Uncertainty in Reactor Lattice Physics Calculations
The Effect of Dilution on the Covariance of Multigroup Cross Sections

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Abstract

Simulation results are of little use if nothing is known about the uncertainty in the results. In order to assess the uncertainty in a set of output parameters due to uncertainty in a set of input parameters, knowledge of the covariance between input parameters is required. Current practice is to apply the covariance between multigroup cross sections at infinite dilution to all cross sections including those at non-infinite dilutions. In this work, the effect of dilution on multigroup cross section covariance is investigated as well as the effect on the covariance between the few group homogenized cross sections produced by lattice code DRAGON.

1. Introduction

There are many stages between the acquisition of nuclear data from experiments and its use in a full core reactor simulation. Any parameter measured experimentally will have some uncertainty associated with its true value and this uncertainty will propagate through each stage of the calculation chain. There exist two general methods for propagating the uncertainty in a set of input parameters to a set of output parameters: The Monte Carlo method and sensitivity based methods.

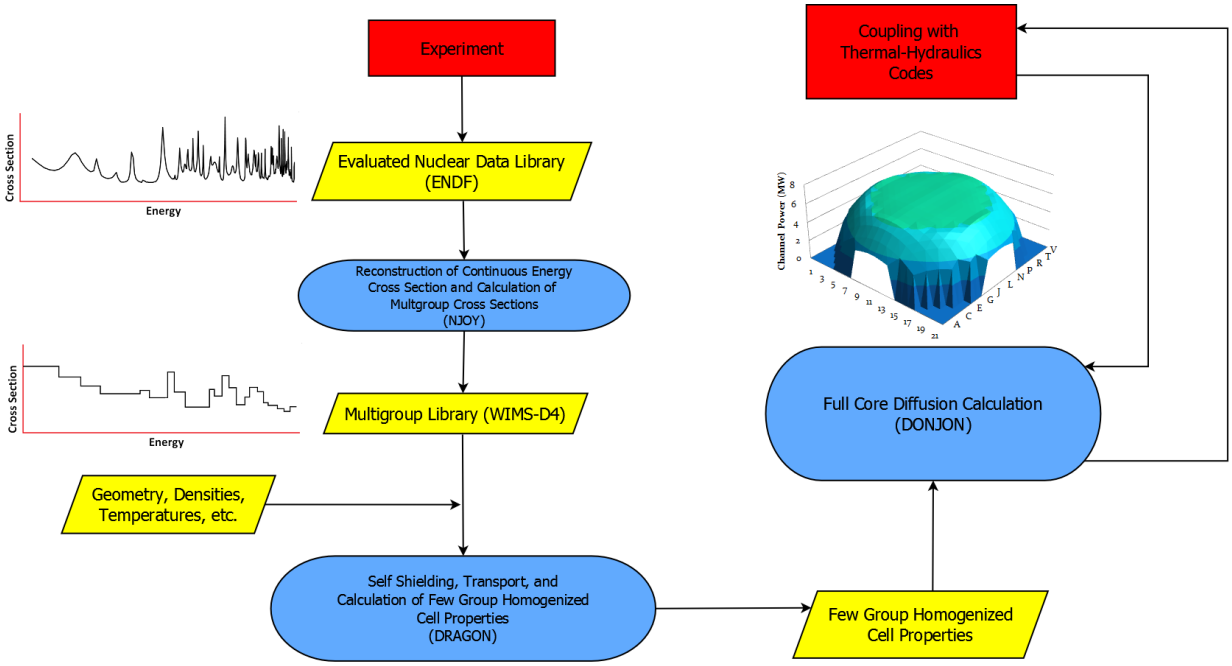

Figure 1 - Reactor Physics Calculation Chain

1.1 Monte Carlo Method

The Monte Carlo method requires that a distribution for each input parameter be defined according to its uncertainty. Note that the choice of distribution is subjective and has the potential to affect the calculated output uncertainty [1]. Samples are then taken from each distribution, taking into account the covariance between parameters and the sampled values are used as input for a simulation. This procedure is repeated until a sufficient number of output values exist to form a distribution from which the standard deviation can be calculated and a confidence interval constructed. This process is summarized in Figure 2.

