Convergence Analysis and Criterion for Data Assimilation with Sensitivities from Monte Carlo Neutron Transport Codes

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ABSTRACT

Sensitivity coefficients calculated with Monte Carlo neutron transport codes are subject to statistical fluctuations. The fluctuations affect parameters that are calculated with the sensitivity coefficients. The convergence study presented here describes the effects that statistically uncertain sensitivities have on first-order perturbation theory, uncertainty quantification, and data assimilation. The results show that for data assimilation, posterior nuclear data were remarkably uninfluenced by fluctuations in sensitivity mean values and by sensitivity uncertainties. Posterior calculated values computed with first-order perturbation theory showed larger dependence on sensitivity mean-value convergence and small uncertainty arising from the sensitivities' uncertainties. A convergence criterion is proposed for stopping simulations once the sensitivity means are sufficiently converged and their uncertainties are sufficiently small. Employing this criterion economizes computational resources by preventing an excess of particle histories from being used once convergence is achieved. The criterion's advantage is that it circumvents the need to set up the full data assimilation procedure, but is still applicable to data assimilation results.

KEYWORDS: Sensitivity Analysis, Uncertainty Quantification, Data Assimilation, Nuclear Data, Serpent2

1. INTRODUCTION

Sensitivity coefficients calculated by Monte Carlo neutron transport codes [1] compare well to sensitivities calculated with deterministic neutron transport codes. Unfortunately, they are more computationally expensive than deterministic perturbation theory. Their expense is a function of the sensitivities' statistical uncertainties. With more Monte Carlo histories, the sensitivities' mean values converge and their statistical uncertainties are reduced thereby leading to more accurate results, but at an increased computational cost. For Monte Carlo calculated sensitivities to be competitive with deterministically calculated sensitivities for data assimilation and uncertainty quantification calculations, the cost of the Monte Carlo simulation must be minimized while still maintaining sufficient statistical accuracy in the sensitivities.

To find this balance between cost and statistics, it is important to end a simulation once a sufficient level of convergence is achieved and the statistical uncertainties are reduced to an acceptable level. By ending the simulation once the sensitivities are acceptable, significant computer time is saved. To be able to end the simulation, what is acceptable in terms of sensitivity convergence and uncertainty needs to be defined and characterized. It is not possible to just examine the individual sensitivity coefficients because there can be hundreds to thousands, some of which are important and others not, and they later take different roles in different formulas. It would be wasteful to continue a simulation until an unimportant sensitivity converged because this sensitivity would not play an important role in the final calculated value. The acceptability of the statistically uncertain sensitivities is the focus of this document and a convergence criterion to stop the sensitivity simulations is proposed based on the results. Previously, simulations were run until some arbitrary criterion specified the user was met, often leading to one to two orders of magnitude more particles than needed being simulated. With the proposed convergence criterion, a systematic approach is presented that can lead to significant computation economizing. While Serpent version 2.1.29 [2] is used in this work, the conclusions are applicable to sensitivities calculated with other Monte Carlo neutron transport codes.

Three sensitivity coefficient applications are evaluated: 1) first-order perturbation theory 2) uncertainty quantification (UQ) and 3) data assimilation (DA) with the generalized linear least squares method [3][4]. The convergence of the sensitivity coefficients affects each application differently, i.e. it affects the convergence of the parameters calculated with the sensitivity coefficients. Therefore, to study the effect of the sensitivity coefficients, the convergence of the applications' calculated parameters will be the focus of this study. With this approach, the convergence of the most important sensitivities is emphasized and less important sensitivities, which may fluctuate greatly and have large uncertainties, are de-emphasized. For UQ, the convergence of the calculated parameter's uncertainty from nuclear data is studied. For DA, the convergence of the posterior nuclear data and their uncertainty, and the posterior calculated values and their uncertainty are examined. DA uses first-order perturbation theory to compute posterior calculated values. Therefore, the convergence of the posterior calculated values in the DA results is examined to evaluate first-order perturbation theory. Ideally, the convergence criterion would not require performing the DA calculations, which can be expensive when large matrices need to be inverted.

