Producing uncertainties and covariance matrix from intermediate data using a Monte-Carlo method.

Greg Henning, Francois Claeys*, Nicolas Dari Bako, Philippe Dessagne, Maelle Kerveno (Université de Strasbourg, Centre National de la Recherche Scientifique, IPHC UMR 7178, F-67000 Strasbourg, France)
(* and CEA, DES, IRESNE, DER, SPRC, LEPh, F-13108 Saint-Paul-lez-Durance, France)

••• Context: (n, n’ γ) cross section measurements

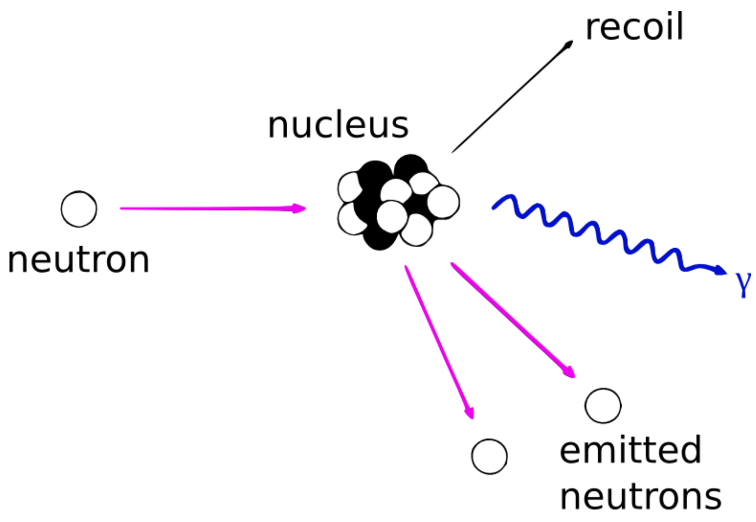
Motivations

- Nuclear reactor developments rely on evaluated databases for numerical simulations.
- However, these databases still present large uncertainties, preventing calculations from reaching the required precision [1].
- An improvement of evaluated databases requires new measurements and better theoretical descriptions of involved reactions.

[1] NEA/WPEC-26, "Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations." (2008)

(n, n’ γ) cross section measurements

- Inelastic neutron scattering are of great importance for the operation of a reactor as they modify the neutron spectrum, the neutron population, and produce new elements.
- Constraining reaction models by measuring precisely exclusive (n, xn γ) cross sections [2].

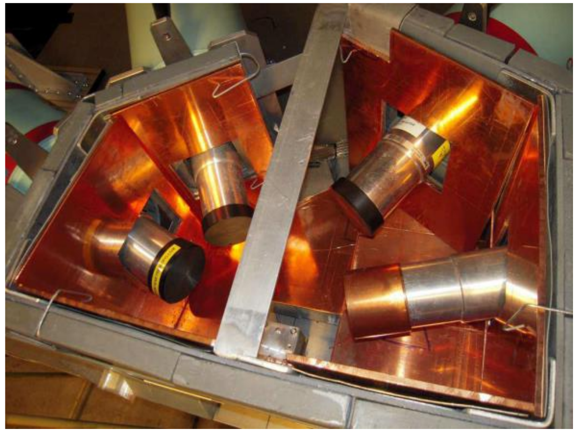


[2] "How to produce accurate inelastic cross sections from an indirect measurement method?" M. Kerveno et al., EPJ Nucl. Sci. Tech. 4, 23 (2018)

Improving (n, n') evaluation with exclusive (n, n' γ) measurements

Measuring (n, n'γ) cross sections with GRAPhEME [1]

- Installed at the Gelina facility (JRC-Geel).
- 30 m flight path.
- Fission Chamber to measure incoming neutron flux.
- 6 planar HPGe, high efficiency and resolution at low E_γ.
- Digital acquisition.
- Measured : ^{235}U, ^{232}Th, ^{nat,182,183,184,186}W, ^{238}U, ^{nat}Zr, ^{233}U, ^{57}Fe, ^{239}Pu

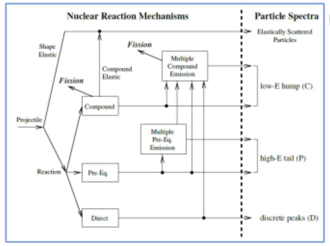


M. Kerveno et al,. EPJ Web of Conferences 239, 01023 (2020)

[1] "GRAPhEME : a setup to measure (n, xn γ) reaction cross sections." Greg Henning, et al.. Adv. in Nuc. Instr. Meas. Met. and App., 2015.

Inferring total (n, n') cross section from (n, n' γ) ones [2]

Reaction models and codes
(input: structure, masses, optical potential, …)



total (n, n') σ computed by the model after constraining them with measurements

Precise (n, n' γ) experimental cross sections

- To be relevant, experimental data must have the lowest possible uncertainties.
- Covariances are key to model constraining by data.

[2] "How to produce accurate inelastic cross sections from an indirect measurement method?" M. Kerveno et al., EPJ Nuclear Sci. Technol. 4, 23 (2018)

••• Extracting (n, n’ γ) cross section from data

- Differential cross section at a given angle : $$\frac{d\sigma_\gamma(E_\mathrm{n})}{d\omega}|_\theta = \frac{1}{4\pi} \times \frac{N_\gamma(E_\mathrm{n})_{|\theta}}{\epsilon_\gamma} \times \frac{1}{N_\mathrm{target}} \times \frac{\epsilon_\mathrm{FC} \times \sigma_{^{238}U(n,f)}(E_\mathrm{n})}{(1-L_\mathrm{n})N_\mathrm{FC}(E_\mathrm{n})}$$

- Angle integrated cross section is obtained via “*Gaussian quadrature method*“

$$\sigma_\gamma(E_\mathrm{n}) = 2\pi\left(w_{110^\circ} \times \frac{d\sigma_\gamma(E_\mathrm{n})}{d\omega}|_{110^\circ} + w_{150^\circ} \times \frac{d\sigma_\gamma(E_\mathrm{n})}{d\omega}|_{150^\circ}\right)$$

- Experimental data come with many parameters (efficiency of detectors, distances, masses, …) with their own uncertainty.
- Data analysis introduces additional uncertainties and correlations (calibration, selection, …).

