ABSTRACT

CLARK, ALEXANDER RICH. Application of Neutron Multiplicity Counting Experiments to Optimal Cross Section Adjustments. (Under the direction of John Mattingly.)

This dissertation presents the first application of model calibration to neutron multiplicity counting (NMC) experiments for cross section optimization that utilizes adjoint-based sensitivity analysis (SA) and first-order uncertainty quantification (UQ). We summarize previous work on SA applied to NMC and describe notable additions. We give the procedure for first-order UQ and Bayesian-inference-based parameter estimation (PE). We then discuss model calibration applied to NMC of a 4.5-kg sphere of weapons-grade, alpha-phase plutonium metal with a neutron multiplicity counter. For bare and polyethylene-reflected configurations of the plutonium sphere, we discuss the sensitivity of the first- and second-moment detector responses (i.e. first and second moments of the NMC distribution, respectively) to the cross sections. We describe the sources of uncertainty in the measured and simulated responses. Specifically, uncertainty in the measured responses is due to both random and systematic sources of uncertainty. Uncertainty in the simulated responses is due to cross section covariances. We describe in detail the adjustment to the cross sections and cross section covariances due to the optimization. Due to the contribution of systematic uncertainties to the measured response uncertainties, the adjustment to the cross sections is similar in trend but larger in magnitude compared to that recommended by previous work. We compare the measured responses to responses simulated with nominal and optimized cross sections, demonstrating that the best-estimate cross sections produce simulations of NMC experiments that are more accurate with reduced uncertainty. We verify that the response variance due to the cross sections computed with sampling-based uncertainty quantification (UQ) is well-approximated by that estimated with first-order UQ.

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Application of Neutron Multiplicity Counting Experiments to
Optimal Cross Section Adjustments

by
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DEDICATION

This work is dedicated to all of my family, friends, colleagues, and especially my wife. My mother and grandparents recognized my interest in both the sciences and music from an early age and did their best to foster my curiosity and creativity. Many hours were spent discussing books, answering a myriad of questions, listening to my favorite musical works, and attending various musical performances. My friends and colleagues from all walks of life encouraged me to always ask questions and to do my best. My wife has loved and supported me through all our years together and she continues to be a source of inspiration and wonder for me.

BIOGRAPHY

Alexander Rich Clark was born in Idaho Falls, Idaho in 1988. He grew up and spent most of his life in Southeastern Idaho, where he met the love of his life in 2012 (and married her soon after). He received a Bachelor of Science degree in Nuclear Engineering with a minor in Music from Idaho State University in May 2014. He began a PhD program at North Carolina State University in August 2014 with Dr. John Mattingly. He received a Consortium for Nonproliferation Enabling Capabilities (CNEC) fellowship in August 2016. He interned at Los Alamos National Laboratory (LANL) with the Nuclear Engineering Nonproliferation Advanced Nuclear Technology (NEN-2) group during Summer 2016 and was mentored by Mark Nelson. He returned to LANL for a year-round internship with the X-Computational Physics Monte Carlo Codes and Applications (XCP-3) group beginning in February 2018 and was mentored by Jeffrey Favorite. His hobbies include choral singing, weight lifting, and video games.

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INTRODUCTION

Neutron multiplicity counting (NMC) is a method for non-destructive analysis of special nuclear material (SNM) frequently employed in nuclear nonproliferation and material safeguards [19, 48, 9, 11, 53, 36, 28]. Kinetic parameters of an SNM assembly, such as neutron multiplication and neutron lifetime, may be inferred by fitting models of NMC distribution moments to measured neutron multiplicity counter responses. How well the inferred kinetic parameters characterize the SNM assembly depends to a large degree on the accuracy and precision of the input nuclear cross sections (e.g. the total and scatter cross sections) and fission parameters (e.g. the fission cross section, the fission spectrum, and the average number of neutrons emitted per fission, $\bar{\nu}$), which for brevity's sake are hereafter collectively referred to as cross sections.

Energy-dependent cross sections are measured from reaction-rate experiments using the time-of-flight technique. Nuclear physics models are fit to measured cross sections from several experiments over many energy regions to obtain evaluated cross sections. High-fidelity benchmark critical experiments are then simulated using the evaluated cross sections to obtain k_{eff} -eigenvalues (integral responses) [54]. If the simulated responses differ significantly from measured responses, the cross sections are adjusted. Cross sections that are deemed appropriate for their intended applications (e.g. criticality safety or reactor analysis) are then released as a library (e.g. ENDF/B-VII.0 [8]).

While evaluated cross sections for plutonium isotopes typically correctly predict the k_{eff} -eigenvalue for plutonium fast metal critical benchmarks [8], they do not adequately predict the NMC distribution for a subcritical assembly of a highly-multiplying sphere of weapons-grade plutonium metal, which implies that the cross sections are over-calibrated. Simulation of plutonium intermediate and thermal solution critical benchmarks are also not adequately predicted [8, 50]. Reference [37] found that the Pu-239 $\bar{\nu}$ in ENDF/B-VII.1 was over-calibrated to a single critical benchmark, Jezebel. Jezebel is a homogeneous bare metal spherical assembly of weapons-grade plutonium alloy [17] and is the principal critical benchmark for evaluation of plutonium fission parameters. In contrast, NMC experiments are used to assay subcritical SNM assemblies that are sometimes reflected or moderated by hydrogenous material. Jezebel is principally sensitive to fast neutrons while assemblies with hydrogenous material are sensitive to all neutron energies. The over-calibration occurs because a bare metal critical benchmark

will only inform cross section adjustments in the fast neutron region; potential inaccuracies in the intermediate and slow region which would not affect simulation of this critical benchmark will have a significant impact on simulation of a subcritical assembly with hydrogenous material.

As shown by Muñoz-Cobo [39], each NMC distribution moment is a function of the cross sections raised to that moment's order; consequently, the higher-order NMC distribution moments are more sensitive to changes in the cross sections than the mean, which is equivalent to the gross neutron count rate. The effect of over-calibration in the cross sections will therefore be more pronounced in the higher-order NMC distribution moments than in the mean.

Cacuci derived a data assimilation procedure that leverages information theory and Bayes' theorem to account for all sources of computational and experimental uncertainty, and he demonstrated that it provides best-estimate model parameters with reduced uncertainty [5]. In the present work, model calibration is the process of using sensitivity analysis (SA) and uncertainty quantification (UQ) to perform optimal adjustment of the nuclear cross sections via parameter estimation (PE). O'Brien [41] developed an adjoint-based SA based on Muñoz-Cobo's [39] stochastic transport equation (STE) that is applicable to the first and higher-order NMC distribution moments. Mattingly [35] demonstrated that each NMC distribution moment may be computed using a standard transport solver with a different fixed, adjoint source, which makes the SA computationally feasible and enables model calibration to be applied to NMC experiments, which will provide cross sections that simulate NMC experiments more accurately with reduced uncertainty.

Miller [37] and Evans [12] identified a discrepancy between cross section evaluations adjusted with critical benchmarks and subcritical experiments. Bare metal critical assemblies are sensitive to fast neutrons, while polyethylene-reflected, subcritical assemblies are sensitive to all neutron energies. The ENDF/B-VII.0 cross sections were adjusted using a bare metal critical benchmark (Jezebel) and were consequently inaccurate for simulating an NMC experiment with polyethylene-reflected plutonium metal. While Evans was able to more accurately predict the mean count rate for the polyethylene-reflected BeRP ball by optimizing the cross sections using a subcritical experiment, the behavior of the subcritical fissile assembly is not sufficiently described by the first NMC distribution moment. The NMC distribution for multiplying material requires higher-order moments to fully describe; therefore, model calibration applied to the first- and higher-order NMC distribution moments will result in cross sections that simulate NMC experiments more accurately with reduced uncertainty.

In this dissertation, we apply a) first-order adjoint-based SA to estimate the sensitivity of the first and second NMC distribution moments to the cross sections, b) first-order UQ to estimate the uncertainties in deterministic transport calculations of the first and second NMC distribution moments, and c) Bayesian inference, implemented using an extended Kalman filter (EKF), to estimate adjustments to the cross sections that will minimize the error in calculation of the first and second NMC distribution moments relative to experiment while simultaneously minimizing the uncertainty in the adjusted cross sections.

1.1 Prior work

1.1.1 Characteristics of neutron multiplicity counting

In NMC experiments, the number distribution of coincident neutron counts is accumulated using a neutron multiplicity counter. The nPod neutron multiplicity counter, pictured in Fig. 1.1, is a polyethylene-moderated array of 15 He-3 proportional counters wrapped in a 0.030-inch thick cadmium lining to minimize room return. The top part of Fig. 1.2a depicts a detector pulse train that is segmented in sequential, equal-width coincidence gates. The bottom part of Fig. 1.2a illustrates the accumulation of the coincident counts. Figure 1.2b is an NMC distribution accumulated with a 1024- μ s coincidence gate width T by counting a highly-multiplying sphere of plutonium metal reflected by polyethylene. A Poisson distribution with the same mean is shown for comparison.

Figure 1.1 The nPod neutron multiplicity counter atop a carbon steel cart.

The counting distribution for independent neutron emissions (e.g. those from (α, n) reactions) is Poisson-distributed, such that all of the higher-order moments are dictated by the mean; in particular, the variance of the distribution is equal to its mean. However, neutrons within a fission-chain reaction are not independent of one another; they appear in bursts that are correlated in time. The counting distribution for multiplying material is therefore a generalized Poisson distribution which requires higher-order moments to fully describe [44]. The width of the NMC distribution in Fig. 1.2b is larger than that of the Poisson distribution; i.e., the variance of the distribution has a contribution from fission

Figure 1.2 a) A detector pulse train is segmented into sequential, equal-width coincidence gates and the frequency of coincident multiplet neutron counts is accumulated to obtain the NMC distribution. b) An NMC distribution accumulated with a coincidence gate width T of 1024 μs by counting a highly-multiplying sphere of weapons-grade plutonium metal reflected by polyethylene and a Poisson distribution with the same mean. The width of the NMC distribution in excess of the Poisson distribution is characteristic of multiplying material.

that is in excess of the Poisson contribution, due to counts correlated within a fission-chain reaction. Assay of SNM via NMC experiments therefore requires the first- and higher-order NMC distribution moments to fully characterize the material.

The order- q NMC distribution moment is expressed as

$$\overline{n^q} = \frac{1}{N} \sum_{n=0}^N n^q f(n), \quad (1.1)$$

where $N = \sum_{n=0}^N f(n)$ is the total number of coincidence gates and $f(n)$ is the NMC distribution accumulated from a detector pulse train, like that shown in Fig. 1.2a. Similarly, the order- q NMC distribution central moment is

$$\mu_q = \frac{1}{N} \sum_{n=0}^N (n - \overline{n})^q f(n). \quad (1.2)$$

The NMC distribution moments are a function of T ; however, in this dissertation, we analyze the asymptotic value of the NMC distribution moments. Feynman defined a measure of variance in the NMC distribution in excess of a Poisson distribution,

$$Y = \frac{\mu_2}{\overline{n}} - 1, \quad (1.3)$$

which was initially used to measure the dispersion of the multiplicity of induced fission neutrons in U-235 [19]. In Eq. (1.3), $\overline{n}$ and μ_2 are the mean and variance of $f(n)$; note that Y vanishes for Poisson-distributed counts. Y is also a function of T , exhibiting asymptotic behavior for wide coincidence gates.

After Feynman's work, Terrell discovered that the cumulative fission multiplicity distribution exhibits a Gaussian shape [55]. Zucker and Holden later evaluated fission multiplicity distributions as a function of energy [61]. The induced fission multiplicity distribution moments used in this work originate from the Zucker and Holden measurements.

1.1.2 Models of neutron multiplicity counting distribution moments

Hage and Cifarelli [9] developed a three-parameter point-kinetics model of NMC distribution moments in terms of singles, doubles, and triples rates, which are the first three reduced-factorial moments¹ of the NMC distribution. Robba, Dowdy, and Atwater [48] (RDA) developed a similar point-kinetics model in terms of the Feynman Y . Hage and Cifarelli [9] demonstrated that the NMC distribution is a generalized Poisson distribution which does not explicitly depend on the mean, enabling Prasad and Snyderman [44] to derive a point-kinetics generating function of NMC distribution moments in terms of a generating function of the fission neutron number distribution moments, which describes the number distribution of neutrons produced from fission chains in the system.

The point-kinetics models developed by Hage and Cifarelli, RDA, and Prasad and Snyderman all assume that the neutron population behavior is separable in space and time. However, in heterogeneous assemblies where the neutron lifetime varies by orders of magnitude in different regions, this assumption does not hold. Consequently, this dissertation employs a more generally applicable model based on neutron transport.

Muñoz-Cobo [39] derived the stochastic transport equation (STE) using a probabilistic description of the neutron population developed by Pál [43] and Bell [2]. The solution of the STE is a generating function whose first moment is the fixed-source adjoint Boltzmann neutron transport equation (NTE). Higher-order moments of the STE generating function are adjoint transport equations; they have the same adjoint transport operator but different fixed, adjoint source terms that are defined in terms of lower-order adjoint fluxes. Therefore, standard transport solvers may be used to compute the higher-order adjoint fluxes and higher-order NMC distribution moments [41]. Davis [20] computed neutron and fission number distribution moments using Pál [43] and Bell's [2] formalism. Mattingly [35] performed deterministic calculations with the multigroup discrete-ordinates code PARTISN [1] to obtain NMC distribution moments by computing moments of Muñoz-Cobo's [39] STE generating function. Humbert [26] computed the NMC distribution itself using Pál [43] and Bell's [2] formalism via deterministic calculations with the multigroup discrete-ordinates code PANDA [25].

1.1.3 Identification of over-calibration in the Pu-239 $\bar{\nu}$

Miller [37] demonstrated that continuous-energy and -angle Monte Carlo code MCNP [59] simulations of a 4.5-kg sphere of weapons-grade, alpha-phase plutonium metal (the BeRP ball²) consistently

¹Factorial and reduced-factorial moments are respectively defined as $\bar{x}_q = \sum_{x=q-1}^{x_{\max}} x(x-1)\dots(x-q+1)f(x)$ and ${}_r\bar{x}_q = \frac{1}{q!} \sum_{x=q-1}^{x_{\max}} x(x-1)\dots(x-q+1)f(x)$, such that ${}_r\bar{x}_q = \frac{\bar{x}_q}{q!}$.

²The plutonium sphere is nicknamed the "Beryllium-Reflected Plutonium (BeRP) ball" because it was originally used in a benchmark with beryllium reflectors [27], but there is no beryllium present in the polyethylene-reflected measurements

overpredicted the mean and variance of the NMC distribution for bare and polyethylene-reflected configurations. Miller investigated and eliminated a variety of assembly and detector properties as potential causes of the discrepancy, and he ultimately demonstrated that a small ($\sim 1\%$) scalar reduction in the value of the ENDF/B-VII.1 Pu-239 $\bar{\nu}$ accurately predicted NMC distribution moments. In the release of the ENDF/B-VII.0³ cross section library, the evaluators noted that the value of the Pu-239 $\bar{\nu}$ was increased by more than two standard deviations below 1.5 MeV to match the Jezebel critical benchmark [8]. It was later noted in the ENDF/B-VII.1 release that the Pu-239 cross sections were such that intermediate and thermal solution benchmarks were not adequately simulated [7].

Evans [12] implemented an energy-dependent adjustment to the Pu-239 $\bar{\nu}$ using Cacuci’s data assimilation procedure applied to three-dimensional multigroup discrete-ordinates Denovo [13] simulations of gross neutron counting of the bare and polyethylene-reflected BeRP ball. Evans’ findings were consistent with those of Miller and with the ENDF/B-VII.0 release notes in that $\bar{\nu}$ should be reduced by one standard deviation above 100 keV and two standard deviations below 100 keV.

Recently, Whewell [60] performed a sampling-based calibration of the ENDF/B-VII.0 Pu-239 $\bar{\nu}$ using MCNP code fixed-source simulations of NMC of the BeRP ball and k_{eff} -eigenvalue simulations of Jezebel. Large deviations in the sampled $\bar{\nu}$ were penalized unless they resulted in a significant improvement in a χ^2 error metric. The calibrated $\bar{\nu}$ reduced the NMC distribution bias but increased the k_{eff} -eigenvalue bias because of large statistical uncertainties. Endo [10] utilized α -eigenvalue measurements to reduce the k_{eff} -eigenvalue uncertainty due to the cross sections. The bias factor and generalized linear least squares methods were applied to PARTISN [1] k_{eff} - and α -eigenvalue simulations of a polyethylene-moderated highly-enriched uranium assembly to calibrate the prompt fission spectrum χ and prompt $\bar{\nu}$. The high degree of correlation between the k_{eff} - and α -eigenvalue measurements and between the prompt and total χ and $\bar{\nu}$ resulted in a smaller k_{eff} -eigenvalue uncertainty than could be obtained with calibration using a k_{eff} -eigenvalue measurement alone.

1.2 Novel contributions

This dissertation presents the first application of model calibration to NMC experiments that utilizes adjoint-based SA, first-order UQ, and Bayesian-inference-based PE. While adjoint-based SA of the first NMC distribution moment (i.e. the mean count rate of a detector) is well-established [22, 12, 18], SA of the second and higher-order NMC distribution moments is relatively new and was demonstrated by O’Brien [41] to be computationally feasible. We therefore utilize adjoint-based SA to perform the first calculation of the variance in the second NMC distribution moment due to cross section covariances using first-order UQ. We also perform sampling-based uncertainty quantification (UQ) to directly compute variance in the responses due to covariance in the cross sections and demonstrate that the response variances are well-approximated by first-order UQ. As a consequence, we further demonstrate that first-order perturbation theory is appropriate for the particular subcritical assembly we analyzed.

discussed in this dissertation.

³ No change was made to the Pu-239 $\bar{\nu}$ between the VII.0 and VII.1 releases. One significant difference in the VII.1 release is the expansion and improvement of cross section covariances, which are utilized in the present work [7, 50].

Bayesian inference is used to perform cross section evaluation and validation [8, 3, 54] and was recently utilized by Evans [12] in optimally adjusting the cross sections to a subcritical experiment. The application of an EKF to NMC experiments for optimal cross section adjustment is novel, however, and is shown in this dissertation to produce best-estimate cross sections such that NMC experiments are more accurately simulated with reduced uncertainty. Additionally, uncertainty in the NMC distribution moments due to both random and systematic sources of uncertainty are included in the model calibration process, whereas Evans' work only accounted for random sources of uncertainty.

1.3 Outline of this dissertation

This dissertation begins by summarizing the model calibration process in Chap. 2. Section 2.2 presents calculation of the detector response moments for an arbitrary geometry in continuous energy and continuous angle. Section 2.3 summarizes the adjoint-based SA and provides notable additions to O'Brien's [41] work. Section 2.4 presents calculation of the detector response moments and their sensitivity to the cross sections with the energy variable discretized via the multigroup approximation and the angle variable in the scatter source treated with a Legendre polynomial moment expansion for a one-dimensional spherical geometry. Notably, Table 2.1 provides the specific form of the adjoint-based sensitivity of the detector response moments to all cross sections. Section 2.5 describes random and systematic sources of uncertainty and discusses their propagation through the measured and simulated detector response moments.

Chapter 3 details the model calibration process applied to NMC of a highly-multiplying sphere of weapons-grade ($\sim 6\%$ Pu-240) plutonium metal in bare and polyethylene-reflected configurations. Section 3.1 presents the EKF algorithm and describes how the response sensitivities and uncertainties affect the optimal adjustment of the cross sections and cross section covariances. We describe in Sec. 3.2 the detector response moment sensitivity to the fission parameters (i.e. moments of the induced fission neutron multiplicity distribution $p(\nu, E)$, the fission cross section σ_f , and the fission spectrum χ) as well as the adjustment to the fission parameters and to their covariances. We compare measured detector response moments to those simulated with the nominal and optimally adjusted cross sections and demonstrate that NMC experiments are more accurately simulated with reduced uncertainty.