2. THEORY

Sensitivities are, speaking simply, tools that are applied to achieve an analysis. They allow simplifying the functional dependence of a calculated value - such as k_{eff} - from neutron transport theory down to a simple linear model, or first-order perturbation theory. The assumed linear relationship between a parameter and the nuclear data used in its calculation is shown in Eq. 1. The first-order derivative, or slope of the linear function, is the sensitivity coefficient matrix $\mathbf{S}$. $\mathbf{C_0}$ is the nominal calculated value with a given neutron transport solver and $\mathbf{C_S}$ is the value calculated with the linear approximation given a change in $\boldsymbol{\sigma}$ ($\Delta\boldsymbol{\sigma}$). The sensitivity coefficients with the linear approximation can be seen as a tool to rapidly scope changes to the nuclear data $\boldsymbol{\sigma}$ without fully solving the neutron transport equation. Here, $\boldsymbol{\sigma}$ is a vector containing the nuclear data with a size $N_\sigma \times 1$, where N_σ equals the number of isotope/reaction pairs $\times$ number of energy groups in the nuclear data. $\mathbf{S}$ is a matrix of dimensions $N_E \times N_\sigma$, where N_E is the number of integral parameters considered. $\mathbf{C_S}$ and $\mathbf{C_0}$ are vectors with a size $N_E \times 1$.

$$\mathbf{C_S} = \mathbf{C_0} + \mathbf{S}\Delta\boldsymbol{\sigma} \tag{1}$$

The linear approximation is often used in uncertainty quantification. By doing linear error propagation on Eq. 1, the uncertainty on $\mathbf{C}$ can be approximated by taking the diagonal elements of the matrix $\mathbf{M_C}$ calculated with Eq. 2. $\mathbf{M}_\sigma$ is a covariance matrix of the nuclear data (size: $N_\sigma \times N_\sigma$).

$$\mathbf{M_C} = \mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T \tag{2}$$

The linear approximation is also used in DA theory to derive the generalized linear least squares (GLLS) technique and has been shown to be effective for linear responses such as k_{eff} [5]. The linear model for $\mathbf{C}$ is fit to experimental values, $\mathbf{E}$, by using Lagrangian multipliers to find the roots that minimize an error function. The roots of $\boldsymbol{\sigma}$ become the posterior nuclear data set $\boldsymbol{\sigma'}$ and are the updated cross sections. The posterior nuclear data set $\boldsymbol{\sigma'}$ is given by Eq. 3. The posterior nuclear data covariance matrix, $\mathbf{M}'_\sigma$, is calculated with Eq. 4. $\mathbf{M_E}$ and $\mathbf{M_M}$ are the experimental and modeling/methodology covariance matrices, respectively, and their dimensions are $N_E \times N_E$. $\mathbf{E}$ and $\mathbf{C}$ are vectors of size $N_E \times 1$.

$$\boldsymbol{\sigma'} = \boldsymbol{\sigma} + \mathbf{M}_\sigma\mathbf{S}^T\big[\mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T + \mathbf{M_E} + \mathbf{M_M}\big]^{-1}\big[\mathbf{E} - \mathbf{C}(\boldsymbol{\sigma})\big] \tag{3}$$

$$\mathbf{M}'_\sigma = \mathbf{M}_\sigma - \mathbf{M}_\sigma\mathbf{S}^T\big[\mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T + \mathbf{M_E} + \mathbf{M_M}\big]^{-1}\mathbf{S}\mathbf{M}_\sigma \tag{4}$$

After DA has been performed, the posterior calculated value, $\mathbf{C}'$, can easily be found if the assumption of its linearity is valid. This is done by using the calculated sensitivity coefficients, and the prior and posterior nuclear data together, as seen in Eq. 5. These values can then be used in the desired application analyses or used to reevaluate the bias between $\mathbf{E}$ and $\mathbf{C}$. Additionally the uncertainty associated with the $\mathbf{C}'$ can be calculated with $\mathbf{M}'_\sigma$ by taking the diagonal elements of matrix $\mathbf{M}'_\mathbf{C}$ calculated as seen in Eq. 6.

$$\mathbf{C}' = \mathbf{C}(\boldsymbol{\sigma}) + \mathbf{S}(\boldsymbol{\sigma'} - \boldsymbol{\sigma}) \tag{5}$$

$$\mathbf{M}'_\mathbf{C} = \mathbf{S}\mathbf{M}'_\sigma\mathbf{S}^T \tag{6}$$

The equations presented in this section show the predominant role that sensitivity coefficients have in these applications. When Monte Carlo neutron transport codes are used to do these analyses, the statistical uncertainties associated with Monte Carlo results will propagate to the results. For example, the calculated values $\mathbf{C_0}$ in Eq. 1 and $\mathbf{C}(\boldsymbol{\sigma})$ in Eq. 3 will have statistical uncertainties that will affect the output values. The sensitivity coefficients used in all of the above equations to calculate $\mathbf{C_S}$, $\mathbf{M_C}$, $\boldsymbol{\sigma'}$, $\mathbf{M}'_\sigma$, $\mathbf{C}'$, and $\mathbf{M}'_\mathbf{C}$ may have important uncertainties that affect the final results. The mean values for $\mathbf{S}$ and $\mathbf{C_0}$ or $\mathbf{C}(\boldsymbol{\sigma})$ need to be sufficiently converged and their uncertainties need to be sufficiently small to have accurate results. What "sufficient" means for the applications and Serpent run times is the subject of the rest of this document.

