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ADJOINT-BASED UNCERTAINTY ANALYSIS FOR ESSENTIAL REACTIONS IN A LASER INERTIAL FUSION ENGINE

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This study establishes a procedure for constructing explicit and adjoint-based implicit sensitivities with MCNP5. Using these methods, an instantaneous sensitivity-based uncertainty analysis is performed on the depleted uranium hybrid LIFE (Laser Inertial Fusion Energy) blanket. Explicit sensitivities and uncertainties are calculated for (n, 2n), tritium production, fission, and radiative capture reaction rates during the fuel lifecycle. Nuclear data uncertainties and Monte Carlo counting precision are compared in a convergence study and the compounding of the two is quantified to gauge the validity of the analysis. A multi-group cross-section library is generated for adjoint calculations and selected adjoint distributions are shown and discussed.

I. INTRODUCTION

A primary purpose of a computational model is to inform design decisions, and in order to make those decisions reliably, the confidence in the results of such models must be known.

Monte Carlo neutron transport and depletion models are often used to inform reactor designers of the ability of a reactor and fuel cycle design to achieve specific goals. These types of models contain several sources of uncertainty that propagate onto the model predictions. The nuclear data that inform a neutron transport model contain experimental and evaluation uncertainties, the results of a Monte Carlo transport code contain statistical counting precision, depletion models bring reaction rate uncertainties onto isotopic masses, and spatial representations of designs are typically not the true engineering geometry.

This work addresses nuclear data uncertainty, which is shown to bound counting precision, and the uncertainties this brings to essential reactions within a Monte Carlo neutron transport model that inform design decisions for the depleted uranium hybrid LIFE (Laser Inertial Fusion Energy) blanket.

II. SENSITIVITY-BASED UNCERTAINTY ANALYSES

Sensitivity-based uncertainty analyses allow for the propagation of dispersions in a model's input data to uncertainties in differential or integral figures of merit, requiring just two pieces of information:[1] (1) some quantification of the dispersion of the uncertain inputs; (2) the sensitivities of the figures of merit of interest to those input data dispersions. For this work, the input data are energy-dependant nuclear cross-sections and their dispersions are quantified by covariance matrices which are typically generated with the nuclear data evaluations. The figure of merit sensitivities are problem-specific and must be generated by the designer. For this work, these are explicit and implicit sensitivity vectors of a few reaction rates to a handful of isotopic cross-sections.

Having quantified the covariances ($\boldsymbol{C}$) and sensitivities (S), the uncertainty (U) can be computed:

$$U = \sqrt{S\boldsymbol{C}S^T}\,. \tag{1}$$

The process not only helps to quantify the confidence in numerical evaluations, but also provides physical insight to the design through the sensitivity functions and can identify the shortcomings in nuclear data that contribute the most to uncertainties.

III. EXPLICIT AND IMPLICIT SENSITIVITIES

Sensitivities are readily defined but can be difficult to quantify. Perturbation theory is used to derive the relative linear response in a figure of merit (R) with respect to the relative perturbation in an input parameter (p):

$$S_{R,p} \equiv \frac{\partial R}{\partial p}\frac{p}{R}\,. \tag{2}$$

For this work, R is assumed to be a linear functional of an operator ($\mathbb{H}$) acting on the angular neutron flux (ψ):

$$R \equiv R\left[\mathbb{H}\left(\vec{r},E,\vec{\Omega}\right),\psi\left(\vec{r},E,\vec{\Omega}\right)\right] = \langle \mathbb{H}\psi \rangle \,, \tag{3}$$

where

$$\langle \quad \rangle \equiv \int_{\vec{r}} d\vec{r} \int_0^\infty dE \int_{\vec{\Omega}} d\vec{\Omega} \,. \tag{4}$$

Essentially, R is a reaction rate and $\mathbb{H}$ is a macroscopic cross-section (Σ).

Instantaneous sensitivities are most generally distributed over all phase space, but can be integrated to generate sensitivity profiles which are functions only of neutron energy. This form is convenient for Eqn. (1) since nuclear data covariances are functions only of neutron energy. Further collapsing of the sensitivity profile generates the total sensitivity, which is a scalar. All following sensitivities are represented in the most differential sense, distributed over all phase space.

