# *Estimation of Covariances on Nuclear Model Parameters with CONRAD: review of all methods*

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## Conrad short description

Conrad



### Functionalities

- Evaluation : analysis of microscopic, semi-integral and integral measurements,
- Bayesian parameters estimations (GLS),
- Uncertainty propagation and evaluation with Monte-Carlo or Analytical methods
- establish a link with reactor physicists : from $\sigma(E)$ to $\sigma_g$

### Nuclear reactions models in Conrad

- Resolved resonance range (MLBW,Reich-Moore,..),
- Unresolved resonance range (average R matrix)
- Statistical models (Hauser-Feshbach, Moldauer, GOE,...)
- Continuum (ECIS wrapper)

From 0eV to 20MeV : all models in the same framework

## Covariance recurrent puzzle



### Generic problems :

- Assigning uncertainties to model parameters involved in the modeling of the neutron induced reactions is a recurrent puzzle
- Significant difficulties became apparent when mass production techniques were developed for adding uncertainty information in Evaluated Nuclear Data Files in response to requests from users involved in fission and fusion reactor development programs.
- Major drawbacks found by reactor physicists
  - most of the time the integral experiments were not taken into account sufficiently soon in the evaluation process,
  - unexpected discrepancies,
  - "Are you sure of these covariances ?"

## Model Parameter Definition



**Between [0eV;200MeV] :**

cross section are based on nuclear reaction models with parameters not always predicted by theory.

**Model parameters : referred as $\vec{x}$ in this presentation**

- Resolved Resonance Range : $E_\lambda, \gamma^i_\lambda, R_{eff}, ...,$
- Unresolved Resonance Range : $D_0, <\Gamma^i>, R_{eff}, ...,$
- Higher energies : Optical model parameters

- parameters used to calculate cross sections covariances.
- Data assimilation technique to estimate the parameters : use of Experiments
- Retroactive methodology, as defined in the SAMMY and CONRAD codes : clearly distinguish the model and nuisance parameters in the uncertainty propagation procedure.

## Nuisance Parameter Definition



*Nuisance parameters : referred as $\vec{\theta}$ in this presentation*

- Experimental parameters : sample composition, the sample temperature, the energy resolution of the facility, the normalization factor and the background corrections.
- Other Model parameters (comming from theory/experiment with uncertainties) whose knowledge is necessary.
- ...

In parameter estimation techniques, these additional ingredients are called nuisance variables whose properties are not of particular interest in itself, but are fundamental for assessing reliable model parameters.

## Solutions



### A-priori work : treating experimental data

- re-analyse experiments from raw data with a proper systematic uncertainty description,
- simulate these uncertainties from Exfor (Conrad) :
  - to take into account a normalization uncertainty : New data = data * N where N = $1 \pm \delta N$,
  - to take into account a background uncertainty : New data = data - B where B = $0 \pm \delta B$

### A-posteriori work : treating during/after adjustment

- Retro-active analysis (Conrad, Sammy)
- Marginalization techniques (Conrad) ; examples :
  - marginalize the normalization parameter : New Theory = Theory/N where N = $< N > \pm \delta N$,
  - marginalize the background parameter : New Theory = Theory + B where B = $< B > \pm \delta B$

## Retro-active techniques



### First introduced in Sammy [1, 2] :

- "retroactively" generate covariance matrix for already evaluated resonance parameters
- calculate the matrix elements knowing the theoretical cross sections, the statistical uncertainty and the nuisance parameters.

### Problems :

- based only on the theoretical curves
- problem of treating "real" statistical uncertainties
- depanding on specific theoretical grid.