3. APPROACH

This document presents the simple benchmark Jezebel Pu-239 to effect this study [6]. Its integral responses include k_{eff} and the spectral indices F28/F25, F49/F25, and F37/F25. Here, spectral indices are referred to as Fij which is the fission of isotope $2jx$ of element $9i$ (i.e. $i = 2, 3, 4$ for U, Np, and Pu, respectively). F37, for example, is the Np-237 fission rate. The COMMARA-2.0 covariance data [7] is used together with the ENDF/B-VII.0 central values [8]. The sensitivity coefficients and nuclear data are discretized in the ECCO 33-energy-group structure [9].

The isotopes Pu-239, Pu-240, and Pu-241 are included in the adjustment. The following nuclear data were explicitly considered: Elastic scattering (MF3/MT2), total inelastic scattering (MF3/MT4), capture (MF3/MT100), fission (MF3/MT18), the average prompt fission neutron multiplicity (MF3/MT456), and the normalized prompt fission neutron spectrum (MF5/MT181). The GLLS calculations use the experimental covariance matrix ($\mathbf{M_E}$) shown in Table I. The correlation factors are taken from the DA analysis in Ref. [4]. For the modeling/modeling covariance matrix ($\mathbf{M_M}$) in GLLS, the variances are the statistical uncertainties of the calculated values from the Serpent simulation.

Table I: Experimental covariance matrix. Diagonal terms are relative standard deviations in percent, off-diagonal terms are correlation coefficients.

	k_{eff}	F28/F25	F49/F25	F37/F25
k_{eff}	0.2%	0.0	0.0	0.0
F28/F25	0.0	1.1%	0.23	0.23
F49/F25	0.0	0.23	0.9%	0.32
F37/F25	0.0	0.23	0.32	1.4%

The Jezebel model is executed in Serpent with 20,000 particles per cycle. Fifteen latent generations are used for the sensitivity calculations. Every ten cycles, the sensitivity coefficients and $\mathbf{C}$ values are written to their respective output files and used to estimate the parameters in the three applications. In this way, the evolution of the calculated parameters in first-order perturbation theory, uncertainty quantification, and DA can be studied as the number of simulated particles increases.

4. RESULTS

4.1. Effects on Linear Approximation and Uncertainty Quantification

The linear model of a calculated parameter is the *raison d'être* of sensitivity coefficients. Subsequently, it is the logical place to start the study. The linear model is also investigated in Section 4.2 when used in DA. This section presents the uncertainty associated with the calculated value of

$\mathbf{C}$ from the linear approximation, or the uncertainty associated with $\mathbf{C_S}$. The uncertainty comes from three sources: the nuclear data, the nominal calculated value $\mathbf{C_0}$ from the Monte Carlo calculation, and from the sensitivities themselves. By investigating the convergence of these sources of uncertainty, it is possible to investigate the effects of the sensitivities' mean values' convergence and of the sensitivities' uncertainties. The nuclear data uncertainty should converge as the sensitivities converge. The uncertainty coming from sensitivities and $\mathbf{C_0}$ should decrease as the number of particles increases. A good convergence criterion for the sensitivity coefficients will be able to consider, simultaneously, these three sources of uncertainty on $\mathbf{C_S}$. Importantly, this analysis ignores the fact that $\mathbf{C_0}$, $\mathbf{S}$, and $\boldsymbol{\sigma}$ may be correlated. This correlation may be important to the overall uncertainty of $\mathbf{C_S}$.

The sensitivity mean values' convergence is investigated by looking at the uncertainty from nuclear data calculated with Eq. 2. This equation directly uses the sensitivity mean values and can be used to assess sensitivity mean value convergence. It is expected that as the number of particles in the simulation increases, important sensitivities (ones that contribute most to calculating the nuclear data uncertainty) will converge, meaning that the nuclear data uncertainty will also converge. Unimportant sensitivities that are not converged will not have a significant effect on nuclear data uncertainty.