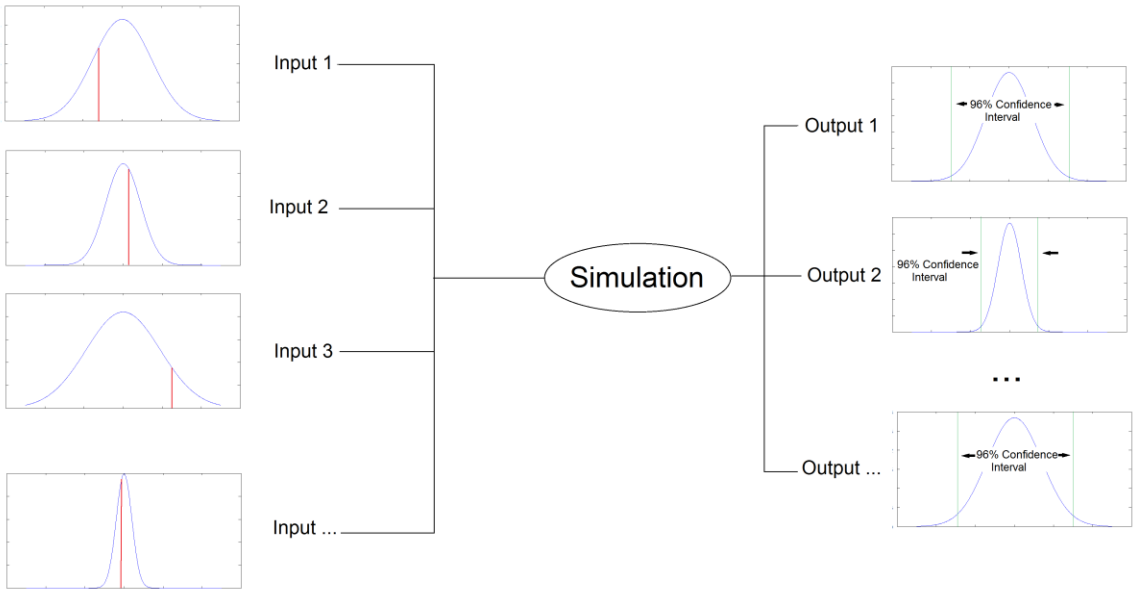

Figure 2 - Monte Carlo Method of Uncertainty Propagation

This method has been implemented in a code created at McMaster University named DINOSAUR [2]. DINOSAUR samples values for either a 69 or 172 group library in WIMS-D4 format using a covariance matrix. A new "perturbed" WIMS-D4 library is then created and used to perform a calculation in DRAGON. This is repeated until a sufficient number of perturbed outputs have been obtained to assess the uncertainty. Tests were performed during the development of DINOSAUR to assess the effect of changing the input distribution and it was found that no statistically significant changes occurred in the results from sampling using a normal distribution versus a uniform distribution [2].

1.1.1 Covariance Decomposition

The Monte Carlo method requires that a vector of random dependant variables be generated to properly replicate how the inputs may realistically vary according to their uncertainty and covariance. This can be done using equation (1).

$$G(\mu,\Sigma) = P(1,\Sigma)^T\ \mu \tag{1}$$

Where G(μ,Σ) is a vector of random dependant variables with covariance Σ and average μ, P(1,Σ) is a vector of perturbation factors with average 1 and covariance Σ, and μ is a vector of average values. The perturbation factors can be calculated using a relative covariance matrix Σ_r and a vector of random independent numbers with average 1 G(1,0) as shown in equation (2).

$$P(1,\Sigma) = \Sigma_r^{\frac{1}{2}}\, G(0,1) + [1.0, 1.0, 1.0, \ldots, 1.0]^T \tag{2}$$

Note that the square root of the relative covariance matrix is required. This can be calculated by decomposing the relative covariance matrix into eigenvalues and eigenvectors V and taking the root of the diagonal matrix D (which is simply a matter of taking the root of each of the diagonal entries).

$$\Sigma = V\ D\ V^T \tag{3}$$

$$\Sigma^{\frac{1}{2}} = V\ D^{\frac{1}{2}}\ V^T \tag{4}$$

So far we have taken for granted the availability of a relative covariance matrix. This is generally the way covariances are stored whether they are from NJOY's ERRORR module [3] or from SCALE [4]. The relative covariance $\Sigma_r(x,y)$ is calculated using an absolute covariance value Σ(x,y) and the expectation value of the two parameters between which the covariance was calculated.

$$\Sigma_r(x,y) = \frac{\Sigma(x,y)}{(\bar{x}\cdot\bar{y})} \tag{5}$$

Finally, the covariance between two random variables x and y is a measure of how likely they are to deviate in the same direction from their expectation values.

$$COV(x,y) = \frac{1}{N-1}\sum_{i=1}^{N}(x_i-\bar{x})(y_i-\bar{y}) \tag{6}$$

1.2 Sensitivity Based Methods

The sensitivity based methods include the one-at-a-time (OAT) method, and the adjoint method. The goal of both of these methods is to determine the sensitivities between input and output parameters. The uncertainty can then be calculated using the sandwich rule [5].

$$\Delta^2 x = S\ \Sigma\ S^T \tag{7}$$

Where S is a vector of partial derivatives between each input parameter and the output parameter x, and Σ is the (absolute) covariance matrix.

