

CHAPTER 11: UNCERTAINTY ANALYSIS IN MCNP

It is important to keep in mind that the statistical error estimated by Monte Carlo calculations is indicative of the precision of the estimated quantities, not its accuracy; that is one can obtain a result with zero variance that is far from the true answer of the problem. The accuracy of the solution depends on the models used in the simulation, uncertainties in the cross sections, the adequacy of the input data as being representative of the problem it intends to simulate, etc. The precision of the problem depends on its nature, the suitability of the tally (estimator) type and, of course, on the number of histories run.

11.1 Fractional Standard Deviation (Relative Error)

All MCNP calculations, normalized to per starting particle history (except for some criticality calculations), are printed together with the fractional standard deviation (fsd), also called the relative error (R). In reporting Monte Carlo results it is important to give both the result and its fsd. A Monte Carlo result, like an experimental result, is not worth reporting without stating with it the value of the associated error. Note that a zero answer implies that no scoring has taken place and consequently fsd will be equal to zero. Acceptable values of the fsd are determined empirically to be as follows:

- For point detectors, an fsd of less than 0.05 (5%) should be obtained; since they are vulnerable to singularities.
- For other estimators, fsd should be less than 0.1 (10%).
- If the fsd is above the values stated above, but less than 0.2 (20%), the results are doubtful.
- If fsd is greater than 0.50 (50% error), the results are completely unreliable.

11.2 Figure of Merit

The fsd may not decrease inversely with the $N^{1/2}$, where N is the number of histories, since infrequent large contributions may cause fluctuations in both fsd and the estimated mean. Therefore, MCNP provides a Figure of Merit (FOM) to assist the user in assessing the statistical behaviour of the obtained answer:

$$\text{FOM} = 1/(\text{fsd}^2 \text{ cpu})$$

where cpu is the computer time for the job. The FOM value is printed every 1000 histories, up to 20,000 histories, and the increment is doubled after every 20,000 histories. The PRDMP card can however change this default increment. A well-behaved estimator will provide a near-constant value of FOM, except early in the problem. An erratic behaviour of FOM indicates that the problem is not converging to the correct solution, that is the estimated quantity is far from

the actual value (even if fsd is small). Another use of FOM is to estimate the time required to attain a desired fsd using $\approx 1/fsd^2$ FOM.

A large value of FOM is desirable as it shortens the execution time. Therefore, one can use this to optimize the efficiency of the calculations by making several short test runs with different variance reduction parameters and then selecting the value of the largest FOM. Note that a good variance reduction technique will tend to reduce the number of non-zero scores in the tally and hence decreases the value of the fsd .

The fsd (R) is related to the second moment of the empirical score's probability density function. Higher order moments provide more sensitive indicators of the fluctuations, and large scores, in the scoring process in a tally. MCNP calculates a parameter called the variance of the variance (VOV), which is the estimated relative variance of the fsd . The value of VOV should be below 0.10 to improve the probability of forming a reliable confidence level. VOV is expected to decrease as $1/N$. Note however that an acceptable value of VOV does not guarantee a high quality confidence interval, because under-sampling of high scores underestimates also the higher score moments. The magnitude of VOV is reported in the "Status of Statistical Checks" table, but the PRDMP card can be used to obtain history-dependent checks of VOV but is a time-consuming process.

11.3 Tally Fluctuation Chart

The essence of the Monte Carlo method is the central limit theorem (CLM), which requires a large number of histories to attain the normal distribution upon which the statistical validity of the above parameters (R, VOV and FOM) is based. One indication that a tally has reached the limit of the CLM is that it converged. MCNP prints at the end of the output, one chart for each tally to give an indication of tally fluctuations; that is how well the tally has converged. This is called the tally fluctuation chart (TFC) and is printed for each tally, at the TFC tally bins. These TFC tally bins by default are the first cell, surface or detector defined in the tally's Fn card, the total rather than uncollided flux, the last user bin (as defined by an FU card), the last segment on the first cell or surface, the first multiplier bin on the tally's FM card, the last cosine bin, the last energy bin and the last time bin. These default bins can be changed by the TF card.

11.4 Empirical Probability Density Function

MCNP attempts also to check that the conditions of the CLT by constructing for each estimator a probability density function (pdf) . This is however an empirical estimate, since the actual pdf of a given tally is not known. A pdf, $f(x)$, where x

s the score from one complete particle history to TFC bin tallies. The quantity $f(x)dx$ is the probability of selecting a history score between x and $x+dx$ from TFC bin tallies. Of course, each TFC tally bin has its own $f(x)$. MCNP automatically covers nearly all TFC bin tallies. The average empirical $f^*(\bar{x}_i)$ between x_i and x_{i+1} is defined by:

$$f^*(\bar{x}_i) = (\text{history score in the } i\text{th score bin}) / \{N(x^{i+1} - x^i)\}$$

where $x^{i+1} = 1.2589 x^i = 10^{0.1} x^i$, chosen to provide 10 equally spaced bins per decade. Ten bins per x decade are used to cover the unnormalized tally range from 10^{-30} to 10^{30} . The user can multiply this range at the start of the problem by the 16th entry of the BCDN card.

Negative scores, that usually arise with neutrons are lumped into one bin below the lowest history score in the built-in $f(x)$ grid (see manual). Unless the BCDN(16) card is negative, then the negative score will be accumulated in the grid and the absolute value of BCDN(16) will be used as the score grid multiplier and the positive history scores will be lumped into the lowest bin.

The CLT theorem requires the first two moments of $f(x)$ to exist, the mean and the variance (R^2). One can also examine the behaviour of $f(x)$ for large history scores to assess if $f(x)$ appears to have been "completely" sampled. The absence of large scores leads to underestimation of the mean value, while its presence results in a large variance.

