A general-purpose code for correlated sampling using batch statistics with MCNP6 for fixed-source problems

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Appendix A
Theoretical Variances for Analog Monte Carlo Calculations

This appendix derives the theoretical variances for the difference of two random tallies and the difference of two random tallies divided by a third random tally for analog Monte Carlo calculations in which every scoring particle makes the same score. These equations are used to verify some of the formulas derived in the main text and their implementation in a computer program.

The sample variance of population x is [Eq. (39) in the main text]

$$s^2 = \frac{\sum_{i=1}^{N} \left(x_i - \overline{x}\right)^2}{N-1}, \tag{A.1}$$

where the population mean is

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

and the mean of the squares is

$$\overline{x^2} = \frac{1}{N}\sum_{i=1}^{N} \left(x_i\right)^2. \tag{A.3}$$

Using Eqs. (A.2) and (A.3), Eq. (A.1) becomes

$$\begin{aligned} s^2 &= \frac{\sum_{i=1}^{N} \left(x_i\right)^2 + \sum_{i=1}^{N} \left(\overline{x}\right)^2 - 2\sum_{i=1}^{N} x_i \overline{x}}{N-1} \\ &= \frac{N\overline{x^2} + N\overline{x}^2 - 2\overline{x}N\overline{x}}{N-1} \\ &= \frac{N}{N-1}\left(\overline{x^2} - \overline{x}^2\right). \end{aligned} \tag{A.4}$$

The variance of the mean of the population is

$$\sigma_{\overline{x}}^2 = \frac{1}{N} s^2 = \frac{1}{N-1}\left(\overline{x^2} - \overline{x}^2\right). \tag{A.5}$$

The variance of the difference of two random variables, Eq. **Error! Reference source not found.** in the main text, is

$$\sigma_{\Delta R}^2 = \sigma_{R_1}^2 + \sigma_{R_0}^2 - 2\,\mathrm{cov}(R_1, R_0), \tag{A.6}$$

where the covariance is

$$\mathrm{cov}(R_1, R_0) = \frac{\sum_{i=1}^{N} \left(R_{1,i} - \overline{R}_1\right)\left(R_{0,i} - \overline{R}_0\right)}{N(N-1)}. \tag{A.7}$$

Expanding the product yields

$$\begin{aligned}\mathrm{cov}(R_1,R_0) &= \frac{1}{N(N-1)}\left(\sum_{i=1}^{N} R_{1,i}R_{0,i} - \sum_{i=1}^{N}\overline{R}_1 R_{0,i} - \sum_{i=1}^{N} R_{1,i}\overline{R}_0 + \sum_{i=1}^{N}\overline{R}_1\overline{R}_0\right)\\ &= \frac{1}{N(N-1)}\left(\sum_{i=1}^{N} R_{1,i}R_{0,i} - \overline{R}_1 N\overline{R}_0 - \overline{R}_0 N\overline{R}_1 + N\overline{R}_1\overline{R}_0\right)\\ &= \frac{1}{(N-1)}\left(\frac{1}{N}\sum_{i=1}^{N} R_{1,i}R_{0,i} - \overline{R}_1\overline{R}_0\right).\end{aligned} \tag{A.8}$$

Using Eqs. (A.5) and (A.8) in Eq. (A.6) yields

$$\begin{aligned}\sigma_{\Delta R}^2 &= \frac{1}{(N-1)}\left(\overline{R_1^2} - \overline{R}_1^{\,2} + \overline{R_0^2} - \overline{R}_0^{\,2}\right) - \frac{2}{(N-1)}\left(\frac{1}{N}\sum_{i=1}^{N} R_{1,i}R_{0,i} - \overline{R}_1\overline{R}_0\right)\\ &= \frac{1}{(N-1)}\left(\overline{R_1^2} + \overline{R_0^2} - \overline{R}_1^{\,2} - \overline{R}_0^{\,2} + 2\overline{R}_1\overline{R}_0 - \frac{2}{N}\sum_{i=1}^{N} R_{1,i}R_{0,i}\right).\end{aligned} \tag{A.9}$$

If every score is 1, then $\overline{x^2} = \overline{x}$ in Eqs. (A.2) and (A.3). Equation (A.9) becomes

$$\sigma_{\Delta R}^2 = \frac{1}{(N-1)}\left(\overline{R}_1 + \overline{R}_0 - \frac{2}{N}\sum_{i=1}^{N} R_{1,i}R_{0,i}\right) - \frac{1}{(N-1)}\left(\overline{R}_1^{\,2} + \overline{R}_0^{\,2} - 2\overline{R}_1\overline{R}_0\right). \tag{A.10}$$

