Annals of Nuclear Energy

An Uncertainty Quantification Method Relevant to Material Test Reactors

--Manuscript Draft--

Manuscript Number:	ANUCENE-D-21-00267
Article Type:	Full Length Article
Keywords:	uncertainty quantification; material test reactors; graphite irradiation; total Monte Carlo
Abstract:	Within material test reactor calculations, spectrum and reaction rate uncertainties are typically not quantified when performing as-run analyses to determine the neutron field experienced by the experiment. Methods to propagate uncertainties through high fidelity simulations are available when sufficient computational power is available. A tool is developed for sampling MCNP inputs from random distributions to determine output uncertainties based on those inputs. Another tool is developed to sample nuclear data cross-section in ACE format using multi-group nuclear data covariances. The Total Monte-Carlo Method and GRS are implemented and compared to one another as well as MCNP sensitivity and uncertainty calculations. The methods were applied to calculate uncertainties in spectrum and reaction rates for the Godiva sphere, UAM-pincell benchmark, and Advanced Test Reactor. The methods agree well, with GRS allowing for an order of magnitude speedup for reaction rate uncertainty calculations and several orders of magnitude for eigenvalue uncertainty calculations.

An Uncertainty Quantification Method Relevant to Material Test Reactors

Vishal Patel[a,*], Jorge Navarro[b], William Windes[c], Pavel Tsvetkov[d]

[a] *2356 W Commodore Way, Seattle, WA 98199*
[b] *P.O. Box 2008 Oak Ridge, TN 37831*
[c] *1955 N. Fremont Ave. Idaho Falls, ID 83415*
[d] *3127 TAMU, College Station, TX 77843-3127*

Abstract

Within material test reactor calculations, energy dependent flux and reaction rate uncertainties are typically not quantified when performing as-run analyses to determine the neutron field experienced by the experiment. When high fidelity Monte-Carlo codes are used in such analyses, straight forward methods to calculated output uncertainties are not available, instead expert opinion is used to postulate computational uncertainties. New methods to propagate uncertainties through these high fidelity simulations are available when sufficient computational power is available. A tool is developed for sampling any part of an MCNP input from random distributions to determine output uncertainties based on those inputs. Another tool is developed to sample nuclear data cross-section in ACE format using multi-group nuclear data covariances. The Total Monte-Carlo Method and GRS are implemented and compared to one another as well as MCNP sensitivity and uncertainity calculations. The methods were applied to the Godiva critical sphere k-eigenvalue, the UAM pincell benchmark energy dependent flux and reaction rates, and the Advanced Test Reactor energy dependent flux within an experimental location. The two methods agree well, with GRS allowing for an order of magnitude speedup for reaction rate uncertainty calculations and several orders of magnitude for eigenvalue uncertainty

*Corresponding author
URL: `www.usnc-tech.com` (Vishal Patel), `www.ornl.gov` (Jorge Navarro), `www.inl.gov` (William Windes), `https://engineering.tamu.edu/nuclear/index.html` (Pavel Tsvetkov)

calculations.

Keywords: uncertainty quantification, material test reactors, nuclear data uncertainties

1. Introduction

Material test research reactors focus on accelerated material degradation experiments in radiation environments and isotope production. Many material changes within the reactor are a function of the energy dependent neutron fluence received over the experiment lifetime, and to correlate neutron damage effects on materials, the fluence must be well known. The reactors have online flux measurements and coolant temperature rise sensors to quantify the total reactor power level. Many experiments are equipped with radiation flux wires to quantify the fluence of neutrons over the total experiment lifetime. Neutronic analysis is also performed after irradiations to predict the neutron flux experienced by the experiment sample. These predicted fluxes are crucial to the derived experiment data because the predicted fluxes are highly detailed whereas the experimental data is quite sparse. Thus it is important to compute the predicted flux well, and to include uncertainties in the results.

The results from online power measurements, counted radiation wires, and computational analysis are combined to determine the actual neutron fluence that the experiment received. The data de-convolution process takes into account uncertainties from all measurement sources to determine the fluence received by an experiment, plus the uncertainty of the result. The computational uncertainty often dominates the total uncertainty of energy dependent fluence because only a few flux wire measurements are available to quantify the neutron spectrum. However, uncertainties from the computational analysis are not well determinable such that expert opinion is used for uncertainty instead of model-based uncertainty. The main difficulties in determining these uncertainties comes from tracking uncertain data inputs (fuel burnup, control positions, changing power levels, ... through computationally intensive Monte-Carlo (MC)

calculations. In order to better understand experiments, the computational uncertainty must be quantified.

Models of material test reactors tend to include as much detail as possible and thus rely upon Monte-Carlo codes where the details can be modeled. Uncertainty quantification (UQ) and sensitivity analysis (SA) methods for Monte-Carlo codes tend to concentrate on k-eigenvalue and not reaction rates. The Monte-Carlo-N-Particle transport code [1] is used in many research facilities, as such, this tool is selected to perform neutronics calculations. A literature review was performed to find an efficient method to propagate uncertainties with MCNP. A cross-section sampling and MCNP input file sampling method was then implemented. MCNP parsers were created to efficiently apply the selected UQ techniques. The UQ method was then compared to the UAM pincell benchmark by means of k-eigenvalue uncertainty calculations.

2. Background

2.1. Neutronic Uncertainty Quantification

2.1.1. Deterministic Methods

The first developments of UQ/SA occurred with respect to the neutron transport equation under the diffusion approximation [2], which was later generalized under the Adjoint Sensitivity Analysis Procedure (ASAP) [3]. Within a multi-group framework, UQ/SA has been performed and implemented in production tools. Specifically, the adjoint multi-group transport equation can be solved with small changes in the physics kernels in both deterministic and Monte-Carlo solutions. For continuous energy adjoint calculations the situation is different. Group to group scattering cross-sections cannot be easily inverted because cross-sections are represented as relations and not discrete points. By representing the scattering matrix as discrete points, the computer memory requirements for calculations grows to unfeasible amounts. For continuous energy codes, other methods have been developed to propagate uncertainties.

2.1.2. Monte-Carlo Based Methods

Effects of perturbations on a response can be directly calculated from forward Monte-Carlo calculations, e.g., no need to run parametric studies for small perturbations. In general, the perturbed parameters are nuclear data related and the response function is the criticality eigenvalue. These calculations predict sensitivity profiles and output uncertainties can be determined from multiplying the magnitude of uncertainties with sensitivities.

The differential operator sampling (DOS) method [4] assumes the effect of the perturbation being made (usually nuclear data) can be represented by a Taylor series expansion around the mean value, generally using a 1st or 2nd order expression. The derivative involved in the series expansion can be calculated using Monte-Carlo means. The original developments did not include all the required steps to get generally correct answers. The fission source was not perturbed during sampling such that a bias was introduced [5]. The methodology without the fission source perturbation will tend to disagree with similar perturbation calculations [6].