Explicit sensitivities respond only to the perturbed input:

$$S_{R,p} = \frac{\Delta \mathbb{H}\,\psi}{\langle \mathbb{H}\psi \rangle}, \tag{5}$$

where

$$\Delta \equiv p\frac{\partial}{\partial p}, \tag{6}$$

while implicit sensitivities also respond to the indirect perturbations of ψ:

$$S_{R,p} = \frac{\Delta \mathbb{H}\,\psi}{\langle \mathbb{H}\psi \rangle} + \frac{\mathbb{H}\,\Delta\psi}{\langle \mathbb{H}\psi \rangle}. \tag{7}$$

Implicit sensitivities are receptive to any input that may alter ψ, whereas explicit sensitivities are zero unless an input is contained explicitly within $\mathbb{H}$. This insensitivity of explicit sensitivities is compensated by the fact that they can be extracted with a single transport calculation, while implicit sensitivities require more sophisticated methods, namely direct Monte Carlo sampling or adjoint-based methods.

Direct Monte Carlo sampling entails directly and randomly perturbing all input parameters for a model within their assumed distributions. This presents a multi-dimensional parameter sample space whose dimensions consist of the value of a cross-section for a certain isotope for a certain reaction type within a certain energy region. For every sample, a transport calculation is run and the resultant figures of merit are tabulated and statistically post-processed. Such analyses consider all figures of merit in parallel, but since precision is limited to the sample size, many transport calculations are required.

Adjoint-based methods consider all possible input data simultaneously, which is why they require only a forward and an adjoint calculation for each figure of merit. Two limitations are that input dispersions are assumed to be normally distributed and only first-order effects are captured from perturbations. The first limitation is reasonable when many experiments are present in a nuclear data evaluation and the second limits the applicability of these analyses to small perturbations. In spite of this, adjoint-based methods are hundreds to thousands of times more computationally efficient than Monte Carlo sampling.

In this work, sensitivities are estimated using the MCNP5 transport code.[2] Since the only type of response analyzed is reaction rates, the inner product in Eqn. (5) is exactly a summation of F^{M4} flux multiplier tallies, which allow for the multiplication of flux with macroscopic cross-sections:

$$\begin{aligned} &\langle \Sigma_{z,x}\psi \rangle \\ &\equiv \int_{\vec{r}} d\vec{r} \int_0^\infty dE \int_{\vec{\Omega}} d\vec{\Omega}\; N_z(\vec{r})\,\sigma_{z,x}(E)\,\psi\left(\vec{r},E,\vec{\Omega}\right) \\ &= \sum_c V_c\, F_{c,z,x}^{M4} \,, \end{aligned} \tag{8}$$

where c, z, and x are the indices for the cell, isotope, and reaction of interest, respectively.

For implicit sensitivities, variational principles performed on Eqn. (7) arrive at an alternate form that introduces the adjoint flux ($\psi^\dagger$) (Ref. 3):

$$S_{R,p} = \frac{\Delta \mathbb{H}\,\psi}{\langle \mathbb{H}\psi \rangle} - \frac{\psi^\dagger \Delta \mathbb{A}\,\psi}{\langle \mathbb{H}\psi \rangle}, \tag{9}$$

where a † superscript denotes the adjoint of a quantity and $\mathbb{A}$ is the transport operator from the inhomogeneous Boltzmann transport equation.

The numerator of the second term in Eqn. (9) is a continuous quantity that cannot be exactly reproduced by MCNP5, but that can be well approximated in discrete regions of phase space by a combination of forward and adjoint F^1 surface current tallies, F^4 cell flux tallies, and F^{M4} cell flux multiplier tallies for neutron losses:

$$\begin{aligned} &\psi^\dagger \Sigma_{c,z,x}\psi \\ &\equiv \int_{\vec{\Omega}} d\vec{\Omega}\; \psi^\dagger\left(\vec{r},E,\vec{\Omega}\right) N_z(\vec{r})\,\sigma_{z,x}(E)\,\psi\left(\vec{r},E,\vec{\Omega}\right) \\ &\approx F_c^{4\dagger}(E)\, F_{c,z,x}^{M4}(E) \sum_i \Delta\mu_i^2\, \alpha_c^\dagger(E,\mu_i)\,\alpha_c(E,\mu_i) \,, \end{aligned} \tag{10}$$