Determining the partial derivative between each input parameter can be done in two ways. The OAT method is the most simple but also the most computationally expensive. Each input parameter is perturbed slightly and the change in output is observed. The partial derivative between the two can then simply be approximated as:

$$\frac{\partial f(z)}{\partial z} \approx \frac{f(z+\delta z) - f(z)}{\delta z} \tag{8}$$

This approximation becomes better and better as δz approaches zero but smaller changes in the input parameter z also elicit a smaller response in f(z) so there is a tradeoff. One must choose a perturbation size that is as small as possible but still gives a large enough response in the output to calculate the partial derivative.

The adjoint method is a much more efficient alternative to the OAT method for calculating sensitivities since it requires only a fraction of the amount of computation. It involves using adjoint functions to determine the sensitivities. The drawback is that it is more difficult to implement since it requires the calculation of adjoints for the relevant equations used in the code through which the uncertainty is to be propagated. If these functions are to be retrofitted into already existing codes, the task becomes more difficult since an understanding of the source code is required in addition to the adjoint functions.

1.3 Problem Statement

Although the Monte Carlo and sensitivity based methods differ in their approach, both rely on knowledge of the covariance between input parameters. Since the uncertainty in the output calculated using both methods depends directly on the input parameter covariance matrix, it is important that these covariances be as accurate as possible. Current practice in uncertainty analysis codes is to apply covariances calculated at infinite dilution to all cross sections, including those at non-infinite dilutions [2]. This includes codes such as SCALE [4], SUSD3D [6], XSUSA (which uses SCALE covariances) [7], and CASMO-5/DP (a modification of CASMO-5 by the Paul Scherrer Institute) [8]. The goal of this work was to investigate the effects of dilution on the covariance between multigroup cross sections as well as on the covariance between the homogenized few group properties that are produced in DRAGON.

2. Methodology

In order to generate multigroup covariance matricies at varying dilutions, a set of perturbed evaluated nuclear data libraries, known as TENDL libraries, in ENDF format were obtained from the Nuclear Research and Consultancy Group (NRG) website[1]. These libraries are created by randomly perturbing

[1] http://www.talys.eu/

parameters used in the reconstruction of continuous energy cross sections [9]. Changing these parameters affects the position, width, and size of resonance peaks. This is known as the Total Monte Carlo approach and differs from Monte Carlo methods which perturb multigroup cross sections because those perturbations account solely for the uncertainty from vertical displacement of the continuous energy cross section and will always estimate a decrease in the uncertainty with dilution [10]. However uncertainty in the positions of resonances and their widths can cause the uncertainty with dilution to increase as is shown later in this work.

The perturbed TENDL libraries were processed into 69 group libraries in WIMS-D4 format using NJOY. The covariance between these cross sections at all energies was then calculated using a python script that was developed for this work known as COCOAPUFFS (Covariance Calculation by Analysis of Perturbed Fundamental Files). Covariances calculated with COCOAPUFFS were validated against a spreadsheet program. Since NJOY can calculate multigroup cross sections at multiple dilutions, it was possible to calculate covariances between cross sections of finite dilution, something which is only possible with the Total Monte Carlo approach. Plots were made of these multigroup covariances for visual comparison.

Only three reactions: Elastic scattering (MT=2), fission (MT=18), and radiative capture (MT=102) were available at multiple dilutions from the NJOY output so covariances for each of these reactions as well as between these reactions were calculated for finite dilutions. The other reactions were only available at infinite dilution. To investigate the effect of dilution on the covariance between the few group homogenized cross sections, DINOSAUR was used to sample from the IAEA library using the calculated covariances. First, the covariances for U235 and U238 at infinite dilution in the DINOSAUR covariance library[2] were replaced with those calculated from the TENDL evaluations. DINOSAUR was then used to run a simulation of a pin cell from the TMI-2 PWR at hot full power as outlined in the Uncertainty Analysis in Modelling (UAM) benchmark created by the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) [11]. The infinite dilution covariances for elastic scattering, fission, and radiative capture (as well the covariances between them) were then substituted with covariances calculated at the closest available dilution to the problem dilution. This corresponded to 1200 barns for U235 and 52 barns for U238. The covariance between the 2 group homogenized cross sections that emerged from DRAGON was then calculated from the output for both the infinite and finite dilution cases.