The adjoint flux can in principle be calculated using Monte-Carlo methods, though efficient methods to do so are difficult to implement for continuous in energy problems. In general to solve the problem would require an inverse random walk from the end of the calculation to the beginning, e.g., a backwards calculation. Recently, the iterated fission probability (IFP) method [7] has been used to determine the adjoint flux from forward monte calculations. This method relies on the physical interpretation of the adjoint flux as an importance weighting[2]; it is the affect of a neutron introduced somewhere in phase space of a critical system. This means during power source iterations, keeping track of what a neutron produced in some iteration i does in a later iteration asymptotic generation n can allow for a creation of the adjoint flux. This adjoint can then be used in typical deterministic manners using the sandwich rule to determine sensitivities. Furthermore, it has been shown [8] that this method of adjoint calculation is equivalent to the differential operator sampling method with fis-

sion source perturbations. A drawback of this method is that a large computer memory is required due to storing of many histories as well as their original birth conditions. The memory requirement is proportional to the number of particles kept track of in each generation and the number of latent generations used to establish an asymptotic case.

Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Track-length importance CHaracterization (CLUTCH) [9] is a similar to the integrated fission probability method was recently implemented in SCALE. This method avoids some pitfalls of the IFP method in that computer memory requirements do not scale directly with the number of particle histories. This is accomplished by following particle histories directly from birth to death and computing relevant MC integrals once a particle dies. The methodology agrees with well multi-group MC methods as well as the IFP [9].

The DOS, IFP, and CLUTCH methods are good at S/U calculations for system wide (integral quantities) such as k_{eff}, and kinetics parameters but has difficulties determining specific tallies like dosimeter calculations because of the large amount of memory required to track all neutrons through generations. The CLUTCH method has the potential to reduce memory requirements and perform sensitivity calculations though has not been completely implemented in any production tool.

The Total Monte-Carlo (TMC) method, first introduced to propagate nuclear data uncertainty through reactor physics calculations [10] is a method to propagate uncertainties with deterministic and MC methods. It is in essence a general sampling method that uses a brute-force approach. Many random inputs to a MC code are created, ran for a long time to get good MC statistics, then uncertainties on outputs from input changes can be found by observing the output distribution and subtracting MC uncertainties. It is an excellent method to propagate input uncertainties through MC calculations, but takes a very long time to perform, needing at least 500 calculations with random inputs, e.g., 500 times longer than a single run. This method is used in this work and will be described in more detail in Sec. 3.1.

The GRS method [11] is similar to TMC where simulations are run many times with inputs randomly selected and outputs stored for statistical analysis to determine uncertainties. However, this method does not have the drawback of needing to run each simulations for a long time. Rather, N simulations with different inputs are run for a short time with a single random number seed, then each N simulation is reran with a different random number seed (totaling about twice the runtime of a single long calculation). The two different random number seed simulations have identical MC (aleatoric) uncertainty distributions. The covariance of the output sets is the epistemic uncertainty of the varying inputs [11] because the MC uncertainty is almost eliminated (goes to zero as MC sample batch sizes increases). This method is used in this work and will be described in more detail in Sec. 3.2.

2.2. Nuclear Data Sampling

A main sources of uncertainty for transport and depletion calculations are based on uncertainties of nuclear data. In general, nuclear data is created from experimental means [12], however to resolve the quickly varying portions of cross-sections as well as temperature dependence, evaluators create evaluations [13]. Cross-sections can also be created from a theoretical basis and corrected with experimental results [14]. Uncertainties in cross-sections are complex because of correlations between different reaction channels as well as variances in channels themselves. These uncertainties are stored in nuclear data evaluations as covariance matrices. Recently, there has been an effort to perturb nuclear data directly through sampling. These created nuclear data are then used in the transport calculation of choice to propagate the nuclear data uncertainty. It should be noted that processing evaluating nuclear data files is not a trivial process with many codes [15, 16, 17] dedicated to the task.

Perturbation theory offers similar calculations with multi-group nuclear data and has been historically the tool of choice for sensitivity and uncertainty quantification, for example SCALE's TSUNAMI [18] uses this method. The nuclear data sampling described is based on Monte-Carlo approaches, thus allowing the

data to be used with any transport approximation instead of just multi-group calculations. An unfortunate aspect of the nuclear data sampling tools are they are either proprietary or in-house implementations, thus not easily available. Open source tools [19] to manipulate nuclear data exist, however concise, reliable APIs to use the methods developed are not yet available. The TENDL-2012 [20] nuclear data library published many iterations of randomly created data and is the largest source of openly available random nuclear data.

2.2.1. Continuous Energy Covariance Based

Evaluated nuclear data comes with multi-group covariance matrices to describe cross-section uncertainties. Tools have been developed to use these covariances to sample nuclear data. Nuclear Data Uncertainty Analysis (NUDANA) [21] and KIWI [22] are two such tools. A drawback of using nuclear data covariances is that covariances are not available for all nuclide and are not all available for all reaction channels. Nonetheless, the available covariances can be used to sample nuclear data.

2.2.2. Multi-Group Covariance Based

Often reactor physics codes use the multi-group approximation to make problems tractable. Continuous data can be collapsed into suitable energy bins by various means to create multi-group nuclear data. Nuclear data covariances can then be used to adjust the multi-group data after collapse. The Cross Section Uncertainty and Sensitivity Analysis (XSUSA) [23] tool implements this method of cross-section sampling. It's built to be create nuclear data with the SCALE covariance matrices for use with the TSUNAMI sequence.

2.2.3. Theoretical Model Based

The TALYS Evaluated Nuclear Data Library (TENDL) [14] is a complete nuclear data library based on theoretical calculations along with specific evaluated data. The use of theoretical calculations allows for evaluations of cross sections that have not been measured and the creation of covariance matrices that have not been measured. The library is created to agree with benchmarked data as

much as possible. It features many isotopes of interests and many, many more covariances than typical libraries that rely more on experimental data. Due to the computational nature of library creation, random nuclear data evaluations can be made using inputs to the theoretical model rather than relying on provided nuclear data covariances. The model inputs are varied until many sets of cross sections are made that are not rejected (e.g., agree with experimental data).

2.2.4. ACE Data Based

A more direct method of sampling is to use vary the ACE (A Compact ENDF) data format that MCNP and other transport codes use. ACE data stores nuclear data in a point-wise manner such that linear interpolations can be made between points to create 'continuous' data. The Nuclear data Uncertainty Stochastic Sampling (NUSS) tool [24] directly perturbs the pointwise data based on multi-group nuclear data covariances. This eliminates the need to manipulate very complex ENDF data, but requires confidence in inputted covariance matrices. A comparison of NUSS and theoretical model based nuclear data perturbations was performed previously [25]. The two methods agreed well for benchmark criticality cases. However, there are cases where the theoretical model produced nuclear data with a non-zero skewness, which are not represented in ENDF data. These skewed data leads to skewed uncertainties which could be important in some safety calculations. The NUSS tool was also extended [26] with better statistical methods to perform global sensitivity analysis based on the group-wise covariances and sampled made. The new method uses a relatively complicated sampling scheme that assumes normal distributions. The sampling method in this paper relies on ACE data with sampling philosophies similar to NUSS.