Next, the effect of the sensitivity uncertainties on $\mathbf{C_S}$ is assessed by using Eq. 7. Examining this parameter allows assessing the effect of sensitivity uncertainties. Eq. 7 comes from linear error propagation on Eq. 1 assuming that the sensitivities are the random variable. $\mathbf{M_S}$ is the covariance matrix of the sensitivity coefficients, where the diagonal is variances of the sensitivities taken from the Serpent output file. It is assumed that the sensitivities are not correlated, i.e. the covariances in $\mathbf{M_S}$ are all zero. The change in the cross section, $\Delta\boldsymbol{\sigma}$, that produces $\mathbf{C_S}$ from the linear model is not known *a priori*. For the purposes of proposing a convergence criterion, it is assumed that the change in the cross sections in 100%, or $\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}$. This will over predict the uncertainty on $\mathbf{C_S}$ coming from sensitivities. However because the aim of this work is to propose a convergence criterion, this will give a conservative estimate of the uncertainty coming from sensitivities. Later when examining DA in Section 4.2, a real $\Delta\boldsymbol{\sigma}$ is used and a more realistic estimate of the effect of sensitivity uncertainties on first-order perturbation theory can be seen. Other values besides $\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}$ could be used, but this value was chosen for its simplicity.

$$\mathrm{var}(\mathbf{C_S}) = \mathrm{diag}\big(\Delta\boldsymbol{\sigma}\mathbf{M_S}\Delta\boldsymbol{\sigma}\big) \tag{7}$$

Figure 1 shows the convergence of the three sources of uncertainty for Jezebel's four responses as the number of particles increases. The values are plotted at intervals of 2,000,000 particles, i.e. one unit on the x-axis is equivalent to 2,000,000 particles. When the number of particles is low, 2-20 million, the uncertainty in $\mathbf{C_S}$ from sensitivities is significant, i.e. close to the uncertainty from nuclear data. Here, the sensitivity coefficients are not yet acceptable for first-order perturbation theory analyses with $\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}$. The uncertainty in $\mathbf{C_S}$ from sensitivities then decreases rapidly within the first 100 units on the x-axis, or 100*2e+6 = 2e+8 particles. By 1,000 units, or 2e+9 particles, the uncertainty in $\mathbf{C_S}$ from sensitivities is roughly equal to that coming from the uncertainty in $\mathbf{C_0}$. Examining the nuclear data uncertainties' convergence, and thereby the sensitivity mean values, shows approximate convergence after $\sim$100 x-axis units (2e+8 particles).
From this set of results, a criterion can be proposed for halting a simulation when the sensitives

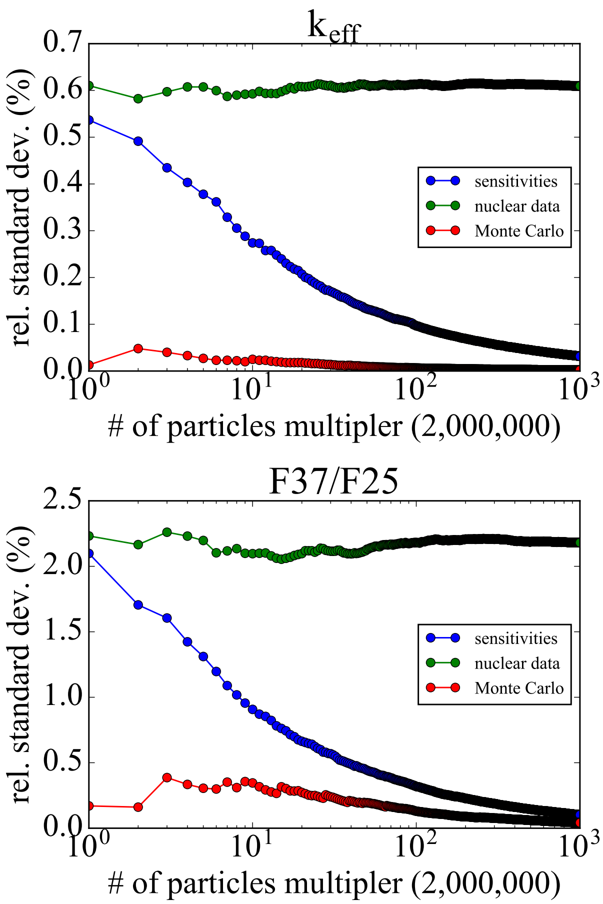

Figure 1: Uncertainties on C calculated with first-order perturbation theory.