- With so many parameters, different kind of uncertainty, correlations, … the usual analytic formula *à la* perturbation theory becomes very complex and may not be enough to characterize the uncertainty and covariance correctly.

$$\sigma^2_{f(x_1,x_2,\ldots x_i)} = \sum_j \left(\frac{\partial f}{\partial x_j}^2 \times \sigma_a^2\right) + \sum_{j\neq k} 2\frac{\partial f}{\partial x_j}\frac{\partial f}{\partial x_k}\sigma_{x_j}\sigma_{x_k}$$

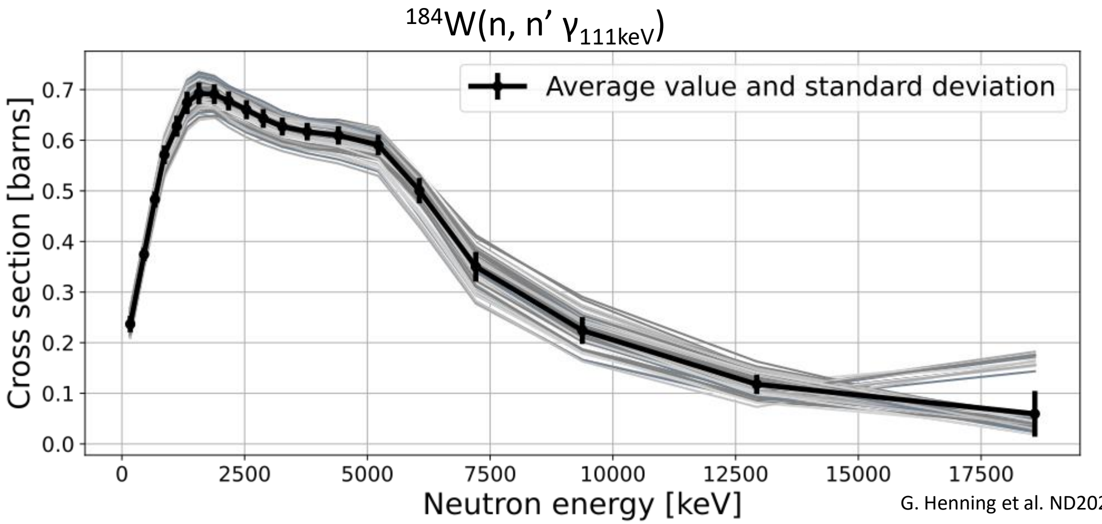
••• The Monte Carlo route

Method

- "Monte Carlo" as in **random sampling**.
- Each parameter comes with its own probability distribution.
- Parameter values are drawn randomly according to their PDF and used to compute a value (such as the final σ).
- This is done many (tens to thousands of) times.
- All values are collected and *stacked*.
- From the *stack* the average value and standard deviation are computed, as well as the correlation matrix.

⚠ ≠ Full Monte Carlo analysis

- Starting from raw histograms.
- Random sampling of efficiencies, target mass, …
- Performing neutron flux extraction, γ peaks fit, ...
- One cross section per iteration : added to the stack.
- Using python `numpy` to produce central values, standard deviation, and correlation matrices from the stack.
- **But** intensive, costly, and needs to be set up from the start.



G. Henning et al. ND2022

Random sampling on intermediate results

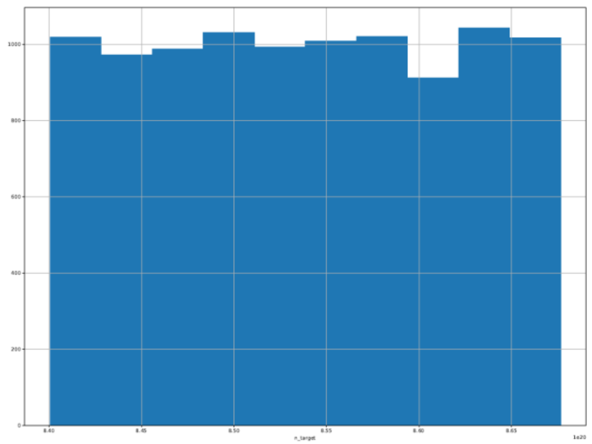
For data that has **already** been **analyzed**

- … using a deterministic (analytical) method.
- Reading intermediate results files and sampling them to *replay* the last step of the analysis many times.
  - Sampling N_γ, $N_n = N_{FC}/\sigma_{U(n,f)}$, …
  - E_n are fixed

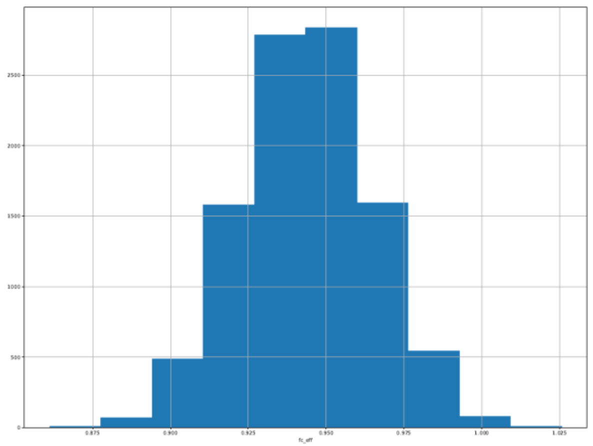
$$\frac{d\sigma_\gamma(E_\mathrm{n})}{d\omega}\Big|_\theta = \frac{1}{4\pi} \times \frac{N_\gamma(E_\mathrm{n})_{|\theta}}{\epsilon_\gamma} \times \frac{1}{N_\mathrm{target}} \times \frac{\epsilon_\mathrm{FC} \times \sigma_{^{238}U(n,f)}(E_\mathrm{n})}{(1-L_\mathrm{n})N_\mathrm{FC}(E_\mathrm{n})}$$

- ⚠ *Systematic* or *statistic* labels on uncertainties loose relevance

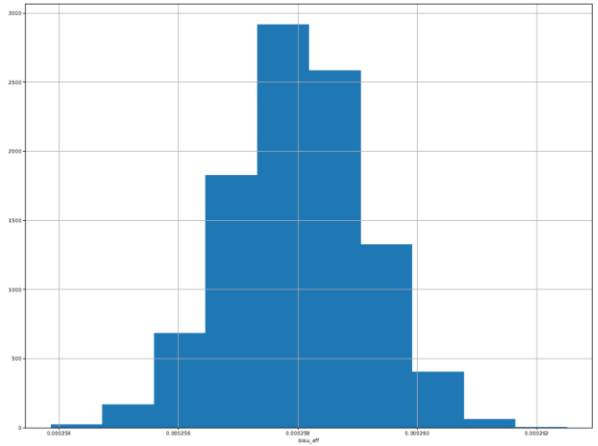
[1] G. Henning et al. ND2022
[2] High accuracy measurements of neutron inelastic scattering cross sections [...]. Ph. Dessagne et al. EU Publications Office (2013).