3. Uncertainty Quantification Methods

3.1. Total Monte-Carlo

The Total Monte-Carlo method refers to a technique to randomly vary fundamental nuclear data parameters to generate many random nuclear data libraries from theoretical models. These random data are used in many long running MC calculations to determine the effects of nuclear data variations. The statistical method to remove the MC statistics from output calculations can be described by breaking up the observed uncertainty into Monte-Carlo and input uncertainties,

$$\sigma_{ob} \approx \overline{\sigma_s^2} + \sigma_i^2 \tag{1}$$

$$\overline{\sigma_s^2} = \frac{1}{N} \sum_{j=1}^{N} \sigma_{s,j}^2, \tag{2}$$

where σ indicates uncertainties, and the subscripts ob, s, i, indicate observed, statistical, input uncertainties, and N is the total number of observations. If a set of observations due to varying inputs can be made along with the associated MC uncertainty, the input uncertainty can be determined using Eq. (1).

A large (500-1000) set of random inputs are generated to create a large set of outputs. Within an MC calculation, each run should have sufficiently low relative MC uncertainty (e.g., $\overline{\sigma_s} \approx 0.05$) such that the total uncertainty observed from the large set of outputs is predominately from epistemic input uncertainties. This method, though easy to implement for most code frameworks, increases calculation time by 500-1000 times that of a single run. This runtime is rather large for personal workstations but quite possible on modern high performance computers where 1000s of processors are available for a single user.

TMC has the added benefit of determining the full covariance of the response [27]. This can be quite useful when performing spectrum adjustments.

Error estimates of the TMC results can be calculating using a bootstrap method. The basic procedure is to take random samples of the random inputs

with replacement. The total number of random samples of the original samples to take should be equal to the original number of samples [28]. The tmc method is then applied to the new sampled inputs along with the corresponding outputs. This whole procedure is repeated many times to create a vector of uncertainty estimates. Confidence intervals can then be calculated by sorting the vector and calculating the lower and upper cutoffs based on a desired confidence interval.

3.2. GRS

The GRS method relies on the statistical distribution of MC outputs in order to determine input uncertainty. By taking two sets of random simulations, two distributions with the same uncertainties are found. The covariance of these distributions is the input uncertainty because statistical errors are the same in both sets and are removed by the covariance operation. In a mathematical sense, given a model, $Y = X(U)$, with input set U that is randomly varied, the average output μ, is,

$$\mu = \mathbf{E}[\mathbf{E}[Y|U]],$$

which given the results of iterated expectations (sometimes called law of total expectation),

$$\mu = \mathbf{E}[Y],$$

with variance, σ^2 as,

$$\sigma^2 = \mathrm{Var}(\mathbf{E}[Y|U]).$$

The square-root of the variance gives the uncertainty of the inputs on the outputs. However, with a single MC run, a very large number of particles would need to be ran (like in TMC) to reduce MC statistics. However, when two sets of MC runs are made with two different random number seeds, two sets of outputs, Y, Y' are created that are conditionally independent and identically distributed, e.g., on average the outputs are the same but comparing individual

results will show differences ($\mu = \mathbf{E}[Y] = \mathbf{E}[Y']$). By using this fact and the following form of the expectation of the two outputs multiplied, the variance of the mean output can be related to the covariance between the two output sets. The expectation of the two outputs multiplied is,

$$\begin{aligned}
\mathbf{E}[YY'] &= \mathbf{E}[\mathbf{E}[YY'|U]], \\
&= \mathbf{E}[\mathbf{E}[Y|U] \cdot \mathbf{E}[Y'|U]], \\
&= \mathbf{E}[\mathbf{E}[Y|U] \cdot \mathbf{E}[Y|U]], \\
&= \mathbf{E}[\mathbf{E}[Y|U]^2]. \qquad (3)
\end{aligned}$$

Inserting Eq. (3) into the definition of covariance,

$$\begin{aligned}
\mathrm{Cov}[Y, Y'] &= \mathbf{E}[YY'] - \mathbf{E}[Y]\mathbf{E}[Y'], \\
&= \mathbf{E}[\mathbf{E}[Y|U]^2] - \mathbf{E}[Y]^2, \\
&= \mathrm{Var}(\mathbf{E}[Y|U|]), \qquad (4)
\end{aligned}$$

shows that the covariance between the two output sets is the variance of the desired mean output given input uncertainties U. This formulation cancels out (or averages) the MC uncertainties such that only the input uncertainties remain. This method avoids Eq. (1) so criteria for $\overline{\sigma}_s^2$ are not required, though MC uncertainties should be reasonably sized and enough particles ran to ensure source convergence.

Covariance information cannot be generated from the GRS method because the method targets the mean variance (diagonal of the covariance) and not covariance information. A bootstrapping uncertainty estimator is also not valid because the GRS method requires unique samples. However different estimators could be used such as jack-knifing, but this is not explored in this work.

4. Sampling Methods

4.1. Nuclear Data Sampling

Randomly generated cross-section files available within TENDL are an excellent resource, however random evaluations for all cross-sections are not available and evaluated covariances are not used when generating the data. While the latter is considered a positive feature of TENDL random data, it is not fully accepted that generated data from fundamental parameters is the correct method of making nuclear data. The ability to generate random data with SCALE based covariance data is a positive feature to overcome issues when data is not available and to sample data based on evaluated distributions. A deficiency in this method of sampling is that the covariance data must be available for the reaction and nuclide of interest to actually sample data. Furthermore, sampling from ENDF formatted covariances directly has a benefit of sampling from any ENDF based data as well as from covariance data that has not yet made it to official SCALE releases.

ASAPy[1] is a tool that was created in this work to perform data sampling from ACE files using SCALE covariance data or ENDF data via NJOY to address the above issues. This tool is similar to the NUSS tool described in Sec. 2.2.4, except it uses the newest SCALE covariance data or newest ENDF data, written in python, and available for use. It also features the ability to use any group structure and/or any user flux weighting functions for covariance collapsing from ENDF sources. The sampling procedures also uses lognormal sampling along with the ability to use any sampling function as long as the percent point function is available.