are acceptable. If $\Delta\boldsymbol{\sigma}\mathbf{M_S}\Delta\boldsymbol{\sigma} + \text{var}(\mathbf{C_0}) << \mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T$, then the simulation can be stopped. This criterion can be applied to perturbation theory analyses and to uncertainty quantification. It will also be tested against DA later. It covers the convergence of $\mathbf{C_0}$ and the acceptability of the $\mathbf{S}$ uncertainties. Because $\mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T$ is converged when $\Delta\boldsymbol{\sigma}\mathbf{M_S}\Delta\boldsymbol{\sigma} + \text{var}(\mathbf{C_0})$ becomes small, it also covers $\mathbf{S}$ mean value convergence. From the data sets presented in this work, the criterion $0.2 * (\Delta\boldsymbol{\sigma}\mathbf{M_S}\Delta\boldsymbol{\sigma} + \text{var}(\mathbf{C_0})) < \mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T$, where $\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}$, was effective in showing convergence for the considered parameters. If another value besides $\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma}$ was used, the results would be consistent and only the constant term 0.2 (where convergence occurs) would be altered. It should also be noted that the $\mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T$ term also has an uncertainty coming from the sensitivity uncertainties that is not described here. The reduction of this uncertainty to an acceptable level would also be covered by the proposed criterion.

4.2. Effects on Data Assimilation Posteriors

The sensitivity coefficients play an important role in the GLLS equations. They are used in Eqs. 3 and 4 in the term $\mathbf{S}\mathbf{M}_\sigma\mathbf{S}^T$ that estimates the variances/covariances of calculated values and in the $\mathbf{S}\mathbf{M}_\sigma$ term that estimates the covariances between calculated values and nuclear data. Additionally, they are used to calculate the posterior moments of the calculated values in Eqs. 5 and 6. First, the effects on the posterior nuclear data calculated with Eqs. 3 and 4 are presented, followed by the calculated values' posterior moments.