N_{target}



Ge Eff.



FC Eff.

••• Implementation

Constrains

- Parameters are positive, we need to avoid division by 0.
- Efficiencies are bound in the range]0; 1]
- Using flat or Gaussian distribution
- N_γ are constrained by total sum
  - Correlated sampling method on the cumulative distribution

Software

- Written in Python 3.7 (compatible with 3.6)
- Libraries requirements:
  - `numpy` and `matplotlib`
  - `Pyyaml` (for configuration reading)
  - Monte Carlo Variable object (`mcvariable`)
  - Ascii Data file reader (`ascii-data-file`)

```yaml
# if uncertainty is negative, it's is relative
name: 635keV

N_iterations: 3000

# Target :
N_target: [6.88e+20, -0.03]

# Loss in the trip from Fission chamber to target
air_loss: [0.018, 0.000001]

# Fission chamber efficiency
fc_eff: [0.94, 0.021]

detectors:
  bleu:
    name: B110
    efficiency: [3.02780E-4, -0.03]
    gamma_file: data/Data_det3_2011_12_13_Unat635keV.yield
    flux_file: data/Flux_det2_2011_12_13_final_Unat_det3_635keV.int_flux
  rouge:
```

- Written to be highly adaptable to many transitions with input and configuration files.

••• Implementation

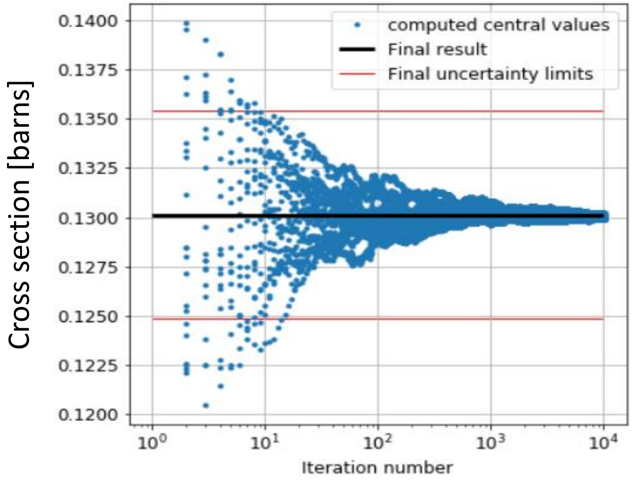
Computing cost

- Computing time mostly proportional to the number of iterations
- ~ one minute for 5000 iterations
- Memory usage also proportional to the number of iterations

Convergence

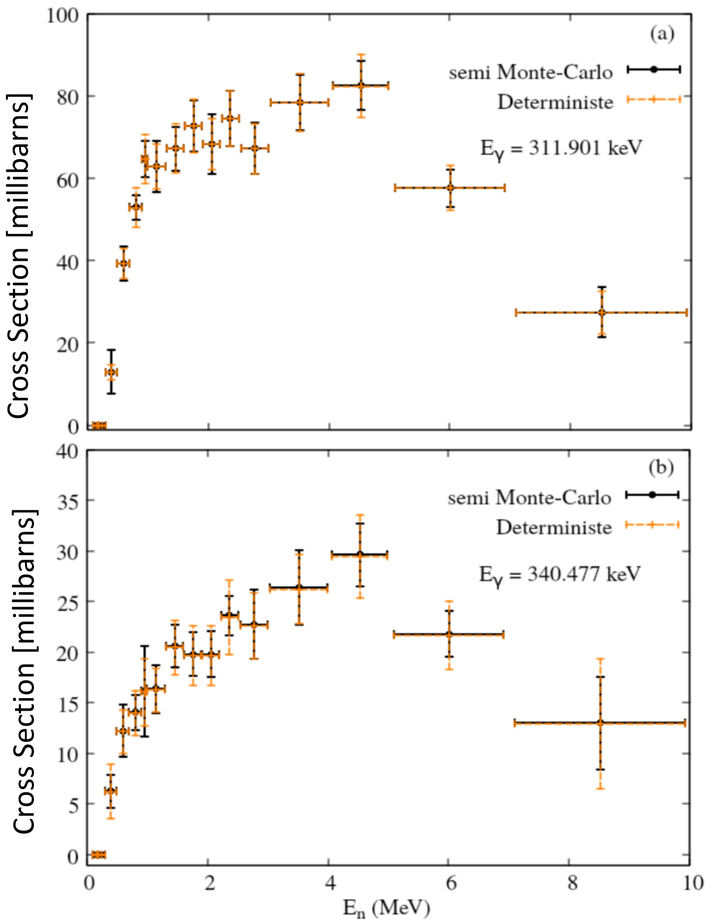
- Checked *a posteriori*
- Testing convergence for central values and standard deviations.
- 2000 iterations is usually largely enough for convergence.

