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Title: One-Group Analytic Test Problems for MCNP5 Perturbation Verification (U)

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SUBJECT: One-Group Analytic Test Problems for MCNP5 Perturbation Verification (U)

Abstract

An analytic monoenergetic fixed-source problem is used to demonstrate a bug in the MCNP5 perturbation feature. The presence or absence of tallies, and the form of the associated FM cards, may lead to silent wrong answers in unrelated perturbed tallies. An analytic monoenergetic k_∞ problem (derived previously) also demonstrates the bug. Input files are listed.

I. Introduction

Recently, verification of the MCNP5 perturbation capability[1] has been done using analytic formulas, direct perturbation calculations, and code-to-code comparisons.[2,3] In this work, bugs have been found. In k_{eff}-eigenvalue problems, the perturbation capability sometimes gives nonzero Δk_{eff} results for fission reactions that do not exist.[3] In fixed-source and k_{eff}-eigenvalue problems, the presence or absence of tallies can change the tally perturbation results.[4]

This paper presents analytic results for a monoenergetic fixed-source problem that may be useful in diagnosing the perturbed tally bug. The analytic k_∞ problem of Ref. 2 is also used to demonstrate the perturbed tally bug as well as the nonzero Δk_{eff} results for fission reactions that do not exist. The monoenergetic cross sections are in continuous-energy format.

The input files, cross-section files, and cross-section directory are listed in an attachment.

II. Fixed-Source Test Problem and Derivatives of the Quantity of Interest

Consider a monoenergetic isotropic point source at the center of a homogeneous sphere of radius R. The material in the sphere has neutron capture and fission, but fission is treated as capture (there is no fission multiplication), and there is no scattering. Thus there is no way to change a neutron's energy, and the cross sections can be specified for one discrete energy. The flux $\psi(r,\hat{\mathbf{\Omega}})$ in direction $\hat{\mathbf{\Omega}}$ at a point r in the sphere is

$$\psi(r,\hat{\mathbf{\Omega}}) = \frac{S}{4\pi}\frac{e^{-\Sigma_t r}}{r^2}, \tag{1}$$

where S is the source strength and Σ_t is the total interaction cross section, given by

$$\Sigma_t = \Sigma_f + \Sigma_c, \tag{2}$$

where Σ_f and Σ_c are the material macroscopic fission and capture cross sections, respectively (the capture cross section Σ_c is MCNP's absorption cross section).

Let the quantity of interest k be the total fission rate in the sphere:

$$\begin{aligned} k &= \int_{4\pi} d\hat{\mathbf{\Omega}} \int_0^R dr\, r^2 \Sigma_f \psi(r,\hat{\mathbf{\Omega}}) \\ &= S\int_0^R dr\,\Sigma_f e^{-\Sigma_t r} \\ &= S\frac{\Sigma_f}{\Sigma_t}\left(1-e^{-\Sigma_t R}\right). \end{aligned} \tag{3}$$

If the material is composed of two isotopes with atom densities N_1 and N_2 such that $\Sigma_x = N_1\sigma_{x,1} + N_2\sigma_{x,2}$, Eq. (3) becomes

$$k = S\frac{N_1\sigma_{f,1} + N_2\sigma_{f,2}}{N_1(\sigma_{f,1}+\sigma_{c,1}) + N_2(\sigma_{f,2}+\sigma_{c,2})}\left(1-e^{-\left[N_1(\sigma_{f,1}+\sigma_{c,1})+N_2(\sigma_{f,2}+\sigma_{c,2})\right]R}\right). \tag{4}$$