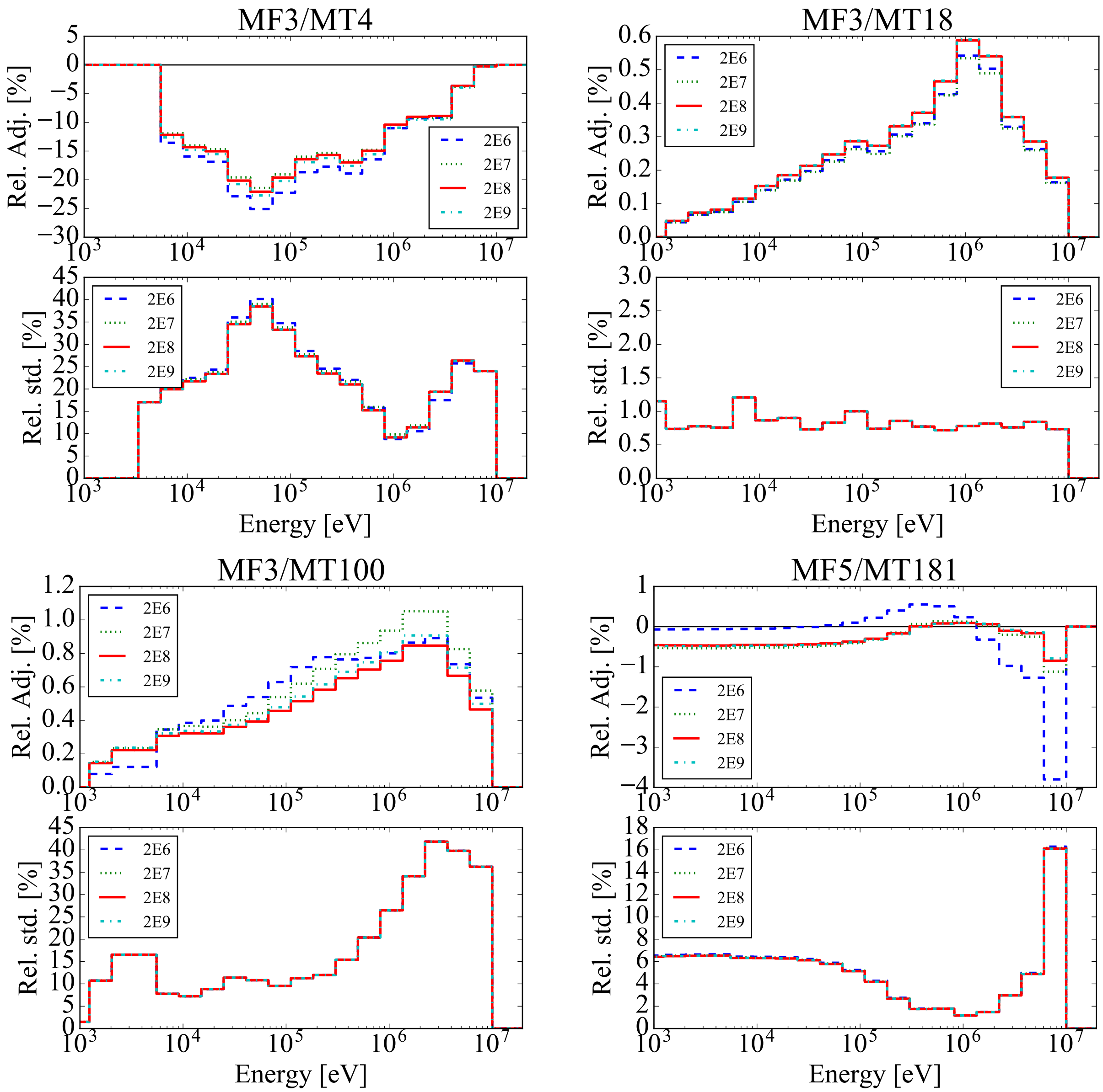

Figure 2: Adjustments to Pu-239 reactions calculated with sensitivity coefficients from different numbers of particle histories (2e+6, 2e+7, 2e+8, 2e+9).

4.2.1. Nuclear Data

The adjustments to select nuclear data at different numbers of particle histories are shown in Figure 2. The adjustments are shown at 2e+6, 2e+7, 2e+8, and 2e+9 particles. For reference with other figures presented in this document, this corresponds to 1, 10, 100, and 1,000 units on their x-axes. The red line representing the adjustment at 2e+8 particles corresponds approximately to where the convergence criterion for first-order perturbation theory presented in Section 4.1 is satisfied. The data are all roughly converged by 2e+8 particles, similar to first-order perturbation theory. This intimates that the proposed criterion may also be suitable for nuclear data adjustment purposes.

Remarkably, the adjustments to the nuclear data are not greatly affected by the sensitivities' uncertainties. The low sensitivity of the posterior nuclear data to the sensitivity coefficient fluctuations is likely related to the other terms in Eqs. 3 and 4. Particularly, the experimental covariance matrix $\mathbf{M_E}$. The values in $\mathbf{M_E}$ are roughly equivalent to those in $\mathbf{S M_\sigma S}^T$. $\mathbf{M_E}$ serves as a ballast as fluctuations in the terms $\mathbf{S M_\sigma S}^T$ and $\mathbf{S M_\sigma}$ may be happening. This restricts the fluctuations in the sensitivities from significantly affecting the adjustments.

4.2.2. Calculated Values

The posterior calculated values are made with in Eqs. 5 and 6, which incorporate the posterior nuclear data and the sensitivities. First, the posterior $\mathbf{C}$ mean values ($\mathbf{C}'$) are shown in Figure 3. $\mathbf{C}'$ shows convergence after 100-300 units on the x-axis, similar to the $\mathbf{C}$ uncertainties shown in Figure 1. For instance, k_{eff} varies at $\sim$2 pcm after 100 x-units. The convergence of $\mathbf{C}'$ seen in Figure 3 corroborates the convergence criterion presented in Section 4.1.

