The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, Tennessee, April 17–21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

MONTE CARLO SAMPLING OF FISSION MULTIPLICITY

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ABSTRACT

Two new methods have been developed for fission multiplicity modeling in Monte Carlo calculations.

The traditional method of sampling neutron multiplicity from fission is to sample the number of neutrons above or below the average. For example, if there are 2.7 neutrons per fission, three would be chosen 70% of the time and two would be chosen 30% of the time. For many applications, particularly ^{3}He coincidence counting, a better estimate of the true number of neutrons per fission is required. Generally, this number is estimated by sampling a Gaussian distribution about the average. However, because the tail of the Gaussian distribution is negative and negative neutrons cannot be produced, a slight positive bias can be found in the average value. For criticality calculations, the result of rejecting the negative neutrons is an increase in k_{eff} of 0.1% in some cases. For spontaneous fission, where the average number of neutrons emitted from fission is low, the error also can be unacceptably large. If the Gaussian width approaches the average number of fissions, 10% too many fission neutrons are produced by not treating the negative Gaussian tail adequately.

The first method to treat the Gaussian tail is to determine a correction offset, which then is subtracted from all sampled values of the number of neutrons produced. This offset depends on the average value for any given fission at any energy and must be computed efficiently at each fission from the non-integrable error function.

The second method is to determine a corrected zero point so that all neutrons sampled between zero and the corrected zero point are killed to compensate for the negative Gaussian tail bias. Again, the zero point must be computed efficiently at each fission.

Both methods give excellent results with a negligible computing time penalty. It is now possible to include the full effects of fission multiplicity without the negative Gaussian tail bias.

Key Words: Monte Carlo, Radiation Transport, Fission Multiplicity, Gaussian Distribution

1 INTRODUCTION

Two new methods have been developed for fission multiplicity modeling in Monte Carlo calculations. Correct fission multiplicity modeling is essential for modeling neutron coincidence counting, which is an important nondestructive assay technique for nuclear safeguards.

1.1 Fission Multiplicity and Coincidence Counting

Fission multiplicity is the number of neutrons released in fission reactions. The prompt neutrons, which are over 99% of the neutrons emitted in fission, are emitted at essentially the same time. The number of neutrons emitted in a single fission can vary from zero to six or more. If a neutron detector counts a number of neutrons at about the same time, inferences can be made about whether the fissionable nuclides are present in an unknown sample material, what the fissionable materials are, and how much fissionable material is present. Such detectors are known as neutron coincidence detectors.

Neutron coincidence counting [1] takes advantage of the great penetrability of neutrons through dense samples. Neutrons are sometimes the only way to assay large, dense samples rapidly. The neutrons usually can measure the entire volume of the item because they are not easily shielded. Passive neutron counting measures the presence of materials that undergo spontaneous fission. Active interrogation counting measures fissions from materials irradiated by an external source of neutrons, photons (photofission), or other particles.

Neutron coincidence counting is complicated by the presence of hydrogenous scattering materials, materials containing neutron poisons (such as boron), sample self-multiplication, and neutrons from other sources [such as (α,n) reactions]. Further, multiplicity counter electronics packages are complex and sum up separately the number of 0, 1, 2, 3, 4, 5, 6, 7, etc., multiples of neutrons within the coincidence resolving time (time gate). Thus, the analysis of multiplicity data is not based directly on the observed multiplicity distribution but on the moments of the distributions.

1.2 Monte Carlo Modeling of Fission Multiplicity

The Monte Carlo method is the preferred tool for the design of neutron multiplicity counters and analysis of coincidence-counting measurements. To be effective, a Monte Carlo code at least must be able to model fission multiplicity and coincident capture. Other capabilities are useful, as well. For example, the MCNPX [2] Monte Carlo radiation transport computer code has special spontaneous fission models, multiple source types, and collision-estimator ^{3}He coincidence capture tallies with time gating and moments.

The traditional Monte Carlo method for sampling neutron multiplicity from fission is to sample the number of neutrons above or below the average. For example, if 2.7 neutrons are produced per fission, 3 would be chosen 70% of the time and 2 would be chosen 30% of the time. This method is the default in MCNPX and the only method available in MCNP4C [3]. For many applications, particularly ^{3}He coincidence counting, a better estimate of the true number of neutrons per fission is required.