For comparison with MCNP5 perturbation results, we will examine the first derivative of k with respect to each of the cross sections of material 1. The derivatives are

$$\frac{dk}{d\sigma_{t,1}} = \left(\frac{N_1}{\sigma_{t,1}}\right)\frac{dk}{dN_1} = S\frac{(\sigma_{f,1}+\sigma_{c,1})}{\sigma_{t,1}}\frac{N_1\Sigma_f}{\Sigma_t}\left\{\left(\frac{\sigma_{f,1}}{(\sigma_{f,1}+\sigma_{c,1})\Sigma_f} - \frac{1}{\Sigma_t}\right)\left(1-e^{-\Sigma_t R}\right) + Re^{-\Sigma_t R}\right\}, \tag{5}$$

$$\frac{dk}{d\sigma_{f,1}} = S\frac{N_1\Sigma_f}{\Sigma_t}\left\{\left(\frac{1}{\Sigma_f} - \frac{1}{\Sigma_t}\right)\left(1-e^{-\Sigma_t R}\right) + Re^{-\Sigma_t R}\right\}, \tag{6}$$

and

$$\frac{dk}{d\sigma_{c,1}} = S\frac{N_1\Sigma_f}{\Sigma_t}\left\{-\frac{1}{\Sigma_t}\left(1-e^{-\Sigma_t R}\right) + Re^{-\Sigma_t R}\right\}. \tag{7}$$

The first-order term of the Taylor series expansion of $\Delta k \equiv k(\sigma_x) - k(\sigma_{x,0})$, where $\sigma_{x,0}$ is the reference value of the cross section, is

$$\Delta k_1 = \left.\frac{dk}{d\sigma_x}\right|_{\sigma_x=\sigma_{x,0}} (\sigma_x - \sigma_{x,0}). \tag{8}$$

The METHOD keyword on the PERT card controls the printing of Taylor terms; Δk_1 is given using METHOD=2.

III. Numerical Results for the Fixed-Source Problem

The isotopes and data used in the fixed-source problem are listed in Table I. The cross sections are one-group macroscopic cross sections from Ref. 5, except that the scattering cross sections were set to zero and the total cross sections recomputed with Eq. (2). In this paper they are treated as microscopic cross sections and the isotopic densities in the homogeneous material are $N_1 = 0.6$ at/bn·cm and $N_2 = 0.4$ at/bn·cm so that the total material atom density $N_1 + N_2$ is 1 at/bn·cm. Nevertheless, we stress that N_1 and N_2 are atom densities, not atom fractions, and N_1 will vary but N_2 will not. These monoenergetic data were put into a continuous-energy format for MCNP using the MAKECE code provided by Bob Little (X-1-NAD). The source strength S was unity.

Table I. Isotopes Used in the Fixed-Source Problem

Index	ν	σ_f (cm^2)	σ_c (cm^2)	σ_s (cm^2)	σ_t (cm^2)
1[a]	3.24	0.081600	0.019584	0.	0.101184
2[b]	2.70	0.065280	0.013056	0.	0.078336

[a] Pu-239 (a), Table 2, Ref. 5.
[b] U-235 (a), Table 9, Ref. 5.

The analytic value of k is 0.251211. The MCNP5 calculation used 4×10^6 source neutrons. The NONU card was used to treat fission as capture. The MCNP5 value of k was 0.251261 ± 0.02%, having an error of 0.02% or 0.99 standard deviations. The cross sections of isotope 1 were each perturbed by +30% independently. Two MCNP5 problems were run. One had a tally only for the quantity of interest k (i.e., the "real" tally) and the other also had a dummy tally with a number smaller than that of the real tally.

Results are shown in Table II. The analytic results were computed using Eq. (8) with the appropriate derivative from Eq. (5), (6), or (7).

Table II. Results for the First-Order Taylor Term Δk_1

			Difference	
	Analytic	PERT Estimate	Rel. to Analytic	Num. Std. Devs.
$\sigma_{t,1}$	4.05596E-02	4.05640E-02 ± 0.02%	0.011%	0.543
$\sigma_{f,1}$	4.22223E-02	–6.93207E-03 ± 0.12% [(a)]	–116.418	5909.05
		4.22277E-02 ± 0.02% [(b)]	0.013%	0.644
$\sigma_{c,1}$	–1.66266E-03	–1.66370E-03 ± 0.12%	0.062%	0.519

[(a)] Only one tally (for k).
[(b)] Also with a "dummy" tally with a number smaller than that of the k tally.

