Data Assimilation of Nuclear Cross Sections Applied to Neutron Multiplicity Counting Experiments

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INTRODUCTION

Data assimilation of nuclear cross sections is the process of updating prior estimates of their value and uncertainty with new information. Data assimilation is currently performed using gross neutron counting experiments [1] which has resulted in biases in expected values of some nuclear parameters, such as Pu-239 nu-bar, and artificially inflated covariances [2]. Neutron multiplicity counting (NMC) experiments would be useful for data assimilation because each moment of the distribution is a function of the cross sections raised to a power denoted by that moment; consequently, calculations of higher order multiplicity moments are more sensitive to the nuclear parameters than the mean, which is equivalent to gross counting. Performing data assimilation using higher order moments of the NMC distribution would therefore lead to more precise estimates of cross sections values and their uncertainty.

Data assimilation is performed in several steps. First, the sensitivity of a detector response (e.g. a specific moment of the NMC distribution) to nuclear cross sections is computed via sensitivity analysis (SA). Previous work has developed perturbation theory-based SA applied to the moments of the NMC distribution, which was derived from the stochastic neutron transport equation (STE) [3]. Second, the sensitivities are used to propagate the uncertainty in the nuclear cross sections through the detector response via uncertainty quantification (UQ). This step is simply an inner product between the sensitivities and covariance data for the nuclear cross sections. Third, a χ^2 (or other appropriate) error metric is calculated using the computed detector response and its uncertainty. This error metric is a variance-weighted sum of squared errors that quantifies how well the computed and observed detector responses agree. The nuclear cross sections are then perturbed and the SA and UQ steps are repeated until the χ^2 error metric is minimized via a parameter estimation (PE) method, e.g., Cacuci's data assimilation formulation [4]. The result is a set of nuclear cross section values that are "optimal" in the sense that the computed detector response most closely matches the observed detector response with the smallest uncertainty.

The forward and adjoint NTE are briefly described and the general form of the sensitivity of the mean detector response is stated. A distinction between "absolute" and "relative" sensitivities is also made. The procedure for propagating the nuclear cross section covariances using the detector response sensitivities is then discussed. The χ^2 error metric is defined and the process for obtaining "optimal" nuclear cross sections is explained.

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THEORY

Sensitivity Analysis

Consider the forward, fixed source neutron transport equation (NTE) [5],

$$\begin{aligned}
&\underbrace{\hat{\Omega}\cdot\nabla\psi(\boldsymbol{r},\hat{\Omega},E)}_{\text{streaming}} + \underbrace{\sigma_t(\boldsymbol{r},E)\psi(\boldsymbol{r},\hat{\Omega},E)}_{\text{total interaction}} \\
&= \underbrace{\int d\Omega' \int dE'\, \sigma_s(\boldsymbol{r},\hat{\Omega}',E'\to\hat{\Omega},E)\psi(\boldsymbol{r},\hat{\Omega}',E')}_{\text{scatter source}} + \\
&\underbrace{\frac{\chi(\boldsymbol{r},E)}{4\pi}\int d\Omega' \int dE'\, \bar{\nu}\sigma_f(\boldsymbol{r},E')\psi(\boldsymbol{r},\hat{\Omega}',E')}_{\text{fission source}} + \\
&\underbrace{\frac{q(\boldsymbol{r},E)}{4\pi}}_{\text{fixed source}},
\end{aligned} \tag{1}$$

which describes a balance of production and loss terms for the expected number of neutrons at some position ($\boldsymbol{r}$), direction ($\hat{\Omega}$), and energy (E). ψ is the neutron angular flux, $\sigma_t, \sigma_f, \sigma_s$ are the total, fission, and scatter cross sections (macroscopic), respectively, χ is the fission neutron spectrum, and $\bar{\nu}$ is the average number of neutrons emitted per fission.