[2] DINOSAUR uses the 44 group SCALE covariance library extrapolated to 69 groups with ANGELO2

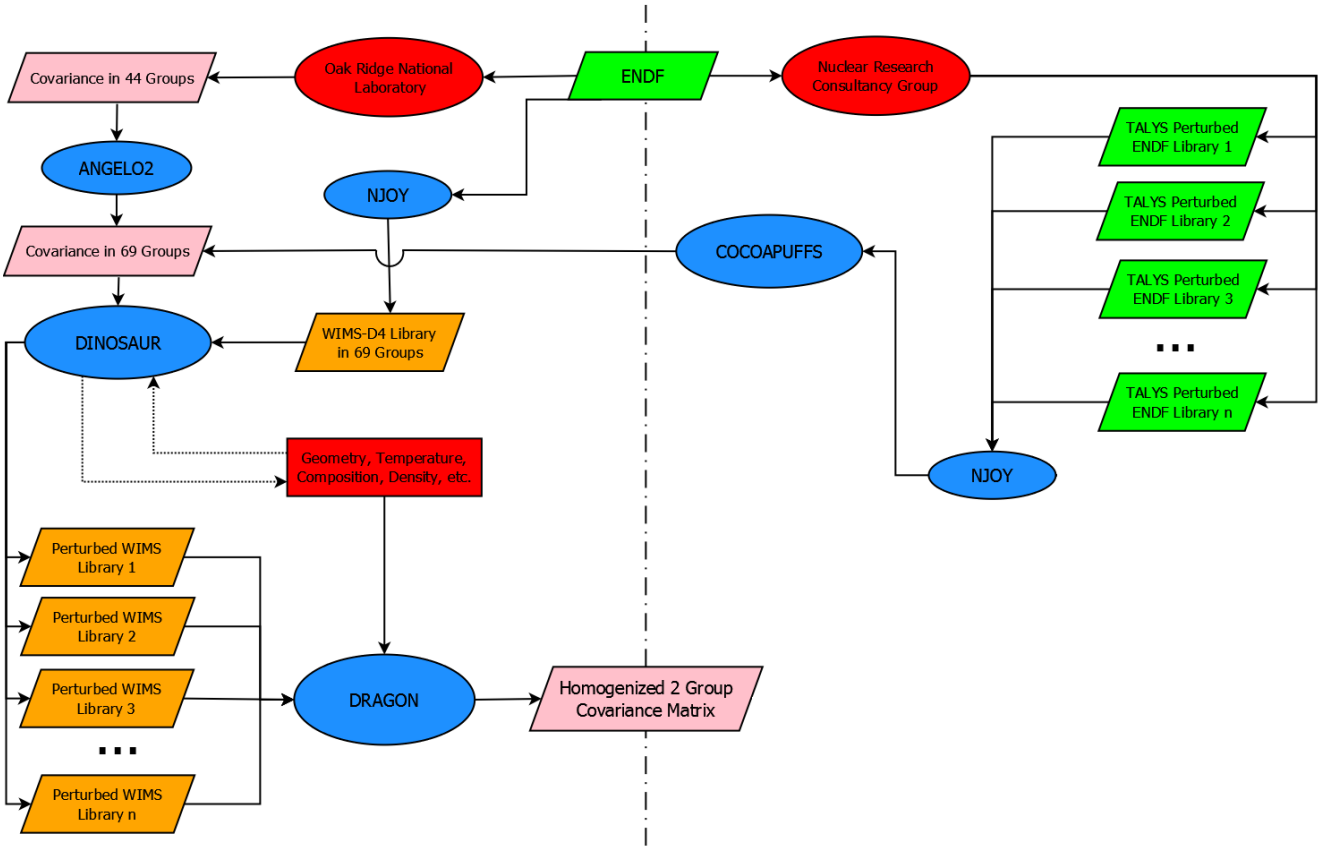

Figure 3 – Methodology for Investigating the Effects of Dilution on Multigroup and Few Group Homogenized Cross Section Covariance

3. Results

The results have been divided into two sections. The first shows the effect of dilution on the 69 group covariance matricies which are used as input to DINOSAUR but could be used in any Monte Carlo or sensitivity based propagation code with modifications to the format. The second shows how using covariance matricies of differing dilution affects the covariance between the homogenized 2 group cross sections that emerge from DRAGON. These cross sections are normally used as input to the full core diffusion code DONJON and so their covariances could be used in codes which propagate the uncertainty through the diffusion calculation whether they be Monte Carlo or sensitivity based.

3.1 Effect of Dilution on Multigroup Cross Section Covariance

As mentioned in the Methodology section, covariance matricies between 69 group cross sections were calculated for U235 and U238 elastic scattering, fission, and radiative capture from the perturbed TENDL evaluations. The results are summarized in the figures that follow.

