New frontiers and challenges for statistical data adjustment methods

M.Salvatores[a,b], G.Palmiotti[b], M.Hermann[c], H.Hiruta[b], P.Oblozinsky[c], M.T.Pigni[c]

[a]CEA-Cadarache; [b]Idaho National Laboratory; [c]Brookhaven National Laboratory

A new frontier: the consistent method

- The **major drawback** of the classical adjustment method is the **potential limitation of the domain of application** of the adjusted data since adjustments are made on **multigroup** data, and both the multigroup structure, the neutron spectrum and the code used to process the basic data file are significant constraints.

- It can be improved by "adjusting" **physical parameters and not multigroup nuclear data.**

- The objective is now to **correlate the uncertainties of some basic parameters** that characterize the neutron cross section description, to the discrepancy between calculation and experimental value for a large number of clean, **high accuracy integral experiments**.

- **In the past a few attempts were made to apply a consistent approach for improving basic nuclear data, in particular to inelastic discrete levels and evaporation temperatures data of Fe56 for shielding applications, and resolved resonance parameters (e.g. gamma and total widths, peak positions etc.) of actinide isotopes.**

- **Although these efforts demonstrated the validity of the approach, they clearly indicated a major drawback related to the way of getting the sensitivity coefficients and the reliability of the covariance data.**

- **Today both challenges can be dealt with and a consistent data assimilation approach becomes practical and feasible.**

The proposed strategy makes use of the product of explicit sensitivity matrices so that the sensitivities of integral experiments to fundamental parameters p_k are defined as:

$$\frac{\Delta R}{\Delta p_k} = \sum_j \frac{\Delta R}{\Delta \sigma_j} \times \frac{\Delta \sigma_j}{\Delta p_k}$$

where R is an integral reactor physics parameter (e. g. k_{eff}, reaction rates, reactivity coefficient, etc.), and σ_j a multigroup cross section (the j index accounts for isotope, cross section type and energy group) and p_k are the basic parameters.

Several experimental configurations and several integral experiments (e.g. k_{eff}, spectral indexes, reactivity coefficients etc) in each configuration can be used. The sensitivity coefficients:

$$\frac{\Delta R}{\Delta \sigma_j}$$

are provided by reactor physics calculations, using the adjoint method according to the Generalized Perturbation Theory.

The following steps are envisaged:

1- Selection of the appropriate reaction mechanisms along with the respective model parameters p_k to reproduce adopted microscopic cross section measurements with the EMPIRE code calculations.

- About 50 or more parameters for each isotope will be considered, including resonance parameters for a few dominating resonances, optical model parameters for neutrons, level density parameters for all nuclei involved in the reaction, parameters entering pre-equilibrium models, and parameters determining gamma-strength functions

2- Determination of covariance matrices for the set of nuclear reaction model parameters obtained in the previous step. This will be achieved by combining initial estimates of parameter uncertainties with uncertainties/covariances for the adopted experimental data.

- Sensitivity of cross sections to the perturbation of the above mentioned reaction model parameters can be calculated with the EMPIRE code in appropriate energy-group structures.

3- Use of the adjoint technique to evaluate sensitivity coefficients of integral reactor parameters to the cross section variations, as described in the previous step. To perform this task, the ERANOS code system can be used.

- Sensitivity coefficients based on generalized perturbation theory can be derived for almost all integral reactor parameters of interest (reactivity coefficients, critical mass, spectrum indexes, power distributions, delayed neutron fraction etc).

4- Perform Monte Carlo calculations of selected experiments

5- Perform consistent data assimilation on basic nuclear parameters using integral experiment analysis

- After the C/E's are available, they will be used together with the sensitivity coefficients coming from the previous step in a data assimilation code that will provide improved parameters for nuclear reaction theory

6- Feedback and checking of the parameters obtained in the previous step

The provisional list of isotopes (~25) of interest is:

Fe-56; Fe-54 …; Cr-52 … ; Ni-59 … ; Na-23; (O-16; C-12)

U-235; U-238; Pu-238; Pu-239; Pu-240; Pu-241; Pu-242

Am-241 ; Am-242 ; Am-243; Np-237; Cm-242; Cm-244; Cm-245

As far as tests, the following strategy is envisaged, with an increasing degree of complexity:

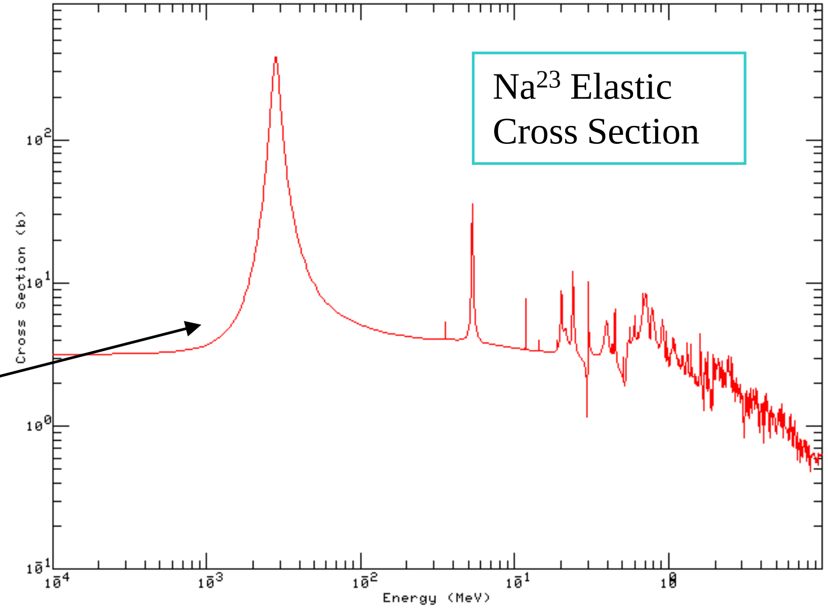
- **Apply the method to the analysis of a neutron propagation experiment in a single-isotope/material medium (e.g. adjustment on a single structural isotope, e.g. Na or Fe-56). This is underway.**
- **Apply the method to the analysis of the JEZEBEL plutonium sphere experiment (adjustment on a single fissile isotope: Pu239)**
- **Apply the method to the analysis of the ZPR-6 Ass. 6A (Enriched U) critical experiments (adjustment on a limited number of fissile and structural isotopes ~10)**

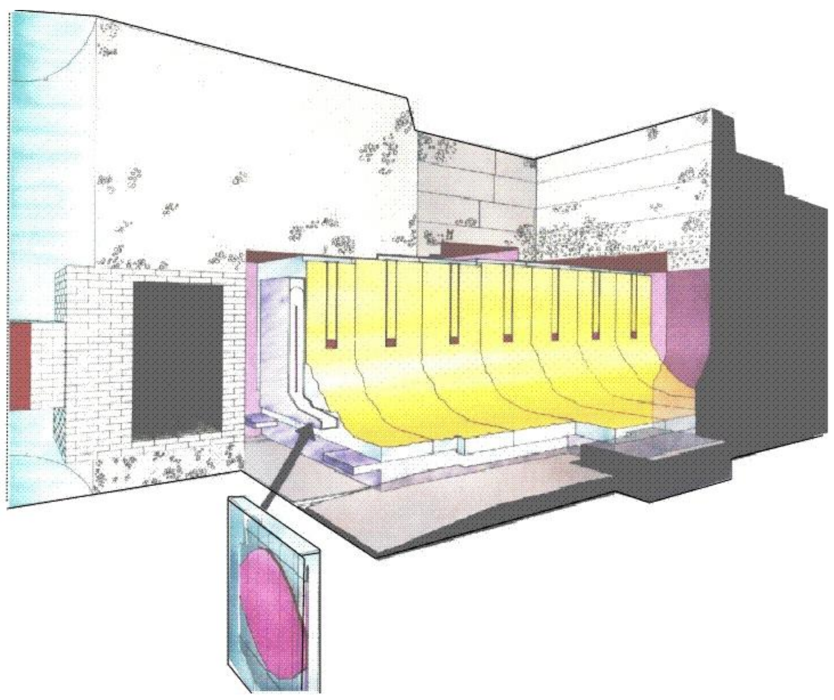
Consistent Data Assimilation: a first step

From Meters to Femtometers

A first attempt of consistent data assimilation is under way using neutron propagation experiments.

