LA-UR-24-28791

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Title: Studying the Random Number Generators in MCNP6 using an Analytic Benchmark

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Intended for: 2024 MCNP User Symposium, 2024-08-19/2024-08-22 (Los Alamos, New Mexico, United States)

Issued: 2024-08-29 (rev.1)

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Studying the Random Number Generators in MCNP6 using an Analytic Benchmark

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2024 MCNP User Symposium
August 22, 2024

LA-UR-24-28791

Abstract

An analytic solution to a previously studied toy problem is derived and used as a code verification benchmark. Using various Random Number Generators (RNGs) in MCNP6, including the newest SFC64 RNG available in MCNP6.3.1, and their various properties (e.g., RNG stride), we show how these RNGs perform and how to correct or workaround potential issues with respect to the analytic benchmark problem.

Hendricks' Spherical Benchmark

In 1991, John Hendricks studied the effects of changing the random number stride in Monte Carlo calculations using a simple test problem [1].

- Static, one-speed transport
- 15-mean-free-path radius sphere
- Isotropic point source at center
- 10% absorbing, 90% scattering (mock cross sections made with `simple_ace.pl` utility)
- Random numbers (RNs) are used for only a few basic functions
  - direction-of-flight: 2 RNs
  - distance-to-collision: 1 RN
  - reaction sampling or rouletting: 1 RN
  - total: 4 RNs per track

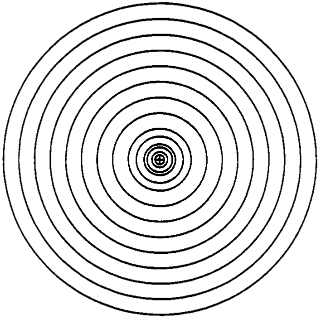


Fig. 4. A 15-mfp spherical geometry test problem. Fluxes are tallied at each of the concentric spheres. A mono-energetic, isotropic point source is at the center, and the scattering medium is 10% absorbing.

Spherical Integral Transport Equation

Hendricks' spherical benchmark is expressed analytically by the static, one-speed, integral neutron transport equation for a homogeneous material in one-dimensional spherical coordinates [2], i.e.,

$$r\phi(r) = \int_0^a r' q(r') \left[E_1 \left(\Sigma_T |r - r'| \right) - E_1 \left(\Sigma_T |r + r'| \right) \right] dr', \tag{1}$$

for a finite or infinite radial boundary a, where

$$q(r') = \frac{\Sigma_S}{2} \phi(r') + \frac{Q(r')}{2} \tag{2}$$

and $E_n(x)$ is defined by the integral

$$E_n(x) = \int_0^1 e^{-x/\mu} \mu^{n-2} d\mu. \tag{3}$$

Numerical Approximation of the Integral

The integral in the transport equation is approximated by an N-point quadrature rule,

$$r\phi(r) = \sum_{j=1}^{N} w_j r_j q(r_j) \left[E_1 \left(\Sigma_T |r - r_j| \right) - E_1 \left(\Sigma_T |r + r_j| \right) \right], \tag{4}$$

where r_j and w_j are the quadrature points and weights, respectively. The scalar flux is evaluated at the quadrature points to form a closed system of equations,

$$r_i\phi_i = \sum_{j=1}^{N} w_j r_j q(r_j) \left[E_1 \left(\Sigma_T |r_i - r_j| \right) - E_1 \left(\Sigma_T |r_i + r_j| \right) \right], \tag{5}$$

where $\phi_i \equiv \phi(r_i)$.

