LA-UR-13-27088
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Intended for: Supercomputing in Nuclear Applications + Monte Carlo, 2013-10-27/2013-10-31 (Paris, France)

Issued: 2013-09-11

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013)
La Cité des Sciences et de l'Industrie, Paris, France, October 27–31, 2013

Monte Carlo Approaches for Uncertainty Quantification of Criticality for System Dimensions

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MCNP6 is used to estimate uncertainties from geometric tolerances using forward and adjoint methods. Results are obtained and the forward and adjoint approaches appear to agree in some cases where the responses are not non-linearly correlated. In other cases, the uncertainties in k disagree for reasons not yet known.

KEYWORDS: MCNP, adjoint, perturbation, sensitivity

I. Introduction

One of the current challenges in nuclear engineering computations is the issue of performing uncertainty analysis for either calculations or experimental measurements. It is often not enough to just know the answer, but also how well that answer is known. In neutron transport, the uncertainty arises from any system parameter: nuclear data, densities, compositions/enrichments, geometry (component dimensions and positions), model approximations, theory assumptions, etc. The dominant source of uncertainty in most neutronics calculations are the nuclear data, e.g., cross sections, fission multiplicities and spectra, etc., and this aspect has been studied extensively. In trying to quantify the uncertainty for measurements of an experimental benchmark, the other system parameters matter. This paper specifically focuses on the issue of estimating the uncertainties arising from geometric tolerances.

There are many sophisticated techniques for uncertainty quantification available. For this paper, only two cases are studied. The first is the forward propagation technique, which can be thought of as a "brute force" approach; uncertain system parameters are randomly sampled, the calculation is run, and uncertainties are found from the empirically obtained distribution of results. This approach need make no approximations in principle, but is very computationally expensive. The other approach investigated is the adjoint-based approach; system sensitivities are computed via a single Monte Carlo calculation and those are used with a covariance matrix to provide a linear estimate of the uncertainty.

An overview of the forward and adjoint approaches is given. Demonstration calculations are performed with MCNP6[(1)] for both. The results show that in many cases the forward and adjoint cases agree, but in others they disagree, suggesting possible errors in the coding or limitations of the adjoint theory applied to geometry.

II. Forward Approach

Forward methods are perhaps the most intuitive. A set of uncertain parameters $X = [x_1, \ldots, x_i, \ldots]$ are defined, each having an underlying probability distribution $f_i(X)$, which may be correlated (perhaps non-linearly or with constraints) with the other parameters.

Each $f_i(X)$ is randomly sampled to generate a random realization of X, which are then used to define a problem geometry. This random realization is run through a code (e.g., MCNP) and a result such as k is obtained for that realization. After numerous realizations N, the distribution of results is obtained, and mean values, variances, normality, or other properties of the output distribution are obtained. The uncertainty in result R is obtained via the standard deviation from basic sample statistics:

$$\delta R = \sqrt{\frac{1}{N-1}\sum_{i-1}^{N}\left(R_i - \bar{R}\right)^2}. \quad (1)$$

This process has the advantage that it is very general and exact within the knowledge of the underlying distributions $f_i(X)$, which may not be known in practice. The main disadvantage is that if the dimensionality of X is large, it may be necessary to perform a very large number of random realizations before the output distribution may become resolved enough to make meaningful inferences.

MCNP provides a utility called *pstudy*[(2)] (a Perl preprocessor script) for forward simulations of uncertainty quantification. The *pstudy* script parses a special MCNP input file (call it the master) containing special macros—the macros are not recognized by MCNP, so it cannot be run directly on the master input file. The script is quite general, allowing for almost any input parameter to be randomly varied, and allowing for user-defined constraints on the random parameters (e.g., to prevent overlaps in parts). When *pstudy* processes the master input file, it creates N derivative input files. Each of these N files is then run, either sequentially or submitted in parallel via batch submit to a cluster. Upon conclusion, MCNP collects the MCTAL output files (a file containing just the tally results and none

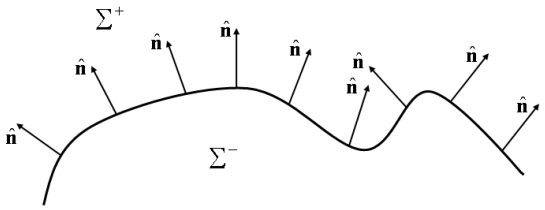

Figure 1: Illustration of surface defined by contour B with corresponding cross sections.

of the details of the calculation found in the standard MCNP output file) and calculates averages and standard deviations of results.

III. Adjoint Approach

The adjoint method arises from an application of perturbation theory, which can be used to compute sensitivity coefficients $s_{R,x}$. The sensitivity coefficient for response R arising from system parameter x is defined as

$$s_{R,x} = \frac{dR/R}{dx/x}, \tag{2}$$

or the ratio of the relative differential change in R arising from the relative differential change in x.