$^{238}U(n, n' \gamma_{635keV})$ @ E_n=2 MeV



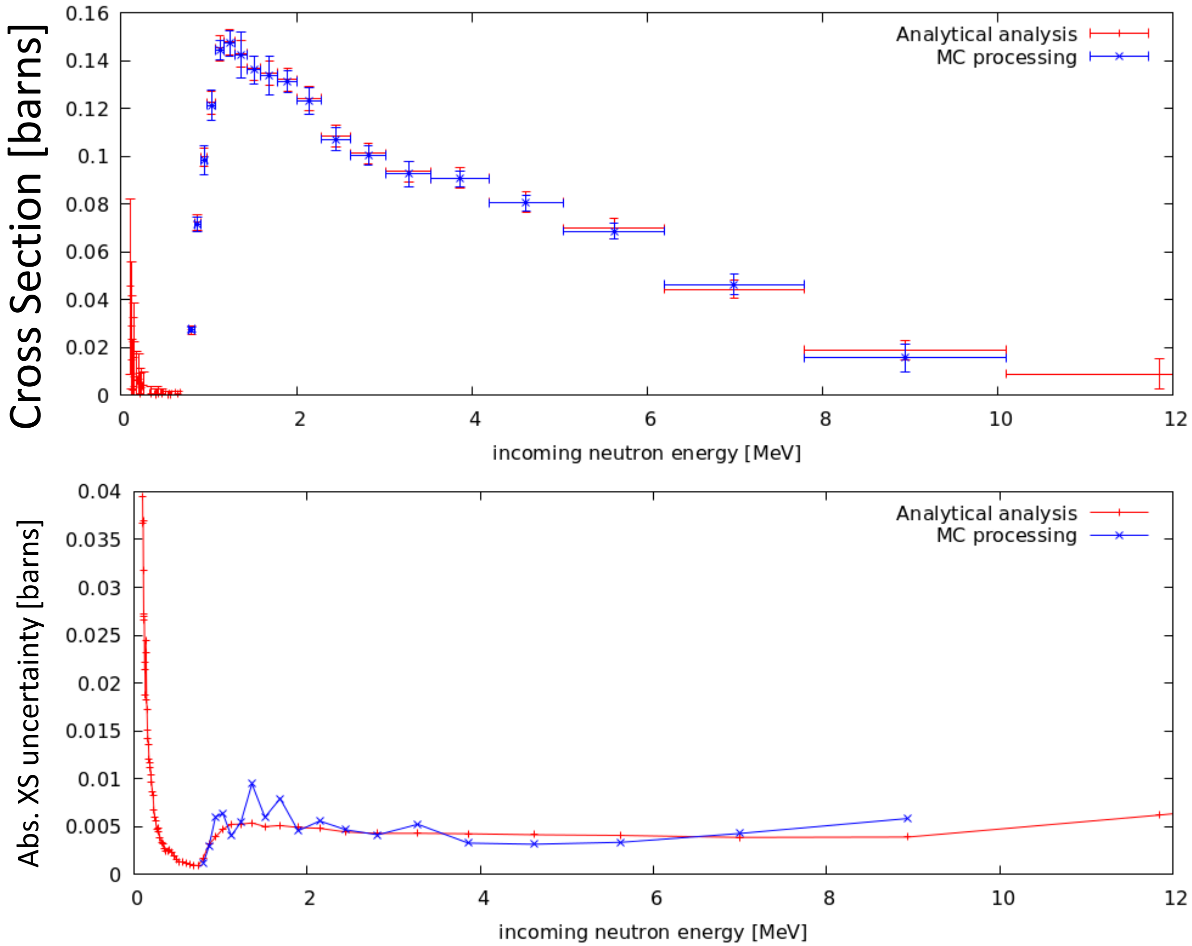
••• Comparison with analytical analysis code

311.9 keV and 340.5 keV γ transitions in ^{233}U



F. Claeys, Thesis, 2023

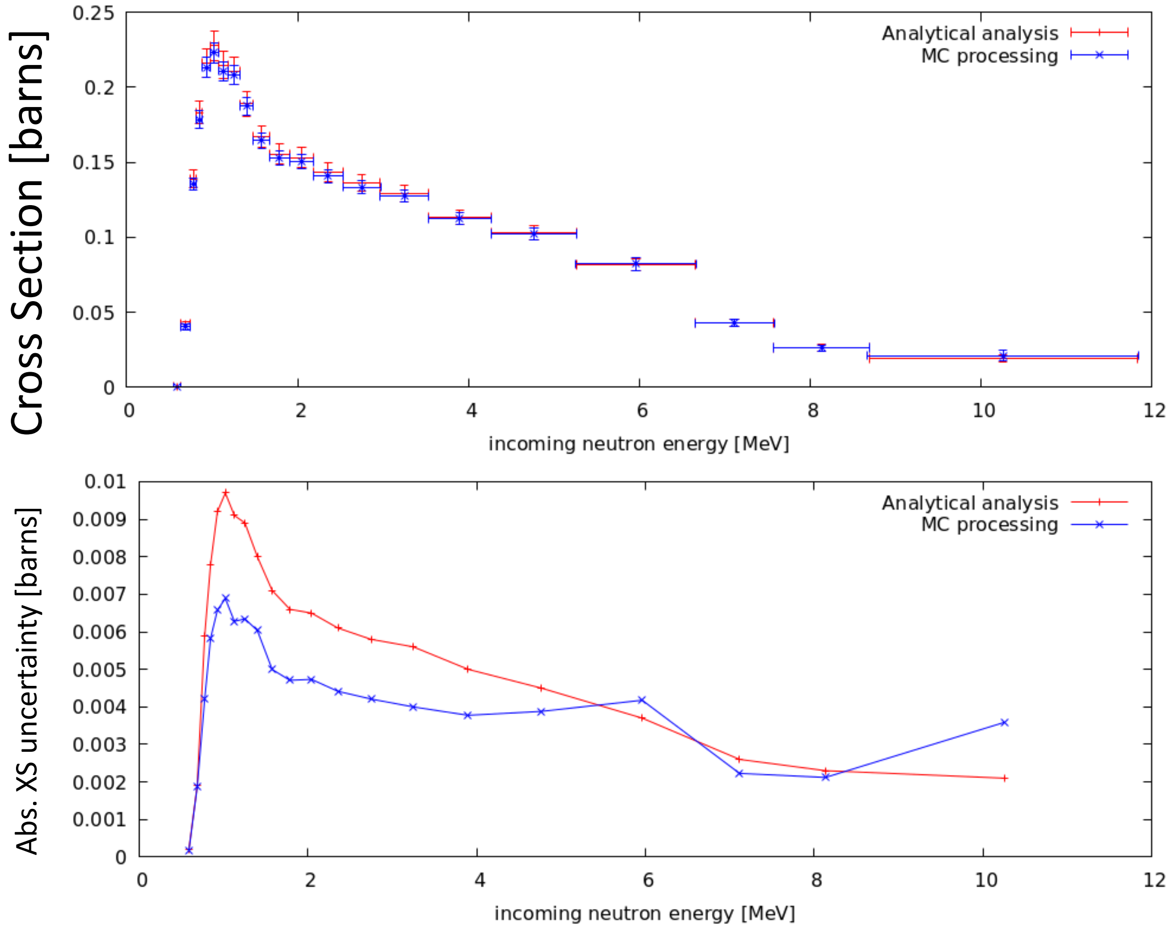
736 keV γ transition in ^{232}Th – (preliminary results)



Central values compatible between the two methods, on the same order for uncertainties.