Fission multiplicity can be sampled from a Gaussian distribution about the average number of neutrons from fission, $\bar{\nu}$, and fission width, w:

$$p(\nu) = e^{-\frac{(\nu-\bar{\nu})^2}{w}} \quad . \tag{1}$$

The Gaussian distribution matches measured data fairly well and also is appealing because it is similar to a normal distribution, or error function, which is what is expected from randomly sampled independent events such as fission. However, the sampled value of ν can have negative values. The negative values are known as the negative Gaussian tail. Because negative neutrons cannot be produced, a slight positive bias is found in the average value. For criticality calculations, the result of rejecting the negative neutrons is an increase in k_{eff} of 0.1% in some cases, which is unacceptable. For spontaneous fission, where the average number of neutrons emitted from fission is low, the error can also be unacceptably large. If the Gaussian width approaches the average number of fissions, 10% too many fission neutrons are produced by not treating the negative Gaussian tail adequately.

Two new methods have been developed for correcting the negative ν values when sampling the fission multiplicity from a Gaussian distribution. These methods have been implemented in the MCNPX Monte Carlo code with excellent results.

The first method to treat the Gaussian tail is to determine a correction offset. This offset then is subtracted from all sampled values of the number of neutrons produced. This offset depends on the average sampled ν value for any given fission at any energy and must be computed efficiently at each fission from the non-integrable error function.

The second method is to determine a corrected zero point so that all neutrons sampled between zero and the corrected zero point are killed to compensate for the negative Gaussian tail bias. Again, the zero point must be computed efficiently at each fission.

Both methods give excellent results with a negligible computing time penalty by using approximate linear fits to the error function integral. The Gaussian shape of fission multiplicity is preserved without biasing the average number of fission neutrons sampled.

2 THEORY

The number of neutrons emitted from fission can be sampled from a Gaussian distribution as

$$\mathrm{P}(\nu) = \frac{1}{w\sqrt{\pi}} \int_{-\infty}^{\nu} p(\nu) d\nu \quad , \tag{2}$$

where

$$p(\nu) = e^{-\left(\frac{\nu - \bar{\nu}}{w}\right)^2} \quad . \tag{3}$$

The normalization constant,

$$C = \frac{1}{w\sqrt{\pi}} \quad , \tag{4}$$

normalizes the distribution to unity as

$$\frac{1}{w\sqrt{\pi}}\int_{-\infty}^{\infty} p(\nu)d\nu = 1 \quad . \tag{5}$$

2.1 Full-Width Half-Maximum

The Gaussian width, *w*, is related to the full-width half-maximum (FWHM) by finding the value of ν at which

$$p(\nu) = \frac{1}{2}p(\bar{\nu}) \quad . \tag{6}$$

That is,

$$e^{-\left(\frac{\nu-\bar{\nu}}{w}\right)^2} = \frac{1}{2}e^{\circ} = \frac{1}{2} \quad . \tag{7}$$

Thus,

$$-\left(\frac{\nu-\bar{\nu}}{w}\right)^2 = ln\frac{1}{2} \quad . \tag{8}$$

Then

$$\nu - \bar{\nu} = w\sqrt{ln2} \tag{9}$$

and

$$\text{FWHM} = 2(\nu - \bar{\nu}) = 2w\sqrt{ln2} \quad . \tag{10}$$

2.2 Changing Variables to a Normal Distribution

The Gaussian distribution function is non-integrable. To calculate the negative tail adjustment efficiently requires a table lookup approximation of the integral. To eliminate the dependence on the width, *w*, in the table lookup, the following change of variables is used to relate the Gaussian distribution to a normal distribution:

$$x = \left(\frac{\nu - \bar{\nu}}{w}\right)\sqrt{2} \quad . \tag{11}$$

Thus, the fission distribution may be represented by the normal distribution, which is independent of width, *w*, as

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad , \tag{12}$$

and

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-x^2/2}\, dx \quad . \tag{13}$$

Further, let

$$x_o = \frac{\sqrt{2}}{w}\bar{\nu} \quad . \tag{14}$$

Then the expectation value of ν is

$$E(\nu) = \mathrm{C} \int_{-\infty}^{\infty} \nu p(\nu) d\nu \quad , \tag{15}$$

$$E(x + x_o) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (x + x_o) f(x) dx \quad , \tag{16}$$

$$E(x+x_o)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}xf(x)dx+\frac{x_o}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)dx \quad , \tag{17}$$

$$E(x+x_o)=0+x_o \quad , \tag{18}$$

$$E(x+x_o)=x_o \quad , \tag{19}$$

and

$$E(\nu)=\nu_o \quad . \tag{20}$$

2.3 The Negative Gaussian Tail Bias

Monte Carlo sampling of the Gaussian distribution causes a bias because negative values of ν are not allowed. That is, the expected value of ν is biased higher because

$$\frac{1}{\sqrt{2\pi}}\int_{-x_0}^{\infty}(x+x_o)f(x)dx=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}(x+x_o)f(x)dx-\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{-x_o}(x+x_o)f(x)dx \tag{21}$$

and

$$>\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}(x+x_o)f(x)dx \quad . \tag{22}$$