To compute the uncertainty the sensitivities are placed in a vector $\mathbf{S} = [s_1, \ldots, s_i, \ldots]$ and convolved with a covariance matrix $\mathbf{C}$ using the so-called "sandwich rule". The sandwich rule involves a vector-matrix-vector multiplication of

$$(\delta R)^2 = \mathbf{SCS}^T. \tag{3}$$

This uncertainty estimate is limited to quantities that vary and are correlated linearly; non-linear variations in the response R from x cannot be captured by this approach. Another limitation specific to this paper, because of the limitations with the method prototyped in MCNP, the uncertainty estimates are further restricted to only the effective multiplication k and for cases where the surface is uniformly expanded or contracted along its surface normal, although extending this to more general responses should be possible.

To illustrate the mathematics behind adjoint-based geometry perturbations, some terminology is needed. The interface between two zones within a geometry is defined by a surface contour B with an outgoing surface normal $\hat{\mathbf{n}}$ as shown in Fig. 1. The zone on the positive side of the surface normal is defined to be the positive zone with respect to the surface, whereas the zone on the negative side is defined as the negative zone. The positive and negative zones have generic macroscopic cross sections Σ^+ and Σ respectively. With these definitions, it is possible to derive an expression for the derivative of k with respect to interface location b located on surface contour B.

Adjoint-based perturbation theory yields the following relationship for the change in k (define $\lambda = 1/k$, where k is that of the unperturbed system, so $d\lambda = -\lambda^2 dk$) with respect to some cross section perturbation:

$$dk = -\frac{1}{M}\left\langle \psi^\dagger, (d\Sigma_t - dS - \lambda dF)\,\psi \right\rangle, \tag{4}$$

where the brackets $\langle ., . \rangle$ indicate an integration over all phase space (position $\mathbf{r}$, direction $\hat{\mathbf{\Omega}}$, and energy E), ψ is the forward angular flux, $\psi^\dagger$ is the corresponding adjoint function, Σ_t is the total macroscopic cross section, S is the scattering operator given by

$$S = \iint dE'\, d\mathbf{\Omega}'\, \Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\mathbf{\Omega}}' \rightarrow \hat{\mathbf{\Omega}}) \tag{5}$$

with Σ_s as the double-differential scattering cross section, F is the fission operator given by

$$F = \frac{1}{4\pi}\iint dE'\, d\mathbf{\Omega}'\, \chi(E' \rightarrow E)\nu\Sigma_f(\mathbf{r}, E') \tag{6}$$

with χ as the fission emission spectrum, ν as the mean number of neutrons produced per fission, Σ_f as the macroscopic fission cross section, and the quantity M is the adjoint-weighted fission source times λ^2 or

$$M = \left\langle \psi^\dagger, \lambda^2 F\psi \right\rangle. \tag{7}$$

Both the forward and adjoint flux correspond to the unperturbed system.

The functional form of a generic cross section in the vicinity of the surface contour B along some ray r crossing the surface at location b in the positive direction is

$$\Sigma(\mathbf{r}) = \Sigma^- + \Theta(r - b)(\Sigma^+ - \Sigma^-), \tag{8}$$

where Θ is the Heaviside step function. Differentiating the cross section with respect to b, the location of the surface crossing, yields

$$\frac{d\Sigma}{db} = -\delta(r - b)(\Sigma^+ - \Sigma^-), \tag{9}$$

where δ is the Dirac delta function. By substituting Eq. (9) into Eq. (4) and rearranging, the following convenient form is obtained:

$$\frac{dk}{db} = \frac{1}{M}\Big[\left\langle \psi^\dagger, (\Sigma_t^+ - \Sigma_t^-)\,\psi \right\rangle_B + \left\langle \psi^\dagger, S^-\psi \right\rangle_B - \left\langle \psi^\dagger, S^+\psi \right\rangle_B + \left\langle \psi^\dagger, \lambda F^-\psi \right\rangle_B - \left\langle \psi^\dagger, \lambda F^+\psi \right\rangle_B \Big]. \tag{10}$$

Subscript B denotes that the volume integral in the inner product is now a surface integral on contour B. The operators with the + and − superscripts are identical to the corresponding definitions except that their constituent cross sections have inherited the corresponding superscript. Recall that the superscripts denote which side the surface the material is on, not the direction that the neutron is traveling. The reason for the particular form chosen in Eq. (10) is seen in the Monte Carlo methodology.