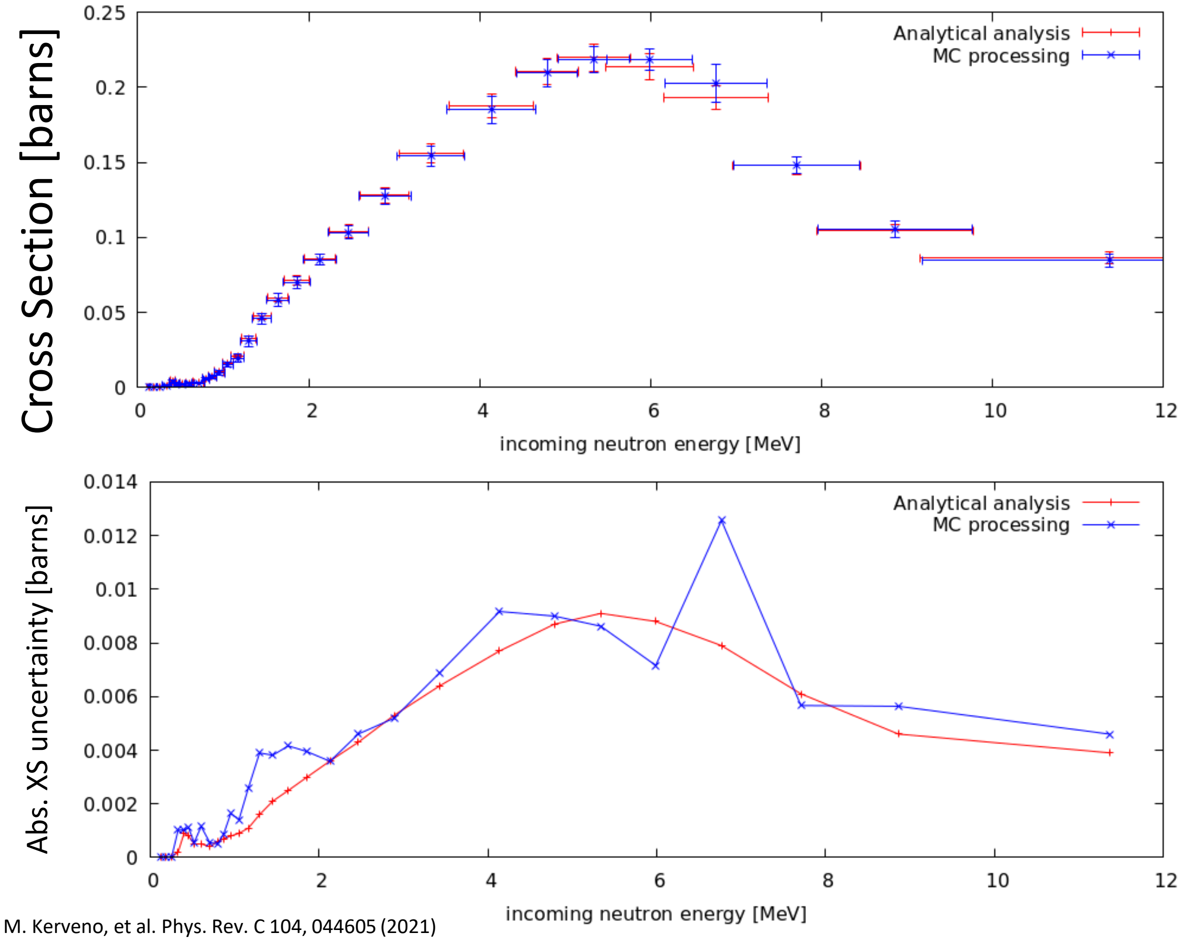
••• Comparison with analytical analysis code

635 keV γ transition in ^{238}U



M. Kerveno, et al. Phys. Rev. C 104, 044605 (2021)

159 keV γ transition in ^{238}U

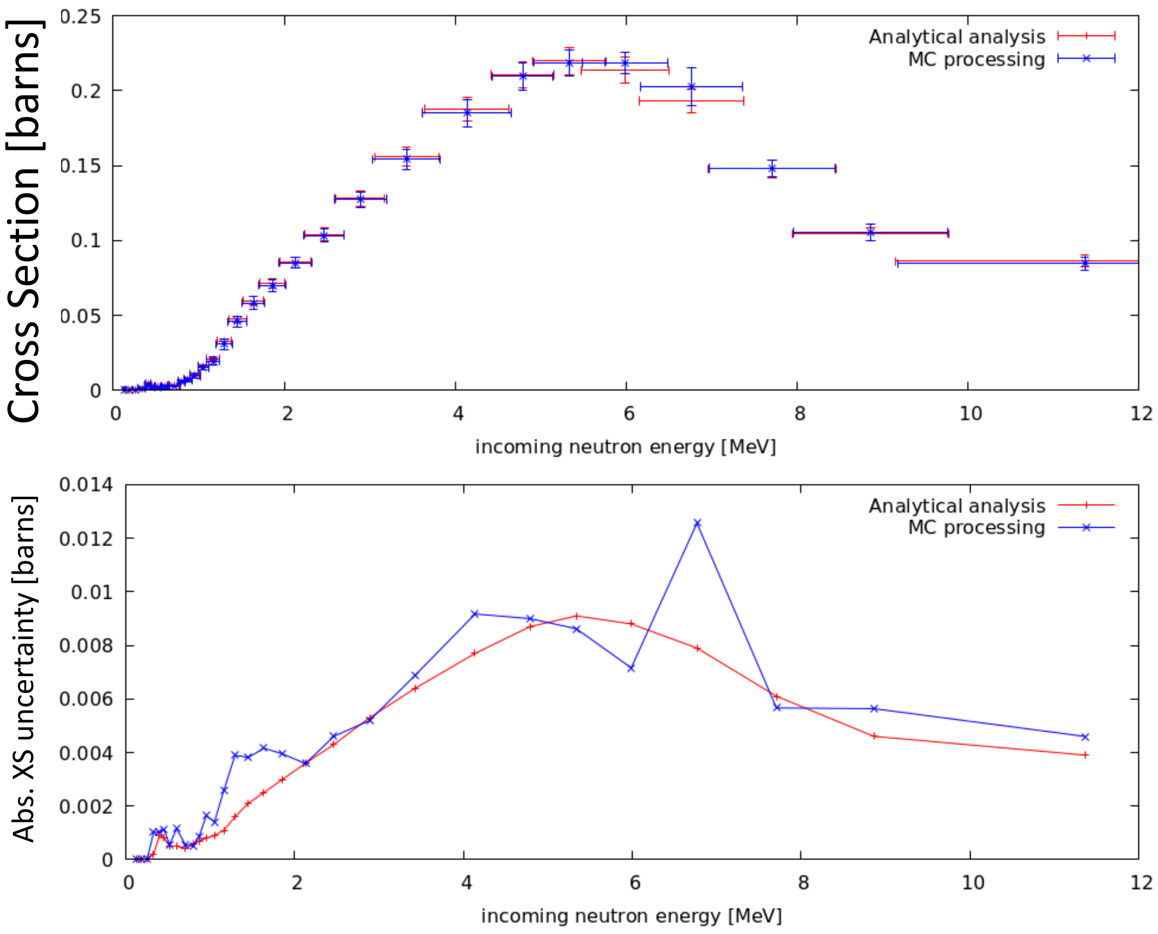


M. Kerveno, et al. Phys. Rev. C 104, 044605 (2021)

Central values compatible. Uncertainties lower for the 635 keV one. Same order for the 153 keV, **but** with additional structure 😮.