4.2. ACE Data Manipulations

The A Compact ENDF file (ACE) format is used for nuclear data within MCNP and other Monte-Carlo codes. It contains all relevant data from ENDF

[1] https://github.com/veeshy/ASAPy/releases/tag/v1.0

files, support random access of data, and specifies all cross-sections on the same unionized energy grid. The ACE data is a formatted data file and readers are available, though writers tend to only translate ENDF data to ACE, with no general method to manipulate the ACE data directly. The ACE data reader within OpenMC [29] was used to read in ACE files. A writer was created based on the structure of ACE files. All data is represented in contiguous arrays, so that if the original data is known (from reading the ACE data), that data can be searched for within the ACE file and replaced with new values as long as the exact same energy grid is specified. This method of adjusting ACE data is implemented in ASAPy. A few nuances when dealing with different data will be discussed.

Cross-Section Perturbation: Nuclear data sampling occurs using multi-group methods while ACE data is stored in a continuous format. Perturbation factors are generated based on taking a ratio of sampled cross-sections and multi-group average cross-sections. These perturbation factors are then applied to the continuous cross-sections by mapping the multi-group structure on the continuous structure. This method can cause difficulties in sampling data when a group boundary happens to occur in a region where the flux or variance changes rapidly. This usually manifests itself in ill-formed covariance information.

ENDF Sum Rules: Many ENDF reactions are subsets of other reactions, so when one cross-section is sampled, others might need to be adjusted for consistency. This is performed within ASAPy by keeping track of all MTs adjusted and comparing against sum rules. Table 1 shows the relevant sum rules from the ENDF manual [13].

$\bar{\nu}$ Data: ENDF data allows for inclusion of total, average number delayed, and prompt fission neutrons. MCNP only uses the total values within ACE files, so only these are modified.

Fission χ Spectrum: The distribution of energy of neutrons born from fission depends on the incident neutron energy. As such, ACE data file stores several tables for a few incident neutron energies. ENDF covariance data does

not have covariance data for each incident neutron so the covariance data within the ENDF file is applied to all incident neutron energy distributions. The distributions are also stored as probability and cumulative distribution functions (PDF and CDF). To sample these, the PDF is perturbed then the CDF is adjusted based on the PDF perturbations then the CDF is re-normalized by adding up the original PDF and perturbation factors to ensure the CDF sums to 1.

4.3. Covariance Data

The most comprehensive resource for covariance data is distributed within SCALE 6.2 [18]. It combines covariance data from several nuclear data sources and experiments. The SCALE based data was generated using a typical LWR flux that include a thermal, epi-thermal, and fast region. A fine 252-group and coarse 56-group structure is available within SCALE. An older 44-group structure exists but contains old data that is not recommended for use. The covariance data can be converted from the internal SCALE binary format to a ASCII format using the SCALE tool AmpxCOVConverter. The resulting data file contains data for material numbers and their relevant reactions correlated with one another. The standard deviations of the specified reactions are given in the relevant group structure followed by the actual correlation matrix. A covariance parser was created within ASAPy to convert the ASCII file to a more general HDF5 store with a hierarchy based on: '/mat1/mt1/mat2/mt2' corresponding to data correlating mat1 MT1 with mat 2 MT2. Often mat 1 and mat 2 are the same, and MT1 and MT2 are the same, specifying self-correlation. Any group structure can be accommodated by the parser such that new evaluations can be easily used within ASAPy.

Covariance data also exists in ENDF files and these covariances can be used to create any group structure as well as use any weighting flux to create covariance matrices to sample with. ENDF data can be parsed with NJOY [15] to generate covariance data. ASAPy implements NJOY input writers along with ENDF readers to minimize the amount of user input to generate covari-

ance data. The minimum input is a path to an ENDF file and the reaction MT numbers to generate covariance data for. A BOXER format reader was also generated in order to read the BOXER formatted covariance files into the previously described HDF5 format.

The covariance data comes in multi-group format which must be mapped to relevant continuous energy bins in ACE data. After sampling data within the multi-group structure, the data is divided by the multi-group mean cross-section to calculate a relative cross-section. These cross-sections are mapped onto the continuous energy group bins then multiplied by the ACE data to generate a sample of data. Two assumptions made are that the group-mean values within the data are very similar to the mean values within the ACE data and that the data within an energy bin are fully-correlated with one another.

No data is shipped with ASAPy, ENDF data is freely available and SCALE data is available with appropriate licenses.

4.4. Nuclear Data Sampling Techniques

A slight deficiency in the ENDF format is the inability for evaluators to convey what type of distribution covariance data should take. Often physical parameters like cross-sections cannot take negative values, but assuming normal distributions are assigned to reported covariances, negative values are possible. An approach often taken is to discard negative data, biasing the sampling scheme. Another method is to assume the distributions are log-normal, which always has positive values. However, without knowing what distributions the covariance data were specified for, errors can occur when large relative errors are present with strong negative correlations [30] due to not transforming the normal-cov to lognormal-cov. In this work, ENDF covariance data is transformed to log-normal covariance data then log-normal sampling is performed ensuring no negative samples are taken.

Nuclear data has strong correlations between energy groups so when sampling data, the full covariance of the data must be taken into account. Multivariate-normal distributions allow for sampling of such data. Given a desired covariance

matrix, C, that is semi-positive definite, and mean values, μ, a multi-variate sample, X_i can be generated as follows. First draw uncorrelated values from the mean using a standard-normal distribution, $\mathcal{N}$ and place the means in a diagonal matrix,

$$x_i = \mathcal{N}[\mu = 0, \sigma = 1],$$

then perform a singular value decomposition of the covariance,

$$C = USV, \tag{4}$$

where U and V are orthogonal matrices, and S is a diagonal matrix containing the singular values of C. A sample can then be drawn as

$$X_i = \mu + x_i S^{0.5} v$$

This method is implemented in Scipy [31] within 'np.random.multivariate_normal'. One may also use eigen or Cholesky decomposition instead of singular value decomposition with similar results.

ENDF based nuclear data sometimes is published with non-semi-positive-definite covariances. In this case the correlation data R must be manipulated to draw samples. An eigen-decomposition of the correlation matrix is made,

$$R = Q\Lambda Q^{-1},$$

where Q contains the eigenvectors of R, and Λ contains the eigenvalues on the diagonal. The negative eigenvalues are set to a small positive number (1e-8) to form $\tilde{\Lambda}$ then the original eigenvectors are multiplied back in to form an adjusted correlation matrix, $\tilde{R}$,

$$\tilde{R} = Q\tilde{\Lambda}Q^{-1}.$$

The correlation matrix is used due to smaller spreads in eigenvalues, however often the small eigenvalues imposed on the matrix cause numerical difficulties when converting the correlation matrix to a covariance matrix so the above procedure may need to be repeated on the converted covariance matrix.

A second method based on a partial Cholesky decomposition [32] that generates a positive semi-definite matrix that equals the original matrix minus an

MT	Description	MTs in Sum
1	Incident Neutron Total cross	2, 4, 5, 11, 16-18, 22-26, 28-37, 41-42, 44-45, 102-117
4	Total of neutron levels	50-91
18	Total fission	19-21, 38
103	Total of proton levels	600-649
104	Total of deuteron levels	650-699
105	Total of triton levels	700-749
106	Total of 3He levels	750-799
107	Total of alpha levels	800-849

Table 1: ENDF Sum Rules

error term was also implemented for correcting non semi-positive definite matrices.