Each inner product of Eq. (10) constitutes an adjoint-weighted tally computed during a random walk simulation. The numerator has five such terms, and accumulation of information for each occurs each time a neutron crosses the surface

for which the sensitivity is desired. The essential component for all these tallies is an estimate of the flux at the surface, which is done by the traditional estimator of

$$\tilde{\psi}_B = \frac{w}{|\mu|}, \tag{11}$$

where $\tilde{\psi}_B$ denotes an individual contribution to the flux estimate at the surface, w is the numerical particle weight, and μ is the cosine of the angle between the particle trajectory and the surface normal.

Each contribution $\tilde{\psi}_B$ must then be multiplied by an estimate of the adjoint function of that particle after having undergone a process representing the differential change in the interface location. The estimate of the adjoint function is obtained by the Iterated Fission Probability (IFP) method,[3] which calculates the forward responses in 10 and assigns each scoring neutron a tag that is passed to subsequent fission generations. After some number of fission generations such that the particle distribution has reached stationarity, an estimate of the population of neutrons arising from the neutron that made that original contribution is made—the population or response after a long time is proportional to the adjoint function—and multiplied by the original scores to form the final score for an adjoint-weighted integral.

The change in the collision rate from the differential surface perturbation is computed by multiplying $\tilde{\psi}_B$ by

$$\tilde{\psi}_B^{\dagger}(\Sigma_t^+ - \Sigma_t^-)/w, \tag{12}$$

where $\tilde{\psi}_B^{\dagger}$ is the estimate of the adjoint function for the particle that just crossed the surface. The factor $(\Sigma_t^+ - \Sigma_t^-)$ arises from the differential change in the collision rate that would have occurred had the surface been moved uniformly an infinitesimal amount at every point in the direction of the surface normal.

The scatter (and fission) source rate derivative terms are computed in a different, and far less efficient, manner. As with the collision rate derivative term, $\tilde{\psi}_B$ is multiplied by

$$\tilde{\psi}_B^{\dagger}\Sigma_s^{\pm}/(\Sigma_s^+ + \Sigma_s^-) \tag{13}$$

for the scattering term, but in this case $\tilde{\psi}_B^{\dagger}$ is the importance of a neutron that would have undergone a scattering process on both sides of the interface had it undergone a differential, uniform perturbation along the surface normal. For the fission term, $\tilde{\psi}_B$ is multiplied by

$$\tilde{\psi}_B^{\dagger}\nu\Sigma_f^{\pm}/(\nu\Sigma_f^+ + \nu\Sigma_f^-). \tag{14}$$

Unfortunately, unless from happenstance, such neutrons will not exist in the simulation to follow and estimate its adjoint function. This is unlike the collision rate derivative term, where the importance is with respect to the existing neutron that will be followed in the course of the normal random walk. Also consider that the adjoint function poses a "what if" question about a neutron's expected future—the neutron need not actually exist or even be possible to appear in the problem, but it may still have a non-zero importance function. Since this "what if" question is being asked about a neutron that does not normally exist in the random walk, one must be created with unit weight and followed for the sole purpose of making an estimate of its importance, and this must be done in a way that does not influence the results since it is not an actual neutron in the system.

To produce this so-called *pseudoneutron*, the simulated (physical) neutron must undergo an artificial scattering event (a *pseudoscatter*) and the resulting secondary, the pseudoneutron, from that is treated separate from the physical particles. Pseudoneutrons undergo all interactions that a physical neutron would and produce progeny (also pseudoneutrons) from fission, but they do not contribute to any tallies in the problem except for making a single estimate of the adjoint function $\tilde{\psi}_B^{\dagger}$. Pseudoneutrons do not interact with the boundary sensitivity tallies that produced them and therefore their surface crossings do not result in the production of more pseudoneutrons. The main drawback to the pseudoneutron approach is that it adds additional random walks and therefore necessitates increases in computational time that in practice are quite significant. Unfortunately, because this "what if" question must be answered for a neutron that would not normally exist, this computationally expensive operation must be carried out.

Since perturbing the surface results in a gain in the size and material of the negative zone and in a corresponding loss to the positive zone, both the gain (positively weighted collision) and loss (negatively weighted collision) must be accounted for by an individual pseudoneutron. In the case where one of the materials is vacuum, no pseudoneutron for that zone (whether positive or negative) is generated since no collision may occur there. Also, in the case where the materials and densities of the zones are identical, no pseudoneutrons are generated for reasons of efficiency since, on average, the two scatter and fission terms will sum to zero.

IV. Results

Two systems are considered to test how well the forward and adjoint-based methods agree. The first system is a solid, bare cylinder of Pu-metal (Jezebel in cylindrical form) with the radius and height varied both independently and in a way that preserves overall mass. The second system is a can of plutonium-nitrate solution where the solution height and inner and outer radii of the can are varied.