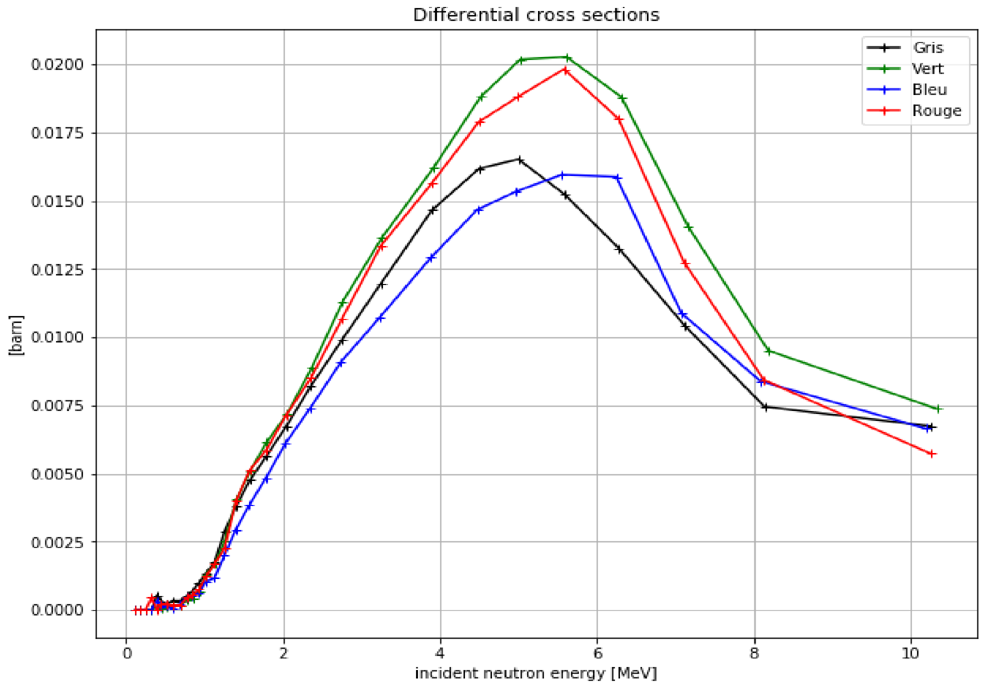
Investigating differences with analytical method

159 keV γ transition in ^{238}U



Central values compatible. Uncertainties lower for the 635 keV one. Same order for the 159 keV, **but** with additional structure.

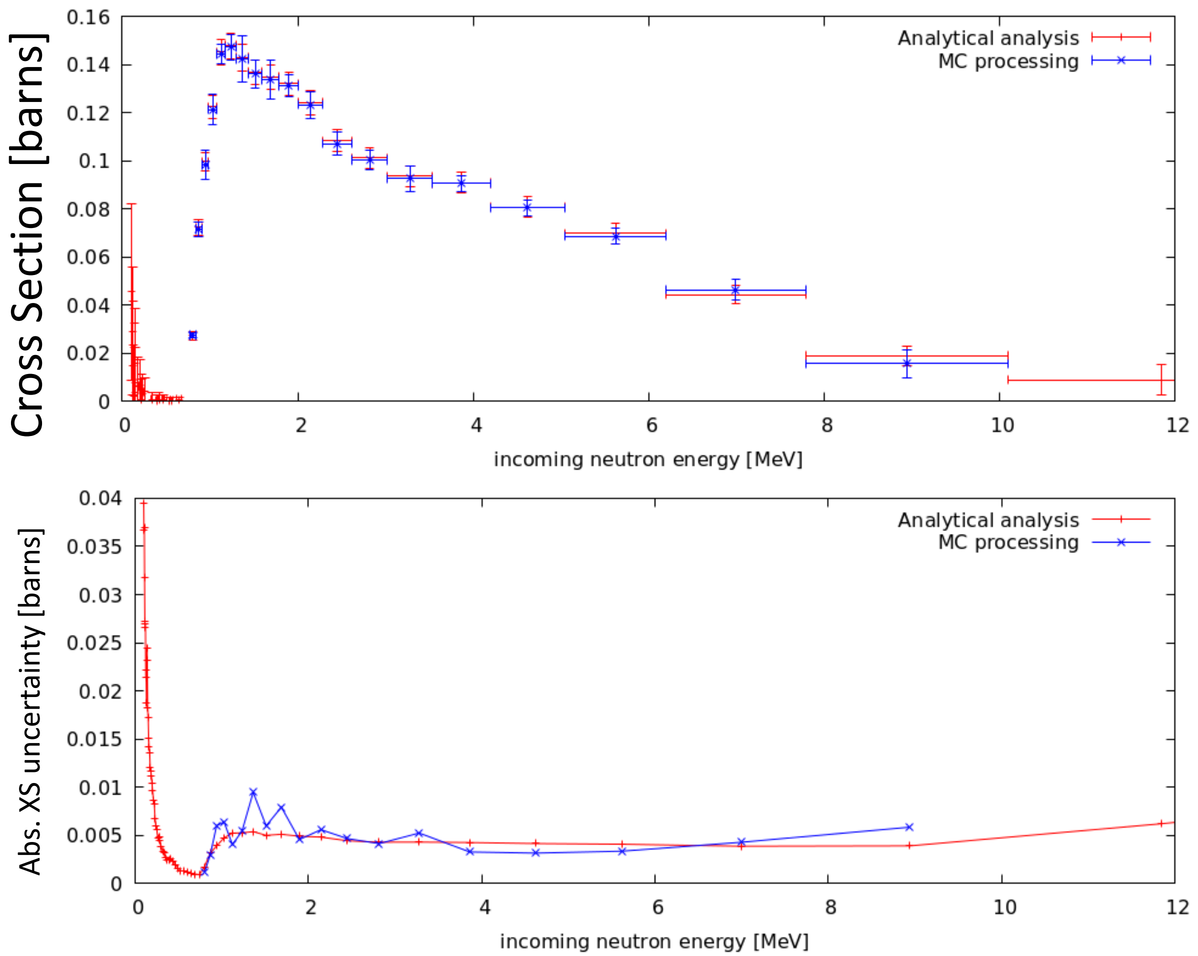
Upon inspection of the input data, the structures appearing in the MC uncertainties actually reflect variations in differential cross section computed for different detectors.

