Uncertainty Evaluation of Nuclear Reaction Model Parameters using Integral and Microscopic Measurements Covariances Evaluation with CONRAD Code

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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 σ_g

Nuclear reactions models in Conrad

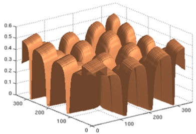
- Resolved resonance range (MLBW,Reich-Moore,..),
- Unresolved resonance range (average R matrix)
- Statistical models (Hauser-Feshbach, Moldauer, GOE,...)
- Continuum (ECIS and TALYS wrapper)

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

Covariance ?

Goals of Covariances Estimations :

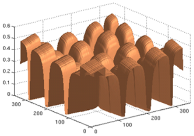
- understanding of experiments

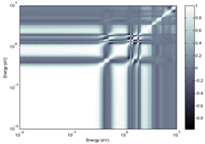


Covariance ?

Goals of Covariances Estimations :

- understanding of experiments
- knowledge of nuclear reaction models and cross sections
- feed Evaluated Nuclear Data Files (ENDF,JEFF,...)





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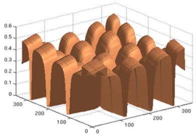
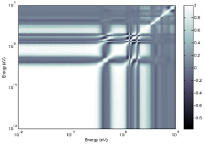
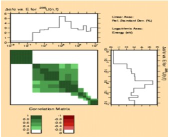


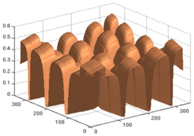


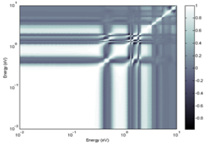


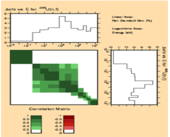
Covariance ?

Goals of Covariances Estimations :

- understanding of experiments
- knowledge of nuclear reaction models and cross sections
- feed Evaluated Nuclear Data Files (ENDF,JEFF,...)
- inputs for applications (reactor physics, fusion, protection, etc ...)
- focusing on nuclear reaction model parameters or cross sections







Covariance ?

Recurrent puzzle :

- take into account ALL uncertainties (including experimental ones) and propagate to
  - nuclear reaction model parameters
  - or cross sections ...
- mass production techniques developed for adding uncertainty information in Evaluated Nuclear Data Files
- low fidelity covariances,
- 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;20MeV] :

Phenomenological 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 : $E_\lambda, \gamma_\lambda^i, R_{eff}, \ldots,$
- Unresolved Resonance Range : $D_0, < \Gamma^i >, R_{eff}, \ldots,$
- Higher energies : Optical model parameters

- parameters used to calculate cross sections covariances.
- Data assimilation technique to estimate the parameters : use of Experiments
- thus ⇒ experimental parameters (with uncertainties)

How to 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) : no experiment during uncertainty analysis
- 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 = $< B > \pm \delta B$

Peele's pertinent puzzle

When ? How ?

- Appears when a full experimental covariance matrix (with systematic uncertainty) is used
- Peele noticed that the minimization of the a least square function could lead to abnormally low results.
- Observation on the ^{239}Pu capture cross section

Analysis of 1st ^{239}Pu resonance with Gwin capture measurement$^{(1971)}$

- data are used until 1 eV,
- no uncertainty in the base EXFOR,
- we chose to associate with this measure a 1% statistical uncertainty and 3% of systematic uncertainty on normalisation,
- adjusted parameters : energy, radiative and neutronic widths.

Peele's pertinent puzzle

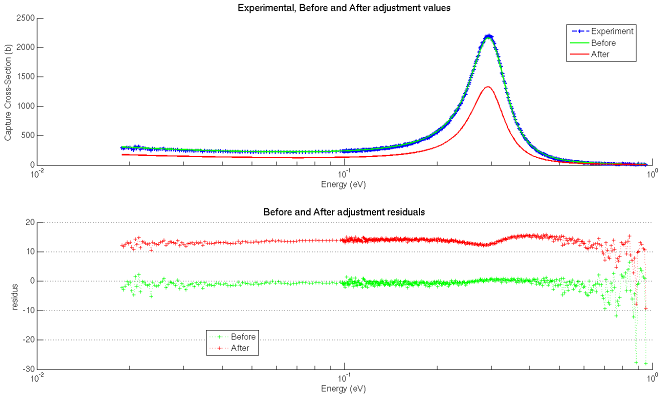


Figure: ^{239}Pu capture cross section (before and after adjustment) and residuals.

