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Title: MCNP1B Variance Error Estimator

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OFFICE MEMORANDUM

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FROM GE ECC Guy Estes and Ed Cashwell

SUBJECT MCNP1B VARIANCE ERROR ESTIMATOR

SYMBOL TD-6-27-78

MAIL STOP 226

A procedure for estimating the error in the MCNP variance (i.e., the standard deviation squared) has been written for MCNP1B and is available in a special version for use by friendly users. Use of the code requires no additional input and will give one additional line of output for each line of tally data output. This line consists of the fractional error estimate for the variance of the mean.

The use of the variance of the variance, or in other words the error in the error, was suggested by Buck Thompson as a possible way to obtain more confidence in tally results. In particular, point detector results can differ statistically from other tally results without any indication that a problem exists. It was felt that the variance of the variance would be useful as an indicator to flag such suspicious tally results.

To date, the variance error estimate has not resulted in a clarification of misleading point detector results, but this is being pursued as time permits. However, experience has shown that this error estimate is very sensitive to "unusual" particles (i.e., those with tally weights much larger than the other particles of the sample population) and as such is valuable as an indicator of modeling problems which lead to these "unusual" particles. These particles produce large perturbations in the variance error estimate. Note that in order to observe these perturbations, the problem must print out tally results at intermediate particle histories by use of the PRDMP card. An example of an "unusual" particle and its effect on the variance error is given in the attachment to this memo.

At present, the significance of the magnitude of the variance error estimate is not fully appreciated. Rather it seems to be more valuable as an indicator of perturbations caused by "unusual" particles. It is expected that, with experience on a variety of problems, the significance of the magnitude of the variance error estimate will become more obvious.

The attachment outlines the derivation of the variance error estimate and presents test problem results which illustrate the experience to date with this technique.

The special version of MCNP1B may be obtained from Hydra disk, OAC = TD6GPE, MCNPVAR. The corresponding UPDATE deck is named UPDVAR.

Please feel free to contact Guy Estes on ext. 2509 for questions. I would be interested in any variance error results obtained.

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MCNP Variance Error Estimate
Derivation of Equations and Sample Problems

Guy Estes and Ed Cashwell

This attachment will outline the derivation of the variance of the variance equations, and will present the results of calculations which have been performed to gain experience with this error estimator.

$\sum_i = N$

Derivation of Equations

In the terminology of Reference 1, the estimate of the sample variance of x is given by the following equations:

$$\sum(x_i^2 - 2x_i\bar{x} + \bar{x}^2) = \sum x_i^2 - 2\frac{\sum x_i \sum x}{N} + \frac{(\sum x_i)^2}{N^2}N$$

$$\bar{\sigma}^2(x) = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2 \qquad = N(\overline{x^2} - 2\bar{x}^2 + \bar{x}^2)$$

$$= \frac{N}{N-1}[\overline{x^2} - \bar{x}^2] \qquad = N(\overline{x^2} - \bar{x}^2)$$

where x = the tally quantity being measured

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\overline{x^2} = \frac{1}{N}\sum_{i=1}^{N} x_i^2 .$$

The variance of the sample mean $\bar{x}$ is given as follows:

$$\bar{\sigma}^2(\bar{x}) = \frac{\bar{\sigma}^2(x)}{N} = \frac{1}{N-1}[\overline{x^2} - \bar{x}^2] .$$

The following expression for the variance of the variance of the sample x is derived in essence in Reference 2:

$$\sigma^2\left(\overline{\sigma}^2(x)\right) = \frac{1}{N(N-1)}\left[(N-1)\,\overline{x^4} - 4\,(N-1)\,\overline{x}\,\overline{x^3} + 8\,(N-3/2)\,\overline{x}^2\,\overline{x^2} - 4\,(N-1)\,\overline{x}^4 + (3-N)\,\overline{x^2}^2\right]$$

where $\overline{x^r} = \frac{1}{N}\sum_{i=1}^{N} x_i^{\,r}$

This equation reduces to the following for large N:

$$\sigma^2\left(\overline{\sigma}^2(x)\right) = \frac{1}{N}\left[\overline{x^4} - 4\,\overline{x}\,\overline{x^3} + 8\,\overline{x}^2\,\overline{x^2} - 4\,\overline{x}^4 - \overline{x^2}^2\right]$$

It follows that the variance of the sample mean $\overline{x}$, $\overline{\sigma}^2(\overline{x})$, is given by the following expression:

$$\sigma^2\left(\overline{\sigma}^2(\overline{x})\right) = \sigma^2\left(\frac{\overline{\sigma}^2(x)}{N}\right) = \frac{1}{N^2}\,\sigma^2\left(\overline{\sigma}^2(x)\right) = \frac{1}{N^3}\left[\overline{x^4} - 4\,\overline{x}\,\overline{x^3} + 8\,\overline{x}^2\,\overline{x^2} - 4\,\overline{x}^4 - \overline{x^2}^2\right]$$

