Sensitivity analysis and cross sections data adjustment for multigroup transport and diffusion

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Abstract

Uncertainties in basic nuclear data and other quantities involved in the characterization of an experiment affect the accuracy of the results when the respective experiment is modelled. The impact of these uncertainties on computed responses can be assessed by combining the sensitivities of these responses to the input parameters with data uncertainties and covariances. Furthermore, best estimates of both the input parameters and recomputed responses, with reduced uncertainties, can be obtained by using data assimilation and adjustment procedures. This paper reports the results of using the data adjustment methodology in conjunction with the well-known Godiva experiment and a partial set of uncertainties from the ZZ-COV-15 library for U-235 and U-238, together with sensitivities computed with APOLLO transport code by the Adjoint Sensitivity Analysis Procedure, to obtain best-estimate values for the k eigenvalue of the system, with reduced uncertainties. In parallel, sensitivities were also computed using COBAYA diffusion code, compared with those produced by APOLLO, and then employed in the adjustment formalism to obtain the adjusted k eigenvalue and its corresponding reduced uncertainty.

1. Introduction

Transport equation numerical solution methods have achieved a good level of maturity, both in deterministic and stochastic versions, meaning that accuracies in the results yielded by the diverse methods are comparable to or lower than the error contained in the input parameters.

Additionally, experimentalists, in charge of the generation of the different cross sections data evaluations, accompany their results by increasingly better estimated uncertainties and covariances.

The level of accuracy reached with transport codes makes possible to combine measured results from integral experiments with numerical results from realistic models, so as to yield better values for the nominal values of the parameters, namely the cross sections, and for the associated uncertainties and covariances. Furthermore, the integral experiment values are also improved, and the uncertainty in the measurements can be reduced.

A sensitivities computation methodology for the diffusion equations based in the Adjoint Sensitivity Analysis Procedure (ASAP) (Cacuci et

al., 1980) has been implemented; and a generalized least squares fitting based in Bayesian inference principle has been applied to a very simple critical system using the computed sensitivities (Cacuci et al., 2007), showing the suitability of the methodology for neutronics problems.

2. Theoretical framework

2.1. Computation of sensitivities by ASAP

The ASAP permits to compute sensitivities of the desired responses to the input parameters and engages in a natural way with deterministic methods both theoretical and computationally. Combination of the first order Gâteaux derivative of the equation or operator considered, together with the relationship between the forward and adjoint operators through the scalar products defined in each subspace, allows avoiding the direct computation of the perturbation in the flux coming from perturbations in the input parameters. Adjoint system must then be solved with the appropriate external source; for instance, if the considered response is the k eigenvalue of the system, then the external source for the adjoint problem must be zero, and (1) is the resulting expression for the sensitivity in the case of the diffusion equation, where each of the effects of the different input parameters can be studied.

$$\delta k = \frac{\left(k^0\right)^2}{\left\langle \vec{\phi}^* \middle| \vec{\chi}^0 \cdot \sum_{\forall g'} \upsilon^{g'0} \cdot \Sigma_f^{g'0} \cdot \phi^{g'0} \right\rangle} \cdot \left[\begin{array}{l} \left\langle \vec{\phi}^* \middle| \nabla \cdot \left(\delta \vec{D} \cdot \nabla \vec{\phi}^0 \right) \right\rangle \\ - \left\langle \vec{\phi}^* \middle| \delta \vec{\Sigma}_a \cdot \vec{\phi}^0 \right\rangle \\ - \sum_{\forall g' \neq g} \left\langle \vec{\phi}^* \middle| \delta \vec{\Sigma}_s^{\rightarrow g'} \cdot \vec{\phi}^0 \right\rangle \\ + \sum_{\forall g' \neq g} \left\langle \vec{\phi}^* \middle| \delta \vec{\Sigma}_s^{g' \rightarrow} \cdot \phi^{g'0} \right\rangle \\ + \dfrac{\left\langle \vec{\phi}^* \middle| \delta \vec{\chi} \cdot \sum_{\forall g'} \upsilon^{g'0} \cdot \Sigma_f^{g'0} \cdot \phi^{g'0} \right\rangle}{k^0} \\ + \dfrac{\left\langle \vec{\phi}^* \middle| \vec{\chi}^0 \cdot \sum_{\forall g'} \left(\delta\upsilon^{g'} \cdot \Sigma_f^{g'0} \cdot \phi^{g'0} + \upsilon^{g'0} \cdot \delta\Sigma_f^{g'} \cdot \phi^{g'0} \right) \right\rangle}{k^0} \end{array} \right] \tag{1}$$