A non-semi positive definite correlation example is the correlation matrix for (n, γ) cross-section of ^{184}W within ENDFB/VIII. The eigen-decomposition and partial Cholesky algorithms were applied to generate 500 samples and the correlation matrices are shown in Fig. 1, where it can be seen that both algorithms perform well compared to the original correlation matrix.

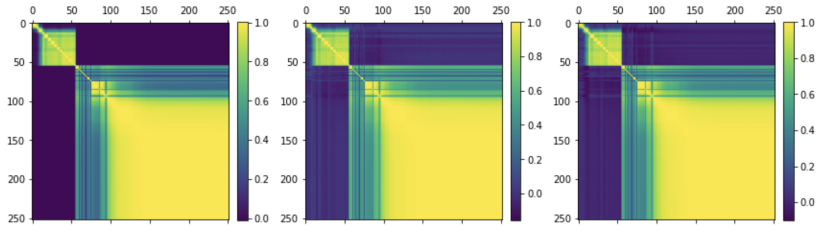


Figure 1: Correlation matrices from (left) the evaluated data file (middle) eigen-decomposition sampling (right) partial Cholesky decomposition sampling

4.5. MCNP Input Sampling

mcACE is a tool developed to perform UQ using MC methods. It is used to manipulate MCNP input files to create random perturbations based on changing any line given variables to change and distributions to sample from. It also handles data post-processing, data transfer, MCNP/ORIGEN coupling, and performs statistics on relevant results. ORIGEN coupling is not discussed in this paper but it is available in the code to help propagate uncertainties through time. The typical flow of mcACE is shown in Fig. 2.

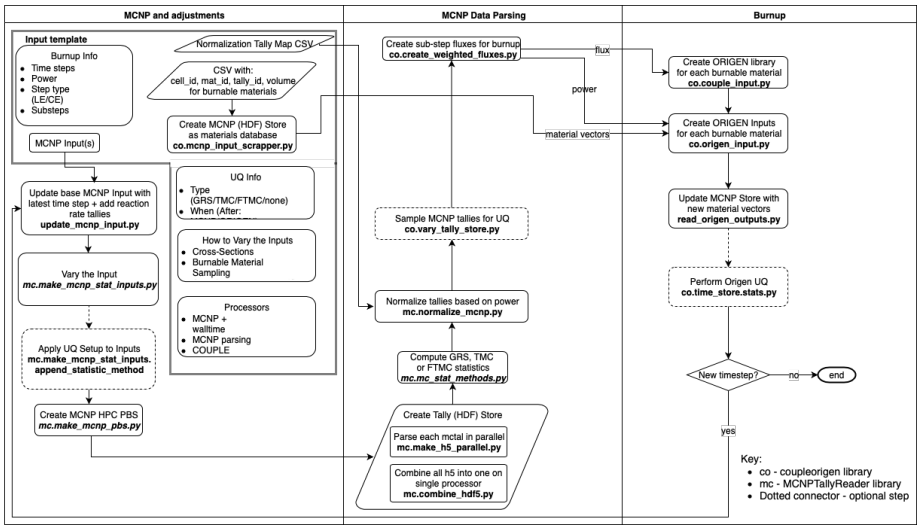


Figure 2: mcACE Flow Diagram

The goal of mcACE was to apply to many reactor designs rather than only work with a single reactor. This goal necessitated writing a program that could understand MCNP syntax. Particularly, MCNP cell lines can be parsed for cell numbers, material numbers, densities, and volumes; MCNP problem lines can be parsed for material numbers and materials. More subtle MCNP features are also handled such as MCNP single line comments (C comment), end of line comments (valid line $ comment), and both types of continuation lines (lines starting with 5 spaces and lines following a &). This allows for reading as well as writing back MCNP files that can be ran with MCNP directly. The whole

input file is parsed into a python class that allows access to the MCNP title, cell, surface, and problem blocks. Find and replace functions help sampling procedures vary inputs.

Any parameter in the MCNP input can be sampled using the mcACE input. This is similar to MCNP-PSTUDY [33], however more general samplers are available. Given the original line and a properly formatted version of that line, sampling can be performed. An example to vary density is shown in Fig. 1, where the first line is the original MCNP line in pseudo-code format, and the second line is the original line with the 'density' number replaced with a python string formatter with index 0. The index 0 corresponds to the position in the 'sampling_scheme' list. The 'sampling_scheme' allows for many sampling functions like uniform, normal, latin-normal, repeating the last sampled value, giving an exact value for a simple find/replace, or a user generated math function. This interface provides good flexibility to sample MCNP files. The mcACE input allows for repeated sampling blocks so sets of parameters can be varied as needed.

Listing 1: Sample mcACE MCNP Line Sampling SNippet

```
mcnp_lines=cellnum matnum density surf cards imp:n=1,
lines_to_vary_with=cellnum matnum {0:.6f} surf cards imp:n=1,
sampling_scheme=latin ,
sampling_values=0.1 0.05,
```

4.6. MCNP Tally Reader

MCNP prints relevant outputs to '.o' files, and optionally '.mctal' files. The '.o' files contain a wealth of information, particularly about statistics and problem run information as well as relevant outputs like tallies and eigenvalue. The '.mctal' files contain a subset of the information in the '.o' files but the information is very structured, allowing for efficient readers to be created. mcACE implements an '.mctal' reader to read eigenvalues, problem information, and

most tallies (i.e., F#:particle, FC, E, T, C, FM, DE/DF, and SD), missing is a mesh-tally reader though one could be added. MCNP '.o' files can also be read for information that is not present in a '.mctal' file such as kinetics parameters and sensitivity coefficients.

4.7. mcACE Storage

The UQ process implemented generates a large amount of output depending on the relevant output parameters. In a typical run with 500 MCNP in eigenvalue mode, 5 tallies with 100 energy bins would result in 2.5e5 outputs to track. In a burnup calculation that uses a 238-group structure and 100 unique materials, a minimum of 11.9e6 outputs must be tracked. Storing this data in typical text files or csv's is not efficient and error prone. mcACE opts to use the HDF5 storage format along with Pandas [34] dataframes to store data as tables in HDF5 format. After relevant outputs are parsed for each MCNP run, all of the similar results are combined into a dataframe with multiple index as tally info as needed and a run number index, with columns as energy bins or other specific names such as 'keff'. This format also makes it easier to perform statistics on the outputs.