Solution : Marginalization

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 the CONRAD code :

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

Analytical marginalization equation :

Additional hypothesis : pdf are gaussians.

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

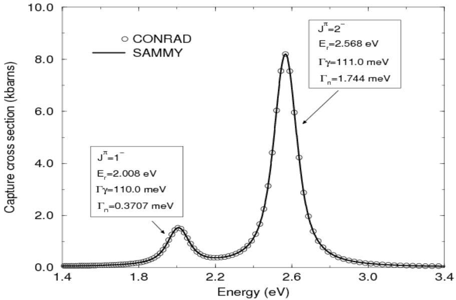
where G is the theoretical derivative matrix : $G = \begin{pmatrix} G^x \\ G^\theta \end{pmatrix}$

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



For this work, we have selected 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,γ) reaction. The analysis is restricted to a small energy range between 1.4 eV and 3.4 eV.

Virtual experiment

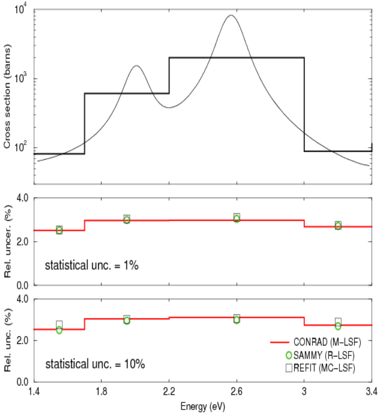
Comparisons of various techniques

Comparison of the uncertainties provided by the analytic and stochastic for a 3% normalization marginalization.

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%)
Γ_γ=110.00 meV	0.12	(0.11%)	0.37	(0.34%)	0.37	(0.34%)
Γ_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%)
Γ_γ=111.00 meV	0.09	(0.08%)	0.18	(0.16%)	0.16	(0.14%)
Γ_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%)
Γ_γ=110.00 meV	0.49	(0.45%)	0.60	(0.57%)	0.60	(0.54%)
Γ_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%)
Γ_γ=111.00 meV	0.39	(0.35%)	0.43	(0.38%)	0.41	(0.34%)
Γ_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%)
Γ_γ=110.00 meV	0.96	(0.86%)	1.02	(0.93%)	1.03	(0.94%)
Γ_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%)
Γ_γ=111.00 meV	0.77	(0.69%)	0.80	(0.72%)	0.77	(0.69%)
Γ_n=1.7440 meV	0.0542	(3.11%)	0.0550	(3.15%)	0.0545	(3.13%)

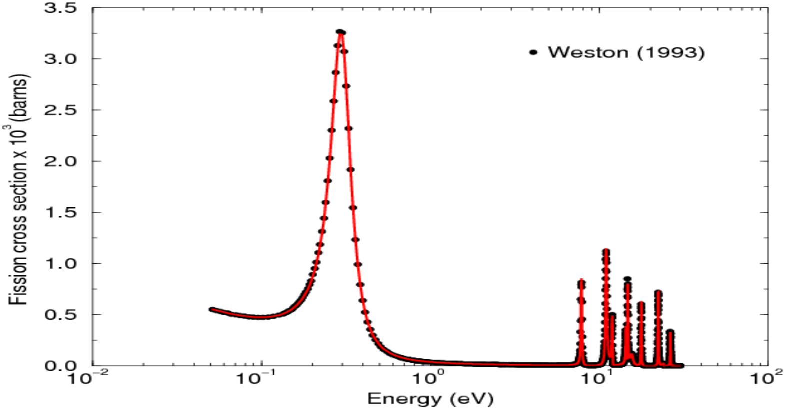
Covariance matrices for group-average cross sections

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).



