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

C. McEwan[1], M. Ball[1] and D. Novog[1]
[1] McMaster University, Hamilton, Ontario, Canada
mcewac2@mcmaster.ca

A Master's Level Submission

Summary

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.

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 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].

1.2 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 [3].

$$\Delta^2 x = S\,\Sigma\,S^T \tag{1}$$

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

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 all the relevant equations used in the code.

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 [5], XSUSA (which uses SCALE covariances) [6], and CASMO-5/DP (a modification of CASMO-5 by the Paul Scherrer Institute) [7]. 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 parameters used in the reconstruction of continuous energy cross sections [8]. 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 [9]. 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.

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

The perturbed TENDL libraries were processed into 69 group libraries in WIMS-D4 format using NJOY [10]. 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.

3. Results I - Effect of Dilution on Multigroup Cross Section Covariance

The calculated covariance matricies for elastic scattering in U235 and U238 using the perturbed TENDL evaluations are shown below.

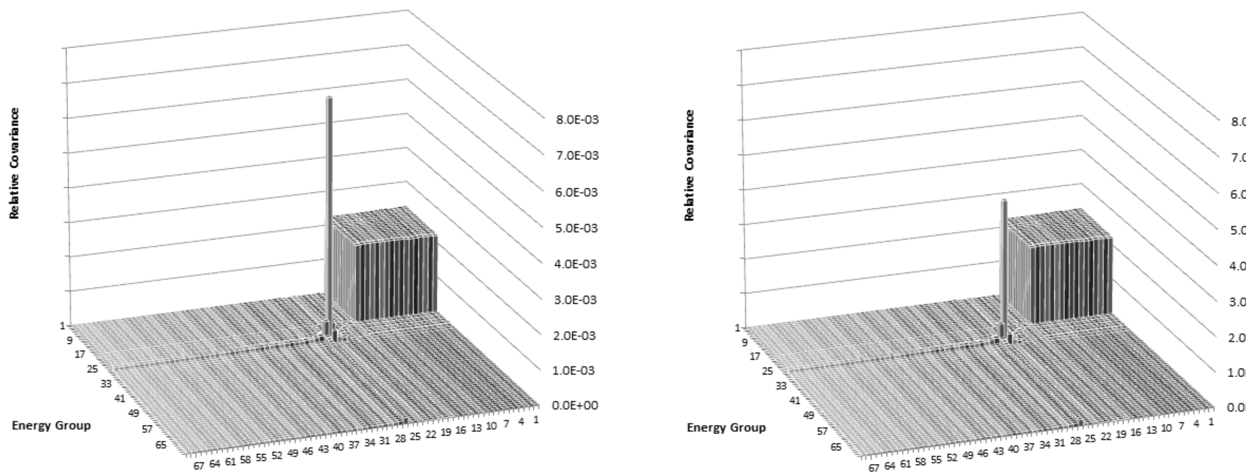

Figure 1 - 69 Group Covariance of U235 Elastic Scattering at ∞ Dilution (left) and 1200 Barns (right)

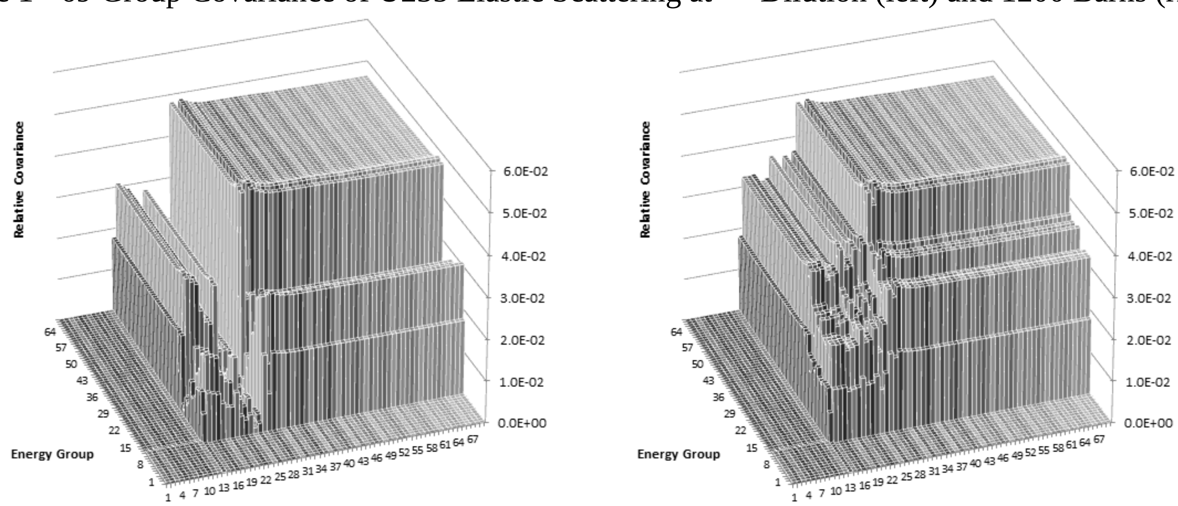

Figure 2 - 69 Group Covariance of U238 Elastic Scattering at ∞ Dilution (left) and 52 Barns (right)

4. Results II - The 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 [11], 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. 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[2]. 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 3.