## Marginalization techniques



### Basics of parameter estimation with Bayes' theorem

When the analysis of a new data set $\vec{y}$ is performed:

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

U : "background/prior" information and $p(\vec{y}|\vec{x}, U)$ : likelihood

Fitting procedure : estimation of the first two moments of $p(\vec{x}|\vec{y}, U)$

### Marginalization techniques

With nuisance parameters :

- evaluate the influence of $\vec{\theta}$ parameters during the estimation of $\vec{x}$ parameters.
- Bayesian marginalization of the $\vec{\theta}$ parameters [4] :

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

Marginalization : estimation of the first two moments of $p_{\vec{\theta}}(\vec{x}|\vec{y}, U)$

## Marginalization techniques



### Two methods implemented in CONRAD :

- Monte-Carlo : calculate first two moment of marginalized distribution [4, 3]
- Analytical

### Analytical marginalization equation :

Additional hypothesis : pdf are gaussians.

$$M_x^{Marg} = \left(G^{x\,T} G^x\right)^{-1} G^{x\,T} G M_x G^T G^x \left(G^{x\,T} G^x\right)^{-1}\ [a]$$

where G is the theoretical derivative matrix : $G = \begin{pmatrix} G^x \\ G^\theta \end{pmatrix}$

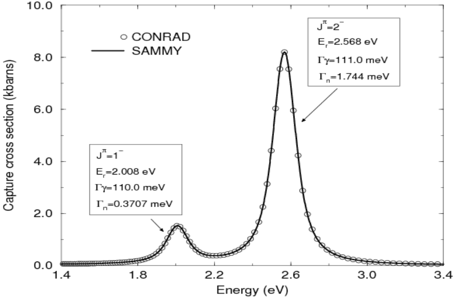
and $M_X$ is the covariance matrix : $M_X = \begin{pmatrix} M_x & M_{x,\theta} \\ M_{\theta,x} & M_\theta \end{pmatrix}$

[a] $G^{x\,T} G^x$ is a square matrix whose size is equal to the number of model parameters, this product can be inverted if the matrix $G^x$ has a rank equal to the number of model parameters. In practise, $N_{exp} \geq N_{parameters}$

This formulae is to be used after the fitting procedure.

## $^{155}$Gd test case Description






- selection of two *s*-wave resonances ($E_r = 2.0$ eV and $E_r = 2.6$ eV) observed in the low energy part of the $^{155}$Gd(n,$\gamma$) reaction
- small energy range between 1.4 eV and 3.4 eV,
- test SAMMY/REFIT/CONRAD

*Full $^{155}$Gd treatment on the way (G. Noguere)*

## Comparisons of various techniques



### Preliminary tests : uncertainty magnitude

- See dependence of realistic statistical uncertainties

| | | | | CONRAD |
|---|---|---|---|---|
| With statistical uncertainty of 1% : | | | | |
| $E_r(1^-) = 2.0080$ | $\pm$ | 0.000047 | eV | (0.0033%) |
| $\Gamma_\gamma(1^-) = 110.00$ | $\pm$ | 0.10 | meV | (0.12%) |
| $\Gamma_n(1^-) = 0.3707$ | $\pm$ | 0.0002 | meV | (0.08%) |
| $E_r(2^-) = 2.5680$ | $\pm$ | 0.000039 | eV | (0.0021%) |
| $\Gamma_\gamma(2^-) = 111.00$ | $\pm$ | 0.08 | meV | (0.10%) |
| $\Gamma_n(2^-) = 1.7440$ | $\pm$ | 0.0010 | meV | (0.08%) |
| With statistical uncertainty of 10% | | | | |
| $E_r(1^-) = 2.0080$ | $\pm$ | 0.00047 | eV | (0.033%) |
| $\Gamma_\gamma(1^-) = 110.00$ | $\pm$ | 0.95 | meV | (1.20%) |
| $\Gamma_n(1^-) = 0.3707$ | $\pm$ | 0.0022 | meV | (0.82%) |
| $E_r(2^-) = 2.5680$ | $\pm$ | 0.00039 | eV | (0.021%) |
| $\Gamma_\gamma(2^-) = 111.00$ | $\pm$ | 0.77 | meV | (0.98%) |
| $\Gamma_n(2^-) = 1.7440$ | $\pm$ | 0.0097 | meV | (0.80%) |