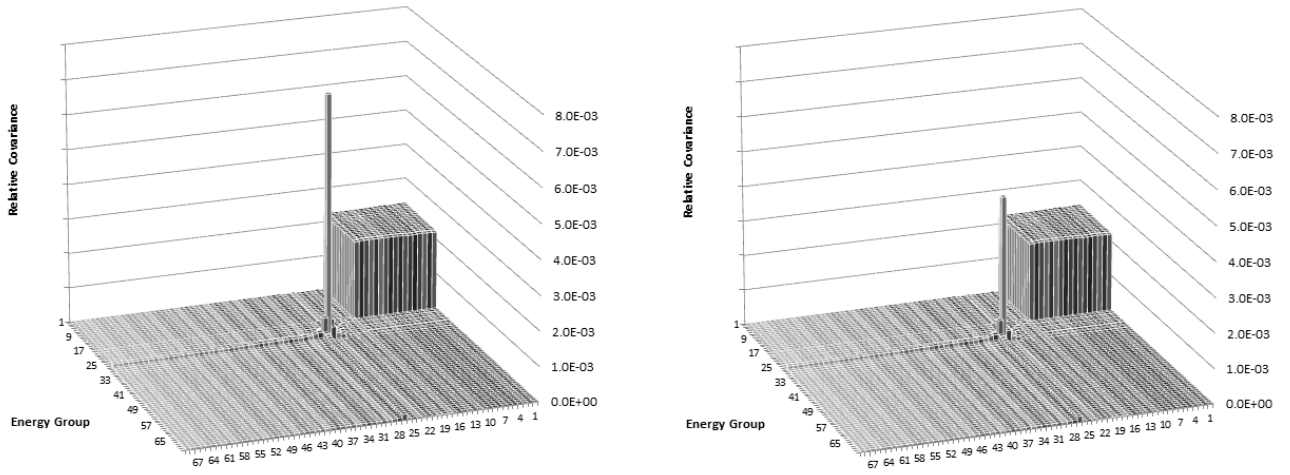

Figure 4 - 69 Group Covariance of U235 Elastic Scattering at ∞ Dilution (left) and 1200 Barns (right)

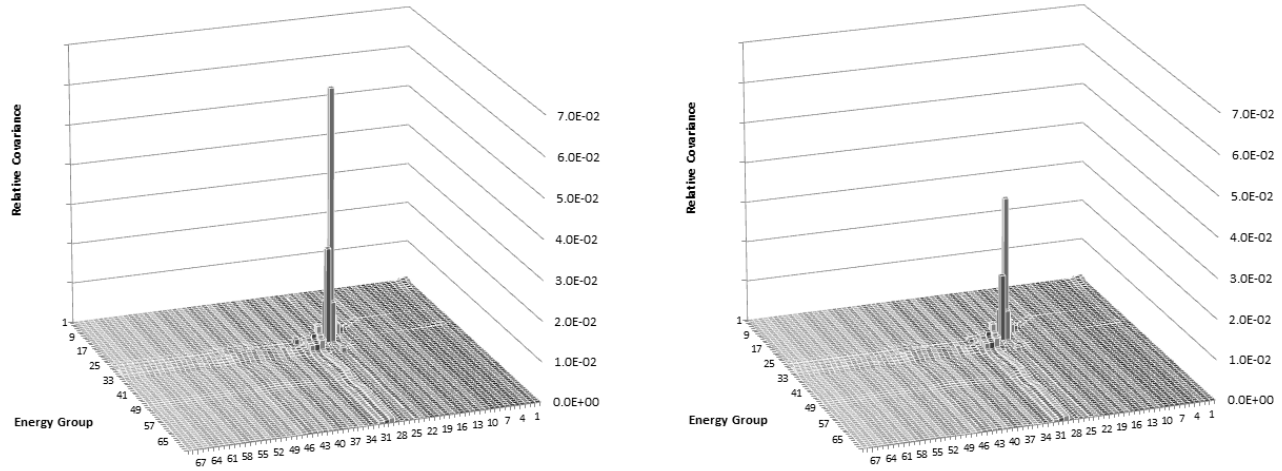

Figure 5 - 69 Group Covariance of U235 Fission at ∞ Dilution (left) and 1200 Barns (right)