In addition, if every particle that scores in configuration 1 also scores in configuration 0, then $\sum_{i=1}^{N} R_{1,i}R_{0,i} = \sum_{i=1}^{N} R_{1,i} = N\overline{R}_1 \le N\overline{R}_0$; likewise, if every particle that scores in configuration 0 also scores in configuration 1, then $\sum_{i=1}^{N} R_{1,i}R_{0,i} = \sum_{i=1}^{N} R_{0,i} = N\overline{R}_0 \le N\overline{R}_1$. In other words,

$$\frac{1}{N}\sum_{i=1}^{N} R_{1,i}R_{0,i} = \min\left(\overline{R}_0, \overline{R}_1\right). \tag{A.11}$$

Equation (A.10) becomes

$$\sigma_{\Delta R}^2 = \frac{\left|\overline{R}_1 - \overline{R}_0\right| - \left(\overline{R}_1 - \overline{R}_0\right)^2}{N-1} = \frac{\left|\Delta R\right| - \Delta R^2}{N-1}. \tag{A.12}$$

More generally, if every scoring particle in configuration n scores the total source rate for configuration n, Q_n, and N_n is the number of particles that score in configuration n, then

$$\overline{R}_n = Q_n \frac{N_n}{N} \tag{A.13}$$

and

$$\overline{R_n^2} = Q_n^2 \frac{N_n}{N} = Q_n \overline{R}_n. \tag{A.14}$$

In addition,

$$\begin{aligned}\frac{1}{N}\sum_{i=1}^{N} R_{1,i}R_{0,i} &= Q_1 Q_0 \frac{1}{N}\min(N_1, N_0)\\ &= Q_1 Q_0 \min\left(\frac{\overline{R}_1}{Q_1}, \frac{\overline{R}_0}{Q_0}\right).\end{aligned} \tag{A.15}$$

Equation (A.9) becomes

$$\sigma s_{\Delta R}^2 = \frac{1}{(N-1)}\left(Q_1\bar{R}_1 + Q_0\bar{R}_0 - 2Q_1Q_0 \min\left(\frac{\bar{R}_1}{Q_1},\frac{\bar{R}_0}{Q_0}\right) - \Delta R^2 \right). \tag{A.16}$$

If $Q_1 = Q_0 = 1$, then Eq. (A.16) reduces to Eq. (A.12).

If there is variance reduction or multiplication, then it will not be true that every particle score is the same. Also, it turns out that Eq. (A.11) is quite difficult to satisfy; it is more likely that

$$\frac{1}{N}\sum_{i=1}^{N} R_{1,i}R_{0,i} < \min\left(\bar{R}_0, \bar{R}_1\right). \tag{A.17}$$

The versions of Eqs. (A.12) and (A.16) that apply to uncorrelated tallies are

$$\sigma_{\Delta R}^2 = \frac{1}{(N-1)}\left(\bar{R}_1 + \bar{R}_0 - \bar{R}_1^{\,2} - \bar{R}_0^{\,2}\right) \tag{A.18}$$

and

$$\sigma_{\Delta R}^2 = \frac{1}{(N-1)}\left(Q_1\bar{R}_1 + Q_0\bar{R}_0 - \bar{R}_1^{\,2} - \bar{R}_0^{\,2}\right), \tag{A.19}$$

respectively.

The variance of a numerical derivative involving three random variables, Eq. **Error! Reference source not found.** in the main text, is

$$\begin{aligned}\sigma_{S_{R,x}}^2 \approx{}& \left(\frac{c_2}{R_0}\right)^2 \left(s_{R_+}^2 + s_{R_-}^2 - 2\,\mathrm{cov}(R_+,R_-)\right) + \left(\frac{S_{R,x}}{R_0}\right)^2 s_{R_0}^2 \\ &- \frac{2c_2S_{R,x}}{R_0^2}\left(\mathrm{cov}(R_+,R_0) - \mathrm{cov}(R_-,R_0)\right).\end{aligned} \tag{A.20}$$