Equation (1) may be recast in operator form,

$$L\psi = Q, \tag{2}$$

with forward transport operator,

$$\begin{aligned}
L =& \hat{\Omega}\cdot\nabla + \sigma_t(\boldsymbol{r},E) - \\
&\int d\Omega' \int dE'\, \sigma_s(\boldsymbol{r},\hat{\Omega}',E'\to\hat{\Omega},E) - \\
&\frac{\chi(\boldsymbol{r},E)}{4\pi}\int d\Omega' \int dE'\, \bar{\nu}\sigma_f(\boldsymbol{r},E'),
\end{aligned} \tag{3}$$

and forward, isotropic fixed source,

$$Q \equiv \frac{q(\boldsymbol{r},E)}{4\pi}. \tag{4}$$

The adjoint NTE,

$$L^+\psi^+ = Q^+, \tag{5}$$

with adjoint source term, Q^+, may be defined such that the value of an inner product is preserved; i.e.,

$$\langle L\psi, \psi^+ \rangle = \langle \psi, L^+\psi^+ \rangle, \tag{6}$$

where the inner product is defined as

$$\langle f, g \rangle \equiv \int d\boldsymbol{r} \int d\Omega \int dE\, f(\boldsymbol{r}, \hat{\Omega}, E) g(\boldsymbol{r}, \hat{\Omega}, E). \tag{7}$$

The adjoint transport operator that satisfies Equation (6) is

$$\begin{aligned} L^+ \equiv &- \hat{\Omega}\cdot\nabla + \sigma_t(\boldsymbol{r}, E) - \\ &\int d\Omega' \int dE'\, \sigma_s(\boldsymbol{r}, \hat{\Omega}, E \to \hat{\Omega}', E') - \\ &\bar{\nu}\sigma_f(\boldsymbol{r}, E) \int d\Omega' \int dE'\, \frac{\chi(\boldsymbol{r}, E')}{4\pi}. \end{aligned} \tag{8}$$

If the adjoint source term is chosen to be a detector response function, i.e., $Q^+ = \sigma_d$, the adjoint flux ψ^+ may be interpreted as the "importance" of source neutrons to the the mean detector response or mean count rate of a detector. The mean count rate may therefore be computed by taking the inner product of the adjoint flux and forward source term, or equivalently [3], the forward flux and the adjoint source term,

$$R \equiv \langle \psi, \sigma_d \rangle = \langle \psi, Q^+ \rangle = \langle \psi^+, Q \rangle. \tag{9}$$

Higher order moments of the NMC distribution may be computed using the STE. Each NMC distribution moment has the same form as Equation (5) but with a special fixed adjoint source [3],

$$L^+\psi_k^+ = Q_k^+, k = 1, 2, ..., K, \tag{10}$$

where K is an arbitrary maximum moment-order. $k = 1$ would denote the usual adjoint NTE while $k > 1$ would denote higher NMC distribution moments. Higher order detector response moments have a form similar to that of Equation (9),

$$R_k \equiv \left\langle \psi, Q_k^+ \right\rangle + \left\langle S, Q_{sk}^+ \right\rangle, \tag{11}$$

with an extra term (the second inner product) that accounts for the contribution of spontaneous fission to the observed NMC distribution moments. In the special case where $k = 1$, $Q_{sk}^+ \equiv 0$ such that $R_1 = R$ is the mean detector response.

For $k = 2$, the adjoint source term becomes,

$$Q_2^+ = \overline{\nu(\nu-1)}\sigma_f I_1^2, \tag{12}$$

where the "importance" of fission neutrons to the detector response is,

$$I_1 \equiv \int d\Omega' \int dE' \frac{\chi(\boldsymbol{r}, E')}{4\pi} \psi^+(\boldsymbol{r}, \hat{\Omega}', E'), \tag{13}$$

such that R_2 in Equation (11) is part of the second moment of the NMC distribution in excess to that of the Poisson contribution. The complete second NMC distribution moment is then [3],

$$\overline{n(n-1)} \equiv R_2 + R_1^2 \tag{14}$$

In other words, For a Poisson distributed process, such as (α, n) reactions, $\overline{\nu(\nu-1)} \equiv 0$ and therefore $R_2 \equiv 0$ also, such that the complete second NMC distribution moment is equal to the square of the mean detector response. A non-Poisson distributed process, such as a fission chain-reaction, has a nonzero value for $\overline{\nu(\nu-1)}$ and thus its second NMC distribution moment contain contributions in excess of a Poisson distributed process.