Chapter 4 provides a detailed comparison between model calibration applied to one-dimensional (spherical) simulations of gross neutron counting of the plutonium sphere and data assimilation applied [12] to three-dimensional simulations of the same source-detector configuration. We demonstrate that the loss of detail in a one-dimensional simulation has not significantly impacted the accuracy of the simulated responses. We also demonstrate that performing model calibration with both random and systematic sources of uncertainty produce cross section adjustments that are similar in trend but increased in magnitude compared to that provided by model calibration with random sources of uncertainty only.

Chapter 5 compares the detector response moment uncertainties due to cross section covariances estimated via first-order UQ to that estimated via sampling-based UQ. We demonstrate that first-order

UQ adequately estimates the response variances due to the cross section covariances. We further show that first-order perturbation theory is appropriate for NMC of a highly-multiplying sphere of weapons-grade plutonium metal in bare and polyethylene-reflected configurations.

Chapter 6 provides conclusions and recommended future work. We emphasize that the model calibration process can include more cross sections than are analyzed here, provided their nominal values and covariances are available. The model calibration process may therefore be extended to NMC experiments with assemblies of differing composition.

SENSITIVITY ANALYSIS AND UNCERTAINTY QUANTIFICATION APPLIED TO NEUTRON MULTIPLICITY COUNTING

This chapter provides a derivation of the adjoint-based SA applied to NMC, as well as a discussion of the sources of random and systematic uncertainty in the detector response moments. After outlining the model calibration process in Sec. 2.1, Secs. 2.2 and 2.3 respectively present calculation of the detector response moments and their sensitivity to the cross sections for a general geometry in continuous energy and continuous angle. Sec. 2.4 then presents the responses and sensitivities with energy discretized via the multigroup approximation and with the angle variable in the scatter source treated with a Legendre polynomial expansion for a one-dimensional spherical geometry. Section 2.5 discusses the sources of random and systematic uncertainties and describes how each may be reduced.

2.1 Model calibration process

Model calibration of nuclear cross sections is performed in three steps, illustrated in Fig. 2.1.

1. The sensitivity of a detector response moment to the cross sections is computed using an adjoint-based approach. Previous work by O'Brien [41] utilized Muñoz-Cobo's [39] STE to compute NMC distribution moments and their sensitivity to the cross sections.
2. The sensitivities are then used to propagate covariance between the nuclear cross sections through the detector response moments via linear propagation of uncertainty. This step is an inner product between the sensitivities and cross section covariances.
3. The sensitivities and response covariances are then used to inform optimization of the cross sections and their covariances via parameter estimation (PE). The result is a set of cross section values that are "optimal" in that the error between measured and simulated detector responses is minimized in a least squares sense.

Figure 2.1 Flowchart of the model calibration process. Detector response moment sensitivities to the cross sections and detector response moment covariances due to cross section covariances are used to inform cross section optimization via model calibration.

2.2 Calculation of detector response moments

O’Brien demonstrated that the sensitivity of each NMC distribution moment (i.e. detector response moment) may be computed with adjoint-based methods applied to moments of the STE generating function [41]. Because each NMC distribution moment is derived from an inner product of the solution to an adjoint transport equation with a special fixed, adjoint source, standard deterministic transport solvers may be used to compute the higher-order detector response moments. Adjoint-based methods are advantageous because they require few transport solves compared to numerical differentiation, making SA of the higher-order NMC distribution moments computationally inexpensive. This SA framework is utilized in this dissertation to perform model calibration of nuclear cross sections applied to the first and second NMC distribution moments.

What follows is the calculation of the NMC distribution moments and a summary of O’Brien’s SA, with some notable additions:

1. O’Brien treated the fission and scatter cross sections, which appear in both the total loss operator and their respective source terms in the NTE, as independent of the total cross section. The derivations in this paper account for the relationship of the fission and scatter cross sections to the total cross section.
2. O’Brien defined a scalar, relative sensitivity rank as the product of the group-averaged cross section and group-summed derivative of the response with respect to the cross section. What is given here instead are scalar, relative sensitivity totals, which are a more standard [22] way of comparing the effect of a change in the cross sections on the responses.
3. The specific form of the response sensitivities are provided in Table 2.1 and are derived by considering the derivative of the group response with respect to a group cross section (Sec. 2.4).

This section and Sec. 2.3 derive the detector response moments and their sensitivity to the cross sections, respectively, for an arbitrary geometry in continuous energy and continuous angle. Section 2.4 presents the response and sensitivity equations with the energy variable discretized via the multigroup approximation and the angle variable in the scatter source treated by Legendre polynomial expansion for a one-dimensional spherical geometry.

Higher-order detector response moments (i.e. higher-order NMC distribution moments) may be computed using the STE generating function to derive higher-order adjoint NTEs with non-reentrant boundary conditions [39]. Each equation for a higher-order adjoint flux,

$$L^* \psi_q^* = Q_q^*, \quad q = 1, 2, \dots, \quad (2.1)$$

has the standard, adjoint transport operator L^* , defined as

$$\begin{aligned} L^* = & -\hat{\Omega} \cdot \nabla + \Sigma_t(\vec{r}, E) \\ & - \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(\vec{r}, \hat{\Omega}, E \rightarrow \hat{\Omega}', E') \\ & - \nu \Sigma_f(\vec{r}, E) \int_{4\pi} d\Omega' \int_0^\infty dE' \frac{\chi(\vec{r}, E')}{4\pi}, \end{aligned} \quad (2.2)$$

with a special fixed, adjoint source Q_q^* . $q = 1$ denotes the standard adjoint NTE for a fixed source subcritical problem while $q > 1$ denotes higher-order adjoint flux and adjoint source terms. The material cross sections are defined as

$$\begin{aligned} \Sigma_t(\vec{r}, E) &= \Sigma_c(\vec{r}, E) + \Sigma_f(\vec{r}, E) + \Sigma_s(\vec{r}, E) = \text{total cross section,} \\ \Sigma_c(\vec{r}, E) &= \text{capture cross section,} \\ \Sigma_f(\vec{r}, E) &= \text{fission cross section,} \\ \Sigma_s(\vec{r}, E) &\equiv \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(\vec{r}, \hat{\Omega}, E \rightarrow \hat{\Omega}', E') = \text{scatter cross section,} \\ \frac{\chi(\vec{r}, E)}{4\pi} &= \text{fission neutron spectrum,} \\ \nu \Sigma_f(\vec{r}, E) &= \text{fission neutron production} \\ &\quad \text{cross section,} \end{aligned} \quad (2.3)$$

and have units of $[\frac{1}{\text{cm}}]$, except for the material fission spectrum, which has units of $[\frac{1}{\text{MeV}}]$. Setting the first-moment adjoint source term Q_1^* to be the detector response function Σ_d means that the mean count rate R_1 of the detector may be computed by taking the inner product of the standard forward flux ψ and the adjoint source term,

$$R_1 = \langle \psi, Q_1^* \rangle = \langle \psi, \Sigma_d \rangle, \quad (2.4)$$

where the inner product is defined as

$$\langle f, g \rangle = \int_V dV \int_{4\pi} d\Omega \int_0^\infty dE f(\vec{r}, \hat{\Omega}, E) g(\vec{r}, \hat{\Omega}, E). \quad (2.5)$$

ψ is computed by solving the standard forward NTE,

$$L\psi = Q, \quad (2.6)$$

with non-reentrant boundary conditions and the standard forward transport operator L , defined as

$$\begin{aligned} L = & \hat{\Omega} \cdot \nabla + \Sigma_t(\vec{r}, E) \\ & - \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(\vec{r}, \hat{\Omega}', E' \rightarrow \hat{\Omega}, E) \\ & - \frac{\chi(\vec{r}, E)}{4\pi} \int_{4\pi} d\Omega' \int_0^\infty dE' \nu \Sigma_f(\vec{r}, E'), \end{aligned} \quad (2.7)$$

and forward source term Q . R_1 in Eq. (2.4) is identical to the mean of the NMC distribution divided by the coincidence gate width T ; i.e.,

$$R_1 = \frac{\bar{n}}{T}. \quad (2.8)$$

Similar to Eq. (2.4), higher-order detector response moments may computed as

$$R_q = \langle \psi, Q_q^* \rangle + \langle S, Q_{q, sf}^* \rangle, \quad (2.9)$$

where the two inner products account for the contribution of induced and spontaneous fission to the detector response moment; S is the spontaneous fission rate density and spectrum of the fixed source with units of $\left[\frac{\text{spontaneous fissions}}{\text{s cm}^3 \text{ MeV}} \right]$. In the special case where $q = 1$, $Q_{q, sf}^* \equiv 0$, such that R_1 is the mean count rate.

For $q = 2$, the adjoint source terms are defined as

$$Q_2^*(\vec{r}, E) = \overline{\nu(\nu-1)\Sigma_f(\vec{r}, E)} I_1^2(\vec{r}), \quad (2.10)$$

$$Q_{2, sf}^{*,j}(\vec{r}) = \overline{\nu(\nu-1)}_{sf}^j I_{1, sf}^2(\vec{r}), \quad (2.11)$$

and are the importance of correlated pairs of induced and spontaneous fission neutrons, respectively, to R_2 . The importance of induced and spontaneous fission neutrons to the mean count rate are

$$I_1(\vec{r}) = \int_{4\pi} d\Omega' \int_0^\infty dE' \frac{\chi(\vec{r}, E')}{4\pi} \psi_1^*(\vec{r}, \hat{\Omega}', E'), \quad (2.12)$$

$$I_{1, sf}(\vec{r}) = \int_{4\pi} d\Omega' \int_0^\infty dE' \frac{\chi_{sf}(\vec{r}, E')}{4\pi} \psi_1^*(\vec{r}, \hat{\Omega}', E'), \quad (2.13)$$

where χ_{sf} is the spontaneous fission neutron spectrum.

Note that Eq. (2.10) is defined for a material while Eq. (2.11) is defined for a nuclide j . While the material cross sections given in Eq. (2.3) have standard [23] definitions given by

$$\Sigma_x(\vec{r}, E) = \sum_{j=1}^J N^j(\vec{r}) \sigma_x^j(E), \quad (2.14)$$

$$\nu \Sigma_f(\vec{r}, E) = \sum_{j=1}^J N^j(\vec{r}) \nu \sigma_f^j(E), \quad (2.15)$$

for an assembly composed of J nuclides with nuclide atom density $N^j(\vec{r})$ and microscopic cross sections $\sigma_x^j(E)$ and $\nu \sigma_f^j(E)$, the cross sections in Eqs. (2.10) and the second inner product in Eq. (2.9) require special consideration (calculation of the material fission spectrum is discussed in note 3). The material fission neutron dispersion cross section in Eq. (2.10) is defined as

$$\overline{\nu(\nu-1)} \Sigma_f(\vec{r}, E) = \sum_{j=1}^J \overline{\nu(\nu-1)}^j(E) N^j(\vec{r}) \sigma_f^j(E). \quad (2.16)$$

Similarly, the material source neutron dispersion cross section is defined as

$$\overline{\nu(\nu-1)}_{sf} S(\vec{r}, E) = \sum_{j=1}^J \overline{\nu(\nu-1)}_{sf}^j S^j(\vec{r}, E), \quad (2.17)$$

such that the second inner product in Eq. (2.9) is computed as

$$\langle S, Q_{2,sf}^* \rangle = \left\langle \sum_{j=1}^J \left[\overline{\nu(\nu-1)}_{sf}^j S^j(\vec{r}, E) \right] I_{sf}^2(\vec{r}) \right\rangle. \quad (2.18)$$

$\overline{\nu(\nu-1)}^j(E)$ and $\overline{\nu(\nu-1)}_{sf}^j$ are the second factorial moments of the induced and spontaneous fission multiplicity distributions $p^j(\nu, E)$ and $p_{sf}^j(\nu)$, respectively, and are respectively defined as

$$\overline{\nu(\nu-1)}^j(E) = \sum_{\nu=1}^{\nu_{\max}} \nu(\nu-1) p^j(\nu, E), \quad (2.19)$$

$$\overline{\nu(\nu-1)}_{sf}^j = \sum_{\nu=1}^{\nu_{\max}} \nu(\nu-1) p_{sf}^j(\nu), \quad (2.20)$$

where ν represents the number of neutrons emitted per fission, $\nu_{\max}$ is the maximum number of neutrons emitted per fission (typically $\nu_{\max} \sim 8$), and E is the energy of an incident neutron.

It is clear from Eqs. (2.10) and (2.12) that because Q_2^* is computed with the square of I_1 , R_2 is a function of cross sections squared. Because the second-moment adjoint source terms Q_2^* and $Q_{2,sf}^*$ are defined in terms of the standard adjoint flux ψ_1^* , R_2 is fully calculable using a standard transport solver. R_2 is related to the NMC distribution variance; i.e.,

$$R_2 = \frac{\mu_2 - \bar{n}}{T}. \quad (2.21)$$

For a Poisson-distributed process, $\mu_2 = \bar{n}$ and $R_2 = 0$. It is therefore evident from Eq. (2.21) that R_2 is the part of the NMC distribution variance in *excess* of the Poisson contribution.

2.3 Sensitivity analysis of the detector response moments

The sensitivity of the mean count rate R_1 to a cross section α in the set $\alpha = \{\bar{\nu}, \overline{\nu(\nu-1)}, \chi, \sigma_f, \sigma_s, \sigma_c\}$ using adjoint-based methods described by O'Brien [41] may be expressed as

$$\frac{\partial R_1}{\partial \alpha} = \left\langle \frac{\partial Q_1^*}{\partial \alpha}, \psi \right\rangle + \left\langle \psi_1^*, \frac{\partial Q}{\partial \alpha} - \frac{\partial L}{\partial \alpha} \psi \right\rangle. \quad (2.22)$$

Because the variance in the NMC distribution in excess of the Poisson contribution R_2 can be computed with the second-moment adjoint source term Q_2^* , which is defined by the standard adjoint flux (see Eqs. (2.10) and (2.12)), adjoint-based SA may also be utilized to express the sensitivity of R_2 to α as [41]

$$\begin{aligned} \frac{\partial R_2}{\partial \alpha} = & \left\langle \psi_2^*, \frac{\partial Q}{\partial \alpha} - \frac{\partial L}{\partial \alpha} \psi \right\rangle + 2 \left\langle \Phi, \frac{\partial Q_1^*}{\partial \alpha} - \frac{\partial L^*}{\partial \alpha} \psi_1^* \right\rangle \\ & + \left\langle \frac{\partial Q_2^*}{\partial \beta}, \psi \right\rangle + \left\langle \frac{\partial Q_{2,sf}^*}{\partial \beta}, S \right\rangle + \left\langle Q_{2,sf}^*, \frac{\partial S}{\partial \alpha} \right\rangle, \end{aligned} \quad (2.23)$$

where $\beta = \{\overline{\nu(\nu-1)}, \overline{\nu(\nu-1)}_{sf}, \sigma_f, \chi, \chi_{sf}\}$ is a cross section in the subset of α that appears explicitly in the adjoint source terms and calculation of Φ is discussed below.

For example, the derivative of Q_2^* with respect to α has two components due to the product rule,

$$\frac{\partial Q_2^*}{\partial \alpha} = \frac{\partial Q_2^*}{\partial \beta} + F^* \frac{\partial \psi_1^*}{\partial \alpha}. \quad (2.24)$$

The first term,

$$\begin{aligned} \frac{\partial Q_2^*}{\partial \beta} = & \frac{\partial}{\partial \beta} (\overline{\nu(\nu-1)} \Sigma_f(\vec{r}, E)) I^2(\vec{r}) \\ & + 2 \overline{\nu(\nu-1)} \Sigma_f(\vec{r}, E) I(\vec{r}) \int_{4\pi} d\Omega' \int_0^\infty dE' \frac{\partial \chi(\vec{r}, E')}{\partial \beta} \psi_1^*(\vec{r}, \Omega', E'), \end{aligned} \quad (2.25)$$

contains only derivatives with respect to the cross sections that appear explicitly in Eq. (2.10), with no derivatives of the flux. The second term contains a new adjoint operator F^* ,

$$F^* = 2 \overline{\nu(\nu-1)} \Sigma_f(\vec{r}, E) I(\vec{r}) \int_{4\pi} d\Omega' \int_0^\infty dE' \chi(\vec{r}, E'), \quad (2.26)$$

that operates on the derivative of the adjoint flux with respect to the cross sections. To avoid computing the flux derivative, Anistratov [41] used the relationship between forward and adjoint transport operators in an inner product to derive a new forward flux, $\Phi = \Phi_1 + \Phi_{1,sf}$, which appears in the second term of Eq.

(2.23) and represents the flux of induced (Φ_1) and spontaneous ($\Phi_{1,sf}$) fission neutrons that contribute to the second-moment detector response, respectively. They are computed by solving the new forward transport equations

$$L\Phi_1 = I_1 Q_{f1}, \quad (2.27)$$

$$L\Phi_{1,sf} = I_{1,sf} Q_{f1,sf}, \quad (2.28)$$

with the standard forward transport operator L of Eq. (2.7), non-reentrant boundary conditions, and special fixed, forward source terms [41],

$$Q_{f1}(\vec{r}, E) = \frac{\chi(\vec{r}, E)}{4\pi} \int_{4\pi} d\Omega' \int_0^\infty dE' \overline{\nu(\nu-1)} \Sigma_f(\vec{r}, E') \psi(\vec{r}, \hat{\Omega}', E'), \quad (2.29)$$

$$Q_{f1,sf}(\vec{r}, E) = \frac{\chi_{sf}(\vec{r}, E)}{4\pi} \int_{4\pi} d\Omega' \int_0^\infty dE' \overline{\nu(\nu-1)}_{sf} S(\vec{r}, E), \quad (2.30)$$

that are the source of correlated neutron pairs from induced and spontaneous fission, respectively.

Instead of solving Eqs. (2.27) and (2.28) individually, they may be combined into a single equation (also with non-reentrant boundary conditions) because they have the same forward transport operator,

$$L\Phi = L\Phi_1 + L\Phi_{1,sf} = I_1 Q_{f1} + I_{1,sf} Q_{f1,sf}. \quad (2.31)$$

A single transport solve using the combined forward fixed source term given by Eq. (2.31) may then be used to compute Φ . Because the source terms for the second-moment adjoint flux ψ_2 and the second-moment forward flux Φ are defined in terms of the standard adjoint and forward fluxes, the sensitivity of R_2 to the cross sections is fully calculable using a standard transport solver.

2.4 Multigroup approximation and Legendre polynomial expansion applied to detector response moments and their sensitivity to the cross sections

The forward and adjoint NTE may be discretized in energy via the multigroup approximation [1],

$$f_g(\vec{r}, \hat{\Omega}) = \frac{\int_{\Delta E_g} dE W(E) f(\vec{r}, \hat{\Omega}, E)}{\int_{\Delta E_g} dE W(E)}, \quad g = 1, \dots, G, \quad (2.32)$$

where $W(E)$ is a weighting function. Multigroup cross sections (Σ_t , Σ_s , Σ_f , and $\nu\Sigma_f$) may be defined by choosing $W(E)$ to be the forward, scalar flux.¹ Multigroup fluxes, sources, and isotopic fission spectra

¹A mathematically exact expression for the multigroup cross sections is obtained by choosing the weight function to be the angular flux ψ ; however, the angular flux is not known prior to the transport solve. Additionally, this definition of the multigroup cross sections would introduce an angular bias as a result of the discrete ordinates approximation. An approximation to the

χ^j are obtained by setting $W(E)$ to unity (calculation of the multigroup material fission spectrum χ is discussed in note 3).

The Zucker and Holden [61] $p(\nu)$ distribution moment $\overline{\nu(\nu-1)}$ is defined for the coarse grid of incident neutrons energies, 0, 1, ..., 10 MeV [61]. To obtain an arbitrary multigroup $\overline{\nu(\nu-1)}$, a quadratic model in energy was fit to the $\overline{\nu(\nu-1)}$ reported by Zucker and Holden. The value of $\overline{\nu(\nu-1)}$ for the desired group structure was then obtained by applying the multigroup approximation to the model. Fits of the quadratic model in energy to the U-235, U-238, and Pu-239 $\overline{\nu(\nu-1)}$ are plotted in Fig. 2.2 for reference.

Figure 2.2 Fits of a quadratic model in energy to Zucker and Holden data for the U-235, U-238, and Pu-239 $\overline{\nu(\nu-1)}$.