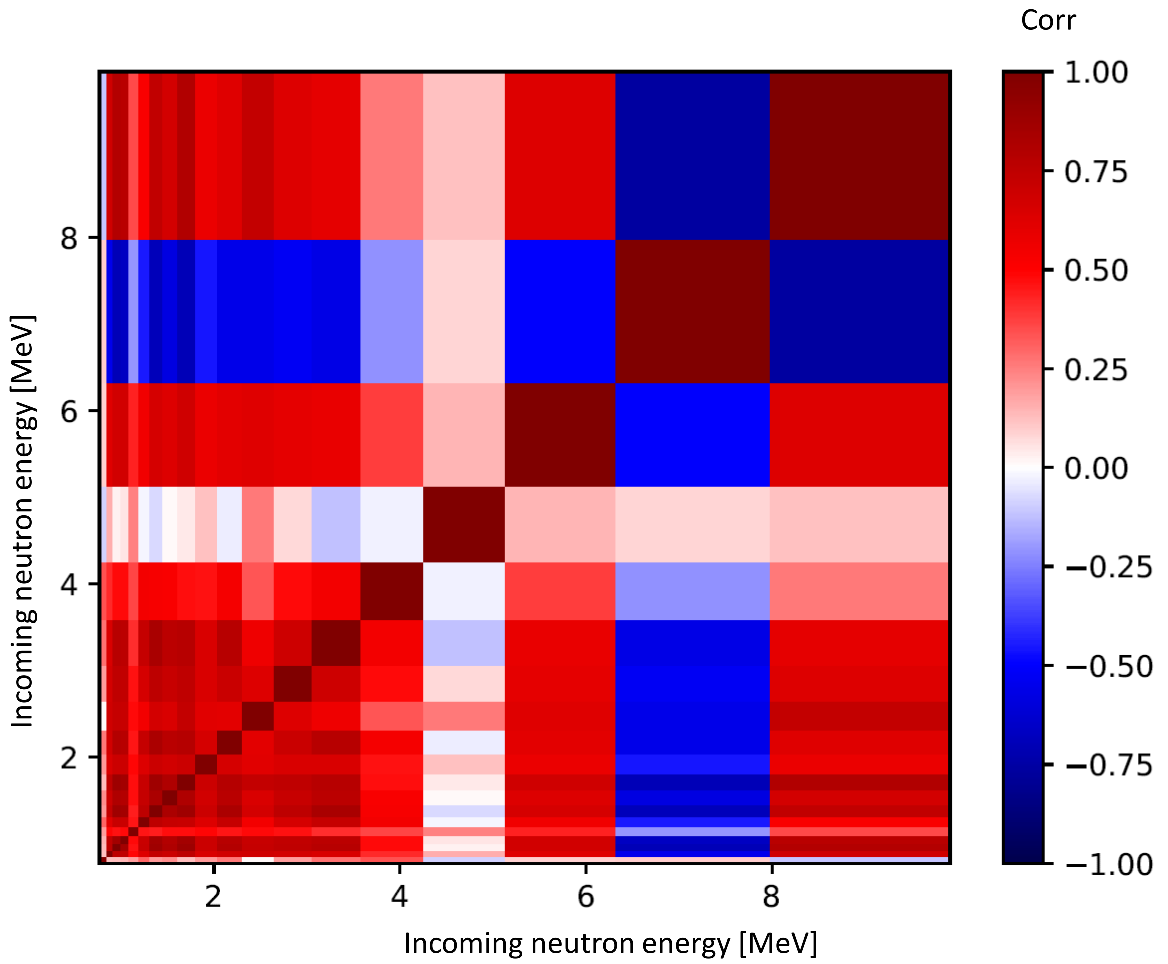


MC processing takes into account this scattering of data, which analytical method just averages out.

••• Main benefit of the MC method: Production of Covariance & Correlation matrices

736 keV γ transition in ^{232}Th – (preliminary results)