Linear dependence of the variance with the statistical uncertainty[1]

[1] Equivalent results are obtained with SAMMY and REFIT

## Comparisons of various techniques



### Preliminary tests : nb of bins

Resonance parameters and uncertainties as a function of the number of bins in the energy grid. The statistical uncertainty used in the calculations is 1%.

| Resonance parameter | Uncertainty for 2140 energy bins | | Uncertainty for 214 energy bins | |
|---|---|---|---|---|
| $E_r(1^-)$=2.0080 eV | 0.000047 | (0.0023%) | 0.000149 | (0.0074%) |
| $\Gamma_\gamma(1^-)$=110.00 meV | 0.10 | (0.09%) | 0.30 | (0.27%) |
| $\Gamma_n(1^-)$=0.3707 meV | 0.0002 | (0.05%) | 0.0007 | (0.19%) |
| $E_r(2^-)$=2.5680 eV | 0.000039 | (0.0015%) | 0.000122 | (0.0048%) |
| $\Gamma_\gamma(2^-)$=111.00 meV | 0.08 | (0.07%) | 0.25 | (0.22%) |
| $\Gamma_n(2^-)$=1.7440 meV | 0.0010 | (0.06%) | 0.0031 | (0.18%) |

The expected discrepancies between the two calculations of about $\sqrt{10}$ makes questionable the use of retroactive techniques only based on theoretical considerations with an arbitrary energy mesh.

## Comparisons of various techniques



### Preliminary tests : conclusions

In the light of the results reported in previous Tables :

- experimental conditions as close as possible of the original one turns out for necessary ingredients within a reliable application of the retroactive approach.
- If such experimental information are missing, the present technique remains valid when the nuisance parameter uncertainties dominate the final results.

## Comparisons of various techniques

### Analytical marginalization :

Illustrate the problem with the normalization factor :

- normalization uncertainty of 3%
- statistical uncertainties of 1%, 5% and 10%.
- Results provided by CONRAD (M-RLSF)[a]

| | CONRAD (M-RLSF) | | |
|---|---|---|---|
| With statistical uncertainty of 1% : | | | |
| $E_r(1^-) = 2.0080$ ± | 0.000047 | eV | (0.0023%) |
| $\Gamma_\gamma(1^-) = 110.00$ ± | 0.12 | meV | (0.11%) |
| $\Gamma_n(1^-) = 0.3707$ ± | 0.0114 | meV | (3.07%) |
| $E_r(2^-) = 2.5680$ ± | 0.000039 | eV | (0.0015%) |
| $\Gamma_\gamma(2^-) = 111.00$ ± | 0.09 | meV | (0.08%) |
| $\Gamma_n(2^-) = 1.7440$ ± | 0.0533 | meV | (3.06%) |
| With statistical uncertainty of 10% | | | |
| $E_r(1^-) = 2.0080$ ± | 0.00047 | eV | (0.023%) |
| $\Gamma_\gamma(1^-) = 110.00$ ± | 0.96 | meV | (0.86%) |
| $\Gamma_n(1^-) = 0.3707$ ± | 0.0116 | meV | (3.13%) |
| $E_r(2^-) = 2.5680$ ± | 0.00039 | eV | (0.015%) |
| $\Gamma_\gamma(2^-) = 111.00$ ± | 0.77 | meV | (0.69%) |
| $\Gamma_n(2^-) = 1.7440$ ± | 0.0542 | meV | (3.11%) |

[a] similar results with SAMMY method

## Comparisons of various techniques



### Analytical marginalization : Covariances

Results provided by CONRAD :