The forward and adjoint fluxes and the scatter cross section may be treated in angle via a Legendre polynomial expansion [1]. The order- m forward fluxes, adjoint fluxes, and scatter cross section moments (for one-dimensional geometry) are respectively defined as

scalar flux spectrum is typically easier to obtain and provides multigroup cross sections that preserves the values of reaction rates (e.g. $\sum_{g=1}^G \nu \Sigma_{f,g} \phi_g$) [1].

$$\phi^m(\vec{r}, E) = \frac{1}{2} \int_{-1}^1 d\mu P^m(\mu) \psi(\vec{r}, E, \mu), \quad (2.33)$$

$$\varphi^m(\vec{r}, E) = \frac{1}{2} \int_{-1}^1 d\mu P^m(\mu) \Phi(\vec{r}, E, \mu), \quad (2.34)$$

$$\phi_q^{*,m}(\vec{r}, E) = \frac{1}{2} \int_{-1}^1 d\mu P^m(\mu) \psi_q^*(\vec{r}, E, \mu), q = 1, 2, \quad (2.35)$$

$$\Sigma_s^m(E \rightarrow E') = \frac{2m+1}{2} \int_{-1}^1 d\mu P^m(\mu) \int_{-1}^1 d\mu' P^m(\mu') \Sigma_s(\mu \cdot \mu', E \rightarrow E'), \quad (2.36)$$

where P^m is a Legendre polynomial of order m . $m = 0$ denotes an isotropic flux or scatter cross section while $m > 0$ denotes increasing orders of anisotropy. The inclusion of the $2m + 1$ normalization factor in Eq. (2.36) is consistent with the scatter cross section moments generated by the code package SCALE [46].

The equations for the forward and adjoint fluxes and their respective operators and sources are recast after applying the multigroup approximation and Legendre polynomial expansion for a one-dimensional geometry.² The standard group forward NTE, new group forward NTE, and the standard group forward transport operator are respectively recast as

$$L_g \psi_g = Q_g, \quad (2.37)$$

$$L_g \Phi_{1,g} = I_1 Q_{f1,g} + I_{1,sf} Q_{f1,sf,g}, \quad (2.38)$$

and

$$\begin{aligned} L_g = & \hat{\Omega} \cdot \nabla + \Sigma_{t,g}(\vec{r}) \\ & - \sum_{m=0}^M \sum_{g'=1}^G P^m(\mu) \Sigma_{s,g' \rightarrow g}^m(\vec{r}) \frac{1}{2} \int_{-1}^1 d\mu' P^m(\mu') \\ & - \chi_g(\vec{r}) \sum_{g'=1}^G \nu \Sigma_{f,g'}(\vec{r}) \frac{1}{2} \int_{-1}^1 d\mu'. \end{aligned} \quad (2.39)$$

The first- and second-moment group adjoint NTE and standard group adjoint transport operator are respectively redefined as

$$L_g^* \psi_{q,g}^* = Q_{q,g}^*, q = 1, 2 \quad (2.40)$$

² For the one-dimensional spherical geometry problem that we discuss later in this dissertation, $\hat{\Omega} \cdot \nabla \psi = \frac{\mu}{r^2} \frac{\partial(r^2 \psi)}{\partial r} + \frac{1}{r} \frac{\partial[(1-\mu^2)\psi]}{\partial \mu}$, where r is the radial coordinate, $\mu = \hat{e}_r \cdot \hat{\Omega}$, and $\hat{e}_r$ is a unit-vector in the direction of the radial coordinate.

and

$$\begin{aligned}
L_g^* = & -\hat{\Omega} \cdot \nabla + \Sigma_{t,g}(\vec{r}) \\
& - \sum_{m=0}^M \sum_{g'=1}^G P^m(\mu) \Sigma_{s,g \rightarrow g'}^m(\vec{r}) \frac{1}{2} \int_{-1}^1 d\mu' P^m(\mu') \\
& - \nu \Sigma_{f,g}(\vec{r}) \sum_{g'=1}^G \chi_{g'}(\vec{r}) \frac{1}{2} \int_{-1}^1 d\mu'.
\end{aligned} \tag{2.41}$$

The second-moment induced and spontaneous fission forward source terms are respectively altered to be

$$Q_{f1,g}(\vec{r}) = \chi_g(\vec{r}) \sum_{g'=0}^G \overline{\nu(\nu-1) \Sigma_{f,g'}(\vec{r})} \phi_{g'}^0(\vec{r}) \tag{2.42}$$

and

$$Q_{f1,sf,g}(\vec{r}) = \chi_{sf,g}(\vec{r}) \sum_{g'=0}^G \overline{\nu(\nu-1)_{sf} S_{g'}(\vec{r})}. \tag{2.43}$$

The second-moment adjoint induced fission source term becomes

$$Q_{2,g}^*(\vec{r}) = \overline{\nu(\nu-1) \Sigma_{f,g}} I_1^2(\vec{r}). \tag{2.44}$$

The second-moment adjoint spontaneous fission source term defined in Eq. (2.11) is not a function of energy. The first-moment induced and spontaneous fission importances are respectively changed to

$$I_1(\vec{r}) = \sum_{g'=1}^G \chi_{g'}(\vec{r}) \phi_{1,g'}^{*,0}(\vec{r}) \tag{2.45}$$

and

$$I_{1,sf}(\vec{r}) = \sum_{g'=1}^G \chi_{sf,g'}(\vec{r}) \phi_{1,g'}^{*,0}(\vec{r}). \tag{2.46}$$

If the inner product given by Eq. (2.5) is redefined to only be over position and direction as

$$\langle f, h \rangle = \int_V dV \int_{4\pi} d\Omega f(\vec{r}, \hat{\Omega}) h(\vec{r}, \hat{\Omega}), \tag{2.47}$$

the group detector response moments may be defined as

$$R_{q,g} = \langle \psi_g, Q_{q,g}^* \rangle + \langle S_g, Q_{q,sf}^* \rangle, \tag{2.48}$$

and the sensitivities of R_1 and R_2 at group g to a cross section at group g' have the same form as their respective continuous-energy definitions given in Eqs. (2.22) and (2.23); i.e.,

$$\frac{\partial R_{1,g}}{\partial \alpha_{g'}} = \left\langle \frac{\partial Q_{1,g}^*}{\partial \alpha_{g'}}, \psi_g \right\rangle + \left\langle \psi_{1,g}^*, \frac{\partial Q_g}{\partial \alpha_{g'}} - \frac{\partial L_g}{\partial \alpha_{g'}} \psi_g \right\rangle \tag{2.49}$$

and

$$\begin{aligned} \frac{\partial R_{2,g}}{\partial \alpha_{g'}} = & \left\langle \psi_{2,g}^*, \frac{\partial Q_g}{\partial \alpha_{g'}} - \frac{\partial L_g}{\partial \alpha_{g'}} \psi_g \right\rangle + 2 \left\langle \Phi_{1,g}, \frac{\partial Q_{1,g}^*}{\partial \alpha_{g'}} - \frac{\partial L_g^*}{\partial \alpha_{g'}} \psi_{1,g}^* \right\rangle \\ & + \left\langle \frac{\partial Q_{2,g}^*}{\partial \beta_{g'}}, \psi_g \right\rangle + \left\langle \frac{\partial Q_{2,sf}^*}{\partial \beta_{g'}}, S_g \right\rangle + \left\langle Q_{2,sf}^*, \frac{\partial S_g}{\partial \alpha_{g'}} \right\rangle. \end{aligned} \quad (2.50)$$

The magnitude of the absolute sensitivity defined in Eqs. (2.49) and (2.50) can vary greatly with respect to cross section and energy group, so it is standard practice [22] to define a relative sensitivity as

$$S_{R_{q,g},\alpha_{g'}} = \frac{\alpha_{g'}}{R_{q,g}} \frac{\partial R_{q,g}}{\partial \alpha_{g'}}, \quad (2.51)$$

which is scaled by the cross section and response values themselves. Equation (2.51) describes a linear relationship between a change in the group cross section and a corresponding change in the group detector response. For example, a relative sensitivity of 1 would mean that a 1% increase in the cross section would result in a 1% increase in the detector response.

Equation (2.51) is an element of a matrix of relative sensitivities of dimension $G \times G$, where the rows are the cross section groups g' and the columns are the response groups g . A vector of sensitivities of dimension $G \times 1$ that quantifies the relative sensitivity of the integrated detector response to the group cross sections may be obtained by summing either Eq. (2.49) or Eq. (2.50) over group g and multiplying by the ratio of the group cross section to the integrated detector response; i.e.,

$$S_{R_q,\alpha_{g'}} = \frac{\alpha_{g'}}{R_q} \sum_{g=1}^G \frac{\partial R_{q,g}}{\partial \alpha_{g'}}. \quad (2.52)$$

Scalar sensitivity totals may be obtained by summing the vector of relative sensitivities over group g' ,

$$S_{R_q,\alpha} = \sum_{g'=1}^G S_{R_q,\alpha_{g'}}. \quad (2.53)$$

The relative sensitivity matrix in Eq. (2.51) is used only to derive the relative sensitivity vector in Eq. (2.52). Relative sensitivity vectors for multiple responses (e.g. R_1 and R_2) are columns of a sensitivity matrix that is utilized in the model calibration process (see Sec. 3.1). Plots of relative sensitivity vectors and totals will be given in Chap. 3.

Table 2.1 summarizes the relative sensitivity of the detector response moments to the group microscopic cross sections for nuclide j with number density N^j . Because the fission neutron production cross section is used to compute the material fission spectrum,³ the sensitivity of the responses with respect to χ^j , $\bar{\nu}^j$, and σ_f^j must all reflect this dependence, which is explicitly given in Table 2.1. Because

³In PARTISN, the material fission spectrum,

$$\chi_g(\vec{r}) = \frac{\sum_{j=1}^J \chi_g^j N^j(\vec{r}) \sum_{g'=1}^G \nu \sigma_{f,g'}^j f_{g'}}{\sum_{j=1}^J N^j(\vec{r}) \sum_{g'=1}^G \nu \sigma_{f,g'}^j f_{g'}}, \quad (2.54)$$

is computed as an average of the isotopic fission spectra χ^j weighted by the fission neutron production cross sections with number density N^j . f is an analytic function constructed from a Maxwellian distribution for thermal energies, a $\frac{1}{v}$ spectrum between thermal and fission energies, a Watt fission spectrum peak, and a 14-MeV fusion spectrum peak [33].

the group sum over the fission spectrum must equal unity, the sensitivity of the responses with respect to χ^j has a normalization constraint. This constraint is not given in Table 2.1 but is discussed by Favorite [18] in the context of response sensitivities to material density and composition parameters (e.g. nuclide weight fractions).

An unconstrained group cross section (e.g. the fission cross section) is allowed to vary independent of any adjustment to the other group cross sections. The fission spectrum χ is constrained to sum to unity, however, and so an adjustment to one group χ_g must have a corresponding adjustment to some or all of the other groups in order to enforce the constraint. The sensitivity of a detector response moment to the fission spectrum must therefore reflect the interdependence of the group χ_g . For the fission spectrum, the relationship between the constrained and unconstrained relative sensitivity vectors is given by Favorite [18] as

$$S_{R_q, \chi_g}^C = S_{R_q, \chi_g} - \chi_g \sum_{g'} S_{R_q, \chi_{g'}}, \quad (2.55)$$

where S_{R_q, χ_g}^C and S_{R_q, χ_g} are the constrained and unconstrained relative sensitivity vectors, respectively. One way to think about this relationship is that the unconstrained sensitivity is adjusted by the fraction to which the group parameter contributes to the sensitivity total. For the specific constraint that the fission spectrum must sum to unity, the sum of Eq. (2.55) over group g (i.e. the constrained sensitivity total) is zero. This means that changes in the detector response due to a change in the group fission spectrum at group g are balanced by corresponding changes in the other group fission spectrum terms.

Note that Favorite [16] provided a table of R_1 sensitivity vectors that are nearly identical to the R_1 sensitivities given here but do not express their relationship to the material fission spectrum. The sensitivities given by Favorite are also defined for the fission spectrum as a function of incident and emergent neutron energies.⁴

The sensitivities given in Table 2.1 are defined in terms of inner products between forward and adjoint angular fluxes as well as between their Legendre polynomial expansion moments for a one-dimensional geometry. The scatter cross section is also given in terms of its Legendre polynomial expansion moments.

Inner products between the forward and adjoint flux moments must reflect the fact that they are defined for directions opposite one another. Favorite [14] distinguished between computational moments, which are calculated by transport solvers and defined by Eqs. (2.33), (2.34), and (2.35), and inner product moments, which account for the reversal in the adjoint flux direction [14]. For a one-dimensional spherical or slab geometry, this amounts to a simple correction factor that is positive for the zeroth and even Legendre polynomial moments and negative for odd Legendre polynomial moments. The relationship between computational and inner product moments is given explicitly for the forward and adjoint fluxes as

⁴Data representing the fission spectrum as a function of incident and emergent neutron energies (i.e. $\chi_{g' \rightarrow g}$) are available; however, all of the analysis given in this dissertation will consider the distribution of emergent neutron energies as independent of incident neutron energy (as in Eqs. (2.39) and (2.41)).

$${}^{IP}\phi_g^m = (-1)^m \phi_g^m, \quad (2.56)$$

$${}^{IP}\varphi_g^m = (-1)^m \varphi_g^m, \quad (2.57)$$

$${}^{IP}\phi_{q,g}^{*,m} = (-1)^m \phi_{q,g}^{*,m}, q = 1, 2, \quad (2.58)$$

where IP denotes the inner product moment, such that inner products between forward and adjoint flux moments may be expressed as

$$\langle {}^{IP}\phi_g^m, \phi_{q,g}^{*,m} \rangle = \langle {}^{IP}\phi_{q,g}^{*,m}, \phi_g^m \rangle = \langle (-1)^m \phi_g^m, \phi_{q,g}^{*,m} \rangle, q = 1, 2 \quad (2.59)$$

and

$$\langle {}^{IP}\varphi_g^m, \phi_{1,g}^{*,m} \rangle = \langle {}^{IP}\phi_{1,g}^{*,m}, \varphi_g^m \rangle = \langle (-1)^m \varphi_g^m, \phi_{1,g}^{*,m} \rangle.^5 \quad (2.60)$$

With respect to the R_2 sensitivity to $\bar{\nu}$, $\overline{\nu(\nu-1)}$ is treated as having a quadratic dependence on $\bar{\nu}$, such that $\frac{\partial \overline{\nu(\nu-1)}}{\partial \bar{\nu}}$, which appears in the third inner product in Eq. (2.50), is not zero. $\frac{\partial \overline{\nu(\nu-1)}}{\partial \bar{\nu}}$ also appears when computing the $\overline{\nu(\nu-1)}$ covariance via linear propagation of uncertainty. The relationship between the $p(\nu, E)$ distribution moments, definition of the coefficients b and c in Table 2.1, and calculation of the $\overline{\nu(\nu-1)}$ covariance are discussed in Appendix A. The last inner product in Table 2.1 for $S_{R_2, \bar{\nu}_g^j}$ is a consequence of this relationship.

⁵An inner product between forward and adjoint fluxes moments is given explicitly in the response sensitivity to the scatter cross section given in Table 2.1 that requires use of Eqs. (2.59) and (2.60). These correction factor equations are also required if the inner product between forward and adjoint angular fluxes in the response sensitivities to the fission, scatter, and capture cross sections are approximated with a Legendre polynomial expansion; i.e.,

$$\begin{aligned} \int_{4\pi} d\Omega \psi_g(\vec{r}, \hat{\Omega}) \psi_{q,g}^*(\vec{r}, \hat{\Omega}) &\approx \sum_{m=0}^M (2m+1) \phi_g^m(\vec{r}) \phi_{q,g}^{*,m}(\vec{r}), q = 1, 2, \\ \int_{4\pi} d\Omega \Phi_g(\vec{r}, \hat{\Omega}) \psi_{1,g}^*(\vec{r}, \hat{\Omega}) &\approx \sum_{m=0}^M (2m+1) \varphi_g^m(\vec{r}) \phi_{1,g}^{*,m}(\vec{r}). \end{aligned}$$

Approximating the angular integral with a Legendre polynomial expansion is not recommended unless angular fluxes are not provided by the transport solver.

Table 2.1 (Cont.) Relative sensitivity of detector response moments R_1 and R_2 to the set of cross sections $\chi_g^j, \overline{\nu}_g^j, \overline{\nu(\nu-1)}_g^j, \sigma_{f,g}^j, \sigma_{s,g' \rightarrow g}^{m,j}, \sigma_{c,g}^j$.

Sensitivity	Equation
$S_{R_2, \overline{\nu(\nu-1)}_g^j}$	$\frac{1}{R_2} \left[\int dV N^j(\vec{r}) \overline{\nu(\nu-1)}_g^j \sigma_{f,g}^j I_1^2(\vec{r}) \phi_g^0(\vec{r}) \right]$
$S_{R_1, \sigma_{f,g}^j}$	$\begin{aligned} & \frac{1}{R_2} \left[\int dV I_1(\vec{r}) N^j(\vec{r}) \nu \sigma_{f,g}^j \phi_g^0(\vec{r}) \right. \\ & + \int dV \gamma_g^j(\vec{r}) \{I_1^j(\vec{r}) - I_1(\vec{r})\} \sum_{g'=1}^G \nu \Sigma_{f,g'}(\vec{r}) \phi_{g'}^0(\vec{r}) \\ & \left. - \int dV \int d\Omega N^j(\vec{r}) \sigma_{f,g}^j \psi_{1,g}^*(\vec{r}, \hat{\Omega}) \psi_g(\vec{r}, \hat{\Omega}) \right] \end{aligned}$
$S_{R_2, \sigma_{f,g}^j}$	$\begin{aligned} & \frac{1}{R_2} \left[\int dV I_2(\vec{r}) N^j(\vec{r}) \nu \sigma_{f,g}^j \phi_g^0(\vec{r}) \right. \\ & + \int dV \gamma_g^j(\vec{r}) \{I_2^j(\vec{r}) - I_2(\vec{r})\} \sum_{g'=1}^G \nu \Sigma_{f,g'}(\vec{r}) \phi_{g'}^0(\vec{r}) \\ & - \int dV \int d\Omega N^j(\vec{r}) \sigma_{f,g}^j \psi_{2,g}^*(\vec{r}, \hat{\Omega}) \psi_g(\vec{r}, \hat{\Omega}) \\ & + 2 \int dV I_1(\vec{r}) N^j(\vec{r}) \nu \sigma_{f,g}^j \phi_g^0(\vec{r}) \\ & + 2 \int dV \gamma_g^j(\vec{r}) \{I_1^j(\vec{r}) - I_1(\vec{r})\} \sum_{g'=1}^G \nu \Sigma_{f,g'}(\vec{r}) \phi_{g'}^0(\vec{r}) \\ & - 2 \int dV \int d\Omega N^j(\vec{r}) \sigma_{f,g}^j \psi_{1,g}^*(\vec{r}, \hat{\Omega}) \Phi_g(\vec{r}, \hat{\Omega}) \\ & + \int dV \gamma_g^j(\vec{r}) \{I_1^j(\vec{r}) - I_1(\vec{r})\} I_1(\vec{r}) \sum_{g'=1}^G \overline{\nu(\nu-1)} \Sigma_{f,g'}(\vec{r}) \phi_{g'}^0(\vec{r}) \\ & \left. + \int dV I_1^2(\vec{r}) N^j(\vec{r}) \overline{\nu(\nu-1)}_g^j \sigma_{f,g}^j \phi_g^0(\vec{r}) \right] \end{aligned}$

Table 2.1 (Cont.) Relative sensitivity of detector response moments R_1 and R_2 to the set of cross sections $\chi_g^j, \bar{\nu}_g^j, \overline{\nu(\nu-1)}_g^j, \sigma_{f,g}^j, \sigma_{s,g' \rightarrow g}^{m,j}, \sigma_{c,g}^j$.