2.4 Sampling the Gaussian

The negative Gaussian tail bias cannot be corrected by simply changing the normalization constant [Eq. (4)] because the Gaussian function is sampled by a rejection scheme that does not include the constant. Let ξ_i be the ith random number, $0 \le \xi_i \le 1$. The sampling scheme for the Gaussian function is then

$$r_1=2\xi_1-1 \tag{23}$$

and

$$r_2 = r_1^2 + \xi_2^2 \quad . \tag{24}$$

If $x_2 > 1$, resample r_1, r_2 . (25)

$$r_3 = \sqrt{-2ln(r_2)/r_2} \quad . \tag{26}$$

The spread in ν is Δ:

$$\Delta = wr_1r_3 \tag{27}$$

and

$$\nu = \bar{\nu} + \Delta \quad . \tag{28}$$

3 CORRECTING THE BIAS

Two new methods have been developed to correct the negative Gaussian tail bias.

3.1 Method 1: Adjust All ν Values

The expected value of the sampled ν can be preserved (forced to $\bar{\nu}$) by using a slightly lower value, ν_1. For each value of x_0, iterate x_1 until

$$\frac{1}{\sqrt{2\pi}} \int_{-x_1}^{\infty} (x + x_1) f(x) dx = x_o \quad . \tag{29}$$

Note that $x_1 < x_0$. Then after sampling Δ set,

$$\nu = \nu_1 + \Delta \quad , \tag{30}$$

where

$$\nu_1 = \bar{\nu} - w(x_o - x_1) \quad . \tag{31}$$

For the 31 equally spaced values of x_0 = 1, 1.1, 1.2 … 3.8, 3.9, 4.0, the corrections are $x_0 - x_1$. The values are presented in Table I. Linear interpolation is used between x_0 values.

Table I. Values of $x_0 - x_1$

0.100528d0, 8.02249d-2, 6.38562d-2, 5.06562d-2, 4.00222d-2,
3.14746d-2, 2.46252d-2, 1.91590d-2, 1.48167d-2, 1.13856d-2,
8.69035d-3, 6.58690d-3, 4.95634d-3, 3.70147d-3, 2.74301d-3,
2.01670d-3, 1.47075d-3, 1.06379d-3, 7.63034d-4, 5.42685d-4,
3.82671d-4, 2.67508d-4, 1.85374d-4, 1.27331d-4, 8.66889d-5,
5.84945d-5, 3.91172d-5, 2.59241d-5, 1.70256d-5, 1.10803d-5,
7.14548d-6

The advantages of Method 1 are that the Gaussian shape is preserved and that the expected value of ν is preserved by shifting the mean/median value slightly lower. Method 1 is the recommended user-controlled method for correcting fission multiplicity in MCNPX and is the default when fission multiplicity is turned on.

3.2 Method 2: Increase the Threshold ν Value

Alternatively, the expected value of the sampled ν can be preserved (forced to ν_0) by increasing the lower cutoff from $-\nu_0$ to $-\nu_2$. The expected value can be integrated from $-\infty$ up to $-x_2$ such that

$$\int_{-\infty}^{-x_2} (x + x_o) f(x) dx = 0 \quad . \tag{32}$$

Note that $-x_2 > -x_0$. Then instead of setting $\nu = 0$ whenever $\nu = \nu_0 + \Delta < 0$, set $\nu = 0$ whenever $\nu = \nu_2 + \Delta < 0$; that is, whenever $\Delta < -\nu_2 = -w\, x_2$.

For the 31 equally spaced values of x_0 = 1, 1.1, 1.2 … 3.8, 3.9, 4.0, the values of x_2 are presented in Table II. Linear interpolation is used between x_0 values.

Table II. Values of x_2

0.302631d0, 0.443487d0, 0.579851d0, 0.712453d0, 0.841865d0,
0.968544d0, 1.09286d0, 1.21512d0, 1.33556d0, 1.45442d0,
1.57186d0, 1.68803d0, 1.80308d0, 1.91710d0, 2.03021d0,
2.14248d0, 2.25400d0, 2.36483d0, 2.47502d0, 2.58463d0,
2.69372d0, 2.80231d0, 2.91045d0, 3.01818d0, 3.12552d0,
3.23249d0, 3.33914d0, 3.44547d0, 3.55151d0, 3.65728d0,
3.76280d0

Method 2 preserves the expected value of ν by selecting fewer fissions of multiplicity 1 while preserving the Gaussian for higher multiplicities.