5. Verification and Application

5.0.1. Godiva Eigenvalue

The Godiva core is a well known benchmark model / experimental validation core. It is a bare spherical mass of HEU that has a well quantified uranium material vector and critical dimensions. It's also a simple reactor core to analyze due to it's fast spectrum. The MCNP-IFP method was used to calculate sensitivities for several reaction MTs. Covariances were provided by ASAPy to calculate the total uncertainty on eigenvalue from reaction rates via the sandwich rule. The mcACE UQ process using TMC and ASAPy generated cross-sections was performed using 1000 runs. Table 2 shows good agreement for all studied reaction MTs, all values agree within uncertainty. MCNP-IFP uncertainty was

Correlation	Reaction	Unc. (pcm)	95% σ	MCNP-IFP
Uncorrelated	(n,γ)	479.4	13.3	482.3
	(n,f) + (n,γ)	493.5	13.3	-
	(n,f)	121.2	3.3	119.8
	$\bar{\nu}$	221.1	5.5	218.5
	Fission χ	167.4	5.0	169.3
Correlated	(n,γ)	838.8	24.4	848.9
	(n,f) + (n,γ)	883.3	25.1	-
	(n,f)	269.5	6.8	269.4
	$\bar{\nu}$	546.0	13.9	544.1
	Fission χ	269.0	12.7	276.2

Table 2: Comparing Godiva Uncertainties using ASAPy to MCNP-IFP

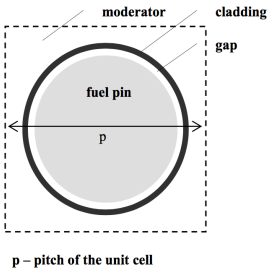
not propagated. This result shows that the TMC method agrees well with the IFP theory in terms of eigenvalue uncertainties. This indirectly shows the GRS method also agrees well with IFP theory in that it agrees well with TMC calculations, which will be shown in Sec. 5.0.2. Reaction rate uncertainties could not currently be calculated within MCNP for further verifications.

5.0.2. UAM Pincell Flux and Reaction Rates

To verify the GRS implementation the TMC (Total Monte-Carlo) method is used as the 'true' result. Furthermore, convergence studies are performed to determine how many runs are needed for GRS cases. The relative errors reported are the uncertainties in the output quantities from input uncertainty, and not the typical MCNP related statistical error. The relative errors of each value are compared by plotting the relative error of the GRS method to the TMC method. If the two methods agree, a point will be on the y=x line.

The UAM Pincell Benchmark [35] at hot-zero power was modeled according to the specifications in Fig. 3. The TMC cases were ran with 7500 particles

/ cycle for 15000 active cycles, the GRS cases used 40 cycles (187.5 times less total particles ran because GRS requires twice as many model runs). In Fig. 4 it can be seen that in general, GRS agrees well with TMC.



Parameter	Value
Unit cell pitch, [mm]	18.75
Fuel pellet diameter, [mm]	12.1158
Fuel pellet material	UO_2
Fuel density, [g/cm^3]	10.42
Fuel enrichment, [w/o]	2.93
Cladding outside diameter, [mm]	14.3002
Cladding thickness, [mm]	0.9398
Cladding material	Zircaloy-2
Cladding density, [g/cm^3]	6.55
Gap material	He
Moderator material	H_2O

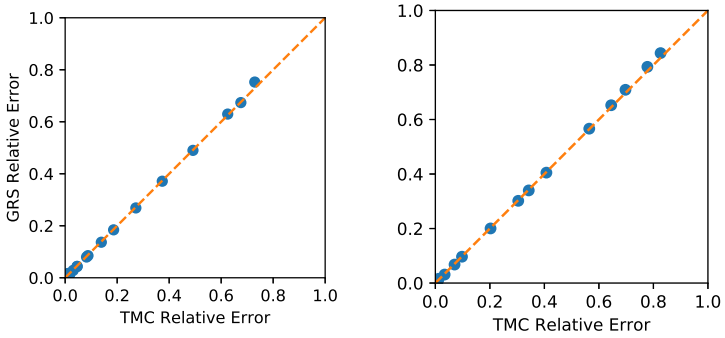
Parameter / Reactor condition	HZP	HFP
Fuel temperature, [K]	552.833	900
Cladding temperature, [K]	552.833	600
Moderator (coolant) temperature, [K]	552.833	557
Moderator (coolant) density, [kg/m^3]	753.978	460.72
Reactor power ,[MWt]	3.293	3 293
Void fraction (%)	-	40

Figure 3: UAM Pincell Dimensions [35]

5.1. Practical Example with Advanced Test Reactor

The Advanced Test Reactor (ATR) [36] is a high powered, high flux material test reactor used for isotope production, fuel qualification, material irradiations, and other experiments. Often the irradiation history of an experiment can be determined through purely experimental means like determining the fission rate of a fueled sample via microscopy or calculating activity via radiation detectors. Other times flux wires must be used along with computer models to determine the irradiation history. When computer models are needed, an estimate of the uncertainty of the relevant computation is important. To show the usefulness of TMC and GRS methods on a real world model, the uncertainty of the flux in an experiment within the ATR was calculated.

The energy dependent flux within graphite shown is very important in determining spectral adjustments based on experiment flux wires. Each model



(a) 238-Group Flux

(b) Reaction Rates

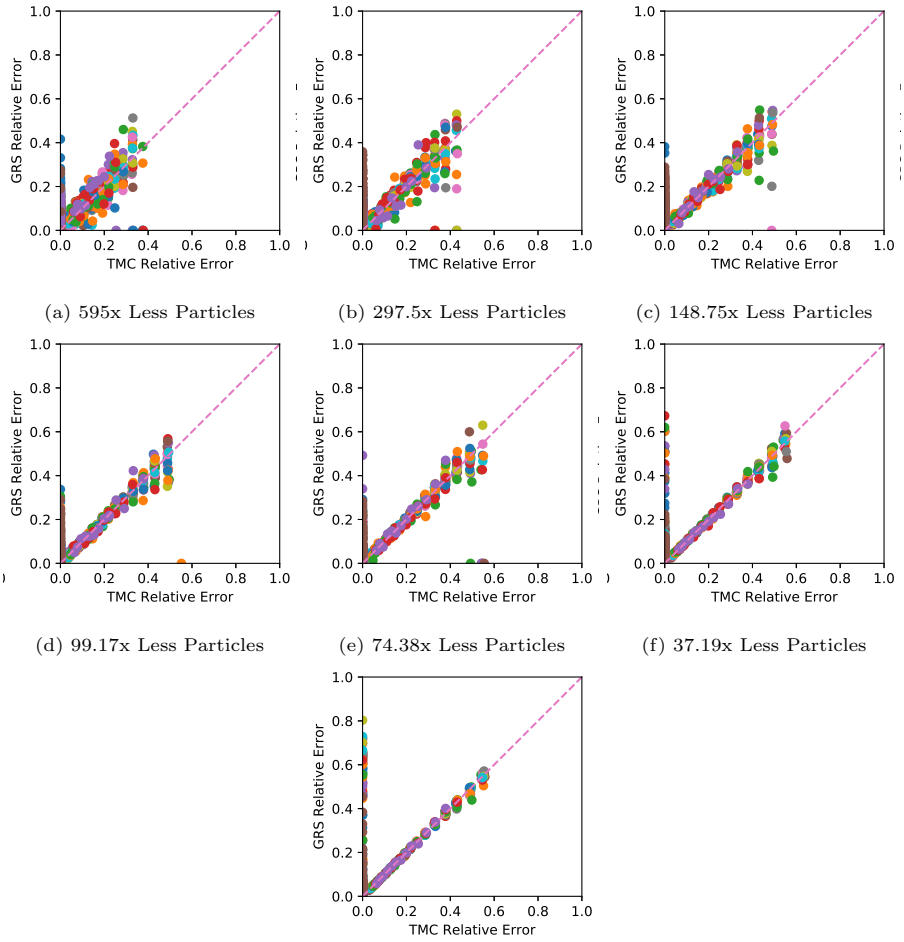
Figure 4: TMC and GRS Relative Uncertainties

