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SNRE EIGENVALUE UNCERTAINTY QUANTIFICATION FROM NUCLEAR DATA SOURCES

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Nuclear thermal propulsion designs include large margins for manufacturing, thermal, and neutronic uncertainties. In the past these uncertainties could be better understood through rapid design and experimental measurements. With shifts to more effort on computational designs and larger computing power available, uncertainties can be quantified using computational means. New nuclear thermal propulsion designs use monte-carlo analysis where well established deterministic uncertainty quantification techniques are not valid. This paper describes a total monte-carlo method that can be applied to determine sensitivities and uncertainties to neutron multiplication factors, neutron spectrum, and burnup from many sources including geometrical, material, and nuclear data. Focus is placed on comparing the Small Nuclear Rocket Engine eigenvalue uncertainty found to the iterated fission probability method.

I. INTRODUCTION

Interest in Nuclear Thermal Propulsion (NTP) design was renewed when NASA [1] suggested NTP as a good choice for a Mars the mission (and beyond). Historically the Rover/Nerva [2] and the SNRE [3] have been well funded programs to build NTP engines. New manufacturing techniques and simulation tools can enable a new NTP design using lessons learned from past programs. This NTP can be tailored for specific missions sets and created to be extendible to other missions. This approach to NTP can allow for new reactor designs that were not possible or thought of in past programs.

Heritage NTP designs relied on engineering approximations that could be validated with many experiments. Many of the tools used to create historical NTP designs are either outdated or unavailable. It is often not clear how the approximations made in historic analyses were created. Next generation modeling tools can be used to determine the validity of historical analysis to guide the creation of new experiments. For any new reactor design, experiments to test understanding of physics must be created before a license for construction can be granted. Experiments requiring nuclear materials tend to be very expensive and difficult to create due to many regulatory and safety concerns. This has lead to the creation of predictive computer codes that are validated by experiments whenever possible.

Uncertainty quantification in neutronics is a well studied area, particularly in deterministic transport problems and for criticality safety calculations. The Adjoint Sensitivity Analysis Procedure [4] allows deterministic codes that can calculate adjoint fluxes to perform uncertainty quantification for any parameter of interest. Monte-carlo methods used in criticality safety calculations have focused on eigenvalue uncertainty. MCNP has several methods to determine eigenvalue uncertainty, particularly the iterated fission probability [5] method is used in this study for comparison purposes. The method used in this study can be applied to any reactor quantity to study uncertainty, whereas the MCNP method has only been applied to the multiplication factor.

The work presented here consists of reviewing a relevant uncertainty quantification method, applying it to an SNRE unit-cell model for eigenvalue uncertainty, and comparing results to MCNP's ksens calculation mode. As applicable examples, a calculation varying moderator radius in the unit cell is also performed to calculate uncertainty of moderator radius on the eigenvalue. The importance of this work is based on the ability to calculate uncertainties of any relevant output (eigenvalue, heating rates, burnup, ...) from any relevant input (cross-sections, material densities, geometries, ...).

II. METHODOLOGY

The Total Monte Carlo method is used to determine the uncertainty of the multiplication factor based on ^{235}U fission cross-section uncertainties. The method to calculate uncertainties and create random data distributions is described here.

II.A. Total Monte Carlo

The Total Monte Carlo method [6] 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 MC calculations to determine the effects of nucelar 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). Though the original version only included nuclear data as sources of uncertainty, any input parameter (geometry, materials impurities, densities, ...) can be varied.

This work focuses on fission-cross section uncertainty. A set of 1000 random inputs are generated to create a large set of computation observations. 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.

II.B. Cross-Section Sampling

Random sampling of nuclear data can be created by sampling the cross-section using their nuclear data covariance distributions. Similar techniques has been performed in the past [7, 8, 9, 10] on continuous and multi-group cross-sections in ENDF [11] or ACE data formats. The sampling here uses continuous energy ACE files with multi-group covariance data. These tools are not available for use such that a new tool, ASAPy, was developed for this work. It should be noted that the TENDL [12] nuclear data library publishes varied nuclear data but only a limited sample is available. Work here is to focus on sampling any ENDF covariance rather than only those available in TENDL.

A multivariate log-normal distribution was used to sample the 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,

$$C = USV,$$

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

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

One may also use eigen or Cholesky decomposition instead of singular value decomposition with similar results. The samples are correlated uniform samples that can be transformed to the desired distribution using the distribution's percent point function.

To edit the ACE files, the ACE reader from OpenMC [13] was used to read the ACE files. Then find/replace functions were created such that the original ACE data could be overwritten based on the sampled data. Correlation data was calculated from ENDFB/VII.1 via NJOY [14].