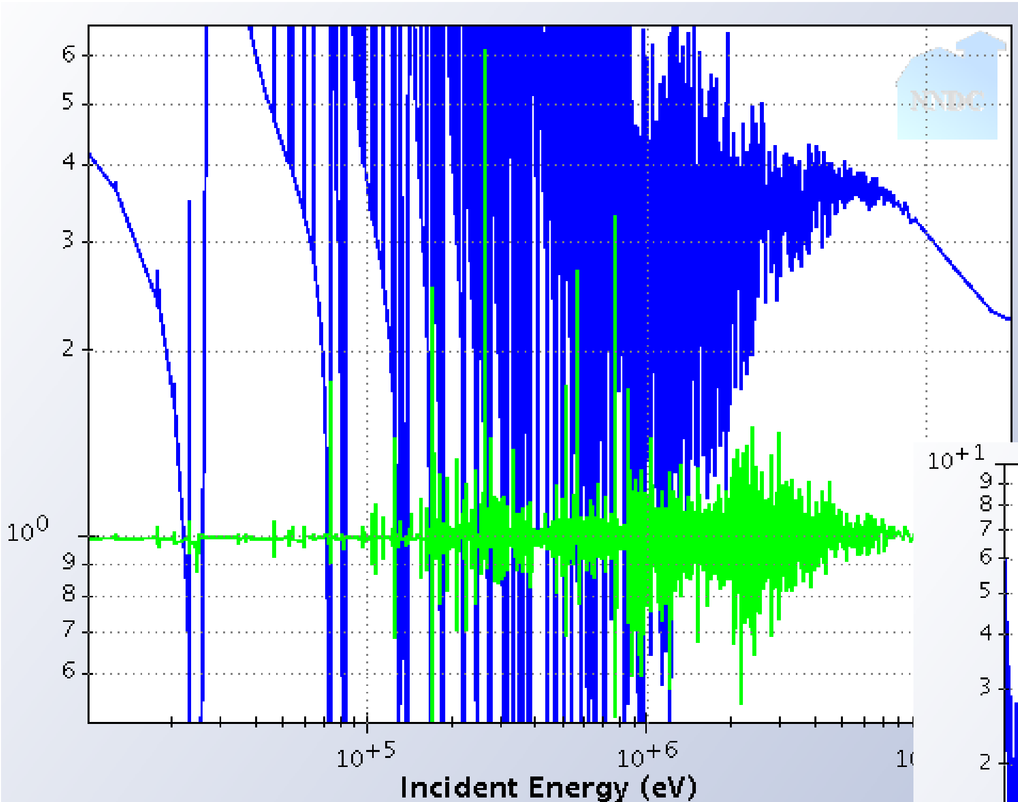
The parameters characterizing 10 major resonances of the sodium elastic cross section and 16 basic nuclear parameters (optical model) will be tuned using the C/E of reaction rates measured in the EURACOS experiment (propagation in 3 meters of sodium).





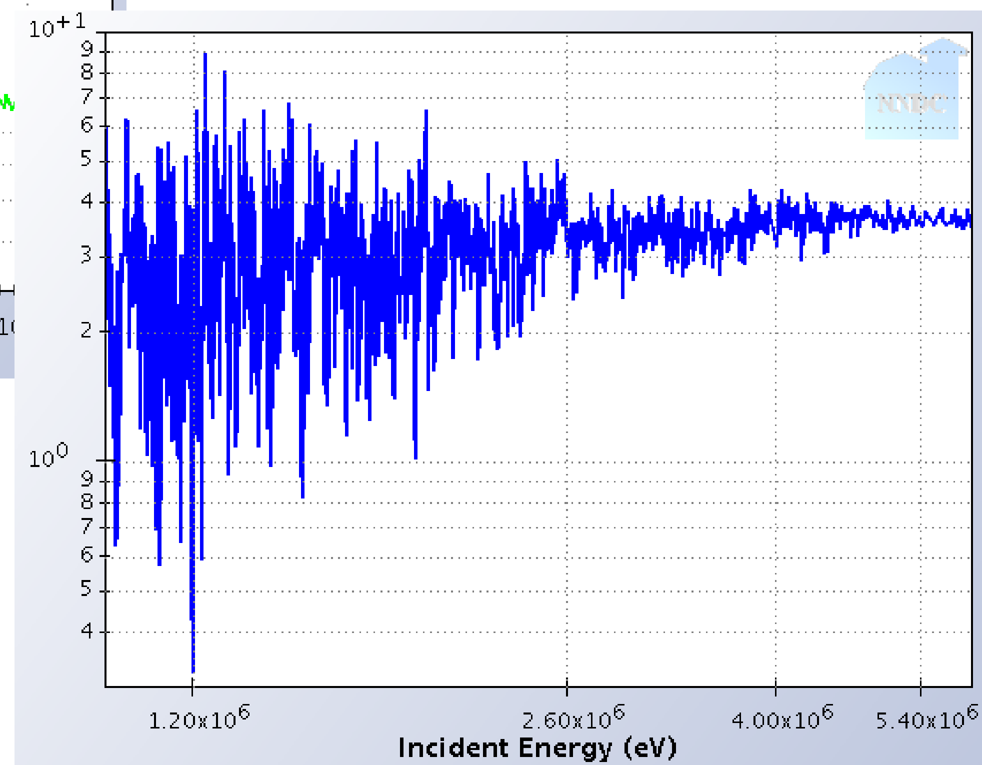
Next step can be a Fe-56 dominated experiment. More challenges foreseen…

56-Fe(n,tot): fluctuations up to 6 MeV



56Fe (n,tot) from ENDF/B-VII.0

Ratio to JENDL-3.3



In Summary:

It is the first attempt to build up a link between the wealth of precise integral experiments and basic theory of nuclear reactions.

A large amount of exceptionally precise integral measurements has been accumulated over last 50 years but these were not utilized for improving nuclear reaction theory and its parameterization.

Recent advances in reaction modeling and transport calculations, combined with the sensitivity analyses methods offer a possibility to obtain feedback on parameters of nuclear reaction models.

This approach is a unique opportunity to meet the objectives of "ab initio" modeling and advanced simulation.