ran has a unique U-235 data library created from TENDL-12 ENDF files [20]. The predicted GRS relative errors (shown in Fig. 5) for the 148.75x case shows reasonable agreement (mosth within 20%) with the TMC values. Grouping of TMC values near the y-axis (x=0) that TMC failed to predict the input errors because of relatively large MC standard deviations or large MC variance to observed variance ratios in the calculated values. This shows that the GRS method is able to predict relative output uncertainties where the TMC method fails. This does not show that the GRS method predicts a similar value to TMC in those cases if TMC were able to predict a value, though it's a reasonable conclusion because the two agree well when TMC is applicable.

The speedup for the GRS method for energy dependent flux is not as great as global values like eigenvalue. Excellent agreement between the TMC and the GRS cases occur when 12.9x less particles are used in GRS than TMC. The 37.19x less particle case has slightly more spread in results but all values where comparable agree with 20%.

6. Conclusions

A process was developed to quantify uncertainty of any output with an established Monte-Carlo neutronic code (MCNP) without any source code modification and built into a new code called mcACE. A review of relevant method



(a) 595x Less Particles

(b) 297.5x Less Particles

(c) 148.75x Less Particles

(d) 99.17x Less Particles

(e) 74.38x Less Particles

(f) 37.19x Less Particles

(g) 12.9x Less Particles

Figure 5: Various Runtimes Predicting Graphite Flux Using GRS

was performed and a combination of sampling techniques and statistical methods were identified to perform uncertainty quantification of relevant outputs for reactor calculations. Comparisons of the selected statistical methods, GRS and TMC were made to confirm their ability to predict similar outputs. GRS showed an decrease of at least 10x computational time relative to TMC when calculating uncertainties of fine-group fluxes in small regions of a reactor model. For larger regions or more global values, 100x or more speedup is possible. The TMC method was shown to also compare well with traditional sensitivity methods when applied to k-eigenvalue calculations.

ASAPy was created to sample ACE data based on ENDF and SCALE covariances using normal and log-normal distributions. ASAPy can generate covariance from ENDF data for any group structure and any spectrum weight. Data is generated as ACE files and methods were developed to update MCNP data tables so that the ACE Files can be used. Generated cross-sections were verified to produce similar uncertainties in the Godiva reactor as adjoint based methods.

Finally the TMC and GRS methods were applied to a real-world model of the Advanced Test Reactor to successfully calculate an energy dependent flux within an experimental location. The two methods agreed well again, with the GRS method being at least 10x faster.

Future work would should include further code-to-code verifications and new nuclear data sampling treatments. In particular, comparisons of reaction rate uncertainties from other codes and energy dependent flux uncertainties are of interest. Sampling methods with built-in sensitivity calculation methods [26] could also be used to add calculations of sensitivity profiles. Sampling methods with decreased sampling requirements [37] could also be implemented.

References

[1] J. T. Goorley, M. R. James, T. E. Booth, F. B. Brown, J. S. Bull, L. J. Cox, J. W. J. Durkee, J. S. Elson, M. L. Fensin, R. A. I. Forster, J. S.

Hendricks, H. G. I. Hughes, R. C. Johns, B. C. Kiedrowski, R. L. Martz, S. G. Mashnik, G. W. McKinney, D. B. Pelowitz, R. E. Prael, J. E. Sweezy, L. S. Waters, T. Wilcox, A. J. Zukaitis, Initial MCNP6 Release Overview - MCNP6 version 1.0, Los Alamos National Laboratory (April 2013).

[2] E. P. Wigner, Effect of small perturbations on pile period, in: Nuclear Energy, Springer, 1992, pp. 540–552.

[3] D. Cacuci, Sensitivity & Uncertainty Analysis, Volume 1: Theory, CRC Press, 2003.
URL https://books.google.com/books?id=6HzSuyJ15AoC

[4] H. Rief, Generalized monte carlo perturbation algorithms for correlated sampling and a second-order taylor series approach, Annals of Nuclear Energy 11 (9) (1984) 455 – 476. doi:http://dx.doi.org/10.1016/0306-4549(84)90064-1.
URL http://www.sciencedirect.com/science/article/pii/0306454984900641

[5] Y. NAGAYA, T. MORI, Impact of perturbed fission source on the effective multiplication factor in monte carlo perturbation calculations, Journal of Nuclear Science and Technology 42 (5) (2005) 428–441. doi:10.1080/18811248.2005.9726411.
URL http://www.tandfonline.com/doi/abs/10.1080/18811248.2005.9726411

[6] Comparison of the Monte Carlo adjoint-weighted and differential operator perturbation methods.

[7] B. C. Kiedrowski, F. B. Brown, P. Wilson, Calculating kinetics parameters and reactivity changes with continuous-energy monte carlo, Tech. rep., Los Alamos National Laboratory (LANL) (2009).

[8] H. J. SHIM, C. H. KIM, Adjoint sensitivity and uncertainty analyses in monte carlo forward calculations, Journal of Nuclear Science and Technol-

ogy 48 (12) (2011) 1453–1461. doi:10.1080/18811248.2011.9711838.
URL http://www.tandfonline.com/doi/abs/10.1080/18811248.2011.9711838

[9] C. M. Perfetti, B. T. Rearden, W. R. Martin, Scale continuous-energy eigenvalue sensitivity coefficient calculations, Nuclear Science and Engineering 182 (3) (2016) 332–353.