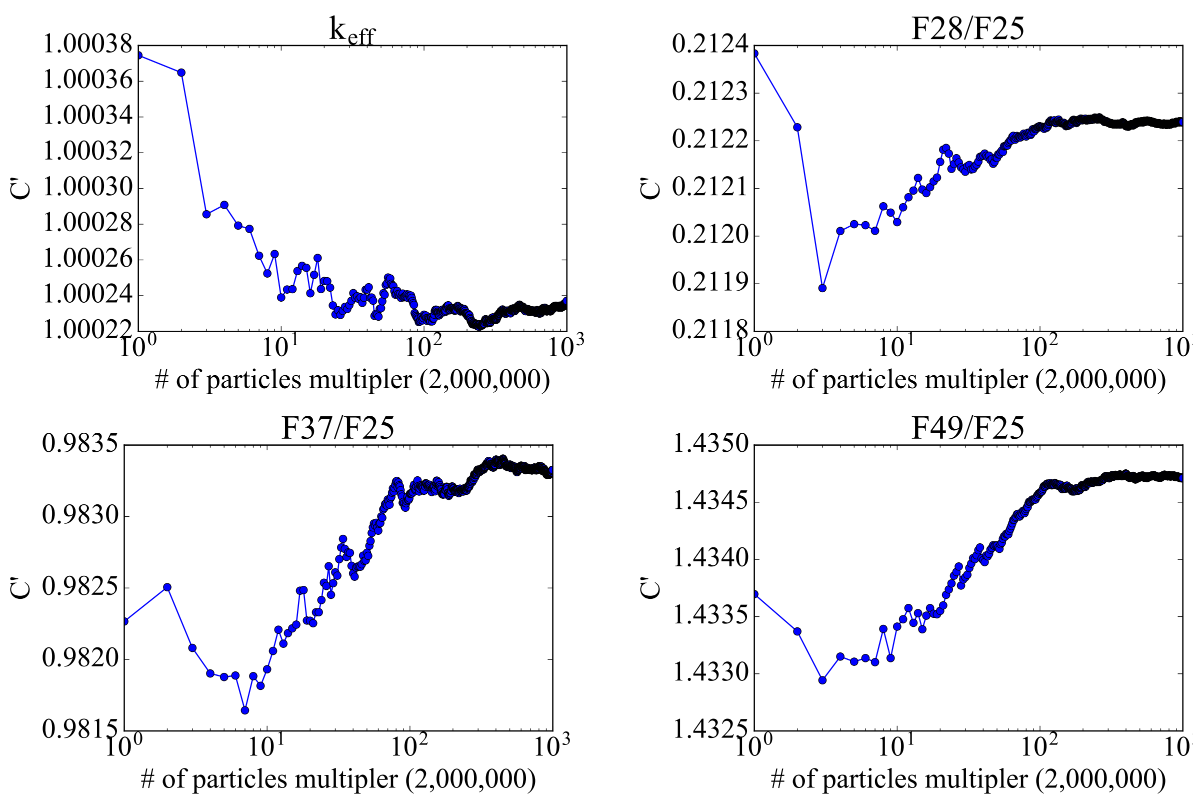

Figure 3: Convergence of posterior calculated values (C′).

The $\mathbf{C}'$ uncertainties from nuclear data and from the sensitivity coefficients are shown in Figure 4. As done for the prior $\mathbf{C}$ values, the uncertainty on $\mathbf{C}'$ coming from the sensitivities' statistical uncertainties can be computed with Eq. 7. In this case, $\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma'} - \boldsymbol{\sigma_0}$ is used instead of $\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma_0}$. This represents a much more realistic estimation of the uncertainty on a $\mathbf{C}$ value calculated with first-order perturbation theory coming from sensitivity uncertainties. Here, it is seen that at 2e+6 particles, the uncertainty from sensitivity uncertainties is roughly one-fifth that coming from nuclear data. By ∼100 units on the x-axis, the uncertainty from sensitivities for all four responses is insignificant compared to that from nuclear data. Additionally, the nuclear data uncertainty is roughly converged at ∼100 units on the x-axis. Figure 4 shows little fluctuations as the number of particles increase, i.e. as the sensitivities become more precise. This behavior reflects that seen for the posterior nuclear data uncertainties seen in Figure 2: Because $\mathbf{M}'_{\mathbf{C}}$ is calculated with $\mathbf{M}'_{\sigma}$, small fluctuations in $\mathbf{M}'_{\sigma}$ will result in small fluctuations in $\mathbf{M}'_{\mathbf{C}}$. Examining these results, the convergence criterion proposed in this work can also be applied to posterior $\mathbf{C}$ uncertainties.

