

LA-UR-26-27617

Approved for public release; distribution is unlimited.

Title: Source Material Density First-Order Sensitivities in MCNP6
Author(s): Favorite, Jeffrey A.
Intended for: Other: MCNP User Symposium, Aug. 24-26, Los Alamos, NM
Issued: 2026-08-24



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Source Material Density First-Order Sensitivities in MCNP6

Jeffrey A. Favorite
Radiation Transport Applications Group (XTD-RTA)
Los Alamos National Laboratory

MCNP User Symposium
Los Alamos, NM
Aug. 24–26, 2026

The Differential Operator (Taylor Series) Perturbation Method in MCNP (PERT)

Proceedings of the 13th International Conference on Radiation Shielding (ICRS-13) & 19th Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society (RPSD-2016) (Paris)

Using the MCNP Taylor series perturbation feature (efficiently) for shielding problems

Jeffrey Favorite*

X-Computational Physics Division, XCP-3, P.O. Box 1663 MS F663, Los Alamos National Laboratory, Los Alamos, NM 87545 USA

Abstract. The Taylor series or differential operator perturbation method, implemented in MCNP and invoked using the PERT card, can be used for efficient parameter studies in shielding problems. This paper shows how only two PERT cards are needed to generate an entire parameter study, including statistical uncertainty estimates (an additional three PERT cards can be used to give exact statistical uncertainties). One realistic example problem involves a detailed helium-3 neutron detector model and its efficiency as a function of the density of its high-density polyethylene moderator. The MCNP differential operator perturbation capability is extremely accurate for this problem. A second problem involves the density of the polyethylene reflector of the BeRP ball and is an example of first-order sensitivity analysis using the PERT capability. A third problem is an analytic verification of the PERT capability.

Transactions of the American Nuclear Society,
116, 997–1000 (2017)
(San Francisco)

Highlights of RPSD-2016/ICRS-13—II

997

Using the MCNP Taylor Series Perturbation Feature (Efficiently) for Shielding Problems

Jeffrey A. Favorite

XCP-3, MS F663, Los Alamos National Laboratory, Los Alamos, NM 87545 USA, fave@lanl.gov

INTRODUCTION

The Taylor series or differential operator perturbation feature [1, 2] was introduced into MCNP [3] in version 4B in the mid-1990s. The perturbation feature has been

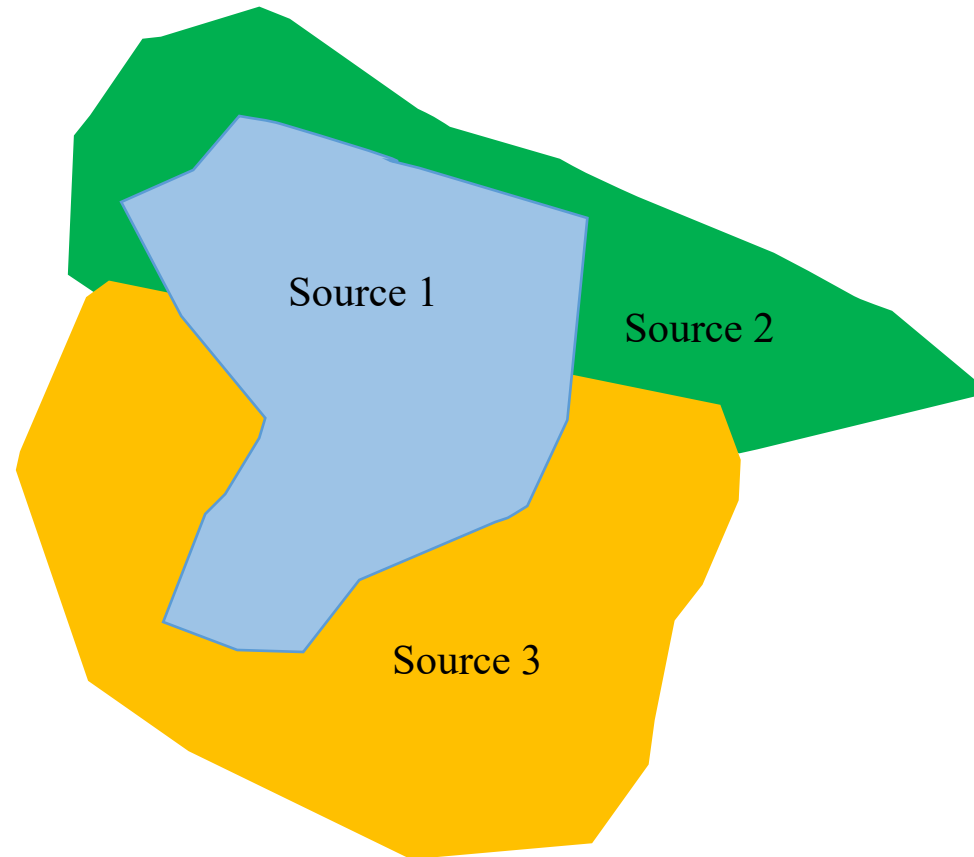
$$\Delta c_2 \equiv \frac{1}{2} \frac{d^2 c}{d\sigma_x^2} \bigg|_{\sigma_{x,0}} (\Delta \sigma_x)^2. \tag{4}$$