Clearly, the *absence* of the dummy tally leads to a serious error (a silent wrong answer) in the perturbation estimate of Δk_1. Also, when the dummy tally has a number greater than the real tally, the effect is the same as if the dummy tally were absent.

The FM card on the dummy tally is also important. When it is "`fm004 (-1 1  -6 -6 -6 -6 -6)`" (reactions are multiplied), the effect is the same as if the dummy tally were absent (it leads to an error in Δk_1), but when it is "`fm004 (-1 1 -6:-6:-6:-6:-6)`" (reactions are added), the real tally perturbation is correct. In addition, if there are four reactions to add in the dummy tally, the effect is the same as if the dummy tally were absent, but with five, the real tally perturbation is correct.

IV. k_∞ Test Problem and Numerical Results

A monoenergetic analytic k_∞ test problem was presented in Ref. 2. There it was shown that the MCNP5 perturbation estimates of the first- and second-order Taylor terms of Δk_∞ were extremely accurate. But Ref. 2 did not look at perturbed tallies.

For completeness, the isotopes and data used in the k_∞ problem are listed in Table III. As in Sec. II, they are treated as microscopic cross sections and the isotopic densities in the homogeneous material are N_1 = 0.6 at/bn·cm and N_2 = 0.4 at/bn·cm so that the total material atom density $N_1 + N_2$ is 1 at/bn·cm. Continuous-energy tables were created using the MAKECE code.

Table III. Isotopes Used in the k_∞ Problem

Index	ν	σ_f (cm^2)	σ_c (cm^2)	σ_s (cm^2)	σ_t (cm^2)
1[a]	3.24	0.081600	0.019584	0.225216	0.32640
2[b]	2.70	0.065280	0.013056	0.248064	0.32640

[a] Pu-239 (a), Table 2, Ref. 5.
[b] U-235 (a), Table 9, Ref. 5.

The analytic value of k_∞ is 2.489362 (there is a typo in this value in Sec. III of Ref. 2). Using a 10-cm sphere of the material with a reflecting boundary and 5000 neutrons per cycle, 30 settle cycles, 100 active cycles, and an initial guess of 1, the MCNP5 track-length estimate of k_∞ was 2.48990 ± 0.00111, having an error of 0.02% or 0.48 standard deviations. The cross sections of isotope 1 were each perturbed by +30% independently. Two MCNP5 problems were run. One had a tally only for the quantity of interest k_∞ (i.e., the "real" tally) and the other also had a dummy tally with a number smaller than that of the real tally.

Results are shown in Table IV. The analytic formulas are given in Ref. 2.

Table IV. Results for Δk_∞ (Sum of Two Taylor Terms)

	Analytic	PERT Estimate	Difference: Rel. to Analytic	Difference: Num. Std. Devs.
$\sigma_{t,1}$	1.96084E-02	1.91346E-02 ± 6.67%	2.416%	0.371
$\sigma_{f,1}$	1.00668E-01	–3.33940E-01 ± 0.16% [(a)]	–431.723	813.41
		1.00659E-01 ± 0.36% [(b)]	–0.009%	0.026
$\sigma_{c,1}$	–9.16860E-02	–9.17190E-02 ± 0.19%	0.036%	0.189

[(a)] Only one tally (for k_∞).
[(b)] Also with a "dummy" tally with a number smaller than that of the k_∞ tally.

The conclusions of the previous section regarding the order of the tallies and the contents of the dummy FM card applied to this problem also.

In the monoenergetic continuous-energy cross sections, fission is given as MT=18, and reactions 19, 20, 21, and 38 do not exist. However, for a perturbation of reactions 19, 20, 21, and 38, the Δk_{eff} results are nonzero. This bug was reported in Ref. 3.