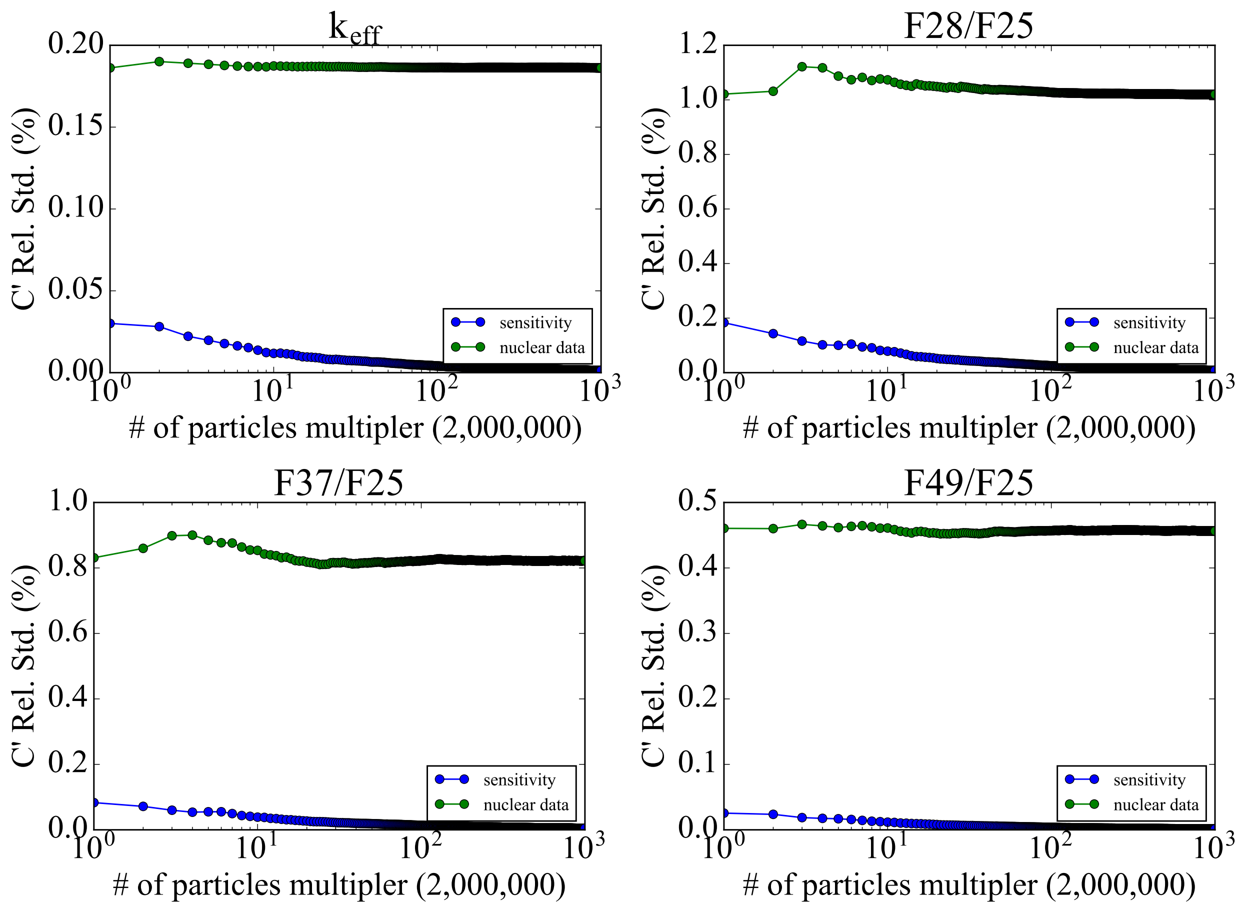

Figure 4: Convergence of the posterior calculated values' (C′) relative standard deviations.

5. CONCLUSIONS

The sensitivity coefficients calculated with Serpent are subject to statistical fluctuations and uncertainty. The statistical fluctuations and uncertainty affect parameters that are calculated with the sensitivity coefficients in first-order perturbation theory, uncertainty quantification, and data assimilation. The convergence study presented here described the effects of sensitivity mean values and uncertainties on these applications. In terms of data assimilation, the posterior nuclear data are remarkably insensitive to the statistical fluctuations of the sensitivity coefficients. This is because of other terms in the equations, such as the experimental covariances, lessen the impact of the fluctuations. For first-order perturbation theory studied by examining the posterior calculated values, convergence was seen within 200,000,000 particles. The posterior calculated values' uncertainties converge rapidly because the posterior nuclear data covariance matrix is not greatly affected by sensitivity uncertainties.

A convergence criterion is proposed for sensitivity calculations when they are used perturbation theory, uncertainty quantification, and data assimilation. The criterion consists of checking, as the simulation is running, the uncertainty on the calculated value with first-order perturbation theory that comes from three sources: the nuclear data, the nominal calculated value from the Monte Carlo calculation, and from the sensitivities themselves. In this work, it was found that once the combined uncertainty from nominal calculated value and from sensitivity coefficients was $\sim$0.2 times smaller than the uncertainty from nuclear data, there was convergence for all parameters calculated with sensitivity coefficients. At this point, the simulation can be stopped. This criterion would ensure that the sensitivities sufficiently well approximated that they would give good results in first-order perturbation theory, uncertainty quantification, and data assimilation. The results presented in this document show that this criterion works well for the three applications investigated and that it could be employed to significantly economize computational resources in future applications. The criterion is advantageous because it is a simple calculation that circumvents the need to setup the full data assimilation procedure, but is still applicable to data assimilation results.

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