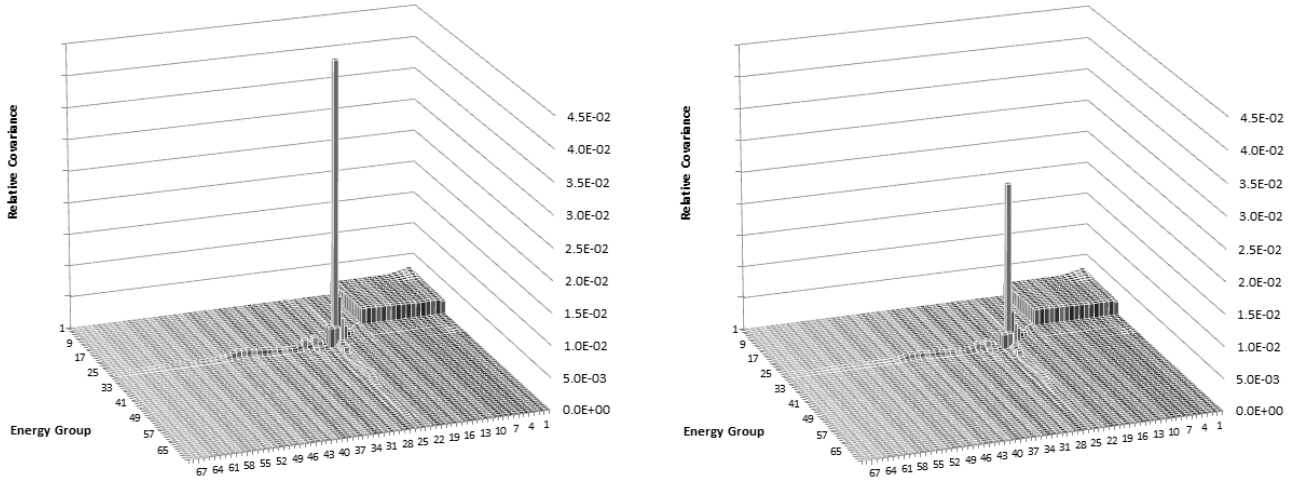

Figure 6 - 69 Group Covariance of U235 Radiative Capture at ∞ Dilution (left) and 1200 Barns (right)

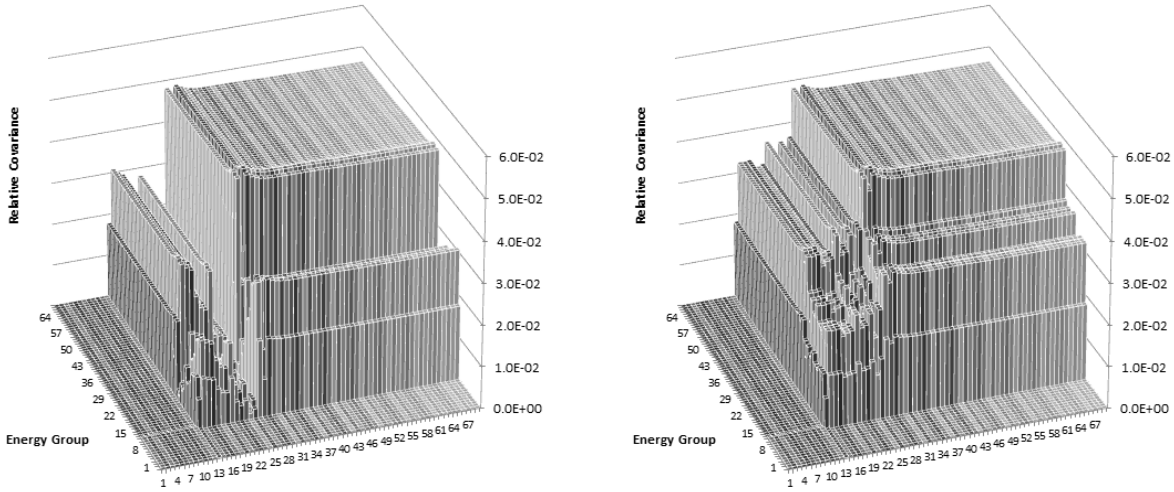

Figure 7 - 69 Group Covariance of U238 Elastic Scattering at ∞ Dilution (left) and 52 Barns (right)