The fractional error in the MCNP variance is defined (somewhat arbitrarily) as follows:

$\left(\frac{\Sigma x_i^2}{N}\right)^2$

$$\text{fractional error} \equiv \frac{\sigma\left(\overline{\sigma}^2(x)/N\right)}{\overline{\sigma}^2(x)/N}$$

$$= \frac{\sqrt{\overline{x^4} - 4\,\overline{x}\,\overline{x^3} + 8\,\overline{x}^2\,\overline{x^2} - 4\,\overline{x}^4 - \overline{x^2}^2}}{\sqrt{n}\,\left(\overline{x^2} - \overline{x}^2\right)}$$

$$\frac{\frac{1}{\sqrt{N}}\sqrt{\frac{\Sigma x_i^4}{N} - 4\frac{\Sigma x_i}{N}\frac{\Sigma x_i^3}{N} + 8\frac{(\Sigma x_i)^2}{N^2}\frac{\Sigma x_i^2}{N} - \frac{4(\Sigma x_i)^4}{N^4} - \frac{(\Sigma}{N}}}{\frac{\sqrt{N}}{N}\left[\frac{\Sigma x_i^2}{N} - \frac{(\Sigma x_i)^2}{N^2}\right]}$$

$$\frac{1}{N}\sqrt{(\Sigma x_i^4) - \frac{4(\Sigma x_i)(\Sigma x_i^3)}{N} + \frac{8(\Sigma x_i)^2(\Sigma x_i^2)}{N^2} - \frac{4(\Sigma x_i)^4}{N^3} - \frac{(\Sigma}{N}}$$

Sample Problems

(a) Test of Point Detector Results

Several MCNP test problems have been run with the coding for the fractional error of the variance. Of particular interest is a spherical concrete shell problem with an isotropic 14 MeV neutron source in the center. The concrete shell has an inner radius of 360 cm and a thickness

$\left[\Sigma x_i^2 - \frac{(\Sigma x_i}{N}\right.$

MCNPLT

$$\Rightarrow \frac{\sqrt{T2}}{T1} = \frac{\sqrt{\frac{TAL(I+3*MXF) - 4*TAL(I)*TAL(I+2MXF)}{N} + \frac{8*TAL(I)**2(TAL(I+MXF))}{N^2} - \frac{4\,TAL(I+3MXF)}{N^3} - \frac{TAL(I\ldots}{N}}}{N\left[TAL(I+MXF) - TAL(I)**2\right]}$$

of 30 cm. A point detector was placed just inside the outer radius of the concrete and the results compared with those from an F2 tally over the outer surface.

Three separate variations of this problem were run.

(1) No variance reduction schemes used (i.e., no source biasing or forced collisions). The results showed a difference in the F2 and F5 tallies of about two standard deviations (19%). The point detector fractional error was ±.089.

(2) Highly biased source to reduce the point detector standard deviation. The results showed a difference of ~12% between the two tallies with the point detector error being ±.029. This, combined with the ±.015 error for the F2 tally, means that the results are about three standard deviations apart.

(3) Highly biased source, forced collisions and very low weight cutoffs were used to obtain agreement to within 4%.

The detailed results (the relative flux ϕ, and the two fractional error estimates) for the three runs are given in Table I.

As can be seen from Table I the variance error estimates for the F5 tally in run #3 did not indicate the substantially better agreement with the F2 tally as expected. No explanation has been found for this. Note however that the variance error estimate does show some small perturbations for the three runs (F2 tally in run #1 between 40,000 & 50,000 particles, and the F5 tallies in runs 2 & 3 between 90,000 & 100,000 particles).

(b) <u>Example of an "Unusual" Particle</u>

A variation of the concrete shell problem was run in which a large perturbation in the variance error estimate was observed in the F2 tally. The two fractional error estimates are shown in Table II for the F1, F2 and F5 tallies. The perturbation increases the variance error estimate by a factor of 6 between 20,000 and 30,000 particles. Note that the error in the sample mean ($\overline{\sigma}/\phi$) did not indicate that a large perturbation had occurred.

The particle which caused this particular problem was investigated. The MCNP default weights (1.0 and 0.5) had been used and the particle had undergone weight cutoff. It survived Russian roulette and had its weight raised to 1.0. In addition, this particle crossed the tally surface at an angle whose cosine was ~.09. The code is programmed to reset the cosine to 0.05 if the actual cosine is less than 0.1. This feature prevents division by zero or by very small cosines since the flux is calculated by dividing the existing particle weight by the cosine for the F2 tally flux. For this case the cosine was set to 0.05 and the final tally weight was 20.0. The average tally weight per source neutron in this job was ~0.1. The fourth moment contribution of the variance error estimate caused the large perturbation observed.