If "complete" sampling has occurred, the largest values of the sampled x 's should have reached the upper bound (if such a bound exists) or should decrease faster than $1/x^3$ so that

$$E(x^2) = \int_{-\infty}^{\infty} x^2 f(x) dx \text{ exists,}$$

where E designates the expected value. Otherwise, N is assumed not to have approached infinity in the sense of the CLT. This is the basis for the use of the empirical $f(x)$ to assess Monte Carlo tally convergence.

11.5 Pareto SLOPE

The slope n in $1/x^n$ of the largest history tallies x is used to determine if and when the largest history scores decrease faster than $1/x^3$. MCNP keeps track of the largest 201 largest scored for each TFC bin tallies. This number is the maximum number of points for a 10% precession in estimating the slope with a generalized Pareto function:

$$\text{Pareto } f(x) = (1+kx/a)^{-1/k-1} / a$$

where a and k are the fitting coefficients. From this functional fit, the slope of $f(x)$ for large x values is defined by $\text{SLOPE} \equiv 1/k+1$. A SLOPE value of zero indicates that not enough large- x tail information is obtained for $f(x)$. The maximum allowed value for SLOPE is ten (10) indicating a "perfect score".

The slope should be greater than three (3) to satisfy the second-moment existence requirement of the CTL. Then, $f(x)$ will appear to be "completely" sampled and hence N will appear to have approached infinity. A printed plot of $f(x)$ is automatically generated in the output file if SLOPE is less than 3, several "S's" appear on the printed plot to indicate the Pareto fit and allow the quality of the fit to the largest history scores to be assessed visually. If the fit does not appear to reflect the best estimate of the largest history scores decrease, a new slope can be estimated graphically.

11.6 Asymmetric Confidence Intervals

The worst situation for forming valid confidence intervals is when the estimated mean is much smaller than the expected value. Then also the estimated variance will be most likely below its expected value, and the confidence interval will cover a smaller than the expected coverage rates. To correct for this, MCNP estimates a statistic shift in the midpoint of the confidence interval to a higher value, without changing the estimated mean. The shifted confidence interval is the estimated mean plus the SHIFT term:

$$\text{SHIFT} = \left\{ \sum (x_i - \bar{x})^3 \right\} / \left\{ 2S^2 N \right\}$$

This SHIFT term attempts to correct for the non-normality (asymmetry) effects in the estimate of the mean. SHIFT is added to the mean to produce the midpoint of the now asymmetric confidence interval about the mean. The estimated standard deviation can then be added to this new midpoint to form the confidence interval about the estimated mean. The estimated mean plus the SHIFT is printed automatically for all TFC bin tallies. The SHIFT should decrease with $1/N$, reaching zero as N approaches infinity. However when $\text{SHIFT} \ll$ half the estimated variance, the CTL conditions can be considered to be "substantially satisfied". SHIFT is printed for the TFC bins (default or as defined by the TF card). The 5th entry of the DBCN card can however be used to produce the shifted value for all tally bins.

11.7 General

A tally fluctuation chart (TFC) table is produced by MCNP after each tally to provide the user with detailed information about the quality of the TFC bin results. It contains the tally value, R, FOM, VOV and SLOPE, as function of the number of history runs.

A conservative (overestimated) estimate of a tally is obtained in MCNP by assuming that the next, $N+1$, history will produce the largest score. The result of this conservative estimate is given also in the TFC bin information table. MCNP performs 10 checks on the TFC bin, on the mean (nonmonotonic behaviour), R (acceptable magnitude, monotonic decrease, $1/N^{1/2}$ decrease), VOV (magnitude <0.1 , monotonic decrease and $1/N$ decrease), FOM (constant value, non-monotonic behaviour) and $f(x)$ (SLOPE >3). All N dependent checks are performed over the last half of the problem.

For non-TFC bins, MCNP provides only the mean and the fsd (R). VOV and the mean+SHIFT can be obtained by DBCN(15). The PRDMP card can be used to print periodically the values of R and VOV. Complete statistical information can be obtained by creating a new tally and selecting the desired tally bin with the TF card. Check the magnitude of R and VOV before forming a confidence interval. SHIFT, if available, should be used to form asymmetric confidence intervals about the mean, to be conservative. History-dependent information on R and VOV should also be assessed. All assessment should be done according to the discussion in this Chapter. Consult also the manual for the statistically pathological output example.

If one does not have enough confidence in the obtained results, several independent runs with different random number sequences (see BDCN card) should be made and the distribution of the obtained results and associated statistical parameters should be examined. A good result will give consistent values. One last note, in spite of all statistical checks used, there is no absolute guarantee that the confidence interval obtained overlaps the true answer. There is always a possibility that some yet unsampled portion of the problem may change the confidence interval if more histories are followed.

10.8 Work Problems

For an MCNP sample problem of your choice, assess the statistical validity of the results of one of the tallies considering:

1. non-monotonic behaviour of the mean values as a function of number histories, N , for the last half of the problem.
 2. acceptable magnitude of the relative error.
 3. monotonic decrease of the relative error as a function of N for the last half of the problem.
 4. $1/N^{1/2}$ decreases in the relative error for the last half of the problem.
 5. acceptable magnitude of VOV (< 0.1).
 6. monotonic decrease of VOV as a function of N for the last half of the problem.
 7. $1/N$ decreases in VOV for the last half of the problem.
 8. statistically constant value of FOM as a function of N for the last half of the problem.
 9. non-monotonic behavior of FOM as a function of N for the last half of the problem.
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