With statistical uncertainty of 1% :

| | | | | | | |
|---|---|---|---|---|---|---|
| $E_r(1^-)$ | 100.0 | | | | | |
| $\Gamma_\gamma(1^-)$ | 18.7 | 100.0 | | | | |
| $\Gamma_n(1^-)$ | -3.1 | 57.9 | 100.0 | | | |
| $E_r(2^-)$ | 8.5 | 11.7 | 1.5 | 100.0 | | |
| $\Gamma_\gamma(2^-)$ | -5.7 | -43.9 | -48.9 | -8.8 | 100.0 | |
| $\Gamma_n(2^-)$ | -3.6 | -58.1 | 100 | 1.3 | -49.9 | 100.0 |

With statistical uncertainty of 10%

| | | | | | | |
|---|---|---|---|---|---|---|
| $E_r(1^-)$ | 100.0 | | | | | |
| $\Gamma_\gamma(1^-)$ | 25.2 | 100.0 | | | | |
| $\Gamma_n(1^-)$ | 4.4 | 3.4 | 100.0 | | | |
| $E_r(2^-)$ | 8.4 | 13.2 | 2.4 | 100.0 | | |
| $\Gamma_\gamma(2^-)$ | -8.2 | -22.0 | -8.8 | -9.2 | 100.0 | |
| $\Gamma_n(2^-)$ | -0.1 | -6.5 | 96.5 | 0.1 | -19.2 | 100.0 |

## Comparisons of various techniques

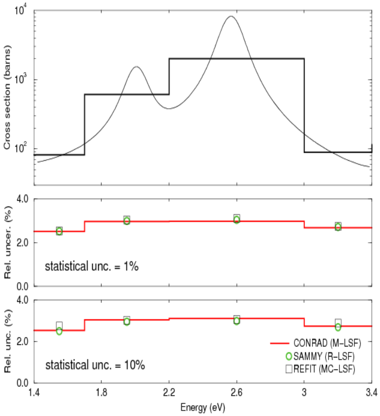
Comparison of the uncertainties provided by the analytic (M-RLSF) and stochastic (MC-RLSF) retroactive models.



| Resonance parameter | Analytic model (M-RLSF) CONRAD | | Monte-Carlo model (MC-RLSF) CONRAD | | Monte-Carlo model (MC-RLSF) REFIT | |
|---|---|---|---|---|---|---|
| Statistical unc. 1% : | | | | | | |
| $E_r$=2.0080eV | 0.000047 | (0.0023%) | 0.000048 | (0.0024%) | 0.000049 | (0.0024%) |
| $\Gamma_\gamma$=110.00 meV | 0.12 | (0.11%) | 0.37 | (0.34%) | 0.37 | (0.34%) |
| $\Gamma_n$=0.3707 meV | 0.0114 | (3.07%) | 0.0114 | (3.07%) | 0.0114 | (3.07%) |
| $E_r$=2.5680 eV | 0.000039 | (0.0015%) | 0.000040 | (0.0016%) | 0.000039 | (0.0015%) |
| $\Gamma_\gamma$=111.00 meV | 0.09 | (0.08%) | 0.18 | (0.16%) | 0.16 | (0.14%) |
| $\Gamma_n$=1.7440 meV | 0.0533 | (3.06%) | 0.0531 | (3.05%) | 0.0537 | (3.08%) |
| Statistical unc. 5% : | | | | | | |
| $E_r(1^-)$=2.0080eV | 0.00024 | (0.012%) | 0.00024 | (0.012%) | 0.00024 | (0.012%) |
| $\Gamma_\gamma$=110.00 meV | 0.49 | (0.45%) | 0.60 | (0.57%) | 0.60 | (0.54%) |
| $\Gamma_n$=0.3707 meV | 0.0114 | (3.07%) | 0.0113 | (3.05%) | 0.0114 | (3.07%) |
| $E_r$=2.5680 eV | 0.00019 | (0.0074%) | 0.00019 | (0.0076%) | 0.00019 | (0.0074%) |
| $\Gamma_\gamma$=111.00 meV | 0.39 | (0.35%) | 0.43 | (0.38%) | 0.41 | (0.34%) |
| $\Gamma_n$=1.7440 meV | 0.0535 | (3.07%) | 0.053 | (3.04%) | 0.0539 | (3.09%) |
| Statistical unc. 10% : | | | | | | |
| $E_r$=2.0080eV | 0.00047 | (0.023%) | 0.00047 | (0.023%) | 0.00047 | (0.023%) |
| $\Gamma_\gamma$=110.00 meV | 0.96 | (0.86%) | 1.02 | (0.93%) | 1.03 | (0.94%) |
| $\Gamma_n$=0.3707 meV | 0.0116 | (3.13%) | 0.0118 | (3.19%) | 0.0116 | (3.12%) |
| $E_r$=2.5680 eV | 0.00039 | (0.015%) | 0.00039 | (0.015%) | 0.0039 | (0.015%) |
| $\Gamma_\gamma$=111.00 meV | 0.77 | (0.69%) | 0.80 | (0.72%) | 0.77 | (0.69%) |
| $\Gamma_n$=1.7440 meV | 0.0542 | (3.11%) | 0.0550 | (3.15%) | 0.0545 | (3.13%) |