where

$$\alpha_c(E,\mu_i) \equiv \frac{\psi_c(E,\mu_i)}{\phi_c(E)} = \frac{\frac{F_c^1(E,\mu_i)}{\mu_i\,\Delta\mu_i}}{\sum_j \frac{F_c^1(E,\mu_i)}{\mu_j}}, \tag{11}$$

and *i* and *j* are discrete direction indices. As the size of the discrete phase space regions shrink to zero, integral terms (like inner products) will approach that of the continuous treatment. It is not yet clear how finely tally bins will have to be discretized across phase space, but future work will study how terms converge with bin size. Also, shrinking bins will reduce the histories contributing to each bin, so a balance will have to be found between discretization error and counting precision.

IV. NUCLEAR DATA LIBRARY COVARIANCES

There are a number of excellent evaluated nuclear data libraries available. Until recently, however, little emphasis has been placed on uncertainty quantification and most libraries lack a sufficient quantity of covariances. Tab. 1 addresses the covariance content of nine libraries, tabulating the total number of covariance matrices and the number of isotopes over which they are distributed.

ENDF/B-VII.1 will partially address covariance deficiencies by increasing the number of covariances to 110 isotopes, but the scheduled release date is December 2011 and covariances will be absent for many isotopes in the library.[4]

TABLE I. Nuclear Data Covariance Availability (November 2010)

Library	Origin (Year)	Size (MiB)	# of Matrices	# of Isotopes / Total
CENDL-3.1	China (2009)	158	87	6 / 240
ENDF/B-VI.8	USA (2001)	108	739	45 / 328
ENDF/B-VII.0	USA (2006)	396	210	24 / 393
ENDF/B-VII.1	USA (2011?)	NA*	NA	110 / NA
JEFF-3.1.1	EU (2009)	249	744	35 / 381
JENDL-3.3	Japan (2002)	116	415	20 / 337
JENDL-4.0	Japan (2010)	572	2155	93 / 406
Low Fidelity	USA (2008)	14	1838	387 / 387
RUSFOND-2010	Russia (2010)	293	83	4 / 686

* NA ≡ not available

For this work, ENDF/B-VII.0-based (Ref. 5) cross-sections are used for transport in MCNP5. Since this library lacks many important covariances, the Low-Fidelity covariance library[6] supplements covariances when necessary. This library is currently the most complete set that is generated with respect to the nominal ENDF/B-VII.0 values. It also tends to have conservatively larger variances than other libraries.

V. DEPLETED URANIUM HYBRID LIFE BLANKET

The design analyzed in this work is the depleted uranium hybrid LIFE blanket.[7-11] The design considered consists of a spherical fusion chamber with a subcritical fission blanket. It strives to close the fission fuel cycle without enrichment or reprocessing, while simultaneously achieving high discharge burnups with reduced proliferation concerns.

The high burnup traversal means that uncertainties are accumulated over many time steps and less certain isotopes are encountered. Tritium fuels the fusion source and fission multiplies the fusion power, so continuous tritium production, fission, and breeding of fissile fuels are all essential to the design.

VI. METHODOLOGY

Explicit nuclear data sensitivities (Eqn. (5)) and uncertainties are calculated for (n, 2n) and tritium production which are related to tritium breeding, fission which is related to thermal power multiplication, and radiative capture which is related to fuel breeding. All coolant, structural, and heavy metal isotopes are considered at five instances: beginning of life (BOL), beginning of full power operation (BOP), maximum plutonium mass (MPU), fifty percent FIMA burnup (F50), and end of full power operation (EOP).

In addition to straight estimates of nuclear data uncertainties (XS), counting precision is calculated for response (MC) and for the nuclear data uncertainty estimate (MC-XS, a variance of a variance). A study determines how these decay or converge with the number of transport histories.