Sensitivity	Equation
$S_{R_1, \sigma_{s,g \rightarrow g'}^{m,j}}$	$\frac{1}{R_2} \left[\int dV \phi_g^m(\vec{r}) N^j(\vec{r}) \sigma_{s,g \rightarrow g'}^{m,j} \phi_{1,g'}^{*,m}(\vec{r}) \right. \\ \left. - \delta_{m,0} \int dV \int d\Omega \psi_g(\vec{r}, \hat{\Omega}) N^j(\vec{r}) \sigma_{s,g \rightarrow g'}^{0,j} \psi_{1,g}^*(\vec{r}, \hat{\Omega}) \right]$
$S_{R_2, \sigma_{s,g \rightarrow g'}^{m,j}}$	$\frac{1}{R_2} \left[\int dV \phi_g^m(\vec{r}) N^j(\vec{r}) \sigma_{s,g \rightarrow g'}^{m,j} \phi_{2,g'}^{*,m}(\vec{r}) \right. \\ - \delta_{m,0} \int dV \int d\Omega \psi_g(\vec{r}, \hat{\Omega}) N^j(\vec{r}) \sigma_{s,g \rightarrow g'}^{0,j} \psi_{2,g}^*(\vec{r}, \hat{\Omega}) \\ + 2 \int dV \varphi_g^m(\vec{r}) N^j(\vec{r}) \sigma_{s,g \rightarrow g'}^{m,j} \phi_{1,g'}^{*,m}(\vec{r}) \\ \left. - 2 \delta_{m,0} \int dV \int d\Omega \Phi_g(\vec{r}, \hat{\Omega}) N^j(\vec{r}) \sigma_{s,g \rightarrow g'}^{0,j} \psi_{1,g}^*(\vec{r}, \hat{\Omega}) \right]$
$S_{R_1, \sigma_{c,g}^j}$	$-\frac{1}{R_1} \left[\int dV \int d\Omega \psi_{1,g}^*(\vec{r}, \hat{\Omega}) N^j(\vec{r}) \sigma_{c,g}^j \psi_g(\vec{r}, \hat{\Omega}) \right]$
$S_{R_2, \sigma_{c,g}^j}$	$-\frac{1}{R_2} \left[\int dV \int d\Omega \psi_{2,g}^*(\vec{r}, \hat{\Omega}) N^j(\vec{r}) \sigma_{c,g}^j \psi_g(\vec{r}, \hat{\Omega}) \right. \\ \left. + 2 \int dV \int d\Omega \psi_{1,g}^*(\vec{r}, \hat{\Omega}) N^j(\vec{r}) \sigma_{c,g}^j \varphi_g(\vec{r}, \hat{\Omega}) \right]$

The importance of induced fission neutrons to the second-moment detector response I_2 in Table 2.1 is defined as

$$I_2(\vec{r}) = \sum_{g'=1}^G \chi_{g'} \phi_{2,g'}^{*,0}(\vec{r}), \quad (2.61)$$

which is similar to the definition of I_1 in Eq. (2.45).

The response sensitivities to the fission parameters (χ^j , $\bar{\nu}^j$, and σ_f^j) contain a ratio of the isotopic to material fission neutron production cross sections weighted with the weighting spectrum f (see note 3),

$$\gamma^j(\vec{r}) = \sum_{g=1}^G \gamma_g^j(\vec{r}) = \sum_{g=1}^G \frac{N^j(\vec{r}) \nu \sigma_{f,g}^j f_g}{\sum_{g'=1}^G \nu \Sigma_{f,g'}(\vec{r}) f_{g'}}, \quad (2.62)$$

as well as the isotopic importance of fission neutrons to R_1 and R_2 ,

$$I_1^j(\vec{r}) = \sum_{g'=1}^G \chi_{g'}^j \phi_{1,g'}^{*,0}(\vec{r}), \quad (2.63)$$

$$I_2^j(\vec{r}) = \sum_{g'=1}^G \chi_{g'}^j \phi_{2,g'}^{*,0}(\vec{r}), \quad (2.64)$$

respectively, similar to the importances given in Eqs. (2.45) and (2.61). Note that if the assembly is composed of a single fissile nuclide, $\gamma^j(\vec{r}) = 1$ and $I_1^j(\vec{r}) = I_1(\vec{r})$.

2.5 Propagation of uncertainty through the detector response moments

Uncertainty in the measured and simulated detector response moments is due to both random and systematic sources [52]. Random uncertainty results from the inherently random nature of neutron counting. The NMC distribution moments and central moments in Eqs. (1.1) and (1.2) are weighted by the frequency $f(n)$ of the number n of coincident neutron counts. The detection of coincident neutron counts can be described by Poisson statistics, so the relative uncertainty in the NMC distribution and its moments decrease as the number of accumulated counts increases [42].

Systematic uncertainty refers to uncertainty in measurement parameters (e.g. properties and configuration of the assembly and detector), errors in the model (discretization of continuous variables and simplifications of the detector and assembly representation), and uncertainty in the cross sections. Measurement parameter uncertainty is difficult to quantify rigorously because it would require the experiment be performed many times. For example, uncertainty in the responses due to the source-detector distance may be determined by varying the source-detector distance and repeating the experiment. Some measurement parameters, for example the detector dead time and assembly mass, cannot be physically varied. The alternative is to vary the measurement parameters in high-fidelity simulations to

determine the response variation due to the measurement parameter variation, which may be thought of as the absolute sensitivity $D_{R_{q,m},p}$ of the order- q measured response to that measurement parameter. If the uncertainty in the measurement parameter itself is known (or if a reasonable estimate may be obtained), the measured response covariance may be computed using linear propagation of uncertainty,

$$[\text{cov}(\mathbf{R}_m, \mathbf{R}_m)]_p = \mathbf{D}_{\mathbf{R}_m, p}^T \text{cov}(\mathbf{p}, \mathbf{p}) \mathbf{D}_{\mathbf{R}_m, p}, \quad (2.65)$$

where the subscript p indicates measured response covariance due to the measurement parameters, $\mathbf{D}_{\mathbf{R}_m, p}$ is a matrix whose columns are the sensitivity of each measured response to the measurement parameters, and $\text{cov}(\mathbf{p}, \mathbf{p})$ is the measurement parameter covariance. The vector of measured responses is denoted by $\mathbf{R}_m$. In general, the measurement parameters may be correlated, but in the absence of prior information, the most conservative estimate is to use a diagonal covariance matrix [5]. Equation (2.65) provides both the variance in and covariance between each of the measured responses due to the measurement parameter covariance. Another way to think about Eq. (2.65) is as a description of the correlation between different experiments with identical features (e.g. the same fissile core counted by the same detector). A more detailed discussion of this topic in the context of fission cross section measurements is provided by Neudecker [40]. This source of uncertainty can be reduced by knowing the measurement parameters more precisely.

Model errors are introduced by discretizing continuous variables (e.g. multigroup and discrete ordinates approximations and choosing a finite number of spatial points on which to solve the NTE) as well as by making simplifications to the representation of the assembly and detector, which may include performing a one-dimensional simulation, treating the detector using an energy-dependent detector response function on the outer boundary of the assembly, and simplifying the model (e.g., reducing the number of nuclides and/or features present in the assembly). Similar to the measurement parameters, quantifying this source of uncertainty requires repeated simulations that vary the discretization and model representation. This source of uncertainty can be reduced by performing higher-fidelity simulations (i.e. finer discretization and more detailed modeling of the geometry and composition of the assembly) at the expense of greater computation time.

Uncertainty in the cross sections and the covariance between them comes from uncertainty in the various reaction-rate measurements across several energy regions used to evaluate them [54]. Similar to the measurement parameters, the relative cross section covariance $\text{relcov}(\alpha, \alpha)$ may be propagated through the simulated detector response using linear propagation of uncertainty,

$$[\text{relcov}(\mathbf{R}, \mathbf{R})]_\alpha = \mathbf{S}_{\mathbf{R}, \alpha}^T \text{relcov}(\alpha, \alpha) \mathbf{S}_{\mathbf{R}, \alpha}, \quad (2.66)$$

where the subscript α indicates simulated response covariance due to the cross sections. The vector of simulated responses is denoted by $\mathbf{R}$. Relative covariance is computed from absolute covariance as

$$\text{relcov}(x, y) = \frac{\text{cov}(x, y)}{x y}, \quad (2.67)$$

where x and y represent a pair of parameters (e.g. cross sections or detector response moments). Similar

to Eq. (2.65), Eq. (2.66) provides the relative variance in and covariance between the simulated responses due to the cross section covariances. Note that there may be covariance between different cross sections (e.g. the capture and fission cross sections) as well as covariance between energy groups of the same cross section. $S_{R,\alpha}$ represents a relative sensitivity matrix whose columns are the relative sensitivity vector for each detector response to the set of cross sections (see Eq. (2.52)). This source of uncertainty can be made smaller by knowing the cross sections more precisely or by performing model calibration.

The measured and simulated response covariances due to the random and systematic sources of uncertainty described above are the quadrature sum of the individual response covariance contributions; specifically,

$$\text{cov}(\mathbf{R}_m, \mathbf{R}_m) = [\text{var}(\mathbf{R}_m)]_N + [\text{cov}(\mathbf{R}_m, \mathbf{R}_m)]_p \quad (2.68)$$

and

$$\text{relcov}(\mathbf{R}, \mathbf{R}) = [\text{relcov}(\mathbf{R}, \mathbf{R})]_\alpha, \quad (2.69)$$

where $[\text{var}(\mathbf{R}_m)]_N$ is the random counting variance in the measured response (denoted by the subscript N). The discretization and model representation error contributions to the simulated response covariance are assumed to be small compared to the cross section covariance contribution. This assumption is justified by the granularity of the phase-space discretization, inclusion of the most significant features of the experiment, and relatively large magnitude of $[\text{relcov}(\mathbf{R}, \mathbf{R})]_\alpha$ (5–40%), all of which will be discussed in Chap. 3.

MODEL CALIBRATION APPLIED TO NEUTRON MULTIPLICITY COUNTING MOMENTS

This chapter discusses application of the model calibration process described in Chap. 2 to NMC measurements of the BeRP ball in bare and polyethylene-reflected configurations [37]. Section 3.1 provides a derivation of the Kalman filter and justifies its use for model calibration applied to NMC experiments. Section 3.2 then describes the application of our model calibration process to NMC of the BeRP ball in bare and polyethylene-reflected configurations. We provide some details regarding both the measurement and simulation of the nPod neutron multiplicity counter counting the BeRP ball in bare and polyethylene-reflected configurations. We discuss the measured detector response moment correlations due to the measurement parameters and the simulated detector response moment correlations due to the cross sections (both nominal and optimally adjusted). We provide the group-wise sensitivity of the detector response moments to the Pu-239 fission parameters ($\bar{\nu}$, $\overline{\nu(\nu-1)}$, σ_f , and χ) and identify significant features. We provide nominal and optimally adjusted fission parameter covariances and discuss their physical interpretation. We discuss the adjustment to the fission parameters and contrast them with those given previously by Evans [12]. We compare the measured detector response moments to those simulated with the nominal and adjusted cross sections and demonstrate that the NMC experiments are more accurately simulated with reduced uncertainty as a result of the model calibration process.

3.1 Parameter estimation applied to neutron multiplicity counting experiments

The sensitivities and response covariances may be used to adjust cross sections such that there is optimal agreement between measured and simulated responses. Bayesian inference utilizes prior information about the cross sections to provide best-estimate cross sections; it is typically used in evaluation of differential cross section measurements as well as cross section adjustments utilizing integral benchmark experiments [30, 31, 8, 3, 54]. The ENDF/B-VII.1 library provides both nominal cross section values as

well as their covariances such that they may be treated as having a multivariate Gaussian distribution.

3.1.1 Origin of the Kalman filter

The Kalman filter is a method of Bayesian inference that can utilize the prior information about the cross sections as well as new information from an experiment (such as an NMC measurement) to provide updated cross sections [57]. The objective of a Kalman filter is to estimate the state $x_k \in \mathbb{R}^n$ of a discrete, stationary, linear stochastic process,

$$x_k = Ax_{k-1} + w_{k-1}, \quad (3.1)$$

using new information from a measurement $z_k \in \mathbb{R}^m$,

$$z_k = Hx_k + v_k, \quad (3.2)$$

where k denotes a discrete iteration, n denotes the number of state space parameters, and m denotes the number of measurements. A is an $n \times n$ matrix that relates the state at iteration $k-1$ to iteration k in the absence of a driving function or noise. H is an $m \times n$ matrix that relates the state to the measurement. w_k and v_k respectively represent the process and measurement noise and are assumed to be independent of one another and described by Gaussian distributions

$$w \sim N(0, Q) \quad (3.3a)$$

and

$$v \sim N(0, R), \quad (3.3b)$$

where Q and R are the process and noise covariances, respectively. The matrices A , H , Q , and R are here assumed to be invariant with respect to k .

If the state is assumed to be independent of the process and measurement noise and described by a Gaussian distribution,

$$x \sim N(\bar{x}, P). \quad (3.4)$$

Eq. (3.1) is called a standard second-order model [49] and can be utilized to obtain a recursive formula that preserves the mean $\bar{x}_k$ and covariance P_k of the state; i.e.,

$$\bar{x}_k = \mathbb{E}[x_k] = A\bar{x}_{k-1} \quad (3.5a)$$

and

$$P_k = \mathbb{E}[(x_k - \bar{x}_k)(x_k - \bar{x}_k)^T] = AP_{k-1}A^T + Q. \quad (3.5b)$$

With prior conditions for the state x_0 and error covariance P_0 , Eqs. (3.5a) and (3.5b) provide respective prior estimates $\hat{x}_k^-$ and P_k^- . We therefore seek a posterior estimate of the state $\hat{x}_k^+$ and error covariance P_k^+ that is conditioned on the set of measurements $Z_k = \{z_0, \dots, z_k\}$; i.e.,

$$\hat{x}_k^- = \mathbb{E}[x_k | Z_{k-1}], \quad (3.6a)$$

$$\hat{x}_k^+ = \mathbb{E}[x_k | Z_k], \quad (3.6b)$$

$$P_k^- = \mathbb{E}[(x_k - \hat{x}_k^-)(x_k - \hat{x}_k^-)^T | Z_{k-1}], \quad (3.6c)$$

and

$$P_k^+ = \mathbb{E}[(x_k - \hat{x}_k^+)(x_k - \hat{x}_k^+)^T | Z_k]. \quad (3.6d)$$

Because the state and measurement are expressed as linear combinations of the jointly Gaussian noise processes, the state and measurement are jointly Gaussian as well. This means that the state estimate conditioned on the measurements is described by a joint Gaussian defined as

$$m = m_x + C_{x,z} C_{z,z}^{-1} (z - m_z) \quad (3.7a)$$

and

$$C = C_{x,x} - C_{x,z} C_{z,z}^{-1} C_{z,x}^T, \quad (3.7b)$$

with mean m and covariance C given by

$$\begin{bmatrix} m_x \\ m_z \end{bmatrix} = \begin{bmatrix} \hat{x}_k^- \\ H \hat{x}_k^- \end{bmatrix} \quad (3.8a)$$

and

$$\begin{bmatrix} C_{x,x} & C_{x,z} \\ C_{z,x} & C_{z,z} \end{bmatrix} = \begin{bmatrix} P_k^- & P_k^- H^T \\ H P_k^- & M \end{bmatrix}, \quad (3.8b)$$

with $M = H P_k^- H^T + R$. Equations (3.8a) and (3.8b) may be substituted into Eqs. (3.7a) and (3.7b) to provide a posterior estimate of the state and state covariance; i.e.,

$$\hat{x}_k^+ = \hat{x}_k^- + P_k^- H^T M^{-1} (z_k - H \hat{x}_k^-) \quad (3.9a)$$

and

$$P_k^+ = (I - P_k^- H^T M^{-1} H) P_k^-. \quad (3.9b)$$

The recursion is made complete by using Eqs. (3.5a) and (3.5b) to project the posterior state and covariance estimate at iteration k into prior estimates for the next iteration; i.e.,

$$\hat{x}_{k+1}^- = A \hat{x}_k^+ \quad (3.10a)$$

and

$$P_{k+1}^- = A P_k^+ A^T + Q. \quad (3.10b)$$

Equations (3.10a) and (3.10b) are often called the iteration update or predictor step and Eqs. (3.9a) and (3.9b) are referred to as the measurement update or corrector step.

One advantage of using a Kalman filter is that it preserves the mean and second central moment of the state distribution. Although other methods of Bayesian inference (e.g. Markov Chain Monte Carlo) estimate the state probability distribution, the ENDF library only provides the nominal cross section values and their covariances. Additionally, the filter requires relatively few model evaluations, making it an excellent choice in obtaining best-estimates of the cross sections and their covariances.

3.1.2 Justification for the extended Kalman filter

The Kalman filter derived in Sec. 3.1.1 is only applicable to linear models; however, the detector response moments derived in Sec. 2.2 are nonlinear functions of the cross sections. Using a nonlinear filter is undesirable because there are a potentially unbounded number of parameters required to describe the state probability distributions. Gaussian distributions are fully described by their mean and second central moment and remain Gaussian under linear transformations, thus making the Kalman filter computationally feasible. We therefore desire a modification to the Kalman filter that linearizes the model about the current state estimate. Consider now a discrete, stationary, *nonlinear* stochastic process f [57],

$$x_k = f(x_{k-1}, w_{k-1}), \quad (3.11)$$

that relates the state at $k-1$ to the state at k and nonlinear measurement process h ,

$$z_k = h(x_k, v_k), \quad (3.12)$$

that relates the state at k to the measurement at k . The process w_k and measurement v_k noises are identical to those defined in Eqs. (3.3a) and (3.3b). The state and measurement are approximated with zero noise using a posterior estimate of the state from a previous time step $\hat{x}_{k-1}^+$,

$$\tilde{x}_k = f(\hat{x}_{k-1}^+, 0) \quad (3.13)$$

and

$$\tilde{z}_k = h(\tilde{x}_k, 0). \quad (3.14)$$

Equations (3.11) and (3.12) are linearized about the state and measurement approximations given in Eqs. (3.13) and (3.14); i.e.,

$$x_k \approx \tilde{x}_k + A(x_{k-1} - \hat{x}_{k-1}^+) + W w_{k-1} \quad (3.15)$$

and

$$z_k \approx \tilde{z}_k + H(x_k - \tilde{x}_k) + V v_k, \quad (3.16)$$

where A and W are matrices of partial derivatives of the stochastic model f with respect to the state and process noise, respectively, and H and V are matrices of partial derivatives of the measurement model h with respect to the state and measurement noise, respectively. Written explicitly, they are

$$A_{[i,j]} = \frac{\partial f_{[i]}}{\partial x_{[j]}}(\hat{x}_{k-1}^+, 0), \quad (3.17)$$

$$W_{[i,j]} = \frac{\partial f_{[i]}}{\partial w_{[j]}}(\hat{x}_{k-1}^+, 0), \quad (3.18)$$

$$H_{[i,j]} = \frac{\partial h_{[i]}}{\partial x_{[j]}}(\tilde{x}_k, 0), \quad (3.19)$$

and

$$V_{[i,j]} = \frac{\partial h_{[i]}}{\partial v_{[j]}}(\tilde{x}_k, 0). \quad (3.20)$$

Defining a prediction error and measurement residual respectively as

$$\tilde{e}_{x_k} = x_k - \tilde{x}_k \quad (3.21)$$

and

$$\tilde{e}_{z_k} = z_k - \tilde{z}_k, \quad (3.22)$$

equations for the respective error processes are approximately given by

$$\tilde{e}_{x_k} \approx A(x_{k-1} - \hat{x}_{k-1}^+) + \epsilon_k \quad (3.23)$$

and

$$\tilde{e}_{z_k} \approx H(x_k - \tilde{x}_k) + \eta_k, \quad (3.24)$$

where ϵ and η are new random variables described by a Gaussian distributions,

$$\epsilon \sim N(0, WQW^T) \quad (3.25a)$$

and

$$\eta \sim N(0, VRV^T), \quad (3.25b)$$

with Q and R as defined in Eqs. (3.3a) and (3.3b). Equations (3.23) and (3.24) closely resemble Eqs. (3.1) and (3.2), for which the original Kalman filter was derived. A second (hypothetical) Kalman filter may be derived using the measurement residual in Eq. (3.22) to estimate the approximate prediction error in Eq. (3.23). This estimate $\hat{e}_k$ could then be used in the prediction error in Eq. (3.21) to estimate the posterior state of the original nonlinear process,

$$\hat{x}_k^+ = \tilde{x}_k + \hat{e}_k. \quad (3.26)$$

Given that ϵ_k and η_k are Gaussian and that $\tilde{e}_{x_k} \sim N(0, \mathbb{E}[\tilde{e}_{x_k} \tilde{e}_{x_k}^T])$ is also Gaussian, the second Kalman filter equation for estimating $\hat{e}_k$ is

$$\hat{e}_k = P_k^- H^T M^{-1} \tilde{e}_{z_k}, \quad (3.27)$$

where P_k^- , H , and M are identical those defined in Sec. 3.1. By inserting Eqs. (3.27) and (3.22) into Eq. (3.26), we recognize that the second Kalman filter equation is not needed to estimate the posterior state of the original nonlinear process. The extended Kalman filter (EKF) equations are therefore

$$\hat{x}_k^- = f(\hat{x}_{k-1}^+, 0), \quad (3.28a)$$

$$P_k^- = AP_{k-1}^+ A^T + WQW^T, \quad (3.28b)$$

$$\hat{x}_k^+ = \hat{x}_k^- + P_k^- H^T M^{-1}(z_k - h(\hat{x}_k^-, 0)), \quad (3.28c)$$

and

$$P_k^+ = (I - P_k^- H^T M^{-1} H) P_k^-. \quad (3.28d)$$

One limitation of the EKF is that the model must still be sufficiently linear near the current state estimate for the filter to converge. Another is that Gaussian distributions are not guaranteed to stay Gaussian under nonlinear transformations. The detector response moments derived in Sec. 2.2 are nonlinear functions of the cross sections; however, as will be shown in Chap. 6, variations in the responses due to small perturbations in the cross sections are sufficiently characterized by a first-order Taylor series expansion. This means that linearization about the state estimate is a good approximation for this problem.