Using Eqs. (A.5) and (A.8) in Eq. (A.20) yields

$$\begin{aligned}\sigma_{S_{R,x}}^2 \approx{}& \frac{1}{(N-1)}\left(\frac{c_2}{\bar{R}_0}\right)^2 \left(\left[\overline{R_+^2} - \bar{R}_+^{\,2} + \overline{R_-^2} - \bar{R}_-^{\,2}\right] - 2\left[\frac{1}{N}\sum_{i=1}^{N} R_{+,i}R_{-,i} - \bar{R}_+\bar{R}_-\right]\right) \\ &+ \frac{1}{(N-1)}\left(\frac{\bar{S}_{R,x}}{\bar{R}_0}\right)^2 \left(\overline{R_0^2} - \bar{R}_0^{\,2}\right) \\ &- \frac{2c_2\bar{S}_{R,x}}{(N-1)\bar{R}_0^2}\left(\left[\frac{1}{N}\sum_{i=1}^{N} R_{+,i}R_{0,i} - \bar{R}_+\bar{R}_0\right] - \left[\frac{1}{N}\sum_{i=1}^{N} R_{-,i}R_{0,i} - \bar{R}_-\bar{R}_0\right]\right),\end{aligned} \tag{A.21}$$

where the sensitivity now has an overbar to be consistent with the notation for the average tallies.

If every score is 1, then $\overline{x^2} = \bar{x}$ from Eqs. (A.2) and (A.3). Equation (A.21) becomes

(A.22)

$$\sigma^2_{S_{R,x}} \approx \frac{1}{(N-1)}\left(\frac{c_2}{\overline{R}_0}\right)^2 \left(\overline{R}_+ - \overline{R}_+{}^2 + \overline{R}_- - \overline{R}_-{}^2 - \frac{2}{N}\sum_{i=1}^{N} R_{+,i}R_{-,i} + 2\overline{R}_+\overline{R}_-\right)$$
$$+\frac{1}{(N-1)}\left(\frac{\overline{S}_{R,x}}{\overline{R}_0}\right)^2 \left(\overline{R}_0 - \overline{R}_0{}^2\right)$$
$$-\frac{2c_2\overline{S}_{R,x}}{(N-1)\overline{R}_0^2}\left(\frac{1}{N}\sum_{i=1}^{N} R_{+,i}R_{0,i} - \overline{R}_+\overline{R}_0 - \frac{1}{N}\sum_{i=1}^{N} R_{-,i}R_{0,i} + \overline{R}_-\overline{R}_0\right).$$

Rearranging and using Eq. (A.11) yields

$$\begin{aligned}\sigma^2_{S_{R,x}} &\approx \frac{1}{(N-1)}\left(\frac{c_2}{\overline{R}_0}\right)^2 \left(\left|\overline{R}_+ - \overline{R}_-\right| - \left[\overline{R}_+ - \overline{R}_-\right]^2\right) \\ &+\frac{1}{(N-1)}\left(\frac{\overline{S}_{R,x}}{\overline{R}_0}\right)^2 \left(\overline{R}_0 - \overline{R}_0{}^2\right) + \frac{2c_2\overline{S}_{R,x}}{(N-1)\overline{R}_0^2}\left(\overline{R}_+ - \overline{R}_-\right)\overline{R}_0 \\ &-\frac{2c_2\overline{S}_{R,x}}{(N-1)\overline{R}_0^2}\left(\min(\overline{R}_+,\overline{R}_0) - \min(\overline{R}_-,\overline{R}_0)\right).\end{aligned} \tag{A.23}$$

Rearranging and using Eq. **Error! Reference source not found.** in the main text yields

$$\begin{aligned}\sigma^2_{S_{R,x}} &\approx \frac{1}{(N-1)}\left(\left[\frac{c_2}{\overline{R}_0}\right]^2 \left|\overline{R}_+ - \overline{R}_-\right| + \frac{\overline{S}^2_{R,x}}{\overline{R}_0}\right) \\ &-\frac{2c_2\overline{S}_{R,x}}{(N-1)\overline{R}_0^2}\left(\min(\overline{R}_+,\overline{R}_0) - \min(\overline{R}_-,\overline{R}_0)\right).\end{aligned} \tag{A.24}$$

If the central difference is an accurate estimate of the derivative, then the three points $(x_0 - \Delta x, \overline{R}_-)$, $(x_0, \overline{R}_0)$, and $(x_0 + \Delta x, \overline{R}_+)$ lie approximately on a line. In that case, the quantity $\min(\overline{R}_+,\overline{R}_0) - \min(\overline{R}_-,\overline{R}_0)$ is either $\overline{R}_+ - \overline{R}_0$ or $\overline{R}_0 - \overline{R}_-$. But that insight does not seem to help simplify Eq. (A.24).