[10] A. Koning, D. Rochman, Towards sustainable nuclear energy: Putting nuclear physics to work, Annals of Nuclear Energy 35 (11) (2008) 2024 – 2030. doi:http://dx.doi.org/10.1016/j.anucene.2008.06.004.
URL http://www.sciencedirect.com/science/article/pii/S0306454908001813

[11] W. Zwermann, B. Krzykacz-Hausmann, L. Gallner, M. Klein, A. Pautz, K. Velkov, Aleatoric and epistemic uncertainties in sampling based nuclear data uncertainty and sensitivity analyses, Tech. rep., American Nuclear Society, Inc., 555 N. Kensington Avenue, La Grange Park, Illinois 60526 (United States) (2012).

[12] N. Otuka, et al., Towards a more complete and accurate experimental nuclear reaction data library (exfor): International collaboration between nuclear reaction data centres (nrdc), Nuclear Data Sheets 120 (2014) 272 – 276. doi:http://dx.doi.org/10.1016/j.nds.2014.07.065.
URL www.sciencedirect.com/science/article/pii/S0090375214005171

[13] M. Herman, A. Trkov, Endf-6 formats manual, National Nuclear Data Centre, BNL, Upton, New York.

[14] A. J. Koning, D. Rochman, Modern nuclear data evaluation with the talys code system, Nuclear data sheets 113 (12) (2012) 2841–2934.

[15] D. Muir, R. Boicourt, A. Kahler, The njoy nuclear data processing system, version 2012, Tech. rep., LA-UR-12-27079 (2012).

[16] D. E. Cullen, Prepro 2015 2015 endf/b pre-processing codes, Tech. rep., IAEA-NDS-39 (2015).

[17] D. Wiarda, M. L. Williams, C. Celik, M. E. Dunn, Ampx: A modern cross section processing system for generating nuclear data libraries, Tech. rep., Oak Ridge National Laboratory (2015).
URL http://www.osti.gov/scitech/servlets/purl/1286858

[18] B. Rearden, M. Jessee, Scale code system, Tech. Rep. ORNL/TM-2005/39, Oak Ridge National Laboratory (2016).

[19] C. Mattoon, B. Beck, N. Patel, N. Summers, G. Hedstrom, D. Brown, Generalized nuclear data: a new structure (with supporting infrastructure) for handling nuclear data, Nuclear Data Sheets 113 (12) (2012) 3145–3171.

[20] S. C. van der Marck, A. J. Koning, D. A. Rochman, Benchmarking tendl-2012, Nuclear Data Sheets 118 (2014) 446–449.

[21] O. Buss, A. Hoefer, J.-C. Neuber, Nuduna: "nuclear data uncertainty analysis", in: Meeting on uncertainty propagations in the nuclear fuel cycle Uppsala University, 2013.

[22] J. Pruet, Kiwi: An evaluated library of uncertainties in nuclear data and package for nuclear sensitivity studies, Tech. rep., Lawrence Livermore National Laboratory (LLNL), Livermore, CA (2007).

[23] W. ZWERMANN, A. AURES, L. GALLNER, V. HANNSTEIN, B. KRZYKACZ-HAUSMANN, K. VELKOV, J. MARTINEZ, Nuclear data uncertainty and sensitivity analysis with xsusa for fuel assembly depletion calculations, Nuclear Engineering and Technology 46 (3) (2014) 343 – 352. doi:http://dx.doi.org/10.5516/NET.01.2014.711.
URL http://www.sciencedirect.com/science/article/pii/S1738573315301297

[24] T. Zhu, Sampling-based nuclear data uncertainty quantification for continuous energy monte carlo codes, Ph.D. thesis, EPFL (2015).

[25] D. Rochman, A. Vasiliev, H. Ferroukhi, T. Zhu, S. van der Marck, A. J. Koning, Nuclear data uncertainty for criticality-safety: Monte carlo vs. linear perturbation, Annals of Nuclear Energy 92 (2016) 150–160.

[26] T. Zhu, A. Vasiliev, H. Ferroukhi, A. Pautz, S. Tarantola, Nuss-rf: stochastic sampling-based tool for nuclear data sensitivity and uncertainty quantification, Journal of Nuclear Science and Technology 52 (7-8) (2015) 1000–1007. arXiv:https://doi.org/10.1080/00223131.2015.1040864, doi:10.1080/00223131.2015.1040864.
URL https://doi.org/10.1080/00223131.2015.1040864

[27] N. Asquith, S. van der Marck, Using total monte carlo to calculate the full covariance matrix of a neutron spectrum, in: Reactor Dosimetry: 16th International Symposium, ASTM International, 2018.

[28] M. Kuhn, K. Johnson, Applied predictive modeling, Vol. 26, Springer, 2013.

[29] P. K. Romano, N. E. Horelik, B. R. Herman, A. G. Nelson, B. Forget, K. Smith, Openmc: A state-of-the-art monte carlo code for research and development, Annals of Nuclear Energy 82 (2015) 90 – 97, joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013, SNA + MC 2013. Pluri- and Trans-disciplinarity, Towards New Modeling and Numerical Simulation Paradigms. doi:https://doi.org/10.1016/j.anucene.2014.07.048.
URL http://www.sciencedirect.com/science/article/pii/S030645491400379X

[30] G. Žerovnik, A. Trkov, D. L. Smith, R. Capote, Transformation of correlation coefficients between normal and lognormal distribution and implications for nuclear applications, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 727 (2013) 33–39.

[31] E. Jones, T. Oliphant, P. Peterson, et al., SciPy: Open source scientific

tools for Python, [Online] (2001–).
URL http://www.scipy.org/

[32] J. Nocedal, S. J. Wright (Eds.), Numerical Optimization, Springer-Verlag, 1999. doi:10.1007/b98874.
URL https://doi.org/10.1007/b98874

[33] F. B. Brown, J. E. Sweezy, R. Hayes, Monte carlo parameter studies and uncertainty analyses with mcnp5, in: PHYSOR-2004, American Nuclear Society Reactor Physics Topical Meeting, 2004.

[34] T. pandas development team, pandas-dev/pandas: Pandas (Feb. 2020). doi:10.5281/zenodo.3509134.
URL https://doi.org/10.5281/zenodo.3509134

[35] K. Ivanov, M. Avramova, S. Kamerow, I. Kodeli, E. Sartori, E. Ivanov, O. Cabellos, Benchmarks for uncertainty analysis in modelling (uam) for the design, operation and safety analysis of lwrs-volume i: Specification and support data for neutronics cases (phase i), Tech. rep., Organisation for Economic Co-Operation and Development (2013).

[36] D. W. Nigg, D. A. Steuhm, Advanced test reactor core modeling update project annual report for fiscal year 2011, Tech. rep., Idaho National Laboratory (INL) (2011).

[37] Z. Sui, L. Cao, C. Wan, X. Zou, Covariance-oriented sample transformation: A new sampling method for reactor-physics uncertainty analysis, Annals of Nuclear Energy 134 (2019) 452–463.

7. Funding

The authors wish to acknowledge that this work was performed by funding from Idaho National Laboratory (INL) by Battelle Energy Alliance, LLC under contract DE-AC07-05ID14517.