MCNP5 can perform adjoint calculations, but only in multi-group (MG) transport mode. The MCNP5 release MG data MGXSNP (Ref. 12) is inadequate for our purposes: it is based upon ENDF/B-V, contains only 30 energy groups and no up-scattering physics, and some isotopes are at 0K while others are at 300K.

Problem-specific data must be generated by processing evaluated data (ENDF/B-VII.0) into ACE format with NJOY99 (Ref. 13) and CRSRD (Ref. 14). A forward neutron flux spectrum is required for multi-group weighting of quantities. Since a LIFE blanket sees many flux spectra during its lifetime, the generality of a MG library constructed from one spectrum is put into question. MG libraries generated with three system-averaged fluxes are compared in forward transport to gauge their generality and to the MCNP5 release point-wise data to gauge their validity.

Adjoint calculations are performed for the four reactions at each time-step. Adjoint distributions of particular interest are shown.

VII. RESULTS AND DISCUSSION

VII.A. Explicit sensitivity and uncertainty

The explicit sensitivities are as expected. (n, 2n) reactions are always roughly 70% sensitive to ^{9}Be and roughly 23% sensitive to lead isotopes. Around 92% of the system tritium production comes from ^{6}Li, with all but ~1% of the rest produced by ^{7}Li. Plutonium produces the bulk of fissions (85%-95%) and is slowly replaced with heavier and heavier isotopes; at the EOP, ^{245}Cm produces 11% of fissions. Radiative capture is provided by heavy metals (58%, 64%, 51%, 35%, 19% at BOL, BOP, MPU, F50, and EOP, respectively) and structural isotopes (35%, 18%, 10%, 12%, 19%), with fission products making up the rest (0%, 15%, 38%, 51%, and 59%).

Tab. 2 shows the total nuclear data uncertainties for the four reactions at the five time-steps. The nuclear data uncertainties in (n, 2n) and tritium production remain roughly constant since they are not strongly affected by the changing flux spectrum (Fig. 1) and buildup of fission products. The uncertainties in fission rates grow with burnup, as less certain isotopes are encountered, and those in radiative capture shrink as emphasis is placed less upon heavy metals and structural isotopes and more on fission products (whose contributions to uncertainty were not considered).

Both forms of counting precision remain within ~5-50pcm; they are always bounded by nuclear data values.

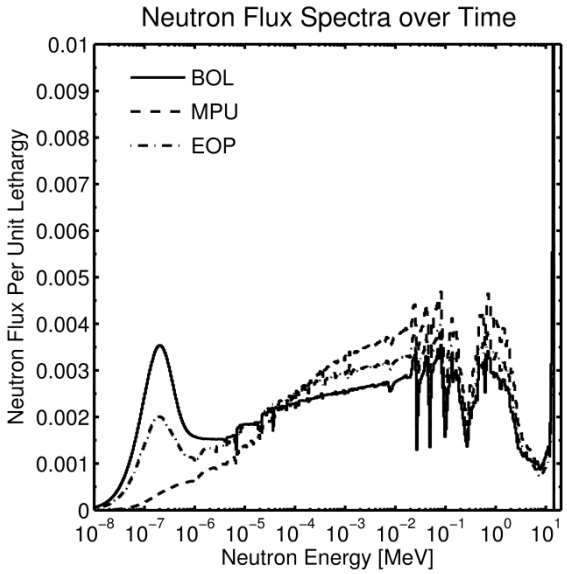

Fig. 1. The system-averaged neutron flux spectrum changes from thermal with no fission products, to fast with some fission products, to thermal with many fission products. The fusion peak varies between 0.02 and 0.025.

TABLE II. Nuclear data relative uncertainties [pcm].