If every scoring particle in configuration *n* scores the total source rate for configuration *n*, then applying Eqs. (A.14) and (A.15) to Eq. (A.21) yields

$$\begin{aligned}\sigma^2_{S_{R,x}} &\approx \frac{1}{(N-1)}\left(\frac{c_2}{\overline{R}_0}\right)^2 \left(\left[Q_+\overline{R}_+ - \overline{R}_+{}^2 + Q_-\overline{R}_- - \overline{R}_-{}^2\right] - 2\left[Q_+Q_- \min\left(\frac{\overline{R}_+}{Q_+},\frac{\overline{R}_-}{Q_-}\right) - \overline{R}_+\overline{R}_-\right]\right) \\ &+\frac{1}{(N-1)}\left(\frac{\overline{S}_{R,x}}{\overline{R}_0}\right)^2 \left(Q_0\overline{R}_0 - \overline{R}_0{}^2\right) \\ &-\frac{2c_2\overline{S}_{R,x}}{(N-1)\overline{R}_0^2}\left(\left[Q_+Q_0 \min\left(\frac{\overline{R}_+}{Q_+},\frac{\overline{R}_0}{Q_0}\right) - \overline{R}_+\overline{R}_0\right] - \left[Q_-Q_0 \min\left(\frac{\overline{R}_-}{Q_-},\frac{\overline{R}_0}{Q_0}\right) - \overline{R}_-\overline{R}_0\right]\right).\end{aligned} \tag{A.25}$$

Simplifying yields

(A.26)

$$\sigma^2_{S_{R,x}} \approx \frac{1}{(N-1)}\left(\frac{c_2}{\overline{R}_0}\right)^2\left(Q_+\overline{R}_+ + Q_-\overline{R}_- - 2Q_+Q_- \min\left(\frac{\overline{R}_+}{Q_+},\frac{\overline{R}_-}{Q_-}\right)\right)$$
$$+\frac{1}{(N-1)}\left(\frac{\overline{S}^2_{R,x}Q_0}{\overline{R}_0}\right)$$
$$-\frac{1}{(N-1)}\left(\frac{2c_2\overline{S}_{R,x}Q_0}{\overline{R}_0^2}\right)\left(Q_+ \min\left(\frac{\overline{R}_+}{Q_+},\frac{\overline{R}_0}{Q_0}\right) - Q_- \min\left(\frac{\overline{R}_-}{Q_-},\frac{\overline{R}_0}{Q_0}\right)\right).$$

Again, if $Q_+ = Q_- = Q_0 = 1$, then Eq.(A.26) reduces to Eq. (A.24).

The versions of Eqs. (A.24) and (A.26) that apply to uncorrelated tallies are

$$\sigma^2_{S_{R,x}} = \frac{1}{(N-1)\overline{R}_0{}^2}\left\{c_2^2\left(\overline{R}_+ - \overline{R}_+{}^2 + \overline{R}_- - \overline{R}_-{}^2\right) + \overline{S}^2_{R,x}\left(\overline{R}_0 - \overline{R}_0{}^2\right)\right\} \tag{A.27}$$

and

$$\sigma^2_{S_{R,x}} = \frac{1}{(N-1)\overline{R}_0{}^2}\left\{c_2^2\left(Q_+\overline{R}_+ - \overline{R}_+{}^2 + Q_-\overline{R}_- - \overline{R}_-{}^2\right) + \overline{S}^2_{R,x}\left(Q_0\overline{R}_0 - \overline{R}_0{}^2\right)\right\}, \tag{A.28}$$

respectively.