3.1.3 Extended Kalman filter applied to optimal adjustment of the cross sections

We apply the EKF derived in Sec. 3.1.2 to optimal adjustment of the cross sections by interpreting the definition of several terms given in Secs. 3.1.1 and 3.1.2. $\hat{x}_k^-$ and P_k^- respectively represent the nominal cross sections and their covariances. H represents the response sensitivities to the cross sections (see Sec. 2.4). $HP_k^- H^T$ and VRV^T respectively represent the simulated and measured response covariances (see Sec. 2.5). z_k and $h(\hat{x}_k^-, 0)$ respectively represent the measured responses and the responses simulated with the nominal cross sections. Although the EKF may be applied iteratively, we only compute a single measurement update step using the nominal cross sections and covariances. The EKF is therefore recast into the following two-step process:

1. Prediction step

$$R_q^0 = \left\langle \psi, Q_q^* \right\rangle \Big|_{\alpha=\alpha^0} + \left\langle S, Q_{q, sf}^* \right\rangle \Big|_{\alpha=\alpha^0}, \quad (3.29)$$

$$\text{cov}(\mathbf{R}^0, \mathbf{R}^0) = \left(\frac{\partial \mathbf{R}^0}{\partial \alpha} \Big|_{\alpha=\alpha^0} \right)^T \text{cov}(\alpha^0, \alpha^0) \left(\frac{\partial \mathbf{R}^0}{\partial \alpha} \Big|_{\alpha=\alpha^0} \right). \quad (3.30)$$

2. Update step

$$\mathbf{K} = \frac{\text{cov}(\alpha^0, \alpha^0) \left(\frac{\partial \mathbf{R}^0}{\partial \alpha} \Big|_{\alpha=\alpha^0} \right)}{\text{cov}(\mathbf{R}^0, \mathbf{R}^0) + \text{cov}(\mathbf{R}_m, \mathbf{R}_m)}, \quad (3.31)$$

$$\alpha^1 = \alpha^0 + K(R_m - R^0), \quad (3.32)$$

$$\begin{aligned} \text{cov}(\alpha^1, \alpha^1) &= \left(I - K \left(\frac{\partial R^0}{\partial \alpha} \bigg|_{\alpha=\alpha^0} \right)^T \right) \text{cov}(\alpha^0, \alpha^0) \\ &= \left(I - K \left(\frac{\partial R^0}{\partial \alpha} \bigg|_{\alpha=\alpha^0} \right)^T \right) \text{cov}(\alpha^0, \alpha^0) \left(I - K \left(\frac{\partial R^0}{\partial \alpha} \bigg|_{\alpha=\alpha^0} \right)^T \right)^T \\ &\quad + K \text{cov}(R_m, R_m) K^T. \end{aligned} \quad (3.33)$$

I denotes the identity matrix of the same dimension as $\text{cov}(\alpha^0, \alpha^0)$ and the superscripts 0 and 1 indicate nominal and updated quantities, respectively. The definition of the Kalman gain or blending factor K is optimal in that it minimizes the updated cross section covariances (i.e. it minimizes the outer product of the error in the updated cross sections) [32]. The covariance term in the denominator of Eq. (3.31) represents the weight of the measured and simulated responses, and the product in the numerator determines how information from the measured and simulated responses should influence the updated cross sections and their covariances.

The first expression in Eq. (3.33) is a frequently encountered form of the equation for the updated cross section covariances. The second expression is applicable for any definition of the gain factor K and is identical to the first expression when K is defined as in Eq. (3.31). We demonstrate this [32] by factoring the parenthetical terms in Eq. (3.33) and utilizing Eq. (3.31). For brevity, we simplify the notation for the sensitivities and covariances by letting $\frac{\partial R^0}{\partial \alpha} \bigg|_{\alpha=\alpha^0} = D_{R,\alpha}$, $\text{cov}(\alpha^x, \alpha^x) = C_{\alpha^x, \alpha^x}$, $x = 0, 1$, $\text{cov}(R^0, R^0) = C_{R^0, R^0}$, and $\text{cov}(R_m, R_m) = C_{R_m, R_m}$. With the new notation, the parenthetical terms in the second expression of Eq. (3.33) are factored as

$$\begin{aligned} C_{\alpha^1, \alpha^1} &= (I - K D_{R,\alpha}^T) C_{\alpha^0, \alpha^0} (I - K D_{R,\alpha}^T)^T \\ &\quad + K C_{R_m, R_m} K^T, \\ &= C_{\alpha^0, \alpha^0} - K D_{R,\alpha}^T C_{\alpha^0, \alpha^0} - C_{\alpha^0, \alpha^0} D_{R,\alpha} K^T + K C_{R^0, R^0} K^T \\ &\quad + K C_{R_m, R_m} K^T, \end{aligned} \quad (3.34)$$

where we recognize that $D_{R,\alpha}^T C_{\alpha^0, \alpha^0} D_{R,\alpha} = C_{R^0, R^0}$. The last two terms of Eq. (3.34) are both an outer product between the gain factor K and another matrix such that they may be combined, resulting in

$$C_{\alpha^1, \alpha^1} = C_{\alpha^0, \alpha^0} - K D_{R,\alpha}^T C_{\alpha^0, \alpha^0} - C_{\alpha^0, \alpha^0} D_{R,\alpha} K^T + K [C_{R^0, R^0} + C_{R_m, R_m}] K^T. \quad (3.35)$$

The bracketed term in Eq. (3.35) is the denominator of the optimal definition of the gain factor K given in Eq. (3.31); thus, Eq. (3.35) simplifies to

$$C_{\alpha^1, \alpha^1} = (I - K D_{R,\alpha}^T) C_{\alpha^0, \alpha^0} - C_{\alpha^0, \alpha^0} D_{R,\alpha} K^T + C_{\alpha^0, \alpha^0} D_{R,\alpha} K^T. \quad (3.36)$$

The last two terms of Eq. (3.36) cancel out, such that Eq. (3.36) is identical to the first expression given in Eq. (3.33).

We implemented the second expression in Eq. (3.33) for the cross section covariance update step in our EKF algorithm because it is more numerically stable than the first expression. This distinction is important because the $\mathbf{K}$ that is actually computed may be sub-optimal due to floating point errors and/or non-Gaussian behavior in the detector response moments. The second expression in Eq. (3.33) is stable under these potential errors while the first expression is only valid if the calculated $\mathbf{K}$ is optimal (i.e. free from numerical and non-Gaussian behavior errors).

In the prediction step, the detector response moments $\mathbf{R}^0$ and their covariance due to the cross section covariances $\text{cov}(\mathbf{R}^0, \mathbf{R}^0)$ are computed using the nominal cross section values and covariances from ENDF/B-VII.1, as described in Secs. 2.2 through 2.5. The update step utilizes new information from the measured responses to compute the gain factor, which uses the measured and simulated response covariances to determine how to weight information from the measured and simulated responses themselves. Responses with less uncertainty will have more weight in estimating the updated cross sections and covariances than responses with more uncertainty. The resulting best-estimate cross sections are such that an NMC experiment will be more accurately simulated. This process may also introduce correlations between cross sections that were not previously known as well as modify existing correlations. These two modifications result in reduced uncertainty in the simulated detector response moments.

3.2 Model calibration applied to neutron multiplicity counting of the BeRP ball

We performed one-dimensional (spherical) PARTISN [1] simulations of NMC measurements of the BeRP ball in bare and polyethylene-reflected configurations [37] to compute the nPod neutron multiplicity counter responses (R_1 and R_2) and their sensitivities to the set of cross sections $\alpha = \{\bar{\nu}_g^i, \overline{\nu(\nu-1)}_g^i, \chi_g^i, \sigma_{f,g}^i, \sigma_{c,g}^i\}$ (see Sec. 2.4). The nPod is pictured in Fig. 1.1 and the BeRP ball nested in polyethylene reflectors is pictured in Fig. 3.1. The BeRP ball is a sphere of weapons-grade ($\sim 94\%$ Pu-239/ $\sim 6\%$ Pu-240) plutonium metal, encased in 305- μm thick stainless steel cladding, with a plutonium mass of 4483.884 g, mean radius of 37.938 mm, and density¹ of $19.655 \frac{\text{g}}{\text{cm}^3}$. The BeRP ball was positioned such that it was 1 m above the concrete floor and more than 4.5 m from the concrete walls of the room. The nPod was positioned such that its front face was 0.5 m from the center of the BeRP ball. The NMC experiment is described in greater detail by Mattingly [34].

The BeRP ball was modeled with a simplified composition of only Pu-239 and Pu-240 and a density of $19.604 \frac{\text{g}}{\text{cm}^3}$. The Pu-240 accounts for nearly all of the spontaneous fission source neutrons that drive

¹Although the density is reported as $19.655 \frac{\text{g}}{\text{cm}^3}$, there is some uncertainty in its true value because the BeRP ball volume is not precisely known. The plutonium metal was immersed in freon prior to its enclosure in its stainless steel cladding, but heating of the plutonium metal occurs because of alpha decay. Using the reported mass and radius results in a density of $19.604 \frac{\text{g}}{\text{cm}^3}$, while the theoretical lower and upper bounds on the density are $19.098 \frac{\text{g}}{\text{cm}^3}$ (if the plutonium sphere were to entirely fill the volume interior to the cladding) and $19.840 \frac{\text{g}}{\text{cm}^3}$ (the theoretical maximum density of alpha-phase plutonium metal), respectively [37].

induced fission in the Pu-239, which is the predominant fissile nuclide in the BeRP ball [37]. The forward intrinsic neutron source Q , calculated using Pu-240 Watt fission parameters [56], is plotted in Fig. 3.2. Although each hemispherical polyethylene reflector has a slightly different density, they were all modeled as having a uniform density of $0.96 \frac{\text{g}}{\text{cm}^3}$. Table 3.1 gives the atom density of the nuclides present in the model. The detector was modeled as a response function on the outer boundary of the assembly and accounts for the source-detector solid angle and the energy-dependent intrinsic efficiency $\epsilon(E)$ of the detector. Mattingly calculated this detector response function by performing a high-fidelity MCNP5 simulation of the nPod [35]. The detector response function was used as the adjoint source Q_1^* in Eq. (2.1) and the intrinsic efficiency of the detector is plotted in Fig. 3.3. Other features of the experiment (concrete floor, stainless steel cladding on the BeRP ball, etc.) were neglected.

Figure 3.1 The BeRP ball nested in polyethylene reflectors.

Figure 3.2 44-group Pu-240 spontaneous fission source integrated over the BeRP ball volume.

Figure 3.3 44-group intrinsic efficiency of the nPod neutron multiplicity counter.

Table 3.1 Atom density of nuclides present in the assembly model.

Nuclide	Atom density $\left(\frac{\text{atoms}}{\text{b cm}}\right)$
Pu-239	$4.60595191 \times 10^{-2}$
Pu-240	$2.90503750 \times 10^{-3}$
H-1	$8.21960442 \times 10^{-2}$
C-12	$4.11308331 \times 10^{-2}$

The ENDF/B-VII.1 cross sections ($\sigma_{t,g}^i$, $\nu\sigma_{f,g}^i$, $\sigma_{s,g\rightarrow g'}^{m,i}$, χ_g^i , $\bar{\nu}_g^i$, σ_f^i , and σ_c^i) for the plutonium metal (Pu-239 and Pu-240) and polyethylene reflector (H-1 and C-12 with $S(\alpha, \beta)$ thermal scattering) were obtained from the code package SCALE [46]. The Pu-239 $\bar{\nu}(\nu-1)$ and the Pu-240 $\bar{\nu}_{sf}$ were both obtained² from the Zucker and Holden distributions (see Secs. 2.2 and 2.4) [61, 56]. The Pu-240 Watt-fission parameters were obtained from the MCNP6 manual [59].

Table 3.2 summarizes the PARTISN transport solve options. The number of discrete ordinates and Legendre polynomial expansion order of the scatter kernel were determined by Favorite [15] to be sufficient such that the forward and adjoint angular fluxes are converged for this particular assembly. The number of energy groups was chosen to be consistent with the group structure of the ENDF/B-VII.1 cross section covariances provided by SCALE. The thickness of cells in the spatial mesh was chosen to be many times smaller than the mean free path of thermal neutrons in plutonium metal and in polyethylene.

Table 3.2 PARTISN transport solve parameters.

Parameter	Value
Number of discrete ordinates	256
Number of Legendre polynomial expansion terms for the scatter kernel	5
Energy groups	44
Spatial cell thickness	50 μm
Source iteration convergence tolerance	1e-06

The measured and simulated response covariances were computed using linear propagation of uncertainty (see Sec. 2.5). The measurement parameter uncertainties were obtained from a nickel-reflected BeRP ball benchmark [47]. The measured response variations were computed using MCNP code simulations of NMC [37] of the bare and polyethylene-reflected BeRP ball with varying source-detector distance, non-paralyzable detector dead time, and BeRP ball radius, mass, and Pu-240 content. The measured response sensitivities to the measurement parameters were then computed with a one-sided finite difference. Calculation of the measured response covariances is discussed in greater detail in Appendix C.

Correlation between the measured responses is plotted in Fig. 3.4 and correlation between the responses simulated with the nominal cross sections is plotted in Fig. 3.5. The measured responses are strongly correlated with one another, which indicates that changes in the measurement parameters will have a significant effect on all of the measured responses. Similarly, the nominal simulated responses exhibit strong correlations (note the difference in scale between Figs. 3.4 and 3.5), which serves to illustrate that a change in the cross sections that significantly affects one response will have a large

²It is worth mentioning here that evaluated $p(\nu, E)$ distributions have recently been made available in the ENDF/B-VIII.0 release [3]. Terrell's [55] formula for the cumulative $p(\nu, E)$ distribution was scaled and adjusted to reproduce the ENDF/B-VIII.0 evaluated $\bar{\nu}$ values for Pu-239 and U-235, 238. The evaluated $p(\nu, E)$ distributions and their first three factorial moments below 10 MeV agree well with Zucker and Holden's original evaluation [61].

impact on all the other responses.

Figure 3.4 Correlations between the measured responses with respect to the measurement parameters.

Figure 3.5 Correlations between the responses simulated with the nominal cross sections.

An EKF was applied to the measured and simulated response moments and their respective covariances to obtain best-estimate cross sections and cross section covariances. The best-estimate cross sections and cross section covariances were then used to recompute the simulated responses and their covariances. The model calibration was also performed with Cacuci's data assimilation code, MULTI-PRED [4]. The EKF and MULTI-PRED returned identical adjustments to the cross sections and cross section covariances.

The cross sections directly adjusted by the EKF were the Pu-239 and Pu-240 χ , $\bar{\nu}$, and σ_f , the Pu-239 $\overline{\nu(\nu-1)}$, and σ_c for Pu-239, Pu-240, H-1, and C-12. The changes made to these cross sections were used to update the principle cross sections (σ_a , $\nu\sigma_f$,³ and σ_t) in the following manner:

$$\Delta\sigma_{a,g}^i = \Delta\sigma_{c,g}^i + \Delta\sigma_{f,g}^i, \quad (3.38a)$$

$$\Delta(\nu\sigma_{f,g}^i) = (\Delta\bar{\nu}_g^i)\sigma_{f,g}^i + \bar{\nu}_g^i(\Delta\sigma_{f,g}^i) + (\Delta\bar{\nu}_g^i)(\Delta\sigma_{f,g}^i), \quad (3.38b)$$

and

$$\Delta\sigma_{t,g}^i = \Delta\sigma_{c,g}^i + \Delta\sigma_{f,g}^i. \quad (3.38c)$$

The adjusted χ^i were renormalized such that $\sum_{g=1}^G \chi_g^i = 1$. Calculation of the material fission spectrum (see note 3 in Chap. 2) ensures that $\sum_{g=1}^G \chi_g = 1$ as well. The differential scatter cross section $\sigma_{s,g \rightarrow g'}^{m,i}$ was not included in the model calibration because its covariance was not available. ENDF/B-VII.1 instead provides covariances for individual elastic and inelastic scatter and $(n, 2n)^4$ reactions summed over emergent neutron energy (outgoing) group. While the model calibration process described in this dissertation could be applied to these individual scatter reactions, the resulting optimal adjustments would not uniquely inform adjustment of the differential scatter cross section, which is utilized in the neutron transport calculations. Alternatively, one could use the sum of the individual scatter reaction covariances as a constraint on an estimate of the differential scatter covariances, which would allow the differential scatter cross section to be directly included in the model calibration. We do not take this approach because the choice of differential scatter cross section covariance that satisfies the sum-rule constraint is not unique.

³Because $\bar{\nu}$, and σ_f were adjusted individually (as opposed to adjusting $\nu\sigma_f$ itself), the updated fission neutron production cross section is computed as

$$\begin{aligned} \widetilde{\nu\sigma}_{f,g}^i &= \widetilde{\bar{\nu}}_g^i \widetilde{\sigma}_{f,g}^i \\ &= (\Delta\bar{\nu}_g^i + \bar{\nu}_g^i)(\Delta\sigma_{f,g}^i + \sigma_{f,g}^i) \\ &= \nu\sigma_{f,g}^i + (\Delta\bar{\nu}_g^i)\sigma_{f,g}^i + \bar{\nu}_g^i(\Delta\sigma_{f,g}^i) + (\Delta\bar{\nu}_g^i)(\Delta\sigma_{f,g}^i) \\ &= \nu\sigma_{f,g}^i + \Delta(\nu\sigma_{f,g}^i). \end{aligned} \quad (3.37)$$

⁴The differential scatter cross section provided by ENDF/B-VII.1 is composed of contributions from elastic and inelastic scatter and (n, xn) reactions. In this manner, the scatter source term of Eq. (2.7) accounts for neutrons produced from non-fission reactions and non-intrinsic sources.

As discussed by Proctor [45], the multigroup covariances provided in the ENDF library are not symmetric positive definite (SPD), which is required for the interpretation of the covariances to be physically meaningful. Symmetric positive semi-definite (SPSD) covariance matrices are typically utilized when SPD matrices are not available but “...represent a lack of sufficient information or poor modeling for the physical system at hand.” Proctor generally found that the multigroup ENDF/B-VII.1 cross section covariances were neither SPD nor SPSPD. We correct the nominal covariances by obtaining the nearest SPSPD matrix [24]. We note that the adjustment to the cross sections and their covariances utilizing either the nominal or the nearest SPSPD covariances are nearly identical because the nominal covariances are close to SPSPD. In other words, the negative eigenvalues for the nominal covariances are small and the majority of the eigenvalues are greater than zero. We discuss computing the nearest SPSPD matrix in Appendix B.