The covariance of ^{235}U sampled data from the ENDFB/VIII.1 covariance file and the original covariance are shown in Fig. 1. It can be seen that the covariances agree well so the sampling procedure was implemented correctly.

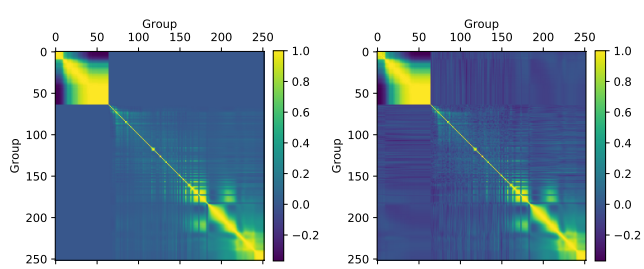

Fig. 1. Correlation Matrix From ASAPy Calculation. (left: ENDFB Actual, right: lognormal samples)

II.C. Iterated Fission Probability Method

MCNP's iterated fission probability method [5] can be used to determine eigenvalue uncertainty based on material cross-section uncertainty. Particularly the sensitivity can be calculated using an adjoint method during the forwards monte-carlo runs, requiring an increased memory footprint and computation time, though not as much as compared to TMC. However, the method is only currently meant for sensitivities due to cross-sections and not any other parameter. Correlation matrices are not built into MCNP and instead NJOY was used to calculate them. The total variance can be calculated via the sandwich rule as,

$$\sigma^2 = SCS^T, \tag{3}$$

where the sensitivity S is calculated with MCNP, and the relative covariance matrix C.

II.D. Sensitivity Information

The goal of uncertainty quantification is to determine output uncertainty from input uncertainty. Sensitivity analysis (SA) seeks to determine how the input uncertainty effects the output uncertainty. Typical goals are to perform factor fixing or to prioritize input importance.

Previous work [15] has used Random Balance Design - Fourier Amplitude Sensitivity Test (RDB-FAST) to perform SA. The RDB method creates a complex input generation requirement and a corresponding input/output relationship that must be accounted for in order to perform SA. This work aims to decoupled the sampling process and the SA process by implemented the EASI [16] method. Another key advantage here is that the EASI method has potential for bootstrapping in order to produce uncertainty estimates of predicted sensitivities.

The EASI method calculates global sensitivity indicies whereas the MCNP IFP method calculates local sensitivity indicies. There has not been work on interpreting global sensitivity indicies for nucelar data applications, particularly when data is highly correlated. It has been shown [15] that highly correlated data tend to have the same variance fraction and that in the case of uncorrelated inputs with linear problems, global sensitivities and local sensitive are the same. The results shown in this paper demonstrate this. Relevant sensitivity profiles are plotted in terms of variance fraction, which is the amount of variance that is attributed to the output from the input. In uncorrelated cases, the sum of variance fractions equals the total variance. In correlated cases this is not the case.

III. RESULTS

A unit-cell model of the SNRE was modeled in MCNP and is shown with relevant dimensions in Fig. 2. This geometry is used in all calculations with 15000 particles per cycle, 1000 cycles, and 30 skipped cycles. The SCALE 44-group energy bounds were used for spectrum calculations and as group boundaries for cross-section sampling.

Label	Component	Radius (cm)	Material
A	Coolant	0.13000	Hydrogen
B	Clad Thickness	0.10000	ZrC
C	Supply	0.20950	Hydrogen
D	Supply Tube	0.26050	Zircaloy-4
E	ZrH	0.58400	ZrH1.89
F	Return	0.67800	Hydrogen
G	Return Tube	0.70500	Zircaloy-4
H	Insulator	0.80650	ZrC 60%
I	Sleeve Half Flat to Flat	0.95650	Graphite

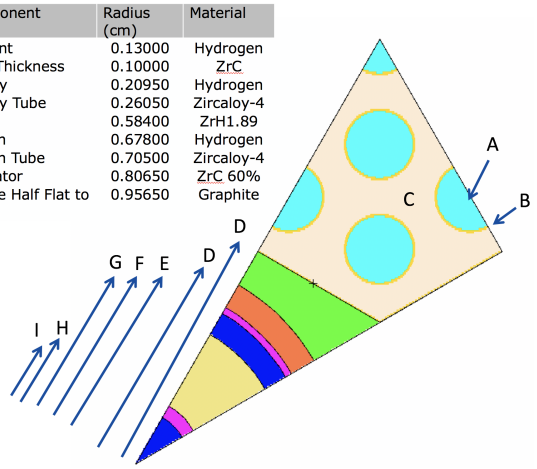

Fig. 2. SNRE Model and Dimensions

III.A. Eigenvalue Uncertainty

Using TMC within ASAPy and sandwich rule with MCNP-IFP, eigenvalue uncertainties from nuclear data were calculated. Table I shows a comparison between ASAPy and MCNP-IFP. All comparable values agreed within a few pcm. These values are considered very close, confirming the cross-section sampling and usage of total monte carlo was successful. An important feature of ASAPy is the ability to sample multiple distributes at once like varying fission and absorption cross-section and the ability to sample the actual mcnp input like in the ZrH varied result. MCNP-IFP has no built in equivalent.