Appendix B
MCNP Base-Case Input File Listing

This is the 999th input file of the 1000 inputs of the base case for Problem 5 and 6 (Secs. **Error! Reference source not found.** and **Error! Reference source not found.**). In the SEED keyword of the RAND card, the number 0999 is replaced by the numbers 0001 to 1000. These cases use implicit capture. The analog cases in the other sections use the same set of random number seeds. The inputs for Problems 1–4 do not have the track-length flux tally. All inputs and outputs from all example problems are available in the repository.

```
He and Su, ANE 2010 and 2011; with F4 tally
C Cell specifications
1 1  -0.67552          -1                                 imp:n = 1 $ Coal inside the ball
2 0                     1 -2                              imp:n = 1 $ void space
3 0                     2                                 imp:n = 0 $ Zero-importance outer world

C Surface specifications
1 so 30.
2 so 45.

C Data cards
mode n
C isotropic point source
sdef erg=d1 pos=0. 0. 0.
sc1 flat energy spectrum from 1 to 14.1 MeV
si1 1. 14.1
sp1 0. 1.
C Material
c begin at.dens., wt.dens.  4.929841407E-02     0.675520000000
c round at.dens., wt.dens.  4.929841406E-02     0.675519999608
m1     nlib=00c
        1001 -3.37682384E-02        1002 -7.76162156E-06
        6012 -4.62712342E-01        6013 -5.42301768E-03
        7014 -6.72886714E-03        7015 -2.63328631E-05
        8016 -1.14527191E-01        8017 -4.63653604E-05
        8018 -2.64843545E-04
       11023 -1.35104000E-03
       12024 -1.05313550E-04       12025 -1.38888268E-05
       12026 -1.59016236E-05
       13027 -2.02656000E-02
       14028 -1.42732593E-02       14029 -7.50998985E-04
       14030 -5.12701709E-04
       16032 -6.39821023E-03       16033 -5.20965872E-05
       16034 -3.04135456E-04       16036 -7.57730967E-07
       17035 -1.51435812E-04       17037 -5.12201883E-05
       19039 -3.13904222E-04       19040 -4.03929083E-08
       19041 -2.38153847E-05
       22046 -2.67509137E-05       22047 -2.46489896E-05
       22048 -2.49419048E-04       22049 -1.86855267E-05
       22050 -1.82555215E-05
       26054 -2.09752812E-04       26056 -3.41447264E-03
       26057 -8.02654714E-05       26058 -1.08690770E-05
       31069 -2.00698629E-03       31071 -1.37061371E-03
phys:n 14.2 0.01
cut:n 1e20 0.05 0.05 0.01 0.01
fc1 current across the coal ball interface
f1:n 1
fc4 total flux in coal ball
f4:n 1
sd4 1.
nps 1e6
prdmp 4j 1e3 1000
idum 1
dbcn 49j 2
print 110 160
rand gen=2 seed=110999000001
```

Appendix C
Modifications to MCNP6.3 to Make the Maximum Number of TFC Entries a User Input

In the unmodified version of MCNP6.3, the variable `mtfc`, the maximum number of TFC entries, is set in setdas.F90 as 100 or 20 based on whether ROC curves are generated in a special tally treatment.**Error! Bookmark not defined.** The maximum applies to the TFC bin of every tally. The idea behind the modification was to let the user input `mtfc` on the PRDMP card.**Error! Bookmark not defined.** A better way to do this would use NPS and the fifth entry on the PRDMP card to set the number of TFC entries, as the manual implies (Section 5.13.5).**Error! Bookmark not defined.** However, in setdas.F90, where `mtfc` is set, the actual value that will be used for NPS is not yet known.

Four files were modified.

In input/mcnp_input.F90, the "5" in the line
```
        cnm(64) = 'prdmp           '; krq(:, 64) = [1, 0, 0, 1, -1, 5, 0]
```
was changed to 6 to allow 6 entries on the PRDMP card.

In input/nxtit0.F90, mtfc was added to the list in "use fixcom, only". The following lines were added:
```
       case (64) NXTIT0_CARDS
       !  >>>>>  print and dump controls                                     prdmp
       if (nwc == 6) mtfc = iitm
```

In imcn.F90, mtfc was added to the list in "use fixcom, only". The lines
```
        if (npp >= 0_I8 .and. ntal /= 0) then
…
            do i = 1, 20
…
                if (nn == 20) n_I8 = npd/2
…
        end if
```
were changed to
```
        if (npp >= 0_I8 .and. ntal /= 0) then
…
            do i = 1, mtfc
…
                if (nn == mtfc) n_I8 = npd/2
…
        end if
```

In setdas.F90, the line
```
        mtfc = 20
```
was changed to
```
        if (mtfc <= 0) then
          mtfc = 20
        end if
```
to retain the default value. Thus, the user input to change the maximum number of TFC entries has no effect if there is a ROC curve calculated.