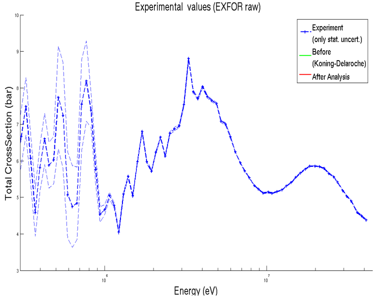
## Covariance matrices for group-average cross sections

Comparison of the point-wise and group-average $^{155}$Gd capture cross section as well as retroactive results provided by CONRAD (M-RLSF), SAMMY (RLSF) and REFIT (MC-RLSF).



## $^{208}Pb$ *test case description*



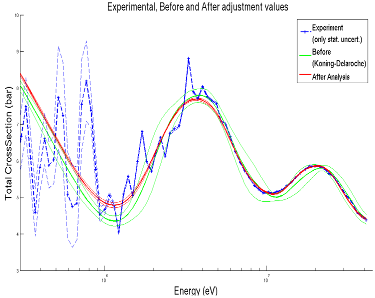



For this work :

- Raw Datas from EXFOR
- Koning-Delaroche Optical potential (with 5% uncertainty on parameter)

## $^{208}Pb$ test case description



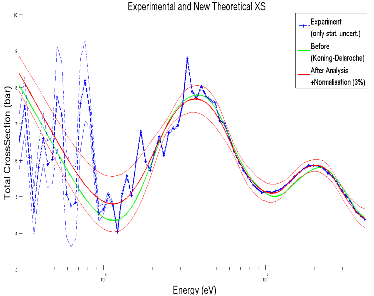



For this work :

- Raw Datas from EXFOR
- Koning-Delaroche Optical potential (with 5% uncertainty on parameter)
- adjust major parameters on experiment (only stat. uncert.)

## $^{208}Pb$ test case description



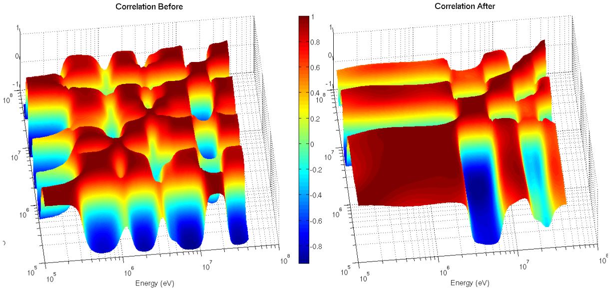



For this work :

- Raw Datas from EXFOR
- Koning-Delaroche Optical potential (with 5% uncertainty on parameter)
- adjust major parameters on experiment (only stat. uncert.)
- adjust major parameters on experiment + marginalization of normalization (3%)

## $^{208}Pb$ test case description



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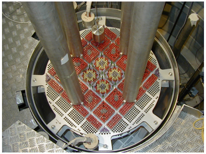
## Integral experiment ?