Where all the symbols are in standard notation, superscript 0 means nominal values and $\left\langle \vec{\phi}_1 \middle| \vec{\phi}_2 \right\rangle = \sum_{\forall g} \iiint_P \phi_1^g(\vec{r}) \cdot \phi_2^g(\vec{r}) d\vec{r}$ is the defined scalar product in the space of the multigroup fluxes. Similar results can be obtained for other typical responses, such as reaction rates or power levels.

2.2. Data adjustment by Bayesian generalized least squares

Bayesian inference principle can be used to combine new information, as the one obtained by numerical simulation of the experiment, with prior knowledge (Cacuci et al., 2007). The new information added leads to a reduction of uncertainties both in system responses and parameters, when the numerical simulation has a good degree of accuracy and the uncertainties have been correctly propagated from the input parameters to the output responses in the computational chain. The procedure involves minimizing the following quadratic objective function (2) subject to the constraints (3).

$$Q(x,y) = \begin{pmatrix} x^T & y^T \end{pmatrix} \cdot \begin{pmatrix} C_p & C_{pr} \\ C_{rp} & C_r \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \tag{2}$$

$$r_{be} = r_c(p_{be}) \approx r_c(p_0) + S \cdot (p_{be} - p_0) \qquad (3)$$

Where x is the difference between the best estimate parameters – referred with subscript be – , and their nominal values – referred with subscript 0 –, and y is the difference between the responses computed with those new parameters, namely the best estimate responses, and the responses computed with the nominal input values. C matrices stand for the covariances between all the values involved and S represents the sensitivities of the results to the input parameters.

3. Problem description

The benchmark model is based on a simplification of a series of experiments performed at LANL during the 50s'. A highly enriched bare uranium sphere denominated Godiva (*International handbook of evaluated criticality safety benchmark experiments,* 2006) is modelled and the k eigenvalue of the system is computed, this is the only response considered. The sphere is composed by 93.71 $^0/_w$ of U-235, 5.27 $^0/_w$ of U-238 and rest of U-234. Its radius is 8.7407 cm, its density is 18.74 g/cm^3 and the experiment was performed at a room temperature of 300 K.

The experiment was conducted with two hemispheres of uranium, one of which was approached to the other till criticality was observed. From that measurements and considering the uncertainties in the dimensions, real configuration and material compositions, Godiva benchmark experiment was defined with its associated uncertainties.

The cross sections used to numerically compute the k eigenvalue contain experimental errors or uncertainties, thus this value is affected by those errors. On the other side, the experimental value is 1.00000 with an uncertainty of ±0.001.

Both experimental and numerical results together with nominal cross sections' values and their uncertainties are used to improve the k eigenvalue estimation, the nominal cross sections, and the uncertainties of all of them, to a better estimation that improves experimental and numerical values.

4. Methodology

In order to obtain the necessary numerical uncertainty in the response, the method of propagation of errors is used. Thus the sensitivities of the k eigenvalue to the cross sections are also needed; these are computed by means of direct recomputations and of forward and adjoint fluxes using ASAP methodology (Cacuci, 2003).

The transport equation was solved by a 1D discrete ordinates method with a P1 approximation for the forward and adjoint equations with the APOLLO2 code (Sánchez et al., 1988) in a 172 energy groups structure. The transport solution was then collapsed to a 15 energy groups structure similar to the one used to provide the uncertainty data contained in the ZZ-COV-15 library (Kodeli, 2006) and homogenized cross sections, diffusion coefficients and interface discontinuity factors were generated with that energy structure.

Sensitivities were computed for the k eigenvalue from the transport solution to the fission cross section and the average number of neutrons per fission, or $\overline{\upsilon}$, for the Uranium 235 and 238 isotopes by recomputation in the given 172 structure and also applying first order perturbation theory, obtaining reasonable agreement. Sensitivities from recomputation were subsequently used.

A diffusion equation solution was also performed with the COBAYA3 code (Aragonés & Ahnert, 1986; Herrero et al., 2007) using the collapsed cross sections from the APOLLO2 computation to the given 15 energy groups structure, and the same sensitivities were computed by first order perturbation theory and compared to the sensitivities obtained with the same methodology by APOLLO2.