On going work in RRR and URR

- ^{155}Gd whole resonance range
- ^{239}Pu 0eV-30eV region analysis with marginalization (capture+fission+transmission)



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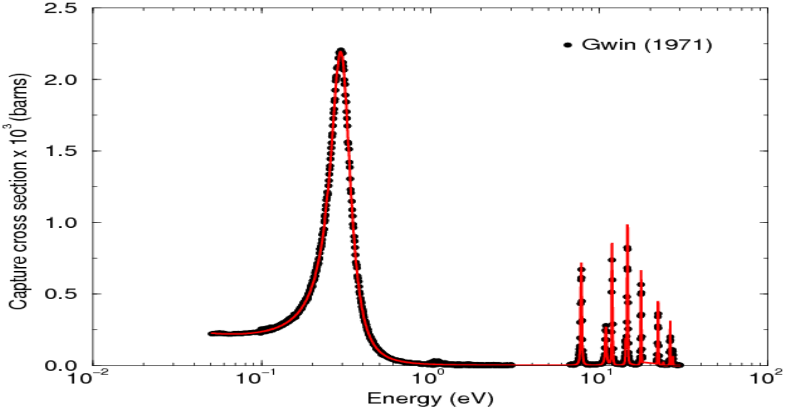

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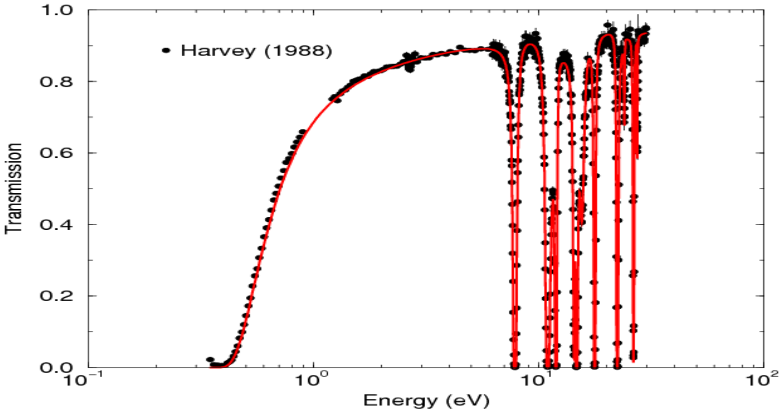

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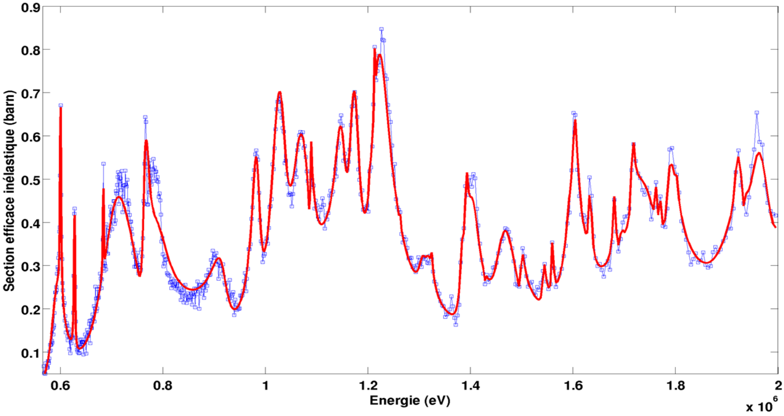
- ^{23}Na whole resonance range + inelastique



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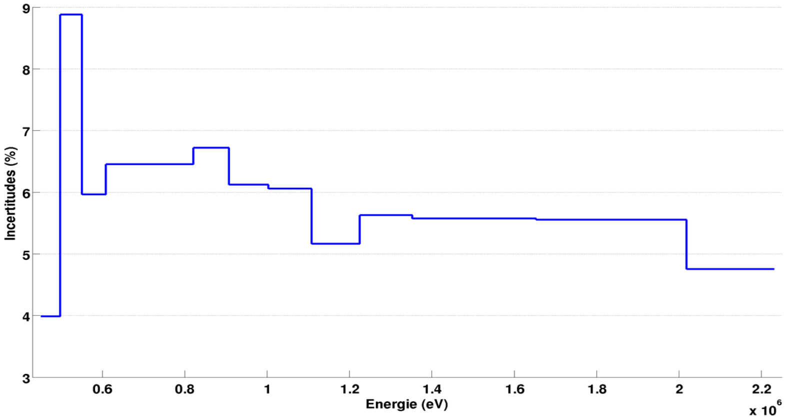