- international benchmark ICSBEP,
- analytic experiments on reactor mock-up (EOLE, MASURCA,...)



- clear reactor irradiations (PHENIX)

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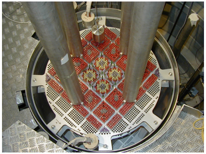

- clear reactor irradiations (PHENIX)

*Not all experiments are good candidates :*

- well described experiment : C/E discrepancies targeted

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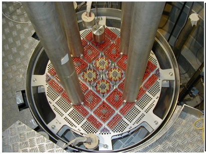
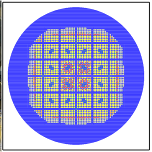




- clear reactor irradiations (PHENIX)

*Not all experiments are good candidates :*

- well described experiment : C/E discrepancies targeted
- experiment must be properly calculated :
  - bias calculated (C/C')
  - sensitivity coefficients available

## Information related to Integral experiments



- From the experiment : $I_E$ and $\delta_E$,
- From the calculation with first order approximation :

$$I = I_0 + \sum_i \frac{\partial I}{\partial \vec{\sigma}_i} \cdot (\vec{\sigma}_i - \vec{\sigma}_i^0) \text{ and } \vec{S}_i = \frac{\partial I}{\partial \vec{\sigma}_i} \cdot \frac{\vec{\sigma}_i^0}{I_0}$$

**Additional term in the cost function :**

$$(\vec{x} - \vec{x}_m)^T M_x^{-1} (\vec{x} - \vec{x}_m) + ... + ((I_E - I)/\delta_E)^2$$

Adjustment process needs gradient of I with respect to the $\vec{x}_m$ parameter set :

$$\frac{\partial I}{\partial \vec{x}_m} = \sum_i \frac{\partial I}{\partial \vec{\sigma}_i} \cdot \frac{\partial \vec{\sigma}_i}{\partial \vec{x}_m}$$

## Application to $^{239}Pu$



- $^{239}$Pu nuclear data accuracy is an important issue for reactor applications
- keff analysis of Pu-fuelled systems showed systematic overestimation of the calculated core reactivity.

| EOLE mock-up | Plutonium Aging | Moderation Ratio (or Void Fraction) | (C-E) ± (δE) (pcm) |
|---|---|---|---|
| MH1.2 (PWR-MOx mixed core) | 4 years | MR=1.2 | 280 ± 250 ($1\sigma_{T4}$=20pcm) |
| MISTRAL-2 (PWR-MOx) | 8 years | MR=1.7 | 630 ± 250 ($1\sigma_{T4}$=20pcm) |
| MISTRAL-3 (PWR-MOx) | 10 years | MR=2.1 | 710 ± 250 ($1\sigma_{T4}$=20pcm) |
| BASALA-Hot (BWR-MOx) | 12 years | 42% void | 610 ± 250 ($1\sigma_{T4}$=20pcm) |
| BASALA-Cold (BWR-MOx) | 13 years | 0% void | 700 ± 250 ($1\sigma_{T4}$=20pcm) |
| FUBILA-Hot (BWR-MOx) | 1 year | 0% void | 250 ± 250 ($1\sigma_{T4}$=20pcm) |

- first paper at ND2007 to propose modification on cross sections (as well as the modification of the mean number of fission neutrons).

## Measurements involved for this paper



### Isothermal Temperature Coefficient

- driven by Moderator Temperature Coefficient: MTC
- 100%-MOx cores in the EOLE facility in cold (20$^o$C-80$^o$C) and hot operation conditions (150$^o$C-300$^o$C).

### Analysis with APOLLO2 code

- a systematic underestimation of the MTC in cold conditions by about (-2.0$\pm$0.3)pcm/$^o$C,
- a well-assessed MTC in hot conditions (+1.0$\pm$2.0)pcm/$^o$C.