Uncertainty data was taken from the JENDL-3.3 evaluation for the 172 energy groups structure in a heuristic way; the change of the energy group structure in the uncertainty data was performed using ANGELO code (Kodeli, 2006) which performs a simple linear interpolation of variance and covariance data between different energy groups structures. On the other hand, uncertainty data for the diffusion computation in 15 energy groups was taken from the ZZ-COV-15 library using the IRDF02 values for the fission cross sections and the ENDF-VI.8 values for $\overline{\upsilon}$. This is in contrast with the use of cross sections from APOLLO2 associated cross section library based

on JEFF-2.2, which states the approximate character of the following results.

The BEST-EST code was then used to propagate uncertainties in the mentioned parameters to get the uncertainty in the response. This same code applied the mentioned Bayesian inference based technique to get the best estimate values for the response and the input parameters.

Thereafter, these best estimate values were used to solve again the transport and diffusion equations in order to assess the performance of the proposed methodology.

5. Numerical results

5.1. Direct and adjoint fluxes

It is of interest to compare the similarity in the direct and adjoint fluxes when they are obtained from a transport or a diffusion solution. In Figure 1, it can be seen the good agreement between the diffusion calculation in 15 energy groups corrected with interface discontinuity factors, and the transport solution collapsed to the same energy groups structure.

On the other hand, as shown in Figure 2, while the adjoint diffusion calculation mostly reproduces the adjoint profile from the transport solution, it does not match the importance levels in all the energy ranges which were arbitrarily normalized to the level of the last energy group.