Removal of the Logarithmic Singularity

The exponential integral has a logarithmic singularity at $r_i - r_j = 0$. It is removed by adding and subtracting $rq(r)$ under the integral,

$$r\phi(r) = \int_0^a \left[r'q(r') - rq(r) + rq(r)\right] \left[E_1\left(\Sigma_T|r - r'|\right) - E_1\left(\Sigma_T|r + r'|\right)\right] dr'. \quad (6)$$

The integral is separated into two parts and the second integral is solved exactly,

$$r\phi(r) = \int_0^a \left[r'q(r') - rq(r)\right] \left[E_1\left(\Sigma_T|r - r'|\right) - E_1\left(\Sigma_T|r + r'|\right)\right] dr' + rq(r)p(r), \quad (7)$$

where

$$p(r) = \frac{1}{\Sigma_T}\left\{2\left[1 - E_2\left(\Sigma_T r\right)\right] - E_2\left[\Sigma_T\left(a - r\right)\right] + E_2\left[\Sigma_T\left(a + r\right)\right]\right\}. \quad (8)$$

Formulation of the System of Equations (1 of 2)

The integral in the transport equation with the logarithmic singularity removed is approximated by an N-point quadrature rule,

$$r_i \phi_i = \sum_{\substack{j=1 \\ j \neq i}}^{N} w_j \left[r_j q(r_j) - r_i q(r_i) \right] \left[E_1 \left(\Sigma_T |r_i - r_j| \right) - E_1 \left(\Sigma_T |r_i + r_j| \right) \right] + r_i q(r_i) p(r_i). \quad (9)$$

This is recast as a $N \times N$ system of equations,

$$\overline{\overline{A}}\,\overline{\phi} = \overline{Q}, \quad (10)$$

Formulation of the System of Equations (2 of 2)

where

$$A_{ij} = r_i \left[1 - \frac{\Sigma_S}{2} p(r_i) \right] + \sum_{\substack{j \neq i \\ j=1}}^{N} w_j r_i \frac{\Sigma_S}{2} \left[E_1 \left(\Sigma_T |r_i - r_j| \right) - E_1 \left(\Sigma_T |r_i + r_j| \right) \right] \tag{11}$$

for $i = j$,

$$A_{ij} = -w_j r_j \frac{\Sigma_S}{2} \left[E_1 \left(\Sigma_T |r_i - r_j| \right) - E_1 \left(\Sigma_T |r_i + r_j| \right) \right] \tag{12}$$

for $i \neq j$, and

$$Q_i = r_i \frac{Q(r_i)}{2} p(r_i) + \sum_{\substack{j \neq i \\ j=1}}^{N} w_j \left[r_j \frac{Q(r_j)}{2} - r_i \frac{Q(r_i)}{2} \right] \left[E_1 \left(\Sigma_T |r_i - r_j| \right) - E_1 \left(\Sigma_T |r_i + r_j| \right) \right]. \tag{13}$$

Isotropic Point Source

The uncollided scalar neutron flux is Q_i/r_i. For a spherical system with an isotropic point source at the center, i.e.,

$$Q(r) = \frac{s_0}{4\pi}\frac{\delta(r)}{r^2}, \tag{14}$$

the uncollided flux is

$$\phi_i = s_0 \frac{\exp\left(-\Sigma_T r_i\right)}{4\pi r_i^2}, \tag{15}$$

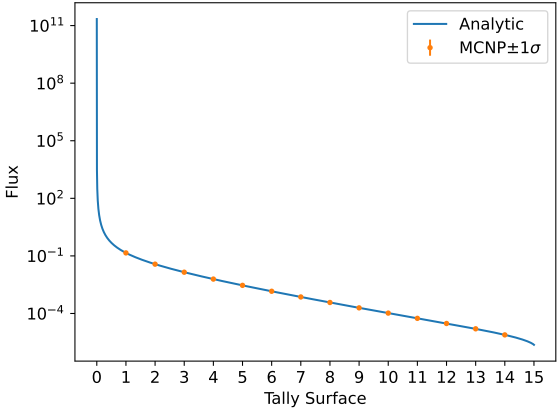
which means that

$$Q_i = s_0 \frac{\exp\left(-\Sigma_T r_i\right)}{4\pi r_i}. \tag{16}$$

Results for 10,000 Gauss-Legendre Quadrature Points

Converged to 6 Significant Figures

Tally Surface	Flux
1	1.43284E-01
2	3.71264E-02
3	1.41400E-02
4	6.19403E-03
5	2.91509E-03
6	1.43307E-03
7	7.25476E-04
8	3.75078E-04
9	1.96984E-04
10	1.04658E-04
11	5.60141E-05
12	2.99863E-05
13	1.57773E-05
14	7.70698E-06



The MCNP6 [3] default random number generator (GEN=1) is used with STRIDE=1.