1. Bare Pu Cylinder

A bare cylinder of Pu metal (same material and density as the Jezebel benchmark[4]) has a nominal radius R of 6.3849 cm and a height H of 9.3269 cm with a nominal k of 1.00116 ± 0.00011. Two different sensitivity/uncertainty studies are performed. The first involves independently perturbing the radius and height. The radius is normally distributed with a standard deviation of 5% the nominal value, and the height is also normally distributed with a standard deviation of 10% its nominal value. the second study involves perturbing the radius (same distribution as before) and fixing the height such that the overall mass is preserved. For the forward method, *pstudy* is employed to run 100 independent random cases the sample standard deviation is computed from the empirical distribution of results. The

	Forward	Adjoint	C/E
Uncorr.	4126	4277	1.037
Corr.	852	938	1.101

Table 1: Comparison of δk (in pcm) from the forward and adjoint calculations for the uncorrelated and correlated studies.

adjoint method generates sensitivities for the radius and one of the planar surfaces defining the cylinder and uses the sandwich rule to compute the estimate of the uncertainty. In the second study, the radius and height are non-linearly correlated, but a linear correlation coefficient is used, which is empirically to be found as -0.9949.

The sensitivity to the radius was calculated to be 0.083628 ± 0.00306 cm^{-1} and the sensitivity of the cylinder height is 0.035823 ± 0.00190 cm^{-1}. Each adjoint calculation was performed in about five minutes a piece, whereas the forward calculations took about two hours each to complete. The computed overall uncertainties in k (in units of pcm where 1 pcm = 10^{-5} are given in Table 1 along with the C/E value to indicate the goodness of agreement; in this case the C/E is the ratio of the uncertainty from the adjoint calculation to the one found empirically from the forward ones. The results of the uncorrelated study agree within 4% error and the results for the non-linearly correlated case agree within about 10%. The agreement for the uncorrelated case is within 1-2σ statistical uncertainties of the computed sensitivities, implying decent agreement. The correlated case is disagrees by about 3σ, but this is expected because the adjoint case may only capture linear correlation, where the variation here is non-linear. Nonetheless, a decent approximation for either can be gained within a matter of minutes with the adjoint case as opposed to hours with the forward case.

2. Pu-Nitrate Solution

The second test case looks at a more complicated variation. The test problem used is a stainless steel can of plutonium-nitrate solution—dimensions and material properties may be found in Chapter 5 of the MCNP Criticality Primer.[5]

Three parameters are varied: the solution volume, the inner radius R_{in}, and the thickness. From these the solution height H_{sol} and the outer radius R_{out} are derived. The volume is varied normally with a standard deviation of 5%, the inner radius is varied normally with a standard deviation of 0.1 cm, and the thickness is varied normally with a standard deviation of 0.02 cm. Table 2 gives the correlation matrix for the inner and outer radii and the solution height. The diagonal terms are the standard deviation in cm, and the off-diagonal terms are the empirically found linear-correlation coefficients.

The results for the sensitivty/uncertainty study are given in Table 3. The δk terms are the uncertainty for each parameter

	R_{in}	R_{out}	H_{sol}
R_{in}	0.104	0.984	-0.352
R_{out}	0.984	0.106	-0.363
H_{sol}	-0.352	-0.363	2.120

Table 2: Correlation matrix for the Pu-Nitrate Solution sensitivity/uncertainty study.

x_i	dk/dx_i (cm^{-1})	δk (pcm)
R_{in}	-4.524×10^{-2}	475
R_{out}	6.460×10^{-2}	688
H_{sol}	1.156×10^{-3}	245
Correl.		-585
Adjoint		274
Forward		663

Table 3: Results for the Pu-Nitrate Solution sensitivity/uncertainty study.

alone; the correlation value is the sum of the off-diagonal terms signed-square rooted. The total uncertainty δk is obtained by taking the signed sum squared of the four other terms in the the table. As seen the forward and adjoint uncertainties disagree by about a factor of 2.4. Not including the correlation terms leads to an adjoint uncertainty of 871 pcm, which then overpredicts the uncertainty by a factor of 1.3.

Clearly, this result is not even close, unlike the bare metal cylinder case. An investigation reveals that there may be some issue with calculating the sensitivity coefficients for the Pu-nitrate cylinder case. The sensitivities compared to those obtained by two separate calculations using a central difference derivative appear to differ significantly. Interestingly, this does not hold true for other cases tested.[6] Investigation continues to explain this large discrepancy.

V. Conclusions

Both forward and adjoint approaches have been applied to calculating geometric uncertainties of k using MCNP6. It appears the results compare favorably for the bare Pu-metal cylinder case, but not so for a stainless steel can of Pu-nitrate solution. The reasons for this are currently under investigation.

Acknowledgments

Funding for this work was provided by the U.S. Department of Energy/National Nuclear Security Agency Nuclear Criticality Safety Program.

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