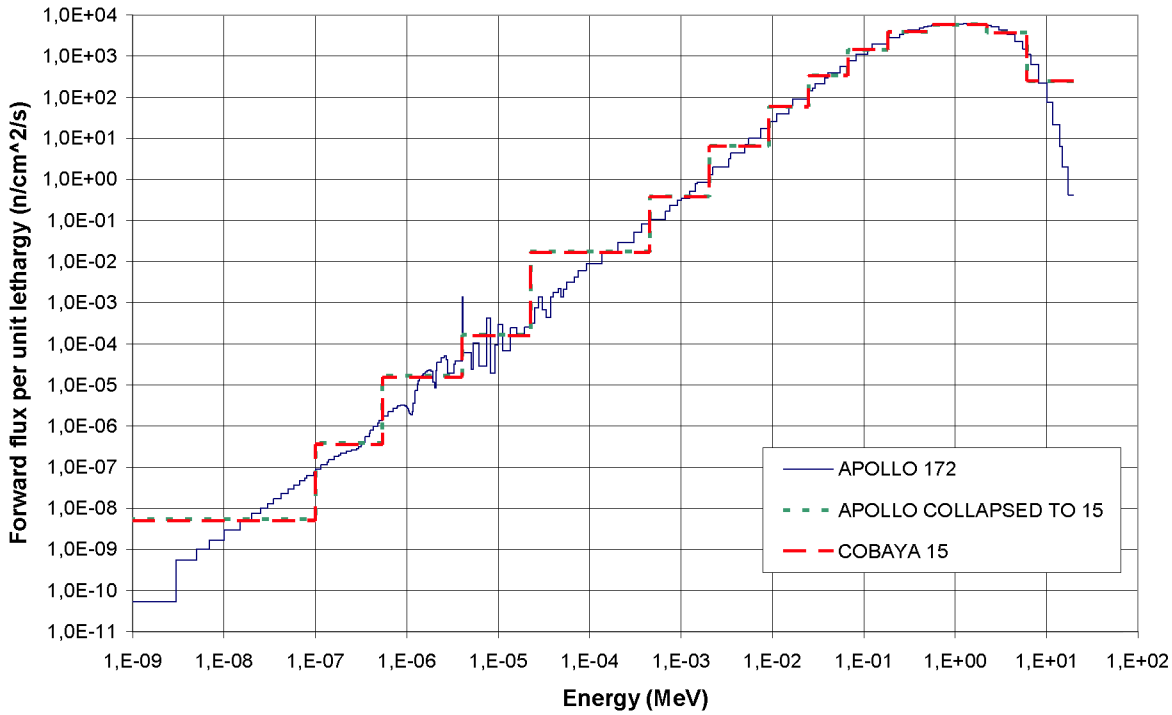

Figure 1. Forward fluxes

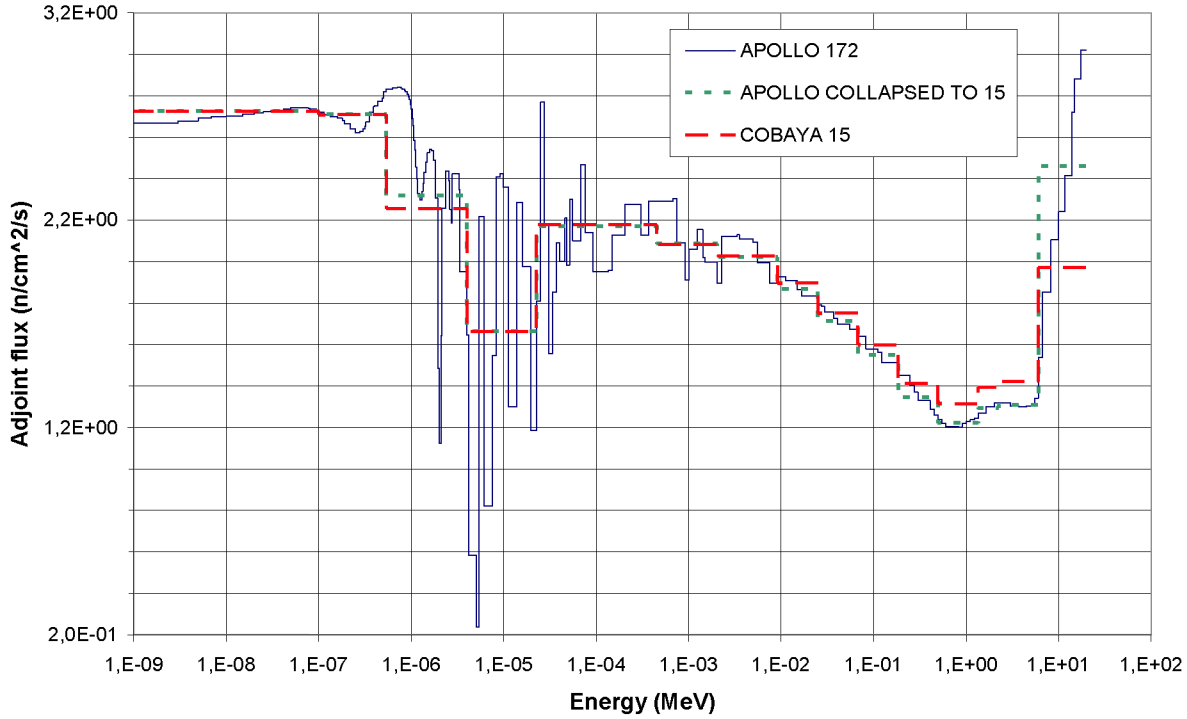

Figure 2. Adjoint fluxes

It is also remarkable the complex structure of the adjoint flux in the resonance region which cannot be reproduced in the coarse group structure considered.

5.2. Sensitivities computations

For the purpose of uncertainty computation and data adjustment, sensitivities of the k eigenvalue to the considered parameters were computed in 172 energy groups for APOLLO and in 15 energy groups for COBAYA, sensitivities from APOLLO were also computed for the 15 energy groups structure with the 172 energy groups solution. Table I and Table II show a comparison for both the transport and the diffusion solution.

There exists a considerable discrepancy around 1 keV for energy group 12 in the sensitivities to the fission cross section, due to the detailed spectrum of the adjoint flux for 172 groups, completely swept in the 15 energy groups structure.