Implications of Exceeding the Random Number Generator Stride

```
warning.  random number stride 1 exceeded 10000000 times.
```

The sample (population) variance is used to calculate the reported standard deviation of the mean, assuming that all histories are independent and uncorrelated. That is,

$$S^2 = \frac{N}{N-1}\left[\frac{1}{N}\sum_{i=1}^{N} x_i^2 - \left(\frac{1}{N}\sum_{i=1}^{N} x_i\right)^2\right]. \tag{17}$$

If the random number stride is exceeded, then the correlations between histories must be taken into account to obtain the proper sample variance and subsequent standard deviation of the mean.

Generalized Population Variance

The sample (population) covariance between neighboring (offset) histories can be defined as,

$$C_{i,i+j} = \frac{N-j}{N-j-1}\left[\frac{1}{N-j}\sum_{i=1}^{N-j} x_i x_{i+j} - \left(\frac{1}{N-j}\sum_{i=1}^{N-j} x_i\right)\left(\frac{1}{N-j}\sum_{i=1+j}^{N} x_i\right)\right], \qquad (18)$$

where $1 \leq j < N$ represents the history offset. For example, if $j = 1$ the sample covariance $C_{i,i+1}$ is the covariance between subsequent histories. If $j = 0$, we recover the sample variance. The covariance-corrected sample variance can then be defined as,

$$\tilde{S}^2 = S^2 + 2\sum_{j=1}^{N-1} C_{i,i+j}, \qquad (19)$$

Computing Sample Covariance

`PTRAC` has a legacy feature where individual history scores can be printed into an easy-to-use column-formatted file:

```
ptrac file=asc write=all max=9e9 coinc=col
      tally=12,22,32,42,52,62,72,82,92,102,112,122,132,142
      value=0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0
```

This produces a `PTRAC` file in the following form:


```
   -1
mcnp6   6                         07/13/24 08/12/24 18:01:16
Analog case, with 1-group cross sections
   1.5000E+01  1.0000E+00  1.0000E+02  0.0000E+00  0.0000E+00  1.0000E+00  1.0000E+00  0.0000E+00  1.0000E+00  1.0000E+04
   0.0000E+00  0.0000E+00  0.0000E+00  1.4000E+01  1.0000E+00  2.0000E+00  3.0000E+00  4.0000E+00  5.0000E+00  6.0000E+00
   7.0000E+00  8.0000E+00  9.0000E+00  1.0000E+01  1.1000E+01  1.2000E+01  1.3000E+01  1.4000E+01  0.0000E+00  1.4000E+01
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.0000E+00  2.0000E+00  1.0000E+00  2.0000E+00  0.0000E+00  0.0000E+00
    4    6    9    7    9    7    9    7    9    7    9    1    4    0    0    0    0    0    0    0
    1    2    5    6    7    8    9   17   18   19   20   21   22   23   24   25   26   27   28    7    8   10   11   17   18   19   20   21   22   23
   24   25   26   27   28    7    8   12   13   17   18   19   20   21   22   23   24   25   26   27   28    7    8   10   11   17   18   19   20   21
   22   23   24   25   26   27   28    7    8   14   15   17   18   19   20   21   22   23   24   25   26   27   28
                        12           22           32           42           52           62           72           82           92          102          112          122          132          142
        2  9.60069E-02  3.72555E-01  9.55163E-02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        3  6.93208E-02  6.73717E-02  1.63702E-02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        4  7.45351E-02  1.76303E-02  1.71822E-02  2.02649E-02  1.22837E-02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        5  5.58696E-01  1.97488E-02  8.07956E-03  2.95310E-02  4.31247E-03  2.19999E-03  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        7  6.93208E-02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        8  1.02161E-01  1.86324E-02  9.95053E-03  5.06158E-03  6.26333E-03  2.89746E-03  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
        9  6.93208E-02  9.97731E-02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
       10  6.93208E-02  1.73302E-02  7.70231E-03  5.93798E-03  1.61951E-02  2.32235E-03  1.61179E-03  1.10629E-03  8.70167E-04  8.14371E-04  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
       11  5.41949E-01  1.48342E-01  8.10403E-03  6.02430E-03  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
       12  7.07133E-02  1.74153E-02  7.71905E-03  4.33784E-03  2.77500E-03  1.92662E-03  1.42305E-03  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
       13  6.93208E-02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
       14  7.29539E-02  2.02809E-02  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
                                                                                                                                          1,1          Top
```