This particular modeling problem was solved by lowering the weight cutoffs to 0.1 and 0.05 from the default values of 1.0 and 0.5.

Conclusions

In summary, the results to date show that the variance error estimate can be valuable in highlighting modeling deficiencies. In fact any particle which has a weight which is much higher than most of the sample population will cause a perturbation in the variance error estimate. Note that in order to observe the perturbations, the user must get printouts of tally results (using the PRDMP card) at a number of intermediate points along the way in running the total sample as shown in Tables I and II.

References:

1. E. D. Cashwell et al., MCN: A Neutron Monte Carlo Code, USAEC Report LA-4751, Los Alamos Scientific Laboratory, January 1972.

2. Z. W. Birnbaum, Introduction to Probability and Mathematical Statistics, Harper and Brothers, New York, 1962.

TABLE I

Run	#particles	F2 Tally ϕ	F2 Tally $\frac{\bar{\sigma}(\phi)}{\phi}$	F2 Tally $\frac{\sigma(\bar{\sigma}^2/N)}{\bar{\sigma}^2/N}$	F5 Tally ϕ	F5 Tally $\frac{\bar{\sigma}(\phi)}{\psi}$	F5 Tally $\frac{\sigma(\bar{\sigma}^2/N)}{(\bar{\sigma}^2/N)}$
I	10K	2.081	.0120	.0069	1.399	.1258	.7734
	20	2.071	.0085	.0048	1.863	.1922	.6721
	30	2.041	.0070	.0040	2.077	.2031	.7000
	40	2.043	.0061	.0035	1.966	.1687	.6420
	50	2.042	.0055	.0041	1.810	.1466	.6417
	60	2.045	.0050	.0038	1.807	.1288	.5852
	70	2.044	.0046	.0037	1.749	.1151	.5744
	80	2.049	.0043	.0035	1.720	.1035	.5632
	90	2.046	.0041	.0032	1.656	.0955	.5631
	100	2.047	.0039	.0030	1.649	.0893	.5310
2	10	2.042	.0478	.0487	1.871	.0939	.6324
	20	2.099	.0334	.0356	1.799	.0546	.5176
	30	2.074	.0275	.0292	1.878	.0652	.4010
	40	2.043	.0240	.0252	1.851	.0521	.3647
	50	2.031	.0215	.0225	1.836	.0439	.3361
	60	2.105	.0194	.0208	1.833	.0383	.3115
	70	2.122	.0179	.0193	1.822	.0342	.2918
	80	2.111	.0168	.0181	1.828	.0310	.2715
	90	2.113	.0158	.0169	1.842	.0287	.2495
	100	2.110	.0150	.0161	1.850	.0287	.2518
3	10	2.049	.0241	.0331	2.046	.1005	.6119
	20	2.036	.0169	.0231	1.963	.0642	.4702
	30	2.031	.0139	.0190	1.934	.0496	.3853
	40	2.022	.0121	.0165	1.880	.0400	.3504
	50	2.043	.0107	.0147	1.907	.0366	.3368
	60	2.050	.0098	.0134	1.954	.0349	.2795
	70	2.054	.0090	.0124	1.935	.0310	.2668
	80	2.054	.0085	.0118	1.950	.0281	.2466
	90	2.058	.0080	.0112	1.941	.0256	.2365
	100	2.056	.0074	.0095	2.145	.0280	.2628

TABLE II

#particles	F1 $\frac{\overline{\sigma}(\phi)}{\phi}$	F1 $\frac{\sigma(\overline{\sigma}^2/N)}{\overline{\sigma}^2/N}$	F2 $\frac{\overline{\sigma}(\phi)}{\phi}$	F2 $\frac{\sigma(\overline{\sigma}^2/N)}{\overline{\sigma}^2/N}$	F5 $\frac{\overline{\sigma}(\phi)}{\phi}$	F5 $\frac{\sigma(\overline{\sigma}^2/N)}{\overline{\sigma}^2/N}$
10K	.0285	.0266	.0288	.0315	.2210	.9558
20	.0197	.0182	.0198	.0205	.1399	.7084
30	.0160	.0148	.0172	.1274	.1002	.6922
40	.0138	.0128	.0147	.0986	.0790	.6882
50	.0123	.0114	.0129	.0801	.1534	.7738
60	.0113	.0104	.0117	.0682	.1304	.6878
70	.0104	.0096	.0108	.0593	.1164	.6809
80	.0098	.0090	.0101	.0526	.1059	.6803