Table I
Absolute sensitivities of k eigenvalue to U-235 fission cross section

Energy groups	Absolute sensitivities (1/barn)		
	APOLLO	COBAYA	(A-C)/A (%)
1	1.0043E-02	1.0229E-02	-1.84
2	1.1084E-01	1.1211E-01	-1.14
3	7.9499E-02	8.0355E-02	-1.08
4	1.5512E-01	1.6052E-01	-3.48
5	9.1625E-02	9.7031E-02	-5.90
6	2.9635E-02	3.1419E-02	-6.02
7	6.2079E-03	6.5471E-03	-5.46
8	9.9313E-04	1.0422E-03	-4.94
9	1.4689E-04	1.5481E-04	-5.39
10	8.2046E-06	8.6849E-06	-5.86
11	6.6597E-07	7.1048E-07	-6.68
12	4.7755E-09	5.6993E-09	-19.35
13	3.6424E-10	3.9186E-10	-7.58
14	3.9492E-12	3.9838E-12	-0.88
15	2.9228E-13	2.9241E-13	-0.05

Table II
Absolute sensitivities of k eigenvalue to U-235 $\overline{\upsilon}$

Energy groups	Absolute sensitivities		
	APOLLO	COBAYA	(A-C)/A (%)
1	7.4288E-03	8.0117E-03	-7.85
2	7.2788E-02	7.7392E-02	-6.32
3	6.1614E-02	6.5396E-02	-6.14
4	1.1230E-01	1.2160E-01	-8.29
5	7.7929E-02	8.4744E-02	-8.75
6	3.3864E-02	3.6529E-02	-7.87
7	9.8228E-03	1.0488E-02	-6.78
8	2.3159E-03	2.4481E-03	-5.71
9	5.6999E-04	5.9718E-04	-4.77
10	7.2092E-05	7.5227E-05	-4.35
11	1.4638E-05	1.5358E-05	-4.92
12	1.3068E-07	1.3570E-07	-3.85
13	1.1119E-08	1.1109E-08	0.09
14	1.4465E-09	1.4447E-09	0.12
15	3.3953E-10	3.3943E-10	0.03

The effect of the adjoint fluxes differences is not so clear in the sensitivities to the average number of neutrons per fission with relative differences below 10 per cent.

5.3. *K eigenvalue uncertainties and best estimate values*

Table III shows k eigenvalues for the transport and diffusion solutions. After data adjustment these results were updated to *best estimate* values also shown.

A goodness of fit test was also performed with the BEST-EST code yielding a χ^2 value of 1.4087 for transport and 133.32 for diffusion. Thus, it is clear that only the transport computation is useful for practical data adjustment as the test result is close to one.

A new computation of the k eigenvalue with best estimate fission cross sections and $\overline{\upsilon}$ for U-235 and U-238 gave the k eigenvalues presented as *recomputation*. The accordance between the newly computed values and the best estimate solution shows the suitability of this methodology to improve nuclear data through numerical solutions of the transport equation.

These results are only indicative of the ability of this methodology to perform data assimilation for nuclear reaction cross sections, correct uncertainties and adjusted cross sections can only be obtained when all the sources of uncertainty, or at least the ones with a higher impact, are included in the computational chain. The computation of uncertainties for the diffusion equation lacks some ingredients to be fully consistent with the uncertainties from the transport equation, namely the uncertainties in all the homogenized cross sections due to the uncertainties in the considered fission cross sections and $\overline{\upsilon}$ values, and the uncertainty due to the simplification of the transport equation. With those values the uncertainty for the diffusion method will be undoubtly higher than the one for the transport method and not of the same order of magnitude; nevertheless these results show the good accordance in the sensitivities from both solutions.

Table III
K eigenvalues and associated uncertainties

	K eigenvalue
Experiment	1.000000 ± 0.00100
APOLLO 172 groups	0.997679 ± 5.786E-3
APOLLO best estimate	0.99939*3* ± 8.590E-4
APOLLO recomputation	0.99939*1*
COBAYA 15 groups	1.089868 ± 6.195E-3
COBAYA best estimate	1.001839 ± 9.872E-4
COBAYA recomputation	0.997758

6. Conclusions

The BEST-EST data adjustment algorithm has been applied to fission data for the highly enriched bare uranium sphere Godiva. Uncertainties propagation was performed by means of the sensitivities computed with forward and adjoint transport solutions and recomputations. Both the transport equation solved with the discrete ordinates method and the diffusion equation solved by a finite differences scheme were tested and results compared, showing that sensitivities and uncertainties computations are consistent, but only the transport solution is suitable for data adjustment with the aim of improving the cross section data sets and their associated uncertainties.

Finally, not all the sources of uncertainty were considered, and it could be possible to solve the transport equation with a higher order of anisotropy. The numerical values presented aim to assess the practical utility of the method, and further developments are needed to perform a data adjustment with full generality.

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