Time-step	(n, 2n)	(n, T)	(n, fission)	(n, γ)
BOL	830	175	65	192
BOP	851	174	438	195
MPU	849	175	424	139
F50	848	174	469	61
EOP	849	179	514	82

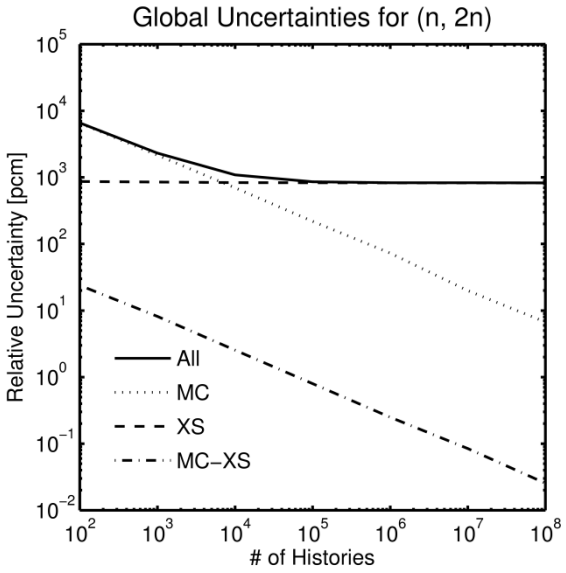

Fig. 2. The contributions to uncertainty are separable. Nuclear data uncertainty dominates above 10^5 and is converged at 10^2 histories for (n, 2n) reactions.

Plotting nuclear data (XS), Monte Carlo counting (MC), and Monte Carlo counting precision of nuclear data (MC-XS) uncertainties versus the number of histories within the MCNP5 simulation (Fig. 2) shows that (1) the individual contributions to overall uncertainty are separable and well-behaved, (2) XS is 10-100 times larger than MC, (3) in an absolute sense MC-XS contributes virtually nothing to overall uncertainty, and (4) XS is essentially converged at 10^2 histories, at which it has a relative uncertainty of ~5%.

VII.B. Multi-group cross-section library

Absorption cross-sections from the three MG libraries compare well to the MCNP5 point-wise cross-sections, whereas scattering cross-sections do not match because up-scattering physics are not yet included. The MG libraries depend weakly on the weighting flux spectrum: all neutron transport results and nuclear data uncertainty estimates lay within 10s of pcm.

To put the dispersion among the MG libraries from different flux spectra into context, Fig. 3 plots the

uncertainty profiles for three quantities involved with ^{6}Li(n, T) uncertainty: the uncertainty in the cross-section (C-LI), the counting precision of the sensitivity (MC-LI), and the standard deviation of the MG representations of the cross-section (MG-LI). The uncertainty in the cross-section bounds counting uncertainty of the sensitivity, which in turn bounds MG dispersion. Since it has already been shown that the integral effects Monte-Carlo counting precision of nuclear data uncertainty are negligible, the dispersion in MG libraries is certainly negligible.

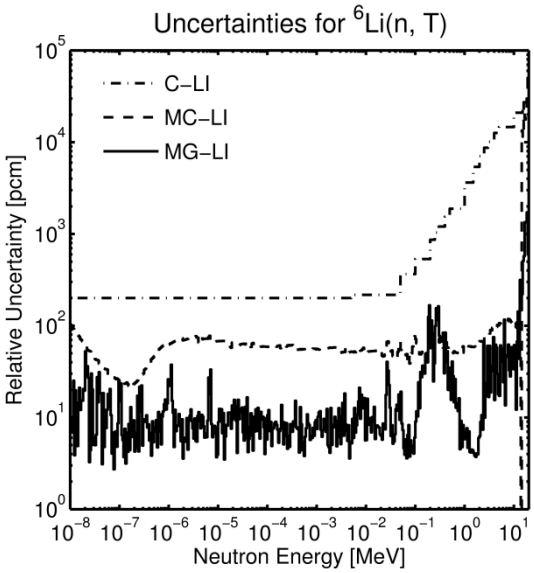

Fig. 3. ^{6}Li(n, T) nuclear data uncertainties bound counting and multi-group uncertainties.

VII.C. Adjoint/importance distributions

Adjoint/importance distributions were generated for the four reactions. Distributions of interest for tritium production are shown in Fig. 4. After some preliminary analysis, some clear physical conclusions can be made: (1) high-energy neutrons are most important at the first wall, (2) thermal neutrons are most important within the fuel layer, (3) and neutrons at the final wall are unimportant. Depressions in the adjoint correspond to a high chance of neutrons at those energies being captured before they can produce tritium.