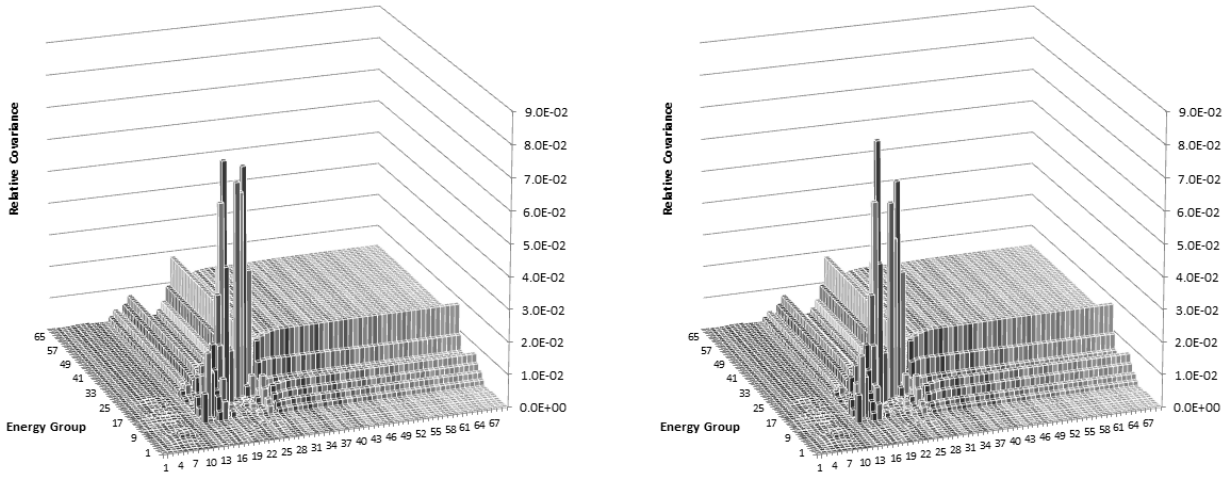

Figure 8 - 69 Group Covariance of U238 Fission at ∞ Dilution (left) and 52 Barns (right)

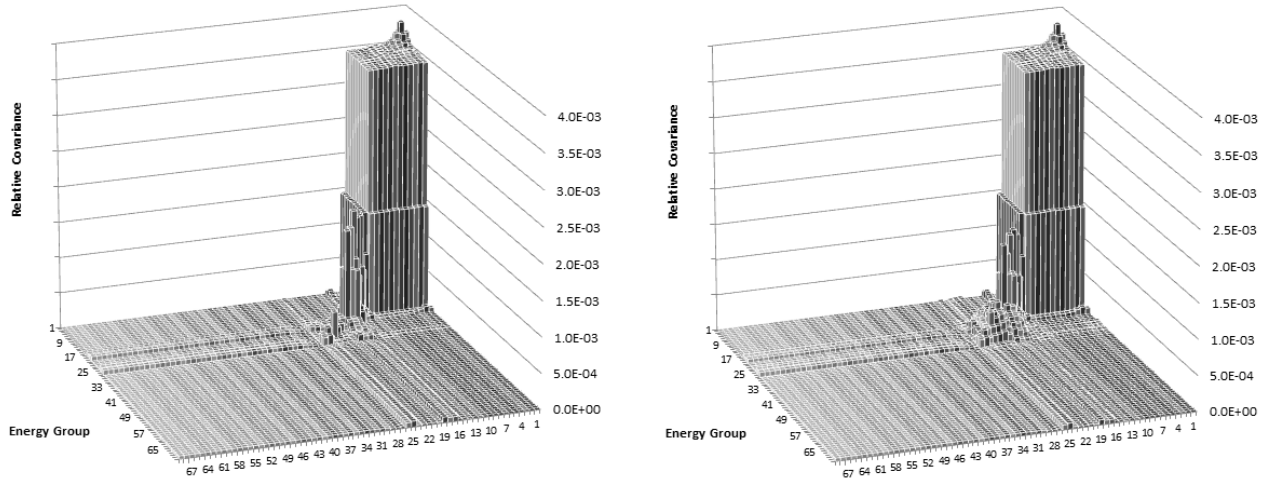

Figure 9 - 69 Group Covariance of U238 Radiative Capture at ∞ Dilution (left) and 52 Barns (right)

The general trend for U235 was a decrease in covariance with dilution. Conversely, U238 cross section covariances increased in some sections while decreasing in others. In particular, elastic scattering and radiative capture showed increases in covariance in the resonance region. As expected, no change in covariance occurred outside of the resonance region since these cross sections are not affected by the dilution calculation performed in NJOY. The energy boundaries of the groups in the resonance range are given in Table 1.

Table 1 – Energy Boundaries of the Resonance Groups in the WIMS-D4 69 Group Library

Group	Energy Range	Group	Energy Range
15	5.53E+3 - 9.12E+3	22	7.55E+1 - 1.49E+2
16	3.52E+3 - 5.53E+3	23	4.81E+1 - 7.55E+1
17	2.24E+3 - 3.52E+3	24	2.77E+1 - 4.81E+1
18	1.43E+3 - 2.24E+3	25	1.60E+1 - 2.77E+1
19	9.07E+2 - 1.43E+3	26	9.88E+0 - 1.60E+1
20	3.67E+2 - 9.07E+2	27	4.00E+0 - 9.88E+0
21	1.49E+2 - 3.67E+2		