Define p_x as the relative cross-section change,

The PERT Card Works Great But Its Application is Limited

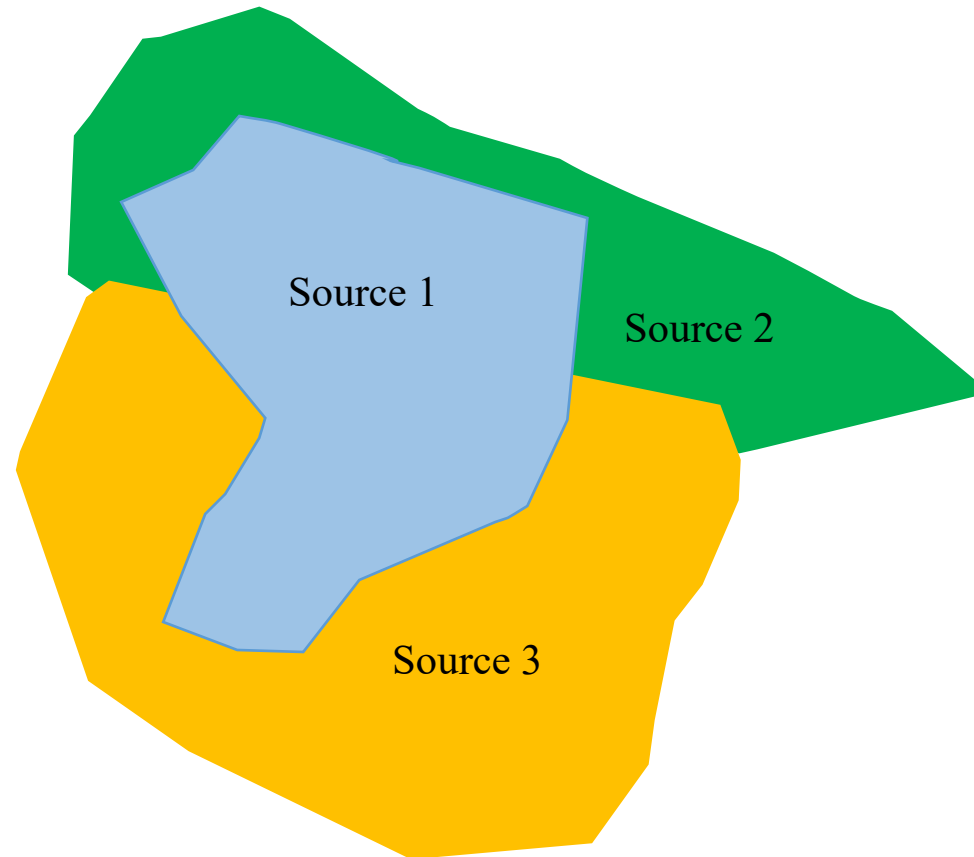
- No point detectors
 - No pulse-height tallies
 - No mesh geometries
 - No second-order Taylor series cross terms
 - No source perturbations
- + When neutrons or gamma rays are emitted due to radioactive decay, the source rate density depends intrinsically on the nuclide densities in the source material.
- + When the PERT capability in MCNP6 is used to compute sensitivities of a response to nuclide and material densities, those sensitivities do not include the effect of the source.
- + This paper shows how to fix that limitation.