V. Summary and Conclusions

In this paper, an analytic monoenergetic fixed-source problem was used to demonstrate a bug in the MCNP5 perturbation feature. A previously derived analytic monoenergetic k_∞ problem was also used. The bug is that perturbed tally results depend on the presence or absence of unrelated tallies and their FM cards. The k_∞ problem also shows that the perturbation capability sometimes gives nonzero Δk_{eff} results for fission reactions that do not exist.

Difficulties with the MCNP5 estimate of k_{eff} sensitivities to scattering cross sections have been observed.[2,3] The analytic fixed-source problem of this paper has no scattering, so it cannot be used to test perturbations of scattering cross sections. The analytic k_∞ does not depend on scattering,[2] so although it has non-zero scattering it too cannot be used to test perturbations of scattering cross sections. However, the bugs identified in this testing may be affecting the sensitivities to scattering. Work is continuing to figure out why the MCNP5 perturbation capability has trouble with scattering in k_{eff} problems.

Extreme caution should be used with the MCNP5 perturbation capability until these bugs are fixed.

References

1. X-5 Monte Carlo Team, "MCNP–A General Monte Carlo N-Particle Transport Code, Version 5," Vol. I, LA–UR–03–1987, and Vol. II, LA–CP–03–0245, Los Alamos National Laboratory (April 24, 2003; Rev. October 3, 2005).

2. Jeffrey A. Favorite, "Comparison of MCNP5 Perturbation Estimates of *k*-Eigenvalue Sensitivities with Exact Results for One-Group and 30-Group Problems (U)," Research Note X-1–RN(U)09–03, LA–UR–09–0499, Los Alamos National Laboratory (January 26, 2009).

3. Jeffrey A. Favorite, "A Comparison of MCNP5 Perturbation Estimates of k_{eff} Sensitivities with TSUNAMI-3D Results for a Homogeneous Thermal Sphere (U)," Research Note X-1–RN(U)09–05, LA–UR–09–1724, Los Alamos National Laboratory (March 17, 2009).

4. Jeffrey A. Favorite, email to Jeffrey S. Bull, Dec. 9, 2008 and March 30, 2009.

5. Avneet Sood, R. Arthur Forster, and D. Kent Parsons, "Analytical Benchmark Test Set For Criticality Code Verification," *Progress in Nuclear Energy*, **42**, *1*, 55-106 (2003).

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ATTACHMENT

INPUT FILES AND CROSS-SECTION FILES

These files are available electronically from the author.

Input file for the fixed-source problem:

```
message: xsdir=xsdir1

tally pert bug, fixed-source, one-group.
10   1   1.    -10    imp:n=1
99   0          10    imp:n=0

10  so   4.

mode n
sdef  pos=0. 0. 0.
nps 4e6
prdmp j 4e5 -1
nonu
m1   90240.43c 0.6   90240.63c 0.4
m2   90240.43c 0.78  90240.63c 0.4
c
c ------------------------------------------------------------
c analytic results:
c   tally 104, unpert: 0.251211
c   pert201:  0.040560
c   pert202:  0.042222
c   pert203: -0.0016627
c   pert204:  0.0 (there is no scattering in xs43 or xs63)
c   pert205:  0.0 (because xs43 and xs63 have fission as mt=18)
c   pert206:  0.042222
c
c mcnp5 results:
c   pert202 is wrong. pert201, 203, 204, and 205 are right.
c   when f4 is not included, pert206 is the same as pert202, as
c   it should be, but they are both wrong.  when f4 is included,
c   pert206 is correct but pert202 is still wrong.
c
c ------------------------------------------------------------
c fc004  dummy
c  f004:n 10
c fm004 (-1 1  -6:-6:-6:-6:-6)
fc104  real, sigf
 f104:n 10
fm104 (-1 1  -6)
sd104 1.
pert201:n cell=10 rho=1.18 mat=2 rxn=1                method=2
pert202:n cell=10 rho=1.18 mat=2 rxn=18               method=2
pert203:n cell=10 rho=1.18 mat=2 rxn=102              method=2
pert204:n cell=10 rho=1.18 mat=2 rxn=22               method=2
pert205:n cell=10 rho=1.18 mat=2 rxn=19 20 21 38      method=2
pert206:n cell=10 rho=1.18 mat=2 rxn=-6               method=2
print

end of input
```