Correlations Between Histories

The normalized correlation coefficient can be used to visualize the magnitude of any issues when exceeding the stride:

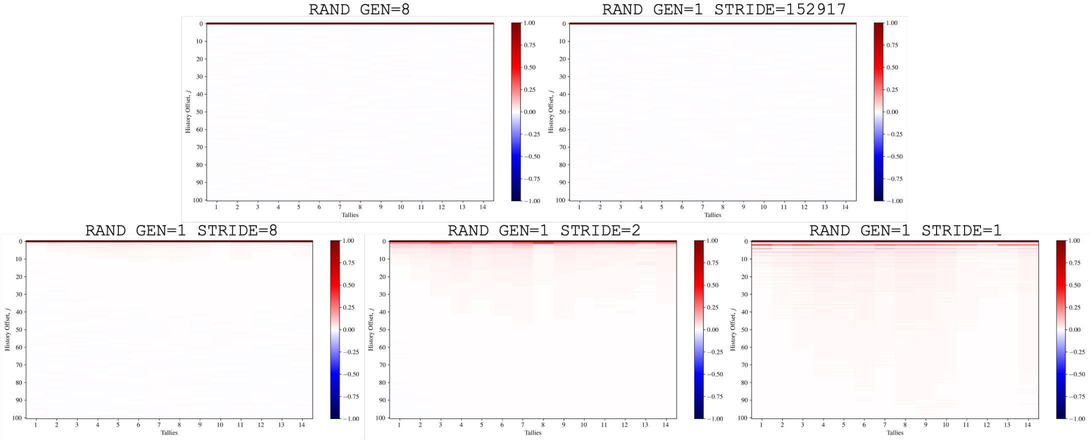
$$\rho_{i,i+j} = \frac{C_{i,i+j}}{\sqrt{C_{i,i} C_{i+j,i+j}}} \tag{20}$$

The history-offset correlations are computed using the MCNP6 default and the new SFC64 random number generator [4] in MCNP6.3.1 and later.

- SFC64 (`RAND GEN=8`) has no stride. Each history uses an independent stream of random numbers.
- 48-bit LCG (`RAND GEN=1`) with strides of 1, 2, 8, 16, 100, 1,000, and 152,917 (default stride).

Numerical Results: Correlations

Positive correlation values between neighboring histories can be seen in red when the random number generator stride is exceeded.