The Problem



- There are 3 source materials.
- Suppose you perturb the density of Source 1 with the PERT card.
- The calculated tally perturbation will include changes in the cross sections, but not changes in the source emissions.

The Problem



- There are 3 source materials.
- Suppose you perturb the density of Source 1 with the PERT card.
- The calculated tally perturbation will include changes in the cross sections, but not changes in the source emissions.

In MCNP,

```
sdef cel=d1 pos=fcel d2 rad=fcel d3 ext=fcel d4 axs=fcel d5 erg=fcel d6 wgt=W  
si1 1 c1 c2 c3  
sp1 d s1 s2 s3
```

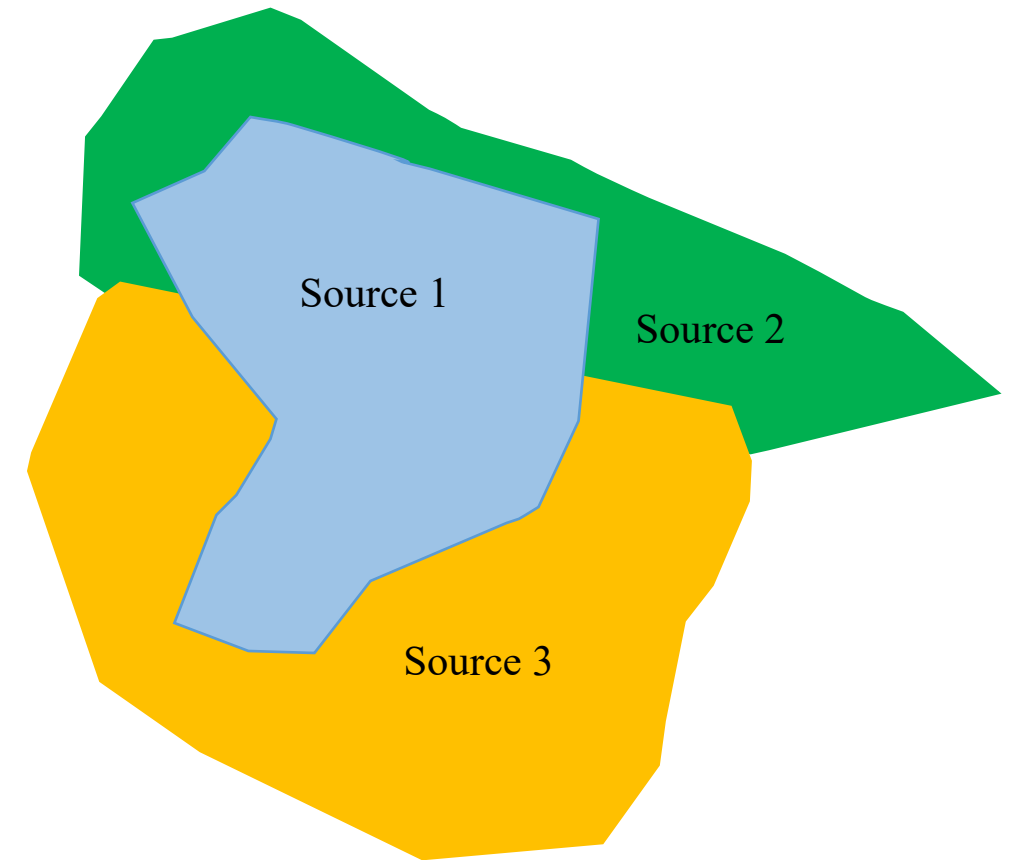
List of cells

Source rates (neutrons/s)

$$W = s1 + s2 + s3$$

Transport Equation and Sensitivity

- The transport equation is $A\Psi = Q$.
- The response is $R = \langle \Sigma_d \Psi \rangle$.
- If there are Z sources,
 - + $A\Psi_z = Q_z, z = 1, \dots, Z$.
 - + The total source rate is $Q_w = \sum_{z=1}^Z Q_z V_z$.
 - + The total response is $R = \sum_{z=1}^Z R_z$ where $R_z = \langle \Sigma_d \Psi_z \rangle$.
- We will calculate the relative sensitivity of the total response R with respect to the density ρ_z of source z : $S_{R, \rho_z} = \frac{\rho_z}{R} \frac{\partial R}{\partial \rho_z}$

