approach in a “true” evaluation: 1st true evaluation made on $^{23}$Na (Jeff3.2)

Major Isotopes: Big 3 + Additional
Covariances Matrices evaluation methodologies using integral experiments on $^{238}\text{U}$ and $^{239}\text{Pu}$ Determination of Matrices
\[ \chi^2_{GSL} = (\bar{x} - \bar{x}_m)^T M_x^{-1} (\bar{x} - \bar{x}_m) + (\bar{E} - \bar{C}(\sigma(\bar{x})))^T M_E^{-1} (\bar{E} - \bar{C}(\sigma(\bar{x}))) \]

\[ \bar{y} \rightarrow \bar{E} \rightarrow \text{Intégrales Exp.} \]

\[ \bar{G} = \frac{\partial \bar{C}}{\partial \bar{x}} = \frac{\partial \bar{C}}{\partial \bar{\sigma}} \otimes \frac{\partial \bar{\sigma}}{\partial \bar{x}} \]

CONTRAINTS: INTEGRAL EXPERIMENTS

Data Assimilation framework for evaluation using integral experiments

AP2/CRONOS2, ERANOS/PARIS, APOLLO3, MCNP, Tripoli-4

ND Treatment
Validation and/or Data Assimilation

\[ \tilde{x} = \{ \gamma_{a\lambda}, E_{\lambda}, a_c, R', OMP, \ldots \} \]

and/or

\[ \sigma^r_g \text{ and } \chi_g, \nu \ldots \]

and/or + TRENDS

“Public” Integral Experiments
- Mini-Inca (ILL)
- ICSBEP/IRPHe
- ...

Additional Integral Experiments
- Irradiation Exp. PROFIL/MANTRA
- Oscillation Exp. MINERVE/DIMPLE
- ...

Used as validation for evaluation \( \rightarrow C/E \sim 1 \)

Using benchmark in relative (see ND2013) to focus on some reaction (\(^{238}\text{U} (n,n')\) )

Take care of experimental correlation between ICSBEP series

High Precision (Oscillation: 1-3%; PROFIL: ~2%)

Flexibility in terms of neutronic spectrum

\( \rightarrow \) Deconvolution of energy domain

SG39 ↔ SG40
"Public" Integral Experiments

ICSBEP (JEZEBEL)
Additional Integral Experiments

PROFIL
Additional Integral Experiments

- CERES Program in MINERVE/DIMPLE
Reduction of Uncertainties with dedicated integral experiments is major (Factor 5-10)

Work presented here on multigroup Cross sections $\rightarrow$ nuclear parameters are also be in the game (especially for thermal benchmarks ; see NEMEA-5, C. De Saint Jean et al.) + on going work on PROFIL)

Choice of integral experiments is crucial to disentangle nuclear data sensitivities

- Use integral experiments sensitive to different reactions or parameters
- Relative integral experiments (reflector effect instead of reactivity, see D. Bernard et al., ND2013)

Difficulty arises if :
- Parameters are not well chosen or forgotten (PFNS, angular distributions …etc…)
- Spurious Integral experiment (as for microscopic ones) with hidden error
- Correlation between experiments are neglected (ICSBEP series …)

Traditional questions arises $\rightarrow$ “old” experiments, effect is diluted on several ND,.. etc

Sometimes true but CIELO and SG39 could give answers
Several kind of Nuclear Data
Several kind of Nuclear Reaction Models
Several kind of Experiments
Several kind of Covariance Matrices
Several kind of International experts (😊)

- CIELO could allow progress on methodologies related to:
  - Data assimilation for traditional evaluation
  - Data assimilation for evaluation using specific integral experiments (IDA)
  - Data assimilation for evaluation with physical constraints
    - Systematic uncertainty constraints effect on several models
    - Lagrange multipliers in the cost function
  - ....
To understand discrepancies → BENCHMARKS with sensitivity calculations

To understand covariances methodologies → List a limited set of ingredients (exp., syst. Unc.,...) and do benchmarking (same inputs → compare results)

To obtain first whole energy range covariances → list a less limited set of experiments (micro + integral) + model parameters + “new” methods + Codes?

For CEA/Cadarache, files are not the finality; methods and understanding of discrepancies on evaluation and related covariances is the major interest

Work on evaluation and covariances for Big 3 and Fe, O, ....