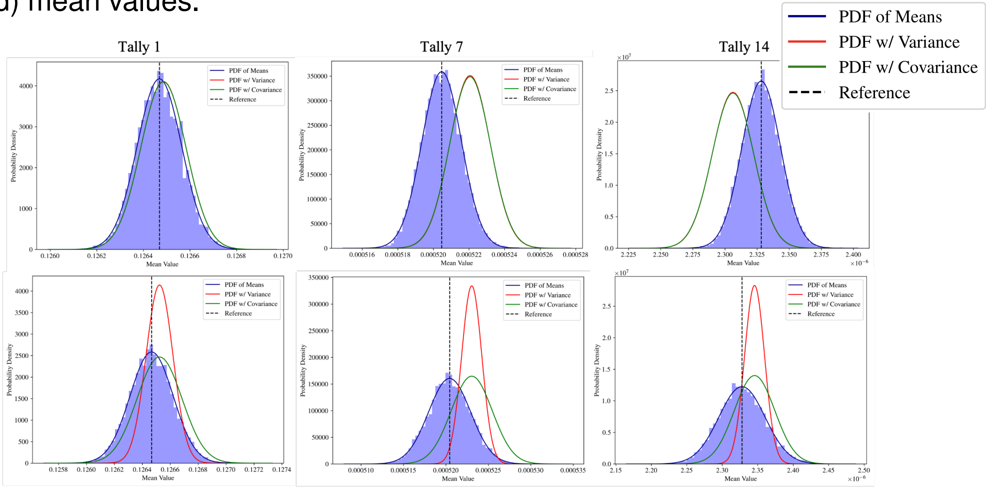


Numerical Results: Probability Density Functions

Each histogram and curve in blue represent 10,000 independent (varying random number seed) mean values.

RAND GEN=8

RAND GEN=1
STRIDE=1

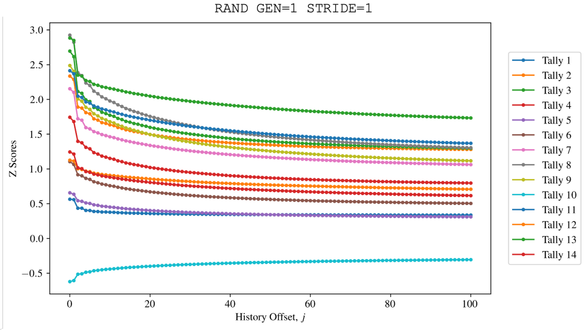


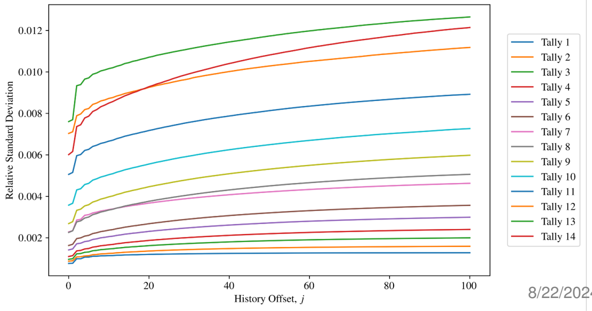
Numerical Results: Z Scores and Relative Standard Deviations

A metric to determine how close the distribution is to the reference solution is the Z score, defined as

$$Z = \frac{\mu - x}{\sigma}, \qquad (21)$$

where x is the semi-analytic reference flux.





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Summary

- A semi-analytical solution to a simple benchmark is provided along with consistent MCNP6 results.
- The standard deviation of the mean of the tallies can be underestimated if the random number generator stride is exceeded; the mean of the tallies are unaffected.
- The covariance-corrected standard deviation can be computed to obtain more appropriate confidence intervals.
- **The best way to avoid any stride exceedance issues is to use the new SFC64 (`RAND GEN=8`) random number generator in MCNP6.3.1 and later.**

References

[1] John S. Hendricks. "Effects of Changing the Random Number Stride in Monte Carlo Calculations". In: *Nuclear Science and Engineering* 109.1 (Sept. 1991), pp. 86–91. DOI: 10.13182/NSE91-A23846. URL: http://www.ans.org/pubs/journals/nse/a_23846.

[2] James J. Duderstadt and William Russell Martin. *Transport Theory*. New York, NY, USA: John Wiley & Sons, 1979.

[3] Joel Aaron Kulesza et al. *MCNP® Code Version 6.3.0 Theory & User Manual*. Tech. rep. LA-UR-22-30006, Rev. 1. Los Alamos, NM, USA: Los Alamos National Laboratory, Sept. 2022. DOI: 10.2172/1889957. URL: https://www.osti.gov/biblio/1889957.

[4] Colin James Josey. *Reassessing the MCNP Random Number Generator*. Tech. rep. LA-UR-23-25111, Rev. 1. Los Alamos, NM, USA: Los Alamos National Laboratory, Sept. 2023. DOI: 10.2172/1998091. URL: https://www.osti.gov/biblio/1998091.