The general form of the sensitivity of the mean detector response to a parameter α using adjoint-based perturbation theory is then,

$$\frac{\partial R}{\partial \alpha} = \left\langle \frac{\partial Q^+}{\partial \alpha}, \psi \right\rangle + \left\langle \psi^+, \frac{\partial Q}{\partial \alpha} - \frac{\partial L}{\partial \alpha}\psi \right\rangle. \tag{15}$$

where $\boldsymbol{\alpha} = \{\alpha\}$ is the set of parameters i.e. nuclear cross sections. Analogous expressions may be derived for the higher order detector response moments [3].

If the inner product given by Equation (7) is redefined to only be over space and direction,

$$\langle f, h \rangle \equiv \int d\boldsymbol{r} \int d\Omega\, f(\boldsymbol{r}, \hat{\Omega}) h(\boldsymbol{r}, \hat{\Omega}). \tag{16}$$

and the forward and adjoint NTE are discretized in energy via the multigroup approximation [5], the group detector response may be defined as,

$$R_g = \left\langle \psi_g^+, Q_g \right\rangle. \tag{17}$$

and the sensitivity of the response at group g to a parameter at group g' has the same general form as Equation (15),

$$\frac{\partial R_g}{\partial \alpha_{g'}} = \left\langle \frac{\partial Q_g^+}{\partial \alpha_{g'}}, \psi_g \right\rangle + \left\langle \psi_g^+, \frac{\partial Q_g}{\partial \alpha_{g'}} - \frac{\partial L_g}{\partial \alpha_{g'}}\psi_g \right\rangle, g, g' = 1, ..., G, \tag{18}$$

The magnitude of the "absolute" sensitivity defined in Equation (18) can vary greatly with respect to parameter type and energy group, so it is useful to define a "relative" sensitivity that is scaled by the parameter and response values themselves,

$$\frac{\delta R_g}{R_g} = S_{R_g,\alpha_{g'}} \frac{\delta \alpha_{g'}}{\alpha_{g'}}, \tag{19}$$

or written another way,

$$S_{R_g,\alpha_{g'}} = \frac{\alpha_{g'}}{R_g}\frac{\partial R_g}{\partial \alpha_{g'}}, \tag{20}$$

The relative sensitivity in Equation (20) relates a fractional change in the group parameter value to one in the group response value. For example, a relative sensitivity of 1 would mean that a 1% increase in the parameter value would result in a 1% increase in the detector response.

Equation (18) describes an element of a matrix of sensitivities of dimension G x G, where the rows are the parameter groups g' and the columns are the response groups g. a vector of sensitivities of dimension G x 1 that quantifies the sensitivity of the *integrated* detector response to the group parameters may be obtained by summing Equation (18) over group g. Scalar sensitivities or ranks may be obtained by using Equation (18) to compute sensitivities using the one-group NTE.

Uncertainty Quantification

The uncertainty in the parameters may be propagated through the detector response using linear propagation of uncertainty,

$$C_R \equiv \sum_{m=1}^{M}\sum_{m'=1}^{M} S_{\alpha_m} C_{\alpha_m,\alpha_{m'}} S_{\alpha_{m'}} \tag{21}$$

where C_R is the covariance in the response due to covariance in set of parameters $\boldsymbol{\alpha}$, S_{α_m} is the sensitivity of the detector response to a parameter α_m, and $C_{\alpha_m,\alpha_{m'}}$ is the covariance between those parameters with dimension G x G. Note that there may be covariance between different parameters (e.g. the scatter and fission cross sections) as well as covariance between energy groups of the same parameter. Equation (21) may describe an inner product with either a matrix or a vector of sensitivities, which would result in either a response covariance matrix or a scalar response variance, respectively. In the latter case, the uncertainty in the detector response would simply be,