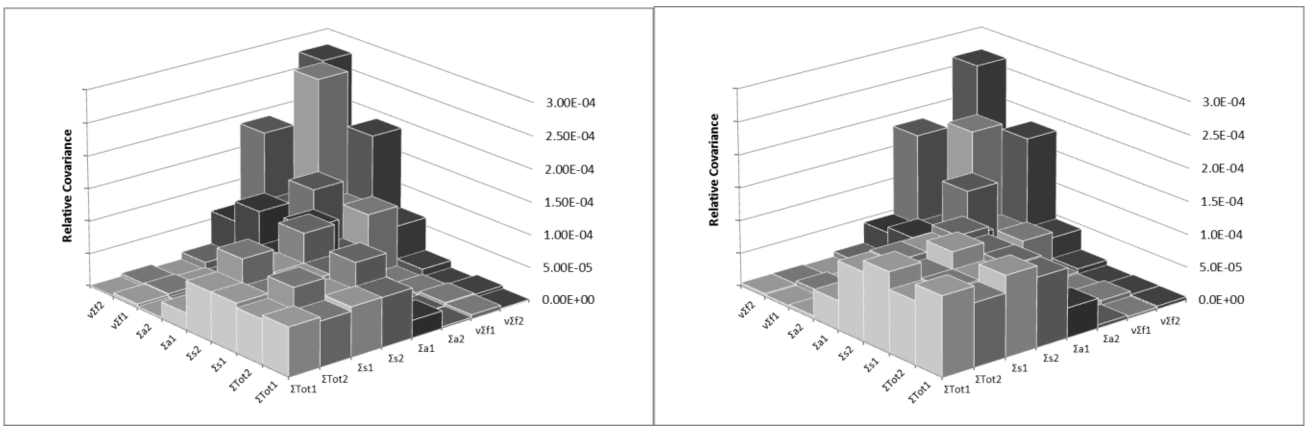

Figure 3 – Homogenized Two Group Cross Section Covariance Calculated using Infinite Dilution Covariances (left) and Finite Dilution Covariances (right)

5. 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%.

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

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.

6. References

[1] D.G. Cacuci and M. Ionescu-Bujor, "A Comparative Review of Sensitivity and Uncertainty Analysis of Large-Scale Systems-II: Statistical Methods," *Nuclear Science and Engineering*, no. 147, pp. 204-217, 2004.

[2] M. Ball, *Uncertainty in Lattice Reactor Physics Calculations*, Hamilton, Canada: Ph.D. Dissertation, McMaster University, 2011.

[3] Z.B.Alfassi, "Uncertainty analysis based on sensitivity analysis," in *Statistical Treatment of Analytical Data*, Oxford, Blackwell Sciences, 2004.

[4] Oak Ridge National Laboratory, "SCALE 5.1 Cross-Section Covariance Libraries," ORNL/TM-2005/39, Rev.1, Vol. 1, Book 3, Sect. M19, Oak Ridge, USA, 2008.

[5] I. Kodeli, "The SUSD3D Code for Cross-Section Sensitivity and Uncertainty Analysis – Recent Development," Vol. 104, No. 1, pp. 791-793, 2011.

[6] W. Zwermann et al., "Uncertainty Analyses with Nuclear Covariance Data in Reactor Core Calculations," *Journal of the Korean Physical Society*, Vol. 59, No. 2, pp. 1256-1259, 2011.

[7] J. Rhodes et al. "CASMO-5 Development and Applications." *ANS Physics of Reactors Topical Meeting (PHYSOR)*, Vancouver, Canada, 2006.

[8] D. Rochman et al. "Exact Nuclear Data Uncertainty Propagation for Fusion Neutronics Calculations," *Fusion Energy and Design*, Vol. 85, No. 5, pp. 669-682, 2010.

[9] M. Ball et al., "The Dilution Dependancy of Multi-Group Uncertainties," *Science and Technology of Nuclear Installations*, [submitted for publication], 2013.

[10] R.E. MacFarlane and D.W. Muir, "The NJOY Nuclear Data Processing System Version 91," Manual LA-12740-M, Chapter X, Los Alamos, USA, 1994.

[11] K. Ivanov et al., "Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation, and Safety Analysis of LWRs, Volume I: Specification and Support Data for the Neutronics Cases (Phase I)," Organization for Economic Cooperation and Development, Paris, France, 2007.