Figures 3.6, 3.7, 3.8, and 3.9 compare the relative sensitivity vectors of R_1 and R_2 to the Pu-239 $\bar{\nu}$, $\bar{\nu}(\nu-1)$, σ_f , and χ for both bare and polyethylene-reflected BeRP ball configurations, respectively (refer to Eq. (2.52)). The sensitivities of R_2 to $\bar{\nu}$, σ_f , and χ are larger than those of R_1 for both configurations. As described in Sec. 2.2, R_2 is a function of the cross sections squared, while R_1 is a function of the cross sections to the first power. Although the magnitude of the R_1 and R_2 sensitivities differ, their shape for each configuration is identical because they are obtained from the same source-detector system (i.e. either the bare or polyethylene-reflected BeRP ball counted by the nPod). While the bare and reflected configuration sensitivities have a similar shape in the fast region, their shapes differ significantly in the intermediate and slow region for all but the response sensitivity to χ . Both detector response moments are more sensitive to the fission parameters for the reflected configuration than for the bare configuration. Additionally, the reflected configuration responses are sensitive to neutrons of all energies, while the bare configuration responses are only sensitive to fast neutrons (the vertical line at 100 keV in Figs. 3.6 through 3.9 indicates the approximate energy at which there is substantial change between the bare and reflected sensitivity profiles for all the fission parameters except for χ). These two properties arise because neutrons that would otherwise escape the BeRP ball may instead be slowed down and reflected by the polyethylene, resulting in a greater number of neutrons available in the system at lower energies, at which neutrons are more likely to induce fission. Assemblies that have a greater neutron multiplication are consequently more sensitive to $\bar{\nu}$, σ_f , and χ .

Figure 3.6 Sensitivity of R_1 and R_2 to the Pu-239 $\bar{\nu}$ for the bare and reflected BeRP ball configuration.

Figure 3.7 Sensitivity of R_2 to the Pu-239 $\overline{\nu(\nu-1)}$ for the bare and reflected BeRP ball configuration. Note that R_1 is not a function of $\overline{\nu(\nu-1)}$ and therefore has no sensitivity to this fission parameter.

Figure 3.8 Sensitivity of R_2 to the Pu-239 σ_f for the bare and reflected BeRP ball configuration.

Figure 3.9 Sensitivity of R_2 to the Pu-239 χ for the bare and reflected BeRP ball configuration.

The R_2 sensitivity to $\overline{\nu(\nu-1)}$ is small compared to the R_2 sensitivity to $\bar{\nu}$. Additionally, the bare and reflected configuration R_2 sensitivities to $\overline{\nu(\nu-1)}$ have similar magnitudes. $\overline{\nu(\nu-1)}$ only appears as a linear term in Q_2^* whereas $\bar{\nu}$ appears implicitly in I_1 (which is squared) and explicitly in the forward and adjoint transport operators. Physically speaking, the number of neutrons emitted by a highly multiplying assembly is primarily determined by the average number of neutrons emitted per fission; consequently, the NMC distribution second moment is much more sensitive to $\bar{\nu}$ than $\overline{\nu(\nu-1)}$. For an assembly where most of the emitted neutrons are from spontaneous fission (e.g. a Cf-252 source or a low-mass plutonium assembly), the dispersion of neutrons emitted per fission would have a more significant impact on the NMC distribution second moment.

For both the bare and polyethylene-reflected configurations, the responses are insensitive to χ for intermediate and thermal emergent neutron energies. Figure 3.10 displays the Pu-239 χ and indicates that neutrons are unlikely to be born with energies of 100 keV or less. While adding polyethylene to the BeRP ball reduces neutron leakage and average neutron incident energy, which consequently increases the likelihood of a fission occurring, the probability of a fission neutron being born with a particular emergent energy is unaffected (given that χ is not a function of incident neutron energy; see note 4 in Chap. 2).

Figure 3.10 Plot of the Pu-239 χ . The majority of neutrons born from fission will have emergent energies ~ 1 MeV.

Figure 3.11 shows the relative sensitivity totals of R_1 and R_2 for the bare and reflected BeRP ball for all cross sections present in the model calibration. Note that the values in the plot are overlapping, not stacked. The sensitivity totals are the sensitivity vectors summed over group (see Eq. (2.53)); they are a convenient way to compare the effect of a change in each of the cross sections between all of the detector response moments. By far, the most influential cross sections on the detector responses are $\bar{\nu}$ and σ_f . This is because they determine the average number of neutrons emitted per fission and the likelihood that induced fission will occur, respectively. All of the sensitivity totals are positive except for

the capture cross sections, which are negative. An increase in the capture cross sections will decrease the detector response moments, while increasing the other cross sections will increase the detector response moments.

Figure 3.11 Relative sensitivity totals of R_1 and R_2 for the bare and reflected BeRP ball configurations.

Figure 3.12 shows the correlation between the Pu-239 fission parameters before (3.12a) and after (3.12b) the optimization. Although ENDF/B-VII.1 provides covariances between the energy groups of each of the fission parameters ($\bar{\nu}_g^i$, χ_g^i , and $\sigma_{f,g}^i$), it does not provide covariances between the fission parameters themselves (e.g. covariance between $\bar{\nu}_g^i$ and χ_g^i) because they are “...evaluated independently with different nuclear physics models and uncorrelated experimental data” [3].

(a)

(b)

Figure 3.12 Correlation between the Pu-239 group fission parameters (χ_g , $\bar{\nu}_g$, $\overline{\nu(\nu-1)}_g$, and $\sigma_{f,g}$) before (3.12a) and after (3.12b) the optimization. The dotted lines delineate individual fission parameter correlation matrices with dimension $G \times G$. The correlations are in transport order from left to right and from top to bottom.

The ENDF library does not provide covariance for moments of the $p(\nu, E)$ distribution higher than the mean ($\bar{\nu}$). However, the second factorial moment of the induced fission neutron multiplicity distribution ($\overline{\nu(\nu-1)}$) is a deterministic, quadratic function of $\bar{\nu}$. This relationship is implicit in Terrell's [55] original analysis of the spontaneous fission neutron multiplicity distribution, where he found the variance (i.e., the second central moment) of the distribution was identical for every spontaneously fissioning nuclide he studied (with the exception of Cf-252), and it is borne out in Zucker and Holden's measurements [61] of the induced fission neutron multiplicity distribution for U-235, U-238, and Pu-239. Therefore, we estimated the uncertainty in $\overline{\nu(\nu-1)}$ by propagating the ENDF/B-VII.1-tabulated uncertainty in $\bar{\nu}$ through this quadratic relationship. We describe this approach for estimating the uncertainty in $\overline{\nu(\nu-1)}$ in detail in Appendix A.

The most striking difference in the $\bar{\nu}$ and σ_f correlations given in Fig. 3.12 is the introduction of negative correlations where there were previously only positive correlations ($\bar{\nu}$) or no correlation (σ_f). This is due to the model calibration being performed with integral responses that are the sum of transport effects over all energy groups. To preserve the value of the integral responses, a change in one group fission parameter must be balanced by changes in other group parameters (similar to the normalization constraint on the response sensitivities to χ). Prior to the model calibration, these fission parameters had either weak or no correlation between high and low incident neutron energies; however, the reflected assembly is sensitive to neutrons of all energies and all of the group parameters contribute to the detector response. The variances in the fission parameters themselves are not significantly reduced by the model calibration, and because the nominal χ covariance already has negative correlations, it was not significantly adjusted.

As with the fission parameter covariances, the model calibration has introduced positive and negative correlations between the fission parameters. Physically speaking, the number and emergent energy distributions of fission neutrons are related both to one another and to the incident energy of the neutron inducing fission. The fission cross section is always multiplied by a $p(\nu, E)$ distribution moment (e.g. $\bar{\nu}$, $\overline{\nu(\nu-1)}$) and the fission spectrum, so only their *product* is a parameter of the STE.

Figures 3.13, 3.14, 3.15, and 3.16 show the adjustment to the Pu-239 $\bar{\nu}$, $\overline{\nu(\nu-1)}$, σ_f , and χ , respectively, in multiples of their nominal standard deviations, as a result of the model calibration. The reduction of $\bar{\nu}$ is significant and consistent with that mentioned by Miller [37] and in the ENDF/B-VII.0 release [8] and is similar in trend, though increased in magnitude, from that recommended by Evans. Similarly, the adjustment to σ_f and χ are similar in trend and increased in magnitude compared to Evans' results. These differences are due primarily to the inclusion of systematic uncertainty in the measured responses. As will be discussed in Chap. 4, when the model calibration is performed using only random counting uncertainties, adjustment to the Pu-239 $\bar{\nu}$, σ_f , and χ are similar to those given by Evans. The adjustment of $\overline{\nu(\nu-1)}$ is significant; however, the assembly is much less sensitive to $\overline{\nu(\nu-1)}$ than to $\bar{\nu}$ (see Figs. 3.6 and 3.7), which means that the adjustment of $\overline{\nu(\nu-1)}$ has less impact on the simulated responses.

The difference in the adjustment of the fission parameters (and the other cross sections) arises from the difference in how information from the measured and simulated responses is weighted by the EKF. The simulated response uncertainty is significantly larger than the measured response uncertainty. This

Figure 3.13 Adjustment to the Pu-239 $\bar{\nu}$ in multiples of its nominal standard deviation. The label “NMC; stat. & sys. unc.” refers to the adjustment made to $\bar{\nu}$ by applying a EKF to NMC experiments, accounting for both random and systematic sources of uncertainty. The label “Gross neutron counting; stat. unc. only” refers to the adjustment to $\bar{\nu}$ by applying Cacuci’s data assimilation process [5] to gross neutron counting experiments, accounting for random uncertainty only.

Figure 3.14 Adjustment to the Pu-239 $\overline{\nu(\nu-1)}$ in multiples of its nominal standard deviation.

means that the EKF will tend to adjust the cross sections such that the simulated responses most closely match the measured responses. However, the measured response systematic uncertainty is significantly larger than the random uncertainty; additionally, the measured responses are strongly correlated with respect to the measurement parameters. By including the systematic covariances, the filter weights information from the measured responses less and information from the simulated responses more, resulting in a difference in the magnitude of the cross section adjustment.

Figure 3.17 displays the measured [37] and simulated detector response moments for the bare and reflected BeRP ball configurations, where the simulated response uncertainty is that due to the cross section covariances and the measured response uncertainty is that due to both random and systematic uncertainties. The results in Fig. 3.17 demonstrate the first application of model calibration applied

Figure 3.15 Adjustment to the Pu-239 σ_f in multiples of its nominal standard deviation. The label “NMC; stat. & sys. unc.” refers to the adjustment made to σ_f by applying a EKF to NMC experiments, accounting for both random and systematic sources of uncertainty. The label “Gross neutron counting; stat. unc. only” refers to the adjustment to σ_f by applying Cacuci’s data assimilation process [5] to gross neutron counting experiments, accounting for random uncertainty only.

Figure 3.16 Adjustment to the Pu-239 χ in multiples of its nominal standard deviation. The label “NMC; stat. & sys. unc.” refers to the adjustment made to χ by applying a EKF to NMC experiments, accounting for both random and systematic sources of uncertainty. The label “Gross neutron counting; stat. unc. only” refers to the adjustment to χ by applying Cacuci’s data assimilation process [5] to gross neutron counting experiments, accounting for random uncertainty only.

to NMC experiments. “Nominal” refers to responses obtained with the nominal cross sections and “adjusted” refers to responses obtained with the optimized cross sections. The uncertainty in the nominal simulated responses for the reflected case as compared to that in the bare case is larger for two reasons. There are a greater number of cross sections in the reflected case (i.e. the addition of polyethylene to the plutonium sphere) and the reflected assembly is more sensitive to the existing cross sections (see Figs. 3.6 and 3.7) than the bare assembly. There is good agreement between the measured and nominal simulated responses for the bare configuration but a significant difference for the reflected configuration. This is

due primarily to over-calibration in the Pu-239 $\bar{\nu}$ as described in Chap. 1. The adjusted responses are in good agreement with the measured responses, and their respective uncertainties overlap; additionally, the simulated response uncertainties are significantly reduced. This indicates that the adjusted cross sections are optimal, based on prior knowledge of the cross sections and their covariances as well as on new information from the measured multiplicity moments and their uncertainty.

Figure 3.17 Measured and simulated R_1 and R_2 for the bare and reflected BeRP ball configurations.

Figure 3.18 is a plot of correlations between the responses simulated with the adjusted cross sections. The response correlations are reduced with respect to the responses simulated with the nominal cross sections but are still significant (note the difference in scale between Figs. 3.5 and 3.18). This change is due to the significant adjustment made to the cross section correlations shown in Fig. 3.12b. The EKF identified many negative correlations between cross sections that were previously considered uncorrelated, which has resulted both in the greatly reduced response uncertainty shown in Fig. 3.17 as well as reduced correlation between the responses.

The response correlations shown in Fig. 3.18 indicate physically meaningful trends. The most highly correlated responses are either different response moments for identical assembly configurations (e.g. R_1 and R_2 for the bare BeRP ball) or the same response moments for different assembly configurations (e.g. R_1 for the bare and polyethylene-reflected BeRP ball). This result is reasonable because these sets of responses have a number of features in common. The former set contains response moments computed from the same NMC distribution, such that both response moments are a function of the same cross sections. The second set contains identical response moments (e.g. R_1) from different NMC distributions. The least correlated responses are different response moments for different assembly configurations (e.g. R_1 for the bare BeRP ball and R_2 for the polyethylene-reflected BeRP ball). This result is also reasonable because the response moments are computed from different NMC distributions obtained by simulating assemblies that do not contain all the same cross sections (i.e. the addition of the polyethylene reflector). It is satisfying to observe that, not only are the NMC experiments more

Figure 3.18 Correlations between the responses simulated with best-estimate cross sections.

accurately simulated with reduced uncertainty, but the response moments themselves are correlated in an intuitive way.

EFFECT OF SYSTEMATIC MEASUREMENT UNCERTAINTIES ON OPTIMAL CROSS SECTION ADJUSTMENT

As discussed in Chap. 3, the adjustment to the Pu-239 $\bar{\nu}$ obtained by applying an EKF to NMC experiments is similar in trend but increased in magnitude compared to that recommended by Evans [12]. The primary reason for this is that the current work accounts for systematic and random sources of uncertainty, while Evans' work accounted for random sources of uncertainty only. To demonstrate the effect of excluding systematic uncertainty in the model calibration process, we performed one-dimensional (spherical) PARTISN simulations of gross neutron counting of the bare and 3.8-cm polyethylene-reflected BeRP ball counted by the SNAP gross neutron counter, which is a single He-3 proportional counter that is moderated by polyethylene and has a removable polyethylene front cover. We then performed model calibration as described in Chap. 2 but only included random sources of uncertainty in the mean count rate R_1 . The SNAP detector with its front cover removed is pictured in Fig. 4.1. The SNAP was positioned such that its front face with the front cover removed was 100 cm from the center of the BeRP ball. The gross neutron counting experiment is described in some detail in [12] and in greater detail in [37].

The BeRP ball model used in the gross neutron counting simulations described here and in the NMC simulations described in Chap. 3 is identical. The cross sections, $p(\nu, E)$ distribution moment $\overline{\nu(\nu-1)}$, and fixed source parameters used in both simulations were likewise obtained from the same sources. The PARTISN transport solve parameters are also identical between the simulations, except for the number of energy groups (27), which was changed to be consistent with Evans' simulation. Similar to the nPod detector response function, we used MCNP6 [59] to calculate the SNAP detector response function, which was used as the adjoint source Q_1^* in Eq. (2.1). The intrinsic efficiency of the SNAP detector is plotted in Fig. 4.2. As described in Chap. 3, the set of cross sections {Pu-239 and Pu-240 χ , $\bar{\nu}$, and σ_f ; Pu-239, Pu-240, H-1, and C-12 σ_c } were directly adjusted by the EKF and Eq. (3.38) was used to update the principal cross sections (σ_a , $\nu\sigma_f$, and σ_t) used to perform the transport solves.

Figures 4.3, 4.4, and 4.5 compare the mean count rate R_1 sensitivity to the Pu-239 $\bar{\nu}$, σ_f , and χ , respectively, for the bare and polyethylene-reflected BeRP ball configurations. Figure 4.6 compares the sensitivity totals for all of the cross sections included in the model calibration applied to gross neutron

Figure 4.1 The SNAP gross neutron counter with its front polyethylene cover removed [12].

Figure 4.2 27-group intrinsic efficiency of the SNAP gross neutron counter.

counting. The main takeaway from these figures is that they follow the same trends as those described in Chap. 3 for the nPod detector mean count rate. The fission parameters are the most highly influential cross sections on the mean count rate of the SNAP and are more so for the polyethylene-reflected BeRP ball than for the bare BeRP ball. With the exception of the capture cross sections, increasing all of the other cross sections tends to increase the SNAP mean count rate.

Figure 4.7 compares the adjustment of the Pu-239 $\bar{\nu}$, which is given in multiples of its nominal standard deviation, between Cacuci's DA process applied to three-dimensional Denovo simulations

Figure 4.3 Sensitivity of R_1 to the Pu-239 $\bar{\nu}$ for the bare and reflected BeRP ball configuration.

Figure 4.4 Sensitivity of R_1 to the Pu-239 σ_f for the bare and reflected BeRP ball configuration.

Figure 4.5 Sensitivity of R_1 to the Pu-239 χ for the bare and reflected BeRP ball configuration.

Figure 4.6 Relative sensitivity totals of R_1 for the bare and reflected BeRP ball configurations.

(DENOVO 3D) and the EKF model calibration process described in Chap. 2 applied to one-dimensional PARTISN simulations (PARTISN 1D). Figures 4.8 and 4.9 are analogous comparisons for the Pu-239 σ_f and χ , respectively. The DENOVO 3D simulations were more detailed than the PARTISN 1D simulations in that they included a model of the SNAP detector, carbon steel cart, and concrete floor. Additionally, the forward intrinsic neutron source contained contributions from both spontaneous fission and (α, n) reactions. Although the DENOVO 3D simulations were limited to cartesian spatial discretization, the spatial cell size was small (~ 1 mm) for the BeRP ball and detector and larger (~ 10 mm) for the distance between the assembly and detector. Other details regarding the DENOVO 3D simulations are given in [12].

The adjustment to the Pu-239 fission parameters in the PARTISN 1D case are more similar to those in the DENOVO 3D case when accounting for random uncertainty only, compared to the adjustments obtained when accounting for random and systematic uncertainties. As discussed in Chap. 3, accounting for systematic uncertainties significantly increases the measured response uncertainty; additionally, the measured responses are strongly correlated. The EKF therefore weights information from measured responses less than the simulated responses, which ultimately changes the magnitude of the cross section adjustment required to minimize the error between the responses in a least squares sense.

Figure 4.10 compares the SNAP detector measured mean count rates [12] to those adjusted in the DENOVO 3D and PARTISN 1D cases. The measured response uncertainty is due only to random uncertainty and the simulated response uncertainty is due to the cross section covariances (See Sec. 2.5). The adjusted responses from both cases agree well with one another and with the measured responses. The accuracy of the PARTISN 1D case adjusted responses demonstrates that the loss of detail in simulating a one-dimensional geometry has not significantly impacted the model calibration process.

Figure 4.10 demonstrates that our one-dimensional (spherical) model of the BeRP ball is a reasonable facsimile of the three-dimensional model. The increased similarity between the fission parameters adjusted using Cacuci's DA process and the EKF model calibration process described in Chap. 2 when accounting for random uncertainties only in the measured responses lends credence to the fission

Figure 4.7 Comparison between adjustments to the Pu-239 $\bar{\nu}$ in multiples of its nominal standard deviation. The legend “stat. unc. only” indicates that the optimal cross section adjustments applied to gross neutron counting experiments account for random uncertainty only. The legend “stat. & sys. unc.” indicates that the optimal cross section adjustments applied to gross neutron counting experiments accounting for random and systematic uncertainties.

Figure 4.8 Comparison between adjustments to the Pu-239 σ_f in multiples of its nominal standard deviation. The legend “stat. unc. only” indicates that the optimal cross section adjustments applied to gross neutron counting experiments account for random uncertainty only. The legend “stat. & sys. unc.” indicates that the optimal cross section adjustments applied to gross neutron counting experiments accounting for random and systematic uncertainties.

parameter adjustments determined by model calibration that accounts for both random and systematic uncertainties. Inclusion of systematic uncertainties significantly increases the measured response uncertainties, which in turn has a pronounced effect on the cross section adjustments required to simulate NMC experiments accurately.