3.2 Effect of Dilution on Few Group Homogenized Cross Section Covariance

Once a set of finite dilution covariance matricies had been developed that approximated the dilutions of U235 and U238 calculated by DRAGON for the TMI-2 PWR, a set of simulations were performed using DINOSAUR and DRAGON. DINOSAUR was used to sample from the 69 group IAEA library first only according to infinite dilution covariances (recall from section 2 that this was the SCALE covariance matrix with all covariances for U235 and U238 replaced by the ones calculated using the TENDL evaluations). The process was then repeated using the U235 and U238 finite dilution covariances calculated from TENDL that most closely resembled the problem dilution calculated by DRAGON in place of their infinite dilution counterparts for elastic scattering, fission, and radiative capture[3]. The covariance between the two group homogenized cross sections produced by DRAGON for the infinite and finite dilution cases was then calculated and the results are shown in Figure 10.

Of particular interest was the change in the fast fission production ($\nu\Sigma_f$) variance, which saw a decrease of 30% when using finite dilution multigroup covariances instead of those at infinite dilution. Conversely, the fast scattering cross section variance increased by a little over 60%, causing an approximately identical increase in the total fast cross section variance when finite dilution covariances were used. It is clear that while some homogenized cross section uncertainties were relatively unaffected, applying covariances calculated for cross sections at infinite dilution to finite dilution cross sections can potentially overestimate or underestimate the true uncertainty.

[3] Infinite dilution covariances were used for all other reactions.

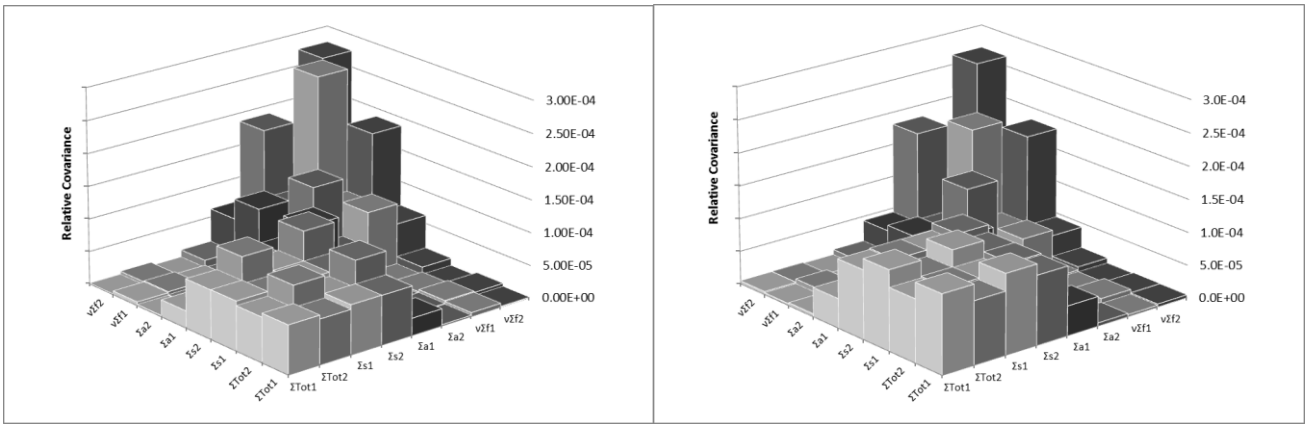

Figure 10 – Homogenized Two Group Cross Section Covariance Calculated using Infinite Dilution Covariances (left) and Finite Dilution Covariances (right)

4. Conclusions

A proper assessment of the uncertainty in simulation results is of great importance since a result is not of much use without knowledge of its accuracy. A key tool for determining the uncertainty in a set of output parameters is the covariance between input parameters. When assessing the uncertainty in lattice physics simulations, current practice is to apply covariances calculated for infinitely dilute cross sections to all cross sections regardless of their dilution. In this work, the effect of dilution on multigroup cross section covariance as well few group homogenized cross section covariance has been assessed. It was shown that the covariance between multigroup cross sections at finite dilution may increase or decrease with reference to the covariance calculated at infinite dilution. To assess the effect on the few group homogenized cross section covariance, a Monte Carlo uncertainty propagation was performed on a TMI-2 PWR pin cell at hot full power using the specifications in the UAM benchmark of the OECD NEA. The results showed that while some covariances are unaffected by the dilution of the input parameter covariance matrix, others can increase or decrease by as much as 60%.

It is the conclusion of the authors that although the few group homogenized cross section covariances do not change drastically with dilution, the subject warrants further investigation. Of particular concern are cases where using infinite dilution covariances in place of those at the proper dilution could cause an underestimation of the uncertainty in the output.

5. References

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