These importances make intuitive sense, as they align with the current understanding of the design. Fast neutrons at the first wall, having a longer mean free path than thermal neutrons, are more likely to penetrate through to the tritium breeding layers to produce a triton, especially after (n, 2n) reactions. Tritium breeding cross-sections are largest at thermal energies, so neutrons in the proximity of tritium breeding layers should be most important when they are thermal. Neutrons at the final wall are likely to leak. Neutrons at resonance energies are likely to be parasitically absorbed before producing tritium.

Adjoint distributions have not yet been analyzed in an energy-direction-correlated sense and have not yet been used to create implicit sensitivities.

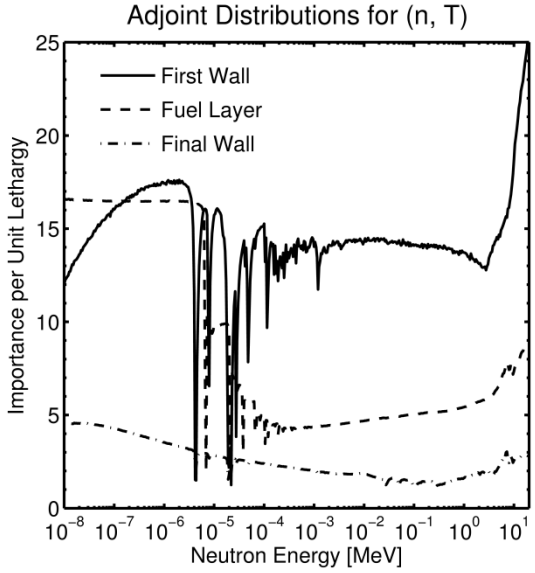

Fig. 4. Adjoint distributions for (n, T) show that (1) fast neutrons are most important at the first wall, (2) thermal neutrons are most important within the fuel layer, and (3) neutrons at the final wall are unimportant.

VIII. CONCLUSIONS AND FUTURE WORK

Equations for explicit and adjoint-based implicit sensitivities were shown and a procedure for their construction with MCNP5 was outlined. Using these methods, an instantaneous sensitivity-based uncertainty analysis was performed on the DU-hybrid LIFE blanket.

Explicit nuclear data, counting, and compounding of counting and nuclear data uncertainties for four reactions were quantified at five instances during a LIFE lifecycle. All total uncertainties were small (0.1-0.8%). This brings validity to the simulations and sets an acceptable level of counting uncertainty of slightly less than the nuclear data uncertainty. There are three enhancements to the analysis, however, that are expected to increase uncertainty estimates: treating uncertainties in a time-dependant sense will allow uncertainties to accumulate over time and both direct consideration of fission products and implicit sensitivities will vastly expand the amount of nuclear data that contribute to overall uncertainties.

Even though three forms of uncertainty contributed to an overall uncertainty estimate, they are completely separable; even in cases when counting precision might be coarse for a figure of merit, estimates of the nuclear

data uncertainty can still be valid. During this study, nuclear data uncertainties bounded counting precision and counting precisions of nuclear data uncertainties were very small.

This work quantified the uncertainty of (n, 2n), tritium production, fission, and radiative capture within the system. While these reaction rates are related to important figures of merit, it would be more useful to quantify the uncertainty of the exact quantities of interest: blanket thermal power multiplication, fissile fuel conversion ratio, and tritium breeding ratio (tritons produced per fusion event). These quantities and others, namely k_{eff}, radiation damage in structural materials, and activation of structural materials will be addressed in future work.

Multi-group cross-section libraries were generated for adjoint calculations. The absorption cross-sections matched point-wise values very well and are only weakly affected by the neutron flux spectrum used for weighting. They, however, lack up-scattering physics. After a thorough validation of the multi-group libraries has been performed for forward calculations, the logical leap will be made that this validity can be directly applied to adjoint calculations; forward validity will be assumed to imply adjoint validity.

Some adjoint distributions have been generated and already provide physical understanding for the design. The generation of more distributions and their insertion into implicit sensitivities will glean even more understanding and enhance the estimates of uncertainty.

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