Figure 4.9 Comparison between adjustments to the Pu-239 χ in multiples of its nominal standard deviation. The legend “stat. unc. only” indicates that the optimal cross section adjustments applied to gross neutron counting experiments account for random uncertainty only. The legend “stat. & sys. unc.” indicates that the optimal cross section adjustments applied to gross neutron counting experiments accounting for random and systematic uncertainties.

Figure 4.10 Comparison between SNAP detector measured and mean count rates adjusted in the Denovo 3D and PARTISN 1D cases. “stat. unc. only” in each legend indicates that the optimal cross section adjustments applied to gross neutron counting experiments account for random uncertainty only.

DIRECT SAMPLING VERIFICATION OF FIRST-ORDER UNCERTAINTY QUANTIFICATION

As discussed in Chap. 2, the simulated response covariance due to cross section covariances is computed using first-order propagation of uncertainty, which is an inner product between the response sensitivity to the cross sections and the cross section covariances. The rationale for this approach comes from first-order perturbation theory [23], which states that the variation in the detector response moment may be approximated by a first-order Taylor series expansion about a small perturbation in the cross sections,

$$R_q|_{\alpha=\alpha^0+\Delta\alpha} = R_q|_{\alpha=\alpha^0} + \sum_{a \in \alpha} \sum_{g=1}^G \left(\frac{\partial R_q}{\partial \alpha_g} \bigg|_{\alpha=\alpha^0} \Delta \alpha_g \right) + \mathcal{O}((\Delta\alpha)^2), \quad (5.1)$$

where $\mathcal{O}$ denotes “order of”. Only the detector response moments $R_q|_{\alpha=\alpha^0}$ computed with the nominal cross sections α^0 , the first derivative of the responses with respect to the cross sections $\frac{\partial R_q}{\partial \alpha_g} \bigg|_{\alpha=\alpha^0}$, and the cross section perturbations $\Delta \alpha_x$ are required. Equation (5.1) is defined such that it describes the response variation due to multiple group cross section perturbations.

First-order perturbation theory is generally applicable when a small cross section perturbation leads to a small change in the response, such that the response variation is approximately linear; i.e., the product of the higher-order derivatives of the response with respect to the cross sections and the cross section perturbations is small enough to neglect. As discussed in Chap. 3, however, the responses change significantly with respect to the Pu-239 $\bar{\nu}$ and fission cross section. Figure 3.11 indicates that a 1% change in these fission parameters results in a 2-9% change in R_1 and a 7-29% change in R_2 . Because both responses are nonlinear in the cross sections (R_2 more so than R_1 ; see Sec. 2.2) and highly sensitive to the fission parameters, the higher-order terms in Eq. (5.1) may be comparable in magnitude to the first-order terms. Depending on the sign of the higher-order terms, first-order UQ may over- or under-predict the response covariance due to the cross section covariances.

Performing sampling-based UQ is one way to determine if first-order UQ is sufficient to characterize variation in the responses due to variation in the cross sections [6]. Sampling-based UQ has the benefit of

making no assumption about how responses vary with respect to the cross sections. It is relatively simple to implement because it only requires that the input cross sections are perturbed, with no modification to the transport solver.

The cross sections in this study were sampled from a multivariate Gaussian distribution,

$$\alpha \sim N(\alpha^0, \text{cov}(\alpha^0, \alpha^0)), \quad (5.2)$$

and used to compute directly perturbed responses i.e. an exact calculation of $R_q|_{\alpha=\alpha^0+\Delta\alpha}$ from Eq. (5.1). α^0 and $\text{cov}(\alpha^0, \alpha^0)$ are the nominal cross sections and their covariances from the ENDF/B-VII.1 library. The variance of the sampled response distribution may then be compared to the response variance computed via first-order propagation. Good agreement between the directly sampled and first-order estimates of the response variance would indicate that first-order perturbation theory adequately characterizes the response variation due to the cross sections.

We performed one-dimensional PARTISN simulations of NMC of the BeRP ball in bare and polyethylene-reflected configurations to compute the detector response moments using both nominal cross sections and cross sections sampled from a multivariate Gaussian distribution. Both the nominal and sampled responses were computed using coarse transport solve options, which are summarized in Table 5.1. We performed low-order simulations to reduce the computational expense of the large number of transport solves required to compute a sufficient number of directly perturbed detector responses. Note that although these simulations result in nominal responses that do not agree well with measured responses, both the nominal and sampled responses are computed with the same transport solve options; therefore, we provide a comparison of first-order UQ and sampling-based UQ applied to NMC of the BeRP ball with the same low-order model.

Table 5.1 PARTISN transport solve parameters for low-order simulations used to perform both first-order and sampling-based UQ.

Parameter	Value
Number of discrete ordinates	8
Number of Legendre polynomial expansion terms for the scatter kernel	1
Energy groups	1
Spatial cell thickness	0.47 cm
Source iteration convergence tolerance	1e-04

One-group cross sections were obtained from SCALE [46], which group-collapsed the 44-group cross sections utilized in the results presented in Chap. 3. The 44-group cross section covariances were collapsed to one group using Proctor’s [45] Python code, Kerberos. The spontaneous fission forward source term Q , nPod neutron multiplicity counter adjoint source term Q_1^* , and $p(\nu, E)$ distribution moment $\overline{\nu(\nu-1)}$ were computed as described in Chap. 3 and group-averaged for a single energy group. The one-group Q and Q_1^* are given in Table 5.2. The BeRP ball model was composed of the same nuclides

as those given in Chap. 3 (Pu-239, Pu-240, H-1, and C-12) but with different atom densities, which are summarized in Table 5.3. The reduction in the number of energy groups and scatter kernel moments results in a significant reduction in the calculated neutron leakage such that the calculated neutron multiplication is artificially high. To avoid simulating a supercritical assembly, the atom densities for Pu-239 and H-1 are reduced from their values given in Table 3.1 to those given in Table 5.3. The atom densities for Pu-240 and C-12 are identical between the simulations described here and in Chap. 3.

Table 5.2 One-group spontaneous fission source term Q and nPod neutron multiplicity counter adjoint source term Q_1^* utilized in the low-order assembly model.

Quantity	Value
Q	$1.2154 \times 10^3 \left[\frac{\text{neutrons}}{\text{cm}^3 \text{ sec}} \right]$
Q_1^*	$4.2140 \times 10^{-3} \left[\frac{\text{counts}}{\text{neutron}} \right]$

Table 5.3 Atom density of nuclides present in the low-order assembly model.

Nuclide	Atom density $\left(\frac{\text{atoms}}{\text{b cm}} \right)$
Pu-239	$2.60595191 \times 10^{-2}$
Pu-240	$2.90503750 \times 10^{-3}$
H-1	$4.21960442 \times 10^{-2}$
C-12	$4.11308331 \times 10^{-2}$

Figure 5.1 gives the sensitivity totals for all of the one-group cross sections. Although the sensitivity totals in Fig. 5.1 generally follow the same trends as those indicated by Fig. 3.11 in the 44-group case, the Pu-239 capture cross section is now slightly less influential than the Pu-239 $\overline{\nu}(\nu-1)$, Pu-240 $\overline{\nu}$ and Pu-240 σ_f . This is due to the reduction from 44 groups to a single energy group. Despite this slight reordering, the sensitivity totals for the Pu-240 $\overline{\nu}$ and σ_f and the Pu-239 $\overline{\nu}(\nu-1)$ and σ_c are all comparable (as they were in the 44-group case). The Pu-239 cross sections are the most highly influential on the detector responses for the one-group problem and indicate that a 1% change in their value will result in a significant change in the detector responses. We therefore expect that the response variation to the Pu-239 cross sections to be the most likely to be inadequately described by first-order UQ. Consequently, we have performed the sampling-based UQ by sampling the Pu-239 $\overline{\nu}$, σ_f , and σ_c cross sections only, while using the nominal values for all other cross sections. We do not sample the Pu-239 $\overline{\nu}(\nu-1)$ because computing the variance in $\overline{\nu}(\nu-1)$ due to the variance in $\overline{\nu}$ requires determining their quadratic relationship (see Appendix A), which cannot be done in a one-group case. Additionally, we demonstrated in Chap. 3 that the detector responses are not sensitive to $\overline{\nu}(\nu-1)$.

The nominal one-group Pu-239 cross section correlations are plotted in Fig. 5.2. The nominal cross

Figure 5.1 Relative sensitivity totals of R_1 and R_2 for low-order simulations of the bare and reflected BeRP ball.

section covariances were used both to compute a first-order estimate of the nominal response variance (see Chap. 2) and to sample the Pu-239 cross sections from a multivariate Gaussian distribution.

Figure 5.2 Nominal cross section correlations for the Pu-239 cross sections used both to compute a first-order estimate of the nominal response variance and to sample the Pu-239 cross sections from a multivariate Gaussian distribution.

The set of sampled cross sections is given by $\alpha_s = \{\alpha_{s,n}\}$, $n = 1, \dots, N$, where each $\alpha_{s,n}$ contains a randomly sampled Pu-239 $\bar{\nu}$, σ_f , and σ_c as well as the nominal value for all of the other cross sections with a sample size of $N = 10^5$. Given the nominal cross sections and nominal cross section covariances, cross sections sampled from a multivariate Gaussian distribution may be computed using [38]

$$\alpha_{s,n} = \mathbf{A}\mathbf{z} + \alpha^0, \quad (5.3)$$

where $z \sim N(0, 1)$ is a vector of samples from a standard Gaussian distribution. The matrix A is related to the nominal cross section covariances via

$$\text{cov}(\alpha^0, \alpha^0) = AA^T. \quad (5.4)$$

One way to determine A is to perform a singular value decomposition (SVD) of the nominal covariance matrix; i.e.,

$$\text{cov}(\alpha^0, \alpha^0) = U\mathbf{W}U^T, \quad (5.5)$$

where U is a unitary matrix whose columns are eigenvectors of $[\text{cov}(\alpha^0, \alpha^0)]^2$ and $\mathbf{W}$ is a diagonal matrix whose elements are the square root of the eigenvalues of $[\text{cov}(\alpha^0, \alpha^0)]^2$. Assuming that the nominal covariance matrix is symmetric positive definite (see Chap. 3 and Appendix C), $\mathbf{W}$ is nonnegative and can be decomposed as

$$\mathbf{W} = \mathbf{W}^{\frac{1}{2}} \mathbf{W}^{\frac{1}{2}}. \quad (5.6)$$

Because $\mathbf{W}$ is diagonal, the elements of $\mathbf{W}^{\frac{1}{2}}$ are the square root of the elements in $\mathbf{W}$. The matrix A can now be expressed as

$$A = U\mathbf{W}^{\frac{1}{2}}, \quad (5.7)$$

such that the sampled cross sections may be computed as

$$\alpha_{s,n} = U\mathbf{W}^{\frac{1}{2}}z + \alpha^0. \quad (5.8)$$

We ensure that the cross sections are correctly sampled from a multivariate Gaussian by respectively computing the mean and covariance of the sampled cross section distribution as

$$\begin{aligned} \bar{\alpha}_s &= \mathbb{E}[\alpha_s] \\ &= \frac{1}{N} \sum_{n=1}^N \alpha_{s,n} \end{aligned} \quad (5.9)$$

and

$$\begin{aligned} \text{cov}(\alpha_s, \alpha_s) &= \mathbb{E}[(\alpha_s - \bar{\alpha}_s)(\alpha_s - \bar{\alpha}_s)^T] \\ &= \frac{1}{N-1} \sum_{n=1}^N \sum_{m=1}^N (\alpha_{s,n} - \bar{\alpha}_s)(\alpha_{s,m} - \bar{\alpha}_s)^T. \end{aligned} \quad (5.10)$$

$\bar{\alpha}_s$ is a vector that contains the mean of the sampled cross section distributions. $\text{cov}(\alpha_s, \alpha_s)$ is a matrix that contains the covariance between the sampled cross sections. Table 5.4 compares the sampled cross section means to the nominal cross section values and Table 5.5 compares the variance of the sampled cross section distributions to the nominal cross section variances. There is good agreement between the nominal cross sections and their variances with the mean and variance of the sampled cross section

distributions, respectively.

Table 5.4 Comparison between the nominal cross sections and the mean of the sampled cross section distributions.

Cross section	Nominal value	Sample mean	Relative difference
Pu-239 $\bar{\nu}$	3.1046×10^0	3.1046×10^0	1.2171×10^{-5}
Pu-239 σ_f	2.0424×10^0	2.0424×10^0	-4.9857×10^{-6}
Pu-239 σ_c	2.2595×10^{-1}	2.2596×10^{-1}	-5.9287×10^{-6}

Table 5.5 Comparison between the nominal cross section variances and the variance of the sampled cross section distributions.

Cross section	Nominal variance	Sample variance	Relative difference
Pu-239 $\bar{\nu}$	2.7965×10^{-4}	2.7790×10^{-4}	6.2649×10^{-3}
Pu-239 σ_f	1.0181×10^{-4}	1.0189×10^{-4}	-7.7441×10^{-4}
Pu-239 σ_c	2.5104×10^{-6}	2.5291×10^{-6}	-7.4712×10^{-3}

Figure 5.3 is a plot of the correlation between the sampled cross sections. Some of the sampled cross sections have a slightly negative correlation where there was previously no correlation (see Fig. 5.2). To determine which of the sampled cross section correlations are statistically significant, we compute the Pearson's correlation coefficient r and its standard error $\text{stdev}(r)$ [21]. r is a measure of how one cross section varies with another and is computed as

$$r = \frac{\text{cov}(x, y)}{\sqrt{\text{var}(x) \text{var}(y)}}, \quad (5.11)$$

where x and y represent a pair of sampled cross sections (e.g. the sampled fission and capture cross sections). The standard error of the Pearson's correlation coefficient $\text{stdev}(r)$ can be computed for a large sample size ($N > 30$) as

$$\text{stdev}(r) = \frac{1 - r^2}{\sqrt{N}}. \quad (5.12)$$

Figure 5.4 presents pairwise plots between the sampled cross sections as well as the Pearson's correlation coefficient with its standard error. The $\text{stdev}(r)$ is larger than r for all but the correlation between the fission and capture cross sections, which indicates that these slight anti-correlations are not statistically significant. In contrast, r is larger than the $\text{stdev}(r)$ for the fission to capture correlation and the value of r agrees well with the nominal correlation in Fig. 5.2. We are therefore confident that the cross sections are being correctly sampled from the multivariate Gaussian distribution.

Figure 5.3 Correlation between the cross sections sampled from the multivariate Gaussian distribution defined by the nominal cross sections and their covariances.

Figure 5.4 Pairwise plots of the sampled cross sections. The Pearson's correlation coefficient and its standard error demonstrate which cross section correlations are statistically significant.

The set of sampled responses is given by $\mathbf{R}_s = \{\mathbf{R}_{s,n}\}$, $n = 1, \dots, N$, where each $\mathbf{R}_{s,n}$ is a vector of responses computed by performing transport solves with the corresponding sampled cross sections $\alpha_{s,n}$. We respectively compute the mean and covariance of the sampled response distribution as

$$\begin{aligned} \overline{\mathbf{R}}_s &= \mathbb{E}[\mathbf{R}_s] \\ &= \frac{1}{N} \sum_{n=1}^N \mathbf{R}_{s,n} \end{aligned} \quad (5.13)$$

and

$$\begin{aligned}\text{cov}(\mathbf{R}_s, \mathbf{R}_s) &= (\mathbb{E}[(\mathbf{R}_s - \bar{\mathbf{R}}_s)(\mathbf{R}_s - \bar{\mathbf{R}}_s)^T]) \\ &= \frac{1}{N-1} \sum_{n=1}^N \sum_{m=1}^N (\mathbf{R}_{s,n} - \bar{\mathbf{R}}_s)(\mathbf{R}_{s,m} - \bar{\mathbf{R}}_s)^T.\end{aligned}\tag{5.14}$$

$\bar{\mathbf{R}}_s$ is a vector that contains the mean of each sampled response distributions. $\text{cov}(\mathbf{R}_s, \mathbf{R}_s)$ is a matrix that contains the covariance between the sampled responses.

We compare the sampled response means to the responses computed with the nominal cross sections to ensure that the sampled responses are being computed correctly. Figures 5.5 and 5.6 respectively plot the incremental means of the sampled response distribution for the bare and polyethylene-reflected BeRP ball as a function of the number of samples, which provides an indication of how many samples are required to compute a response mean that is characteristic of the response distribution. The simplest way to compute the incremental mean of a distribution is to recompute Eq. (5.13) as each new sample is computed. This approach is cumbersome for a large sample size, however, and so we utilize a recursive relation [58] to iteratively compute the incremental mean for the first N' samples; i.e.,

$$\bar{x}_{N'} = \frac{1}{N'} (x_{N'} + (N' - 1) \bar{x}_{N'-1}), 1 < N' \leq N,\tag{5.15}$$

where $x_{N'}$ represents sample N' of one of the responses. The incremental mean of the sampled response distributions in Figs. 5.5 and 5.6 indicate that approximately 10^4 samples are required to converge to a stable value. Additionally, there is good agreement between the nominal responses and the mean of the total set of sampled responses. We are therefore confident that enough sampled responses were generated such that the mean of the sampled response distributions accurately reproduce the nominal response values.

(a)

(b)

Figure 5.5 Incremental mean of the sampled response distributions compared to the nominal responses a) R_1 and b) R_2 for the bare BeRP ball.

(a)

(b)

Figure 5.6 Incremental mean of the sampled response distributions compared to the nominal responses a) R_1 and b) R_2 for the 3.8 cm polyethylene-reflected BeRP ball.

Similarly, we compare the sampled response distribution variances to the response variances computed with first-order UQ. Figures 5.7 and 5.8 plot the incremental variances of the sampled response distribution as a function of the number of samples, which provides an indication of how many samples are required to compute a response variance that characterizes the response distribution. Although a recursive relation analagous to that for the mean exists for iteratively computing the incremental variance, this relation is numerically unstable because small numbers are subtracted from successively larger numbers. Welford [58] instead provides a numerically stable algorithm, which is given by

$$\begin{aligned} M_{2,N'} &= M_{2,N'-1} + (x_{N'} - \bar{x}_{N'-1})(x_{N'} - \bar{x}_{N'}), \\ \text{var}(x)_{N'} &= \frac{M_{2,N'}}{N' - 1}. \end{aligned} \tag{5.16}$$

As with the incremental mean, approximately 10^4 samples are required for the sampled response variance to converge to a stable value. There is good agreement between the response variances computed via first-order and sampling-based UQ, which indicates that, for this problem, first-order UQ adequately characterizes variation in these responses due to variations in the cross sections considered in this chapter.

(a)

(b)

Figure 5.7 Incremental variance of the sampled response distributions compared to the response variance in a) R_1 and b) R_2 computed with first-order UQ for the bare BeRP ball.

(a)

(b)

Figure 5.8 Incremental variance of the sampled response distributions compared to the response variance in a) R_1 and b) R_2 computed with first-order UQ for the 3.8 cm polyethylene-reflected BeRP ball.

It is remarkable that, despite the nonlinearity of the detector response moments with respect to the cross sections, first-order UQ adequately characterizes the response variance due to the cross sections considered in this chapter. In addition to providing justification for computing the response variances with first-order UQ, these results also lend credence to applying the EKF to model calibration to NMC of the bare and polyethylene-reflected BeRP ball. Two shortcomings of this study are that the sampling-based UQ was not applied to more of the one-group cross sections nor to the multigroup cross sections. Expanding the sampling-based UQ in both ways would be more illustrative of the effect of other transport phenomena (e.g. upscattering and downscattering) that arise from perturbing multigroup cross sections that are not present in the one-group problem presented here. The computational expense of sampling-based UQ scales exponentially with the number of parameters, however, making even a moderately-sized multigroup problem prohibitively time-consuming. Regardless, the results presented here indicate that application of first-order UQ and the EKF are appropriate for NMC of the bare and polyethylene-reflected BeRP ball.