Input file for the k_∞ problem:

```
message: xsdir=xsdir1

pu239a and u235a, unpert, kinfinity
10  1    1.             -10    imp:n=1
99  0                    10    imp:n=0

*10  so  10.

mode n
kcode 5000     1.    30    130
prdmp j 100
sdef        pos=0. 0. 0. rad=d2
si2 0. 10.
sp2 -21 2
m1   90240.40c 0.6   90240.60c 0.4
m2   90240.40c 0.78  90240.60c 0.4
c
c ----------------------------------------------------------
c analytic results:
c   tally 54 and 64, unpert: 2.489362
c   pert101:  0.01961
c   pert102:  0.10067
c   pert103: -0.09169
c   pert104:  0.0 (there is no scattering in kinfinity)
c   pert105:  0.0 (because xs40 and xs60 have fission as mt=18)
c   pert106:  0.10067
c
c mcnp5 results:
c when f004 is not included:
c   delta-k, pert 5, is wrong (non-zero), others are right.
c   pert102 and pert 106 are wrong, both tallies.
c   pert101, 103, 104, and 105 are right.
c when f004 is included:
c   delta-k, pert 5, is wrong (non-zero), others are right.
c   pert102, tally 54 is right, tally 64 is wrong.
c   pert106, tally 54 is wrong, tally 64 is right.
c   pert101, 103, 104, and 105 are right.
c
c ----------------------------------------------------------
c
  fc004 dummy
   f004:n 10
  fm004 (-1 1 -6:-6:-6:-6:-6  )
c  f054:n 10
c fm054 (-1 1 -7 18)
c sd054 1.
 f064:n 10
fm064 (-1 1 -7 -6)
sd064 1.
c
pert101:n cell=10 rho=1.18 mat=2 rxn=1            method=1
pert102:n cell=10 rho=1.18 mat=2 rxn=18           method=1
pert103:n cell=10 rho=1.18 mat=2 rxn=102          method=1
pert104:n cell=10 rho=1.18 mat=2 rxn=22           method=1
pert105:n cell=10 rho=1.18 mat=2 rxn=19 20 21 38  method=1
pert106:n cell=10 rho=1.18 mat=2 rxn=-6           method=1
c
print

end of input
```

Cross-section file xs40:

```
 90240.40c 2.40000E+02 0.00000E+00 11/02/97
pu239 a, table 2, unperturbed




      82    90240        2        3        2        0        0        0
       0        0        0        0        0        0        0        0
       1       11       18       21       24       27       30       42
      45       45       47        0        0        0        0        0
       0        0        0        0        0       82        0        0
       0        0        0        0        0        0        0        0
  1.000000000000E-11                100  3.264000000000E-01  3.264000000000E-01
  1.958400000000E-02  1.958400000000E-02                  0                   0
                   0                  0                   2                   0
                   2  1.000000000000E-11                100  3.240000000000E+00
  3.240000000000E+00                 18                  22                 102
                 180                  1                   5                  19
                   1                  0                   1                   5
                   9                  1                   2  8.160000000000E-02
  8.160000000000E-02                  1                   2  2.252160000000E-01
  2.252160000000E-01                  1                   2  1.958400000000E-02
  1.958400000000E-02                  0                   0                   0
                   1                 19                   0                   1
                  10                  0                   2  1.000000000000E-11
                 100                  1                   1                   0
                   2  1.000000000000E-11                100                   2
  1.000000000000E-11                100  1.000000000000E-11                 100
                   0                  1                  28                   0
                   2  1.000000000000E-11                100                   1
                   1                  0                   2  1.000000000000E-11
                 100                  2  1.000000000000E-11                 100
  1.000000000000E-11                100
```