Related to sub-thermal and thermal shapes of the plutonium cross sections.

Focus on the negative resonances and the first positive resonance (at 0.3eV).

## A posteriori $^{239}Pu$ uncertainties estimations



### A Priori

In the previous estimation we choose

- JEFF3.1 + a negative resonance added at -20meV : $\vec{x}_0$
- **NO covariance** $M_x^0$

### Estimation of a-priori with CONRAD

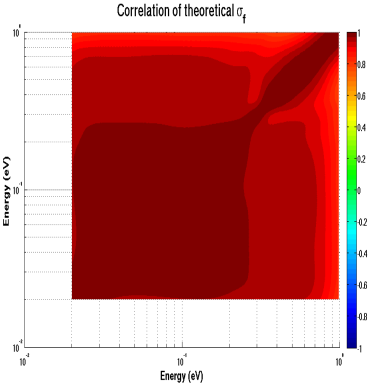
The following experiments were taken into account :

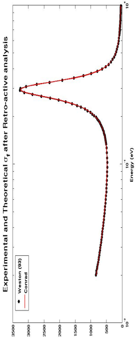
- Weston-1993 fission (add syst. uncert. of 0.6%).
- Gwin-1971 capture (assumed 1% stat. and 3% of syst. uncert.)

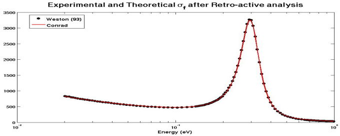
Analysis was performed on the [0eV,3eV] energy domain

# Estimation of a-priori with CONRAD






Conrad

## Results of the adjustment on integral experiment



### Parameter Estimation

- $E = -15.00$meV,
- $\Gamma_\gamma = 6.06$meV,
- $\Gamma_{f1} =$ -31.30meV

$\sigma_{th}$ : values($\Delta$ JEFF3.1)

- $\sigma_f$ : 746.74 b ($_{-0.91\text{ b}}$)
- $\sigma_c$ : 273.18 b ($_{+2.54\text{ b}}$)

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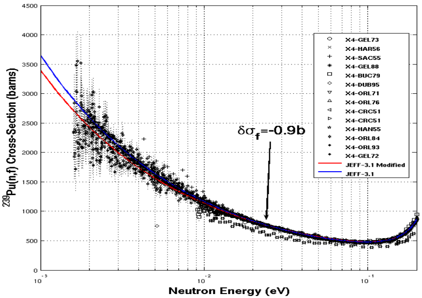

## Results of the adjustment on integral experiment



### MTC discrepancies :

| Experiment | C-E (pcm/°C) | | |
|---|---|---|---|
| (pcm/°C) | JEFF2.2 | JEFF3.1 | This work |
| -15± 0.3 | -2.0 | -1.87 | -1.54 |

MTC discrepancy still too large, $^{239}$Pu thermal shape not enought.

### Conclusion :

- slight improvement of the data
- covariance matrix on the parameters.

## *Marginalization :*

- can be applied in nuclear data evaluation work
- analytic algorithms implemented in CONRAD consistent with SAMMY as well as with Monte-Carlo approaches.
- experimental conditions well reproduced : necessary ingredients for a retroactive approach.

## *Integral experiments :*

- clear integral experiment can/should be used in the evaluation process
- best practises should be used and described
- interaction reactor physicists / nuclear data evaluators should :
  - append in a clear mathematical framework
  - be as far as possible automatic
  - associated with validation benchmarks to avoid non-expected discrepancies

CEA-Cadarache : use of both methodology with Conrad

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- G. Arbanas et al., in Proceedings of PHYSOR-2006 Topical Meeting on Reactor Physics, Vancouver, Canada, 2006 (American Nuclear Society, 2006).
- G. Noguere et al., Nucl. Sci. Eng. 160, 108 (2008).
- C. De Saint Jean et al., Nucl. Sci. Eng. 161, 363 (2009).