CONCLUSIONS AND FUTURE WORK

This dissertation presented the first application of model calibration to NMC experiments for optimal adjustment of nuclear cross sections that utilized adjoint-based SA and first-order UQ. The sensitivity of the first and second moments of the NMC distribution (i.e. first and second detector response moments) are computed using adjoint-based SA and are used to compute a first-order estimate of the response covariances due to covariance in the cross sections. The response covariances due to random and systematic uncertainty were utilized in an EKF, which identified best-estimate cross sections such that NMC experiments were more accurately simulated with reduced uncertainty.

The Pu-239 $\bar{\nu}$ was determined to be the most influential parameter on the detector responses. The adjustment to $\bar{\nu}$ identified by the EKF was consistent with the ENDF/B-VII.0 [7] release notes and with the findings of Miller [37] but our recommended adjustments to the Pu-239 fission parameters ($\bar{\nu}$, σ_f , and χ) are similar in trend but increased in magnitude compared to those recommended by Evans [12]. Our model calibration included both random and systematic uncertainties, while the data assimilation performed by Evans accounted for random uncertainties only, which is the primary cause of the difference in the magnitude of our respective adjustments. In particular, the cross section adjustments recommended by the EKF are more similar to those recommended by Evans when only random uncertainties are considered. Furthermore, we demonstrated that despite our use of a simplified, one-dimensional model of the BeRP ball, the detector response moments were accurately simulated in comparison to Evans' three-dimensional simulations.

The EKF identified new co- and anti-correlations between the group fission parameters as well as the previously unknown correlation between the fission parameters themselves. The adjustment to the cross section covariances resulted in reduced uncertainty in the simulated detector responses. Additionally, the simulated response covariances computed after optimal adjustment of the cross sections indicated physically meaningful relationships. Responses that had the largest number of features in common (e.g. different response moments from the same NMC distribution) were also the most highly correlated.

We performed sampling-based UQ to demonstrate that first-order UQ provides an adequate estimate of the response variation due to perturbations in the Pu-239 cross sections, to which the detector responses are most sensitive. The agreement between the first-order estimate of and directly sampled

response variance provides justification for the application of an EKF to NMC of the BeRP ball in bare and polyethylene-reflected configurations.

As mentioned in Chap. 3, we did not include the differential scatter cross section in our model calibration process because covariances for this cross section were not available. The detector response moments from NMC of the bare and polyethylene-reflected BeRP ball are relatively insensitive to the scatter cross section for all isotopes present in the simulation; consequently, these detector responses would not be significantly impacted by adjustment to this cross sections. However, assemblies with lower neutron multiplication and/or a greater amount of low-Z material could potentially be much more sensitive to the scatter cross sections. We therefore recommend that the differential scatter cross section be included in model calibration applied to NMC if covariances for this cross section become available in future ENDF (or other cross section library) releases or can be estimated in a well-posed manner.

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APPENDICES

PROPAGATION OF UNCERTAINTY IN THE SECOND FACTORIAL MOMENT OF THE INDUCED FISSION NEUTRON MULTIPLICITY DISTRIBUTION

The ENDF library does not currently tabulate covariances for moments of the induced fission neutron multiplicity distribution $p(\nu, E)$ higher than the first moment, i.e., the mean multiplicity $\bar{\nu}$. In this dissertation, the $p(\nu, E)$ distribution second factorial moment ($\overline{\nu(\nu-1)}$) is parameterized in terms of $\bar{\nu}$, such that the $\overline{\nu(\nu-1)}$ covariance may be calculated using linear propagation of uncertainty.

Terrell demonstrated that the spontaneous fission $p(\nu)$ distribution is characterized by $\bar{\nu}$ and a fixed width parameter σ^2 (the second central moment of $p(\nu, E)$), which is identical for virtually all spontaneous fissioning nuclides, except for Cf-252 [55]. The measured induced fission $p(\nu, E)$ distributions published by Zucker and Holden demonstrate that $\overline{\nu(\nu-1)}$ is a smoothly varying quadratic function of $\bar{\nu}$ [61]. Figure A.1 shows the measured $p(\nu, E)$ for Pu-239, Fig. A.2 presents both $\bar{\nu}$ and $\overline{\nu(\nu-1)}$ as a function of energy, and Fig. A.3 illustrates the relationship between $\overline{\nu(\nu-1)}$ and $\bar{\nu}$.

The relationship between $\bar{\nu}$ and $\overline{\nu(\nu-1)}$ can be expressed in multigroup form (see Sec. 2.4) as

$$\overline{\nu(\nu-1)}_g = a + b \bar{\nu}_g + c (\bar{\nu}_g)^2. \quad (\text{A.1})$$

The coefficients a , b , and c are then used to compute the derivative of $\overline{\nu(\nu-1)}_g$ with respect to $\bar{\nu}_g$, yielding

$$\frac{\partial \overline{\nu(\nu-1)}_g}{\partial \bar{\nu}_g} = b + 2c \bar{\nu}_g, \quad (\text{A.2})$$

such that the $\overline{\nu(\nu-1)}$ covariance is computed as

$$\text{cov}(\overline{\nu(\nu-1)}, \overline{\nu(\nu-1)}) = \left(\frac{\partial \overline{\nu(\nu-1)}}{\partial \bar{\nu}} \right)^T \text{cov}(\bar{\nu}, \bar{\nu}) \left(\frac{\partial \overline{\nu(\nu-1)}}{\partial \bar{\nu}} \right), \quad (\text{A.3})$$

where $\frac{\partial \overline{\nu(\nu-1)}}{\partial \bar{\nu}}$ is a diagonal sensitivity matrix whose elements are Eq. (A.2) and $\text{cov}(\bar{\nu}, \bar{\nu})$ is the $\bar{\nu}$ covariance. The sensitivity matrix is diagonal because Eq. (A.1) only relates $\bar{\nu}$ at one energy group to $\overline{\nu(\nu-1)}$

at the same energy group.

Figure A.1 Pu-239 $p(\nu, E)$ plotted as a function of both ν and E [61]. Although the mean of the distribution monotonically increases as a function of energy, the width of the distribution remains constant.

Figure A.2 Pu-239 $\overline{\nu}$ and $\overline{\nu(\nu-1)}$ plotted as a function of incident neutron energy [61]. The fitted models respectively demonstrate that $\overline{\nu}$ and $\overline{\nu(\nu-1)}$ vary linearly and quadratically with respect to energy.

Figure A.3 Pu-239 $\overline{\nu(\nu-1)}$ plotted as a function of $\overline{\nu}$ [61]. $\overline{\nu(\nu-1)}$ is a smoothly varying quadratic function of $\overline{\nu}$ because the width of the induced fission neutron multiplicity distribution is constant with respect to incident neutron energy [55]. A fit of $\overline{\nu(\nu-1)}$ to $\overline{\nu}$ is plotted to demonstrate the quadratic dependence.

COMPUTING THE NEAREST SYMMETRIC POSITIVE SEMI-DEFINITE COVARIANCE MATRIX

A covariance matrix provides a linear, pairwise relationship between several parameters (e.g. cross sections or detector response moments) [51]. The diagonal elements of a covariance matrix represent the variance in a parameter while the off-diagonal elements represent the covariance between pairs of parameters. Positive or negative covariance respectively indicates that a pair of parameters are positively or negatively correlated. Zero covariance means that the parameters do not exhibit linear correlation; however, this does not necessarily imply that they are independent of one another because they may have a nonlinear relationship. A covariance matrix must be both symmetric and positive definite for these relationships to be physically meaningful.

Let $\mathbf{x} = [\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N]$ denote an $M \times N$ matrix of M parameters and N samples, such that each column represents one sample of all of the parameters. The covariance between all of the parameters may then be computed as

$$\begin{aligned} \text{cov}(\mathbf{x}, \mathbf{x}) &= \mathbb{E}[(\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^T], \\ &= \frac{1}{N-1} \sum_{n=1}^N (\vec{x}_n - \bar{\mathbf{x}})(\vec{x}_n - \bar{\mathbf{x}})^T, \end{aligned} \tag{B.1}$$

where the vector of parameter means is computed as

$$\begin{aligned} \bar{\mathbf{x}} &= \mathbb{E}[\mathbf{x}], \\ &= \frac{1}{N} \sum_{n=1}^N \vec{x}_n. \end{aligned} \tag{B.2}$$

The covariance matrix definition given in Eq. (B.1) leads to two important properties. The first is that a covariance matrix is symmetric, which can be easily seen by reversing the order of the parenthetical terms and observing that the computed covariance does not change. The second is that a covariance matrix is at least positive semi-definite (PSD). This property can be seen by taking an inner product between an $M \times 1$ vector of nonzero values $\vec{v}$ and the covariance matrix, which can be expressed as [29]

$$\vec{v}^T \text{cov}(\mathbf{x}, \mathbf{x}) \vec{v} = \vec{v}^T \left[\frac{1}{N-1} \sum_{n=1}^N (\vec{x}_n - \bar{\mathbf{x}})(\vec{x}_n - \bar{\mathbf{x}})^T \right] \vec{v}. \quad (\text{B.3})$$

$\vec{v}$ can be moved inside the sum term and we recognize that

$$\vec{v}^T (\vec{x}_n - \bar{\mathbf{x}})(\vec{x}_n - \bar{\mathbf{x}})^T \vec{v} = ((\vec{x}_n - \bar{\mathbf{x}})^T \vec{v})^2. \quad (\text{B.4})$$

Equation (B.3) can therefore be written as

$$\vec{v}^T \text{cov}(\mathbf{x}, \mathbf{x}) \vec{v} = \frac{1}{N-1} \sum_{n=1}^N ((\vec{x}_n - \bar{\mathbf{x}})^T \vec{v})^2 \geq 0. \quad (\text{B.5})$$

Equation (B.5) is always nonnegative because the summand is squared; therefore, a covariance matrix as defined in Eq. (B.1) is said to be PSD and is guaranteed to have nonnegative eigenvalues.¹ Given that $\vec{v}$ is nonzero and defining $\vec{z}_n = (\vec{x}_n - \bar{\mathbf{x}})$, Eq. (B.5) can only be zero if and only if $(\vec{z}_n)^T \vec{v} = 0$ for each n . If the set of $\vec{z}_n$ are strictly nonzero, the covariance matrix is full rank and all of its eigenvalues will be positive.² A full rank covariance matrix as defined in Eq. (B.1) is therefore said to be positive definite (PD).

As mentioned in Chap. 3, Proctor [45] determined that the multigroup cross section covariances from ENDF/B-VII.1 were neither symmetric positive definite (SPD) nor symmetric positive semi-definite (SPSD). In order to perform model calibration with physically meaningful covariances, we calculate the nearest SPSPD covariance matrix [24]. We first compute elements of a correlation matrix that correspond with the covariance matrix defined in Eq. (B.1) using

$$\text{cor}(x_i, x_j) = \frac{\text{cov}(x_i, x_j)}{\sqrt{\text{var}(x_i) \text{var}(x_j)}}, i, j = 1, \dots, M, \quad (\text{B.6})$$

where x_i and x_j represent a pair of parameters, $\text{var}(x_i) = \text{cov}(x_i, x_i)$, and $\text{var}(x_j) = \text{cov}(x_j, x_j)$. We then compute the eigenvalues and associated eigenvectors of the correlation matrix whose elements are defined in Eq. (B.6). Only the real component of the eigenvalues and eigenvectors are kept, and the eigenvalues that are smaller than a tolerance of 10^{-8} are set to zero. The modified set of eigenvalues and eigenvectors are then used to construct a new correlation matrix, which is termed the nearest SPSPD correlation matrix. The relationship given by Eq. (B.6) is utilized to compute the nearest SPSPD covariance matrix.

We acknowledge that the original ENDF/B-VII.1 cross section covariances are “nearly” SPSPD; that is, the negative eigenvalues are nearly zero and the imaginary components of the eigenvalues and eigenvectors are small. The nearest SPSPD covariance matrix is therefore nearly identical to the original covariance matrix. Our model calibration utilizing the original and nearest SPSPD covariance matrices consequently provide nearly identical adjustments to the cross sections and their covariances.

¹If one of the eigenvalues were negative, there would be some eigenvector $\vec{w}$ such that $\vec{w}^T \text{cov}(\mathbf{x}, \mathbf{x}) \vec{w} < 0$, which is not allowed by Eq. (B.5).

²If one of the eigenvalues were zero, there would be some eigenvector $\vec{w}$ such that $\vec{w}^T \text{cov}(\mathbf{x}, \mathbf{x}) \vec{w} = 0$, which is not allowed by Eq. (B.5) if the covariance matrix is full rank.

PROPAGATION OF MEASUREMENT PARAMETER UNCERTAINTY THROUGH NEUTRON MULTIPLICITY COUNTING DISTRIBUTION MOMENTS

As described in Chap. 2, we computed the measured response covariances due to both random and systematic sources of uncertainty. We briefly described calculation of the measured response covariance due to systematic sources in Chap. 3 and provide greater detail here.

Miller [37] found that the moments of NMC measurements of the BeRP ball in bare and polyethylene-reflected configurations were over-predicted in high-fidelity MCNP simulations. To determine if errors in the source-detector model could account for inaccuracies in the NMC distribution, Miller performed several high-fidelity MCNP simulations of the NMC experiment in which he varied many measurement parameters, including the BeRP ball mass, density, and radius as well as the source-detector distance, paralyzable and non-paralyzable detector dead-times, and Pu-240 content. Miller provided the nominal detector responses¹ as well as the responses for each variation in the measurement parameters. Because the response variation over the range of measurement parameter variations was approximately linear, we computed the measured response sensitivity to the measurement parameters using a one-sided finite difference; i.e.,

$$\left. \frac{\partial R_q}{\partial p} \right|_{p=p_0} = \frac{R_q|_{p=p_0} - R_q|_{p=p'}}{p_0 - p'}, q = 1, 2, \quad (\text{C.1})$$

where $R_q|_{p=p'}$ and $R_q|_{p=p_0}$ are respectively the simulated responses evaluated with the perturbed p' and nominal p_0 sets of measurement parameters. p' and p_0 are respectively a single perturbed and nominal measurement parameter. Only one measurement parameter was varied at a time while the others were kept at their nominal values.

¹The detector responses reported by Miller are the mean and variance of the NMC distribution, which are respectively identical to $\bar{n}$ and μ_2 defined in Eqs. (1.1) and (1.2). The NMC distribution was accumulated with a coincidence gate width of $T = 4096 \mu\text{s}$. We respectively determined the measured R_1 and R_2 using Eqs. (2.8) and (2.21). We then computed the sensitivity of the measured R_1 and R_2 (instead of the reported $\bar{n}$ and μ_2) to the measurement parameters using Eq. (C.1).

The measurement parameter uncertainties were obtained from the ICSBEP benchmark measurement, FUND-NCERC-PU-HE3-MULT-001 [47], which documented the nPod neutron multiplicity counter measurement of the BeRP ball in bare and nickel-reflected configurations. This benchmark included a rigorous UQ of all aspects of the source-detector assembly mass, composition, dimensions, temperature, and positioning as well as effects due to the surrounding features (e.g. the mild carbon steel cart) and the ambient conditions of the room. Although this benchmark was performed with a different reflector material than that used in Miller’s experiment, both measurements were performed with the same fissile core and multiplicity counter. The ICSBEP benchmark included all of the same measurement parameters that Miller considered, which had only to do with the nPod neutron multiplicity counter and the BeRP ball itself (and not to do with the reflector material). The measurement parameter uncertainties determined in the ICSBEP benchmark are therefore applicable to Miller’s experiment.

We computed the measured response covariance due to the measurement parameters with first-order UQ as described in Chap. 2. We constructed a sensitivity matrix ($\mathbf{D}_{\mathbf{R}_m, \mathbf{p}}$ from Eq. (2.65)) whose columns are the measured response sensitivity to all of the measurement parameters computed using Eq. (C.1). We constructed a diagonal measurement parameter covariance matrix ($\text{cov}(\mathbf{p}, \mathbf{p})$ from Eq. (2.65)) whose elements are the measurement parameter variances obtained from the ICSBEP benchmark. The measured response covariance due to the measurement parameters ($[\text{cov}(\mathbf{R}_m, \mathbf{R}_m)]_p$ from Eq. (2.65)) is therefore computed as the inner product between the sensitivity and covariance matrices. The complete measured response covariance due to random and systematic uncertainties is then given by Eq. (2.68).

Tables C.1 and C.2 respectively provide for the bare and polyethylene-reflected BeRP ball a summary of the measurement parameters considered, the response sensitivity to the measurement parameters, figure and table references from which the response sensitivities were estimated, the measurement parameter uncertainties reported in the ICSBEP benchmark, and the response variances due to the measurement parameter uncertainties.

Table C.1 Summary of the measurement parameters p considered, the response sensitivities $\frac{\partial R_q}{\partial p}$, $q = 1, 2$ to the measurement parameters, figure and table references [37] from which the response sensitivities were estimated, the measurement parameter uncertainties $\text{stdev}(p)$ reported in the ICSBEP benchmark [47], and the response variance $\text{var}(R_q)$, $q = 1, 2$ due to each measurement parameter for the bare BeRP ball.

p	$\frac{\partial R_1}{\partial p}$	$\frac{\partial R_2}{\partial p}$	Ref.	$\text{stdev}(p)$	$\text{var}(R_1)$	$\text{var}(R_2)$
source-detector distance (cm)	-2.5798×10^2	-1.6045×10^2	Table VIII	2.8867×10^{-1}	5.5461×10^3	2.1453×10^3
BeRP radius (cm)	-9.4077×10^3	-1.0057×10^4	Table IX	1.9284×10^{-3}	3.2912×10^2	3.7611×10^2
BeRP mass (g)	4.8502×10^0	5.3898×10^0	Table X	5.8000×10^{-2}	7.9137×10^{-2}	9.7724×10^{-2}
dead-time (μs)	-7.1636×10^0	-1.9178×10^1	Fig. 12	2.8867×10^{-1}	4.2763×10^0	3.0648×10^1
Pu-240 content (wt fraction)	1.3615×10^5	4.4515×10^4	Fig. 14	2.0000×10^{-3}	7.4146×10^4	7.9263×10^3

Table C.2 Summary of the measurement parameters p considered, the response sensitivities $\frac{\partial R_q}{\partial p}$, $q = 1, 2$ to the measurement parameters, figure and table references [37] from which the response sensitivities were estimated, the measurement parameter uncertainties $\text{stdev}(p)$ reported in the ICSBEP benchmark [47], and the response variance $\text{var}(R_q)$, $q = 1, 2$ due to each measurement parameter for the 3.8 cm polyethylene-reflected BeRP ball.

p	$\frac{\partial R_1}{\partial p}$	$\frac{\partial R_2}{\partial p}$	Ref.	$\text{stdev}(p)$	$\text{var}(R_1)$	$\text{var}(R_2)$
source-detector distance (cm)	-5.7161×10^2	-1.9084×10^3	Table VIII	2.8867×10^{-1}	2.7228×10^4	3.0348×10^5
BeRP radius (cm)	-3.9322×10^4	-2.0273×10^5	Table IX	1.9284×10^{-3}	5.7499×10^3	1.5284×10^5
BeRP mass (g)	2.4983×10^1	1.2362×10^2	Table X	5.8000×10^{-2}	2.0997×10^0	5.1405×10^1
dead-time (μs) ²	-3.9175×10^1	-1.9501×10^2	Fig. 12	2.8867×10^{-1}	1.2789×10^2	3.1689×10^3
Pu-240 content (wt fraction)	2.4618×10^5	4.0983×10^5	Fig. 14	2.0000×10^{-3}	2.4241×10^5	6.7184×10^5

²While Miller [37] provided response variations for the bare and 3.81 cm polyethylene-reflected BeRP ball configurations with respect to the source-detector distance, BeRP radius and mass, and the Pu-240 content, he instead provided response variations with respect to the dead-time for the bare and 2.54 cm polyethylene-reflected configurations. The ratio of the response sensitivities to the source-detector distance and to the BeRP radius and mass between the 3.81 cm and 2.54 cm cases are about 1.5. We therefore computed the response sensitivity to the dead-time for the 2.54 cm polyethylene-reflected configuration and multiplied it by 1.5 to estimate the response sensitivity for the 3.81 cm polyethylene-reflected case.