$$\sigma_R = \sqrt{C_R}. \tag{22}$$

Parameter Estimation

The sensitivities and response uncertainty are then used to minimize a χ^2 error metric,

$$\chi^2 \equiv \sum_{k=1}^{K}\left(\frac{\overline{R_k} - R_k}{\sigma_{R_k}}\right)^2, \tag{23}$$

where $\overline{R_k}$ is the order-k observed detector response and R_k is the order-k computed detector response moment with uncertainty σ_{R_k}, noting that each term in Equation (23) is a scalar. The detector response due to the perturbed parameters may be efficiently computed using the sensitivities via first order Taylor expansion [3],

$$R_k(\tilde{\alpha}) = R_k(\alpha_0) + \sum_{m=1}^{M}\frac{\partial R_k}{\partial \alpha_m}\delta\alpha_m, \tag{24}$$

where α_0 is the nominal parameter value and $\delta\alpha_m$ is the perturbation. The parameters are adjusted, the SA and UQ steps are repeated, and the perturbed detector response is recomputed until Equation (23) is minimized. Note that in gross neutron counting (i.e. $k = 1$), only a single term is present in Equation (23) that varies linearly with the parameters. By applying data assimilation to NMC experiments (i.e. $k > 1$), the χ^2 minimization has additional terms that vary nonlinearly with the parameters; specifically, each NMC distribution moment is a function of the cross sections raised to a power denoted by that moment. Data assimilation that includes higher order NMC distribution moments should therefore lead to more precise estimates of the parameters.

RESULTS AND ANALYSIS

1D PARTISN [5] simulations of gross neutron counting of the BeRP ball, which is a 4.5 kg sphere of alpha-phase, weapons-grade plutonium metal [6], were used to compute the sensitivity of the nPod neutron multiplicity counter to nuclear cross sections. The BeRP ball was simulated with either no reflector (bare) or a 1.5” polyethylene reflector (reflected). Figure 1 compares the Pu-239 $\overline{\nu}$ relative sensitivity vectors for both the bare and reflected BeRP ball configurations. Figure 2 is an analogous comparisons for the Pu-239 σ_f relative sensitivity vectors.

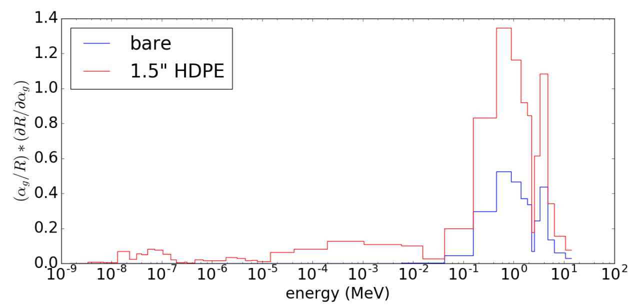

Fig. 1. Pu-239 $\overline{\nu}$ sensitivity for the bare and reflected BeRP ball configurations.

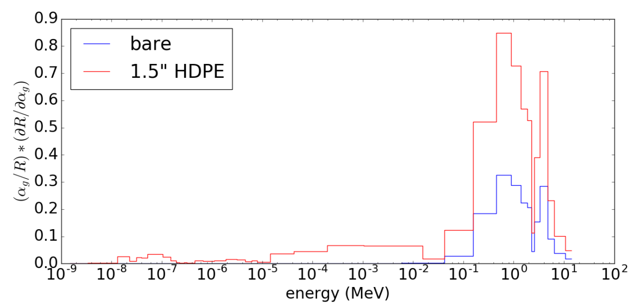

Fig. 2. Pu-239 σ_f sensitivity for the bare and reflected BeRP ball configurations.