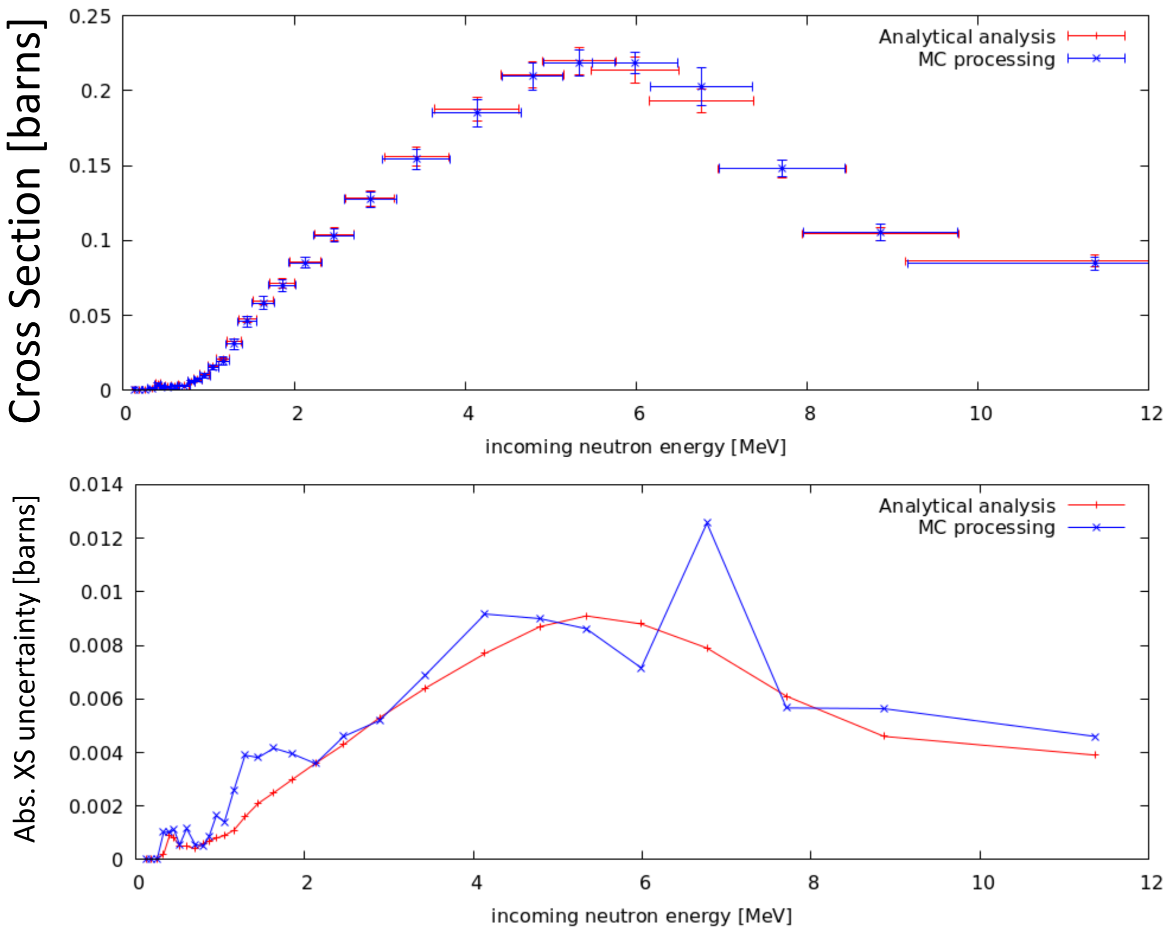


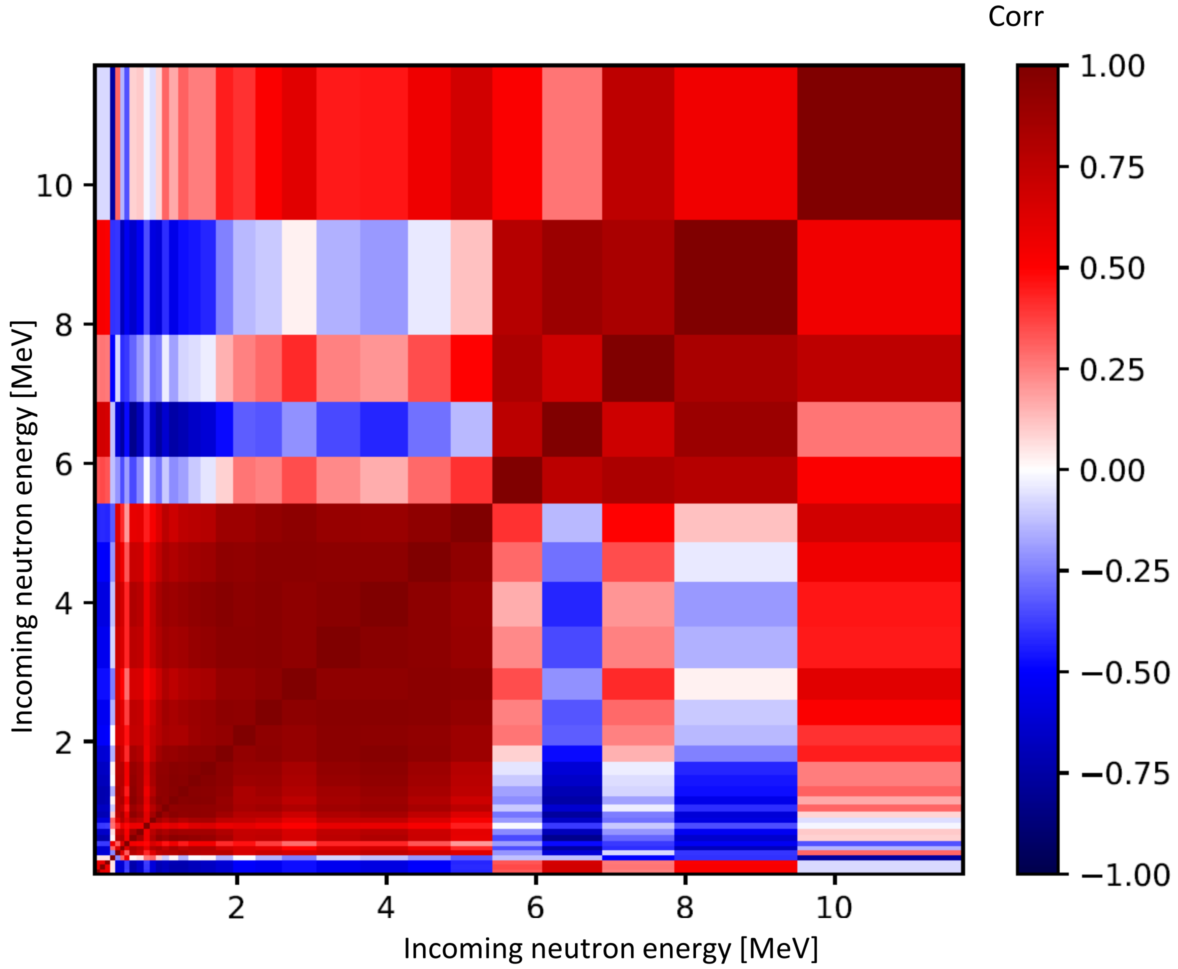


Values mostly positively correlated because the number of scattering centers in the target is the main source of uncertainty.

Main benefit of the MC method: Production of Covariance & Correlation matrices

153 keV γ transition in ^{238}U





± structure matching the structure seen in the input data.

••• Conclusions and perspectives

Importance of (n, n') reactions for applications

Using exclusive channel (n, n' γ) for indirect determination.

Control of uncertainties and correlations is key.

Using Monte Carlo processing on intermediate analysis files to produce uncertainties and covariances.

Central values compatible between MC and analytical methods.

Uncertainties with MC actually better reflect the input data.

MC processing software highly adaptable : all our previous data can be exploited (already ^{233}U, ^{238}U, ^{232}Th).

Highlights the importance of keeping intermediate data available (Open Data)

Study the sensitivity to sources of uncertainty by *turning* them *on* and *off*

Efficient: reusing preprocessed data, easier than reprocessing the raw data in full MC

Better uncertainties, and Cov & Corr matrices produced

Outputs still to be fully exploited (particularly Covariances).

Full Monte Carlo analysis in development for other nuclei.