4 RESULTS

Many problems using a wide variation of combinations of materials have been run to demonstrate the effects of the corrected fission multiplicity. The sampled values of ν are presented using the Method 1 correction, the Method 2 correction, and no correction. The MCNP4C results do not have the correct fission multiplicity but do have the corrected expected value of ν. Finally, values of ν and the width, *w*, are presented for all problems in which all spontaneous fission sources used these values. The correct expected value of ν is the value for those problems where ν is set. Otherwise, the MCNP4C-sampled value of ν is the best. The relative error is presented immediately after each sampled ν value. Some spontaneous fission results are presented in Table III. Some induced fission values are presented in Table IV.

As expected, the MCNP4C-sampled values of ν agree closely with the specified values when the ν values are specified for spontaneous fission, even though the MCNP4C multiplicity is totally wrong. Method 1 and Method 2 also preserve the expected value of ν within statistical uncertainty. The necessity of the two correction methods for fission multiplicity is shown by the uncorrected results. The sampled value of ν is 6%–8% too high for tests inp81, inp87, inp91, and inp92, where nonphysical widths are nearly as large as ν. When actual fission widths and ν values are used, the effect of the Gaussian tail is usually unnoticeable, although it can be as high as 1% for induced fission and slightly higher for spontaneous fission, where ν tends to be smaller. Generally, $1.04 < w < 1.3$ and $1.7 < \nu < 3.4$. The worst case is $\nu / w = 1.6$ for ^{233}U.

Table III. Spontaneous-Fission Results

	Method 1	Method 2	Uncorrected	MCNP4C	ν	w
inp07	2.0050 0.0011	2.0055 0.0012	2.0344 0.0011	2.0065 0.0001		1.8
inp17	2.0063 0.0007	2.0068 0.0007	2.0697 0.0007	2.0067 0.0001		1.5
inp24	2.1798 0.0017	2.1798 0.0017	2.1798 0.0017	2.1798 0.0017		
inp55	2.5880 0.0005	2.5880 0.0005	2.5880 0.0005	2.5880 0.0005		
inp81	1.0088 0.0009	1.0091 0.0010	1.0886 0.0009	1.0100 0.0001	1.01	0.99
inp82	1.0997 0.0006	1.0997 0.0006	1.1021 0.0006	1.0998 0.0003	1.10	0.5
inp83	1.2489 0.0008	1.2488 0.0008	1.2998 0.0008	1.2495 0.0003	1.25	1.0
inp84	1.3493 0.0004	1.3493 0.0004	1.3493 0.0004	1.3495 0.0004	1.35	0.4
inp85	2.2093 0.0005	2.2094 0.0005	2.2186 0.0005	2.2093 0.0002	2.21	1.1
inp86	2.3893 0.0003	2.3893 0.0003	2.3893 0.0003	2.3895 0.0002	2.39	0.6
inp87	3.1436 0.0008	3.1443 0.0009	3.3712 0.0008	3.1498 0.0001	3.15	3.0
inp91	1.5002 0.0008	1.5007 0.0009	1.6021 0.0008	1.4999 0.0003	1.5	1.4
inp92	1.1991 0.0009	1.1989 0.0009	1.2759 0.0008	1.1994 0.0003	1.2	1.1
inp94	2.5880 0.0005	2.5880 0.0005	2.5880 0.0005	2.5880 0.0005		

Table IV. Induced-Fission Results

	Method 1	Method 2	Uncorrected	MCNP4C	
inp04	2.5424 0.0008	2.5425 0.0008	2.5462 0.0008	2.5421 0.0003	
inp05	3.8017 0.0009	3.8018 0.0009	3.8037 0.0009	3.8077 0.0005	
inp07	2.2630 0.0009	2.2648 0.0009	2.3128 0.0009	2.2677 0.0003	1.8
inp17	2.2647 0.0005	2.2647 0.0005	2.3166 0.0005	2.2648 0.0001	1.5
inp24	2.9339 0.0006	2.9346 0.0006	2.9350 0.0006	2.9393 0.0004	

5 CONCLUSIONS

Neutron multiplicity counting is an important tool for nondestructive assay of fissionable materials. Fission multiplicity must be modeled to simulate coincidence detectors in Monte Carlo calculations. Using a Gaussian distribution to model fission multiplicity causes a small bias in the sampled value of ν. Two new methods have been developed that correct the bias. These methods have been implemented into MCNPX and show excellent agreement with the expected results.

6 REFERENCES

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