Conrad and Optical Model Calculation

RIPL Optical Potential : users point of view

- difficult to handle, link to physics ?
- how to define varying parameters with uncertainties ?
- ....a lot of zeros !!!!
- example of ^{208}Pb :

```
   0.001  200.0000
 82   82
208  208
  0     0    1    1    0
  1
 200.000
   1.24400  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0
            0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0
   0.64600  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0
            0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0
  50.60000  0.00000+0  6.90000-3  0.00000+0  1.50000-5  0.00000+0  7.00000-9
            0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0
            0.00000+0  0.00000+0  0.00000+0  0.00000+0 -5.65000+0  0.00000+0
            0.00000+0  0.00000+0  0.00000+0  0.00000+0  1.00000+0  0.00000+0
  1
 200.000
   1.24400  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0
            0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0
   0.64600  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0  0.00000+0

  etc ......
```

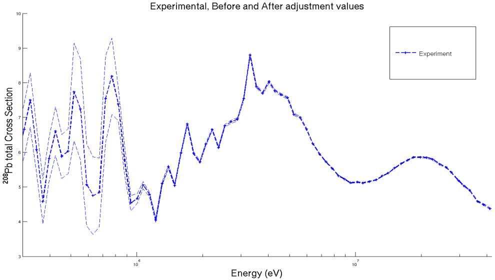
Conrad and Optical Model Calculation

Conrad wrapping ECIS :

- readeable, link to OMP energy dependence
- possible to define varying parameters with uncertainties
- example of ^{208}Pb :

```
[/Theory/NuclearModel]
   NuclearModelType = "ecis"
[/Theory/OpticalModel]
   OpticalModelType = "KoningDelaroche"
   EFermi = -5.65219
   Idr = 0
[/Theory/OpticalModel/RealVolume]
   r_0 = 1.244 +/- 0.0622 *CONSTANT*
   a_0 = 0.646 +/- 0.0323 *FITTED*
   p_0 = 50.6 +/- 2.53 *FITTED*
   p_2 = 0.0069 +/- 0.000345 *FITTED*
   p_4 = 1.5e-05 +/- 7.5e-07 *CONSTANT*
   p_6 = 7e-09 +/- 3.5e-10 *CONSTANT*
   p_17 = -5.65 +/- 0.2825 *CONSTANT*
[/Theory/OpticalModel/ImagVolume]
   p_0 = 15.6 +/- 0.78 *FITTED*
   p_2 = 88 +/- 4.4 *FITTED*
[/Theory/OpticalModel/ImagSurface]
   r_0 = 1.246 +/- 0.0623 *CONSTANT*
   a_0 = 0.51 +/- 0.0255 *FITTED*
   p_0 = 13.8 +/- 0.69 *FITTED*
   p_1 = 0.018 +/- 0.0009 *FITTED*
   p_5 = 13.8 +/- 0.69 *FITTED*
etc .....
```

^{208}Pb test case description



For this work :

- Raw Datas from EXFOR

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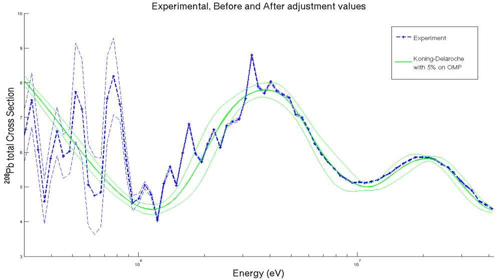

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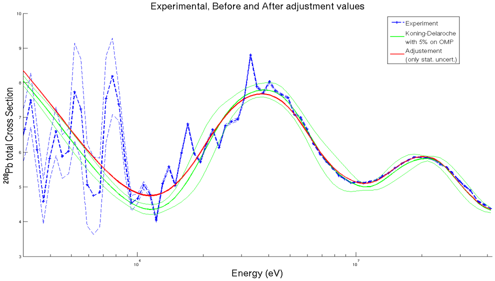

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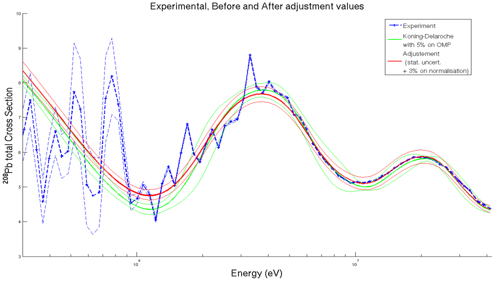

For this work :

