The use of Integral experiments to improve neutron induced cross sections. Mathematical description of CEA activities for Multigroup cross section adjustment and beyond

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SG33 Meeting, Issy-Les-Moulineaux, 2010 June

CEA history with multigroug cross section

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When ? What ? How ?

- In the 70's and 80's, in particular at CEA-Cadarache, physicists decided to use integral experiments to assess multigroup cross sections uncertainties by using adjustment procedure,
- The library ERALIB1 used with the ERANOS system is the result of this methodology,
- Description of the mathematical framework used at that time to take into account properly the information coming from integral experiments done on reactor mock-up or simple integral experiments (e.g. ICSBEP)
- Propose new solutions (beyond multigroup).

General Theory of parameter estimation

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- $\vec{y} = \overrightarrow{y_i}$ $(i = 1 \ldots N_y)$ denote some experimentally measured variables,
- $\vec{x}$ denote the parameters defining the model used to simulate theoretically these variables
- $\vec{t}$ the associated calculated values to be compared with $\vec{y}$.

Using Bayes' theorem and especially its generalisation to continuous variables, one can settle the following relation between conditional probability density functions (written p(.))

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 $p(\vec{x}|\vec{y}, U)$

Deterministic Theory

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To solve this problem, one has to make some assumptions on the prior probability distribution involved.

- Maximum entropy principle : given a covariance matrix and mean values, the choice of a multivariate joint normal for the probability density $p(\vec{x}|U)$ is maximizing the entropy,
- same idea for the likelihood $p(\vec{x}|\vec{y}, U)$,
- Laplace approximation : posterior distribution has same maximum adn curvature than a gaussian.

Generalized χ^2_{GLS}

If the expectation and covariance matrix are $\vec{x}_m$ and M_x, the evaluation of posterior expectation and covariances are done by finding the minimum of the following cost function (a generalized least-square) :

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

Traditional Multigroup cross section adjustment

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In this section, the $\vec{x}$ parameters are indeed the multigroup cross sections themselves.
With the following change in notations :

- $\vec{x} \rightarrow \vec{\sigma}$: vector of size N_σ= Number of Isotopes $\times$ Number of Reactions $\times$ Number of energy groups
- M_σ is the a priori covariance matrix on multigroup cross sections.
- $\vec{y} \rightarrow \vec{E}$: 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,...).

χ^2_{GLS} for multigroup adjustment

The generalized least-square may be written as follows :

$$\chi^2_{GLS} = (\vec{\sigma} - \vec{\sigma}_m)^T M_\sigma^{-1} (\vec{\sigma} - \vec{\sigma}_m) + (\vec{E} - \vec{C}(\sigma))^T M_E^{-1} (\vec{E} - \vec{C}(\sigma))$$

Information related to integral experiments simulation

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Using a first order approximation, one can write :

$$\vec{C}(\sigma) = \vec{C}(\sigma_m) + S \cdot (\vec{\sigma} - \vec{\sigma_m})$$

S is a matrix (size $N_E \times N_\sigma$) of calculated derivatives supposed to be constant (when the cross-sections slighly change) :

$$S_{ij} = \frac{\partial C_i}{\partial \sigma_j}$$

Most of the time, S is referred to sensitivities :

$$S_{ij} = \frac{\partial C_i}{\partial \sigma_j} \cdot \frac{\sigma_j}{C_i}$$

Implemented mathematical solutions

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The first order solution most of the time used is given by :

$$\vec{\sigma} - \vec{\sigma}_m = M_\sigma \cdot S^T \left(M_E + S \cdot M_\sigma \cdot S^T \right)^{-1} \cdot \left(\vec{E} - \vec{C}(\sigma_m) \right)$$

For the posterior covariances on the multigroup cross sections, one obtains :

$$M_\sigma{}' = M_\sigma - M_\sigma \cdot S^T \left(M_E + S \cdot M_\sigma \cdot S^T \right)^{-1} \cdot S \cdot M_\sigma$$

Major drawbacks

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- N_σ= Number of Isotopes × Number of Reactions × Number of energy groups : a lot of parameters
- M_σ is the a priori covariance matrix on multigroup cross sections : comming from ?
- $\vec{E}$, Integral Experiments experimental descriptions ?
- M_E is then experimental covariance matrix :correlations between integral experiments?
- $\vec{C}$: Bias related to calculated values
- dedicated multigroup libraries with condensed integral information : no clear definition of application domain
- macroscopic changes of cross sections :how to perform properly broad to finer energy meshes ?
- a lot of unexpected correlations : unphysical ?

New CEA Activities

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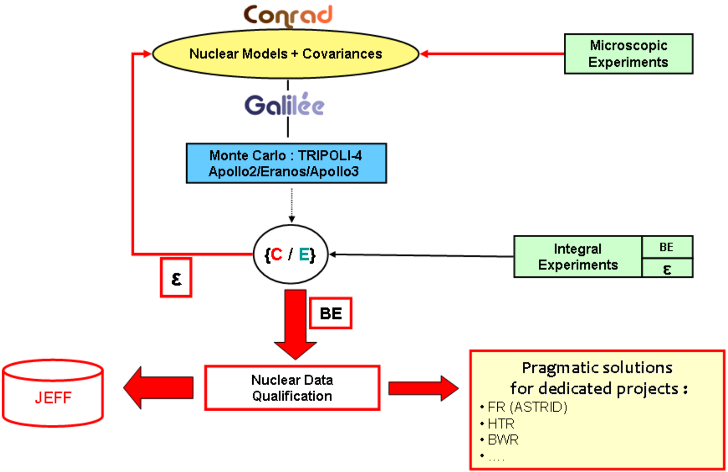

ϵ Integral experiment ?

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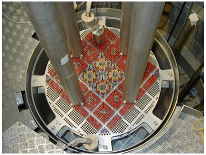
- international benchmark ICSBEP,
- analytic experiments on reactor mock-up (EOLE, MASURCA,...)



- clean reactor irradiations (PHENIX)

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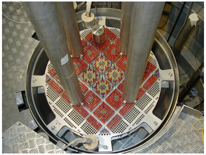

- clean reactor irradiations (PHENIX)

Not all experiments are good candidates :

- well described experiment : C/E discrepancies targeted

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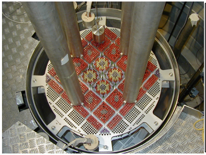
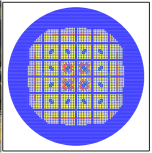
- analytic experiments on reactor mock-up (EOLE, MASURCA,...)





- clean 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

Integration of Integral experiments during the Evaluation process

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

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

$\vec{y}$ 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

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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

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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

Major initial Conditions :

- Nuclear data Evaluation work on Covariances prior
- Use reference codes (deterministic or Monte-Carlo)
- Re-analyse Integral experiments (C/E + δE).

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Integral Experiments

Nuclear Data Oriented

- clear integral experiment can/should be used in the evaluation process
- need interaction reactor physicists / nuclear data evaluators :
- need modern tools

Reactor Concept Oriented

- New covariances from Evaluation shows :
  - 1-5% on cross sections
  - long range correlations
  - $\Rightarrow$ 1000-2000 pcm!
- sg33 activities are thus necessary to :
  - establish a consistent benchmark exercise on multigroup adjustment,
  - use pragmatic solutions to reduce uncertainties