The $\overline{\nu}$ and σ_f sensitivities have the largest magnitude in the fast energy groups and are much smaller for slower energy groups, which indicates that changes in the fast group fission parameters have the greatest effect on the mean count rate. Additionally, the magnitude of the fission parameter sensitivities increases significantly between the bare and reflected cases. Neutrons that would otherwise escape the BeRP ball may instead be reflected and slowed down by the polyethylene reflector, resulting in a greater number of neutrons available in the system at lower energies, at which neutrons are most likely to induce fission. The mean count rate is therefore more highly influenced by changes in the fission parameters in the reflected case than in the bare case.

Table I summarizes the relative sensitivity ranks for the bare and reflected BeRP ball configurations. Although the BeRP ball contains Pu-239 and Pu-240 and the polytheylene reflector contains H-1 and C-12, only the Pu-239 and H-1 ranks are given because the Pu-240 and C-12 ranks are several orders of magnitude smaller.

The fission parameters have a positive rank while the scatter (elastic and inelastic) and capture cross section ranks

TABLE I. Relative sensitivity ranks for the bare and reflected BeRP ball configurations.

	bare	reflected
Pu-239 $\overline{\nu}$	3.03e+00	9.28e+00
Pu-239 σ_f	1.89e+00	5.86e+00
Pu-239 σ_{el}^0	-4.67e-01	-1.05e+00
H-1 σ_{el}^0	-	-2.10e+01
Pu-239 σ_{il}^0	-1.56e-01	-3.06e-01
Pu-239 σ_c	-3.38e-02	-3.74e-01
H-1 σ_c	-	-2.35e-01

are negative. This means that increasing the fission parameters will *increase* the detector response while increasing the scatter and capture cross sections will *decrease* the detector response. Note that all of the ranks increase (in absolute magnitude) significantly between the bare and reflected configurations. As indicated by the sensitivity vectors given in Figure 1 and Figure 2, changes in the NTE parameters have a greater effect on the reflected configuration detector response than on the bare configuration detector response.

Table II summarizes the mean count rate and its uncertainty due to covariance in the nuclear cross sections for the bare and reflected BeRP ball configurations. Note that while the uncertainty in the mean count rate for the bare configuration is relatively small ($< 5\%$), the uncertainty for the reflected case is significantly larger ($\sim 12\%$). This is due to the increased number of parameters, i.e. the addition of polyethylene to the plutonium sphere, as well as the increased sensitivity of the detector response to the existing parameters (see Figure 1 and Figure 2).

TABLE II. Mean detector response (i.e. mean count rate) and its relative uncertainty for the bare and reflected BeRP ball configurations.

configuration	$R\left(\frac{\text{counts}}{\text{sec}}\right)$	$\frac{\sigma_R}{R}$
Bare	8.26e+03	4.33e-02
Reflected	1.93e+04	1.23e-01

CONCLUSIONS AND FUTURE WORK

Because the higher order NMC distribution moments are a function of the cross sections raised to a power denoted by the order of the moment, small variations in the cross sections will have a greater effect on their value; it is therefore expected that performing data assimilation with higher order NMC distribution moments will result in cross section estimates that are more sensitive to uncertainty in the nuclear data than those provided by gross neutron counting alone. The SA and UQ steps are applied to the first moment of the NMC distribution (i.e. the mean count rate) and are demonstrated here. It is observed that the mean detector response varies the most with respect to changes in the fast group fission parameters (i.e. $\overline{\nu}$ and σ_f) for the reflected BeRP ball. The uncertainty in the mean detector response for the reflected configuration is larger than that for the bare configuration for two reasons. There are more cross sections in the reflected configuration, which means that more parameter covariance is propagated through the detector response. The reflected configuration detector response is also more sensitive to the parameters, which means that the inner product given by Equation (21) will be larger.

Future work will include performing the PE step on the mean detector response as well as applying the data assimilation to the second moment of the NMC distribution, which will be sufficient to demonstrate the methodology for the third and higher order NMC distribution moments. Kalman filtering is a natural choice for the PE step because it will use Bayesian inference to update the current estimates of cross section value and uncertainty with previously obtained NMC and covariance data.

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