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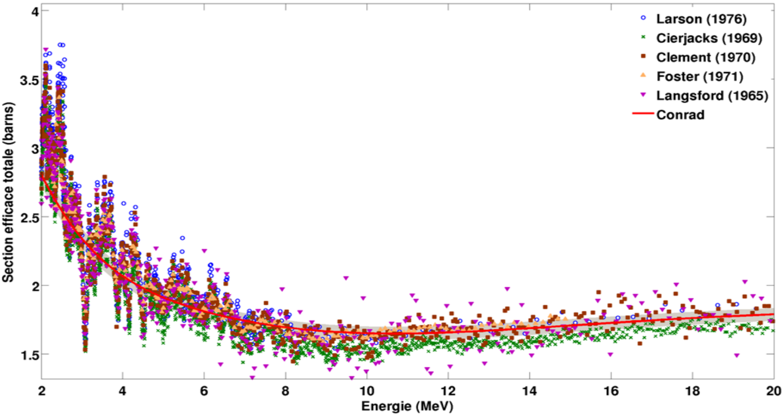
- adjust major parameters on experiment (only stat. uncert.)
- adjust major parameters on experiment + marginalization of normalization (3%)

On going work in Continuum

- ^{23}Na



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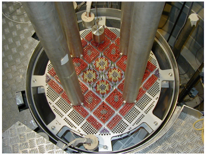
- Integral experiments !

Integral experiment ?

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



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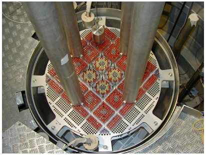

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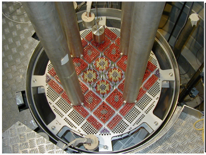
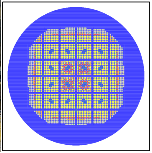

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Not all experiments are good candidates :

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

Information related to Integral experiments

Original Information from Microscopic experiments

- the analysis of microscopic experimental set $\vec{y}$ is performed "giving" the following cost function :

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

Additional Information from Integral experiments

- $\vec{y} \rightarrow \vec{E}$: vector of size N_E = Number of Integral Experiments
- M_E is then experimental covariance matrix
- $\vec{t} \rightarrow \vec{C}$: vector of size N_E = Number of Integral Experiments

$\vec{E}$ is a set of measurements which is related to cross sections (k_{eff}, ...) and $\vec{C}$ its associated set of calculated values (from neutronic codes, for example ERANOS, APOLLO2, TRIPOLI-4,...).

The treatment of Integral experiments

The solution is to mix both microscopic and integral measurements in the same generalized least square :

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

$\vec{y}$ beeing the set of microscopic experiments and $\vec{E}$ the set of integral experiments.

To implement previous equations, one has to calculate the gradient of $\vec{C}$ with respect to the $\vec{x}$ parameter set (nuclear reaction model parameters):

$$G(i,j) = \frac{\partial C_i}{\partial x_j}$$

The treatment of Integral experiments

Three different methods are implemented in the CONRAD framework to calculate the derivative matrix G :

- the low fidelity method, where G will be called G_{lf},
- the coupled method, where G will be called G_{cc},
- the reference or exact method, where the derivative matrix will be denoted as G_{ref}.

The treatment of Integral experiments: reference method

Assuming that there are N_x parameters and N_E integral values, we will create $(2N_x + 1)$ evaluations from CONRAD calculations for the reference method :

- one based on the values of the parameters set $\vec{x}$ used to calculate $\vec{C}$,

Then, for each parameter x_j from $\vec{x}$, we will create two evaluations based :

- on the parameters vectors $\vec{x}_{+\delta x_j} = \{x_0, \ldots, x_j + \delta x_j, \ldots, x_{N_x}\}$
- and $\vec{x}_{-\delta x_j} = \{x_0, \ldots, x_j - \delta x_j, \ldots, x_{N_x}\}$.

With $\vec{x}_{+\delta x_j}$ and $\vec{x}_{-\delta x_j}$, we can calculate $\vec{C}^{+\delta x_j}$ and $\vec{C}^{-\delta x_j}$ Finally, the derivative matrix G_{ref} for the reference method is described as:

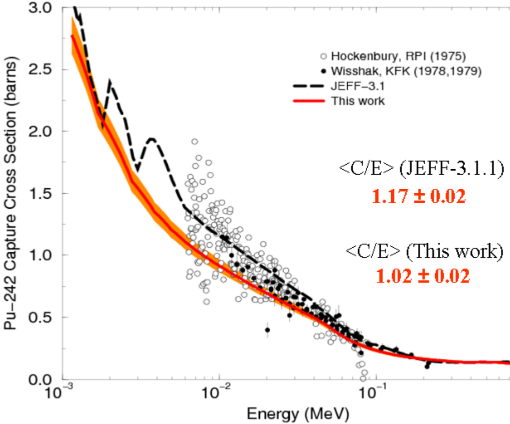
$$G_{ref}(i,j) = \frac{\partial C_i}{\partial x_j} \simeq \frac{C_i^{+\delta x_j} - C_i^{-\delta x_j}}{2\delta x_j}$$

- Major drawback : very time consuming because $(2N_x + 1) \cdot N_E$ neutronic calculations needed
- Advantages : accuracy and can be applied with both deterministic and Monte Carlo codes.
- Challenges : from nuclear reaction parameters to neutronic calculation via nuclear data treatment

Application to ^{242}Pu

- Profil experiments (irradiation in Phenix reactor) give highly fruitful information on capture cross section of minor actinides and several fission products.
- in several samples, $\frac{^{243}Am}{^{242}Pu}$ concentration ratio gives C/E big descrepancies

Isotopic Ratio	Sample	PROFIL C/E-1 (%)	PROFIL-2 C/E-1 (%)
$^{234}U/^{235}U$	^{235}U	-2.1 ± 1.6	0.0 ± 0.4
$^{235}U/^{238}U$	^{235}U	1.1 ± 4.8	0.0 ± 0.4
$^{236}U/^{235}U$	^{234}U		0.5 + 0.4
	^{235}U	0.4 + 0.2	0.4 + 0.1
$^{239}Pu/^{238}U$	^{235}U	0.8 ± 0.8	
	^{238}U	1.1 ± 0.3	2.3 ± 0.2
$^{237}Np/^{238}U$	^{238}U		-6.7 ± 2.9
$^{240}Pu/^{239}Pu$	^{238}U	0.1 ± 0.1	−2.2 ± 0.6
	^{239}Pu	−2.1 ± 0.2	−2.3 ± 0.1
$^{238}Pu/^{239}Pu$	^{239}Pu	-19.1 ± 4.1	-26.7 ± 12.6
$^{239}Pu/^{238}Pu$	^{238}U	1.9 ± 0.8	3.5 ± 0.1
$^{241}Pu/^{240}Pu$	^{239}Pu	4.4 ± 1.1	3.6 ± 0.4
	^{240}Pu	5.2 ± 0.5	3.9 ± 0.6
$^{242}Pu/^{241}Pu$	^{240}Pu	16.6 ± 2.7	11.5 ± 2.9
	^{241}Pu	9.3 ± 0.7	
$^{243}Am/^{242}Pu$	^{242}Pu	20.9 ± 1.8	14.7 ± 2.8
$^{238}Pu/^{237}Np$	^{237}Np		-6.0 ± 1.3
$^{242m}Am/^{241}Am$	^{241}Am	8.7 ± 1.9	7.6 ± 0.2
$^{238}Pu/^{241}Am$	^{241}Am	5.5 ± 1.6	10.7 ± 1.9
$^{242}Pu/^{241}Am$		6.3 ± 1.5	9.7 ± 2.6
$^{242}Cm/^{241}Am$		4.5 ± 1.2	
$^{244}Cm/^{243}Am$	^{242}Pu	0.0 ± 6.7	
$^{245}Cm/^{244}Cm$	^{244}Cm		-2.6 ± 0.3
$^{233}U/^{232}Th$	^{232}Th		-16.4 ± 7.6
$^{234}U/^{233}U$	^{233}U		-8.5 ± 0.1
$^{235}U/^{234}U$	^{233}U		2.8 ± 1.9
	^{234}U		3.1 ± 0.2



Experimental systematic uncertainties :

- peele's pertinent puzzle appears with full experimental matrix
- marginalization can/must be applied in nuclear data evaluation work
- experimental conditions must be well reproduced : necessary ingredients.

Fast range covariance :

- fast range treatment is equivalent to other energy ranges (RRR) : use parameters as vector of uncertainties

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
  - needs modern tool to establish direct link between nuclear models and neutron transport codes

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