TABLE I. k_{eff} Uncertainty From Varied Inputs

Varied Quantity	ASAPy (pcm)	MCNP-IFP (pcm)
Absorption MT=102	671.19	678.67
Fission MT=18	86.35	87.69
Fission + Absorption	677.28	N/A
Fission $\bar{\nu}$ MT=452	585.18	591.76
Fission χ	20.20	22.67
$ZrH_{1.89}$ radius.	623.26	N/A

The $ZrH_{1.89}$ moderator radius was varied using a mean values of 0.584 cm and a normal deviation of 0.03. This demonstrates the ability to vary geometry components using the developed tool. The iterated fission probability method has no analog in MCNP. This calculation does not preserve ZrH1.8 mass such that it will over-predict the geometry effects because more or less moderator is introduced. Features to correlate sampling such that total mass is constrained are possible. The calculated uncertainty was $ZrH_{1.89}$ radius was 623.26 pcm which is quite substantial.

III.B. Energy Dependent Sensitivity

The iterated fission probability method calculates sensitivities directly which are then used with external covariances to determine uncertainty. The sampling approach calculates uncertainties directly so sensitivity information is not directly calculated as described in Sec. II.D.. The variance contributors can still be calculated via the EASI method and sandwich rule. Figure 3 shows the energy dependent variance fractions from ^{235}U capture cross-section uncertainties for uncorrelated data. The IFP and ASAPy (EASI) profiles agree well. However, when data is correlated as in Fig. 4, the profiles do not agree well. The EASI profile attributes similar variance to inputs that are highly correlated.

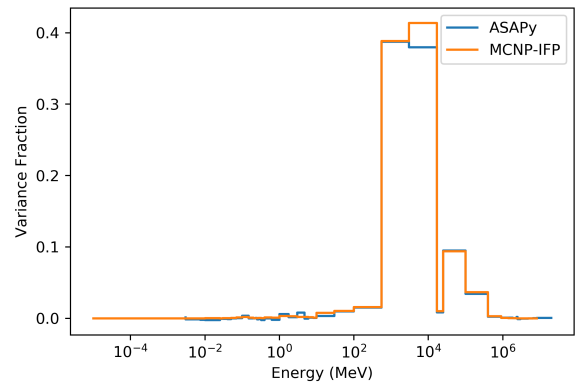

Fig. 3. Uncorrelated Variance fractions from to ^{235}U capture cross-section

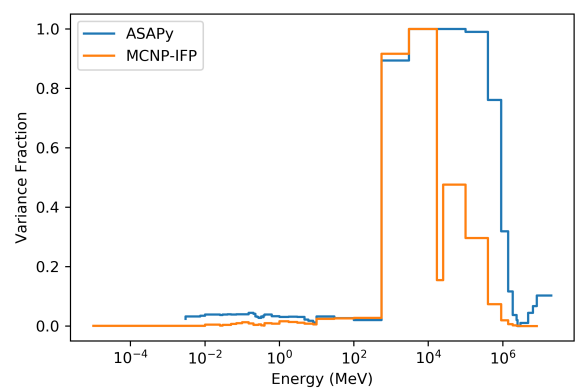

Fig. 4. Correlated Variance fractions from to ^{235}U capture cross-section

IV. CONCLUSIONS

A monte-calro based uncertainty quantification tool is being developed to analyze NTP cores. Nuclear data was sampled based on correlations and ran through many MCNP calculations to determine uncertainty of multiplication factor using the total monte carlo method. This was compared to the built-in MCNP iterated fission probability method of determining eigenvalue sensitivity/uncertainty. It was found that the uncertainties calculated were similar. Another calculation was performed varying a geometrical component to show-case determining uncertainties based on different input uncertainty sources. Variance fraction contributions were also calculated

using the sandwich rule and the EASI method. MCNP and ASAPy results agreed well in uncorrelated data cases but had different results in correlated cases. This is attributed to differences between global and local sensitivity analysis.

Future work includes performing these calculations on a full core rather than just a unit cell and sampling all the uncertainties at once and calculating uncertainties based on those samples. A bootstrapped statistical estimate for uncertainties should also be investigated. The use of global sensitivties also needs further investigation to understand the results better. Furthermore, criticality uncertainty calculations can help reduce potential design margins in NTP systems allowing for higher performance. Uncertainties in heating rates (as well as any relevant output) can also be calculated.

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