Cross-section file xs60:

```
 90240.60c 2.40000E+02 0.00000E+00 11/02/97
u235 a, table 9, unperturbed




      82    90240        2        3        2        0        0        0
       0        0        0        0        0        0        0        0
       1       11       18       21       24       27       30       42
      45       45       47        0        0        0        0        0
       0        0        0        0        0       82        0        0
       0        0        0        0        0        0        0        0
  1.000000000000E-11                100  3.264000000000E-01  3.264000000000E-01
  1.305600000000E-02  1.305600000000E-02                  0                   0
                   0                  0                   2                   0
                   2  1.000000000000E-11                100  2.700000000000E+00
  2.700000000000E+00                 18                  22                 102
                 180                  1                   5                  19
                   1                  0                   1                   5
                   9                  1                   2  6.528000000000E-02
  6.528000000000E-02                  1                   2  2.480640000000E-01
  2.480640000000E-01                  1                   2  1.305600000000E-02
  1.305600000000E-02                  0                   0                   0
                   1                 19                   0                   1
                  10                  0                   2  1.000000000000E-11
                 100                  1                   1                   0
                   2  1.000000000000E-11                100                   2
  1.000000000000E-11                100  1.000000000000E-11                 100
                   0                  1                  28                   0
                   2  1.000000000000E-11                100                   1
                   1                  0                   2  1.000000000000E-11
                 100                  2  1.000000000000E-11                 100
  1.000000000000E-11                100
```

Cross-section file xs43:

```
 90240.43c 2.40000E+02 0.00000E+00 11/02/97
pu239 a, table 2, unperturbed, sigs=0



        54     90240         2         2         1         0         0         0
         0         0         0         0         0         0         0         0
         1        11        18        20        22        24        26        34
        36        36        37         0         0         0         0         0
         0         0         0         0         0        54         0         0
         0         0         0         0         0         0         0         0
  1.000000000000E-11                 100  1.011840000000E-01  1.011840000000E-01
  1.958400000000E-02  1.958400000000E-02                   0                   0
                   0                   0                   2                   0
                   2  1.000000000000E-11                 100  3.240000000000E+00
  3.240000000000E+00                  18                 102                 180
                   5                  19                   0                   1
                   5                   1                   2  8.160000000000E-02
  8.160000000000E-02                   1                   2  1.958400000000E-02
  1.958400000000E-02                   0                   0                   1
                   0                   1                  10                   0
                   2  1.000000000000E-11                 100                   1
                   1                   0                   2  1.000000000000E-11
                 100                   2  1.000000000000E-11                 100
  1.000000000000E-11                 100
```

Cross-section file xs63:

```
 90240.63c 2.40000E+02 0.00000E+00 11/02/97
u235 a, table 9, unperturbed, sigs=0



        54     90240         2         2         1         0         0         0
         0         0         0         0         0         0         0         0
         1        11        18        20        22        24        26        34
        36        36        37         0         0         0         0         0
         0         0         0         0         0        54         0         0
         0         0         0         0         0         0         0         0
  1.000000000000E-11                 100  7.833600000000E-02  7.833600000000E-02
  1.305600000000E-02  1.305600000000E-02                   0                   0
                   0                   0                   2                   0
                   2  1.000000000000E-11                 100  2.700000000000E+00
  2.700000000000E+00                  18                 102                 180
                   5                  19                   0                   1
                   5                   1                   2  6.528000000000E-02
  6.528000000000E-02                   1                   2  1.305600000000E-02
  1.305600000000E-02                   0                   0                   1
                   0                   1                  10                   0
                   2  1.000000000000E-11                 100                   1
                   1                   0                   2  1.000000000000E-11
                 100                   2  1.000000000000E-11                 100
  1.000000000000E-11                 100
```

Cross-section directory file xsdir1:

```
atomic weight ratios
 90240 2.40000E+02
directory
90240.40c  2.40000E+02 xs40     0 1 1   82
90240.60c  2.40000E+02 xs60     0 1 1   82
90240.43c  2.40000E+02 xs43     0 1 1   54 0 0  0.00000E+00
90240.63c  2.40000E+02 xs63     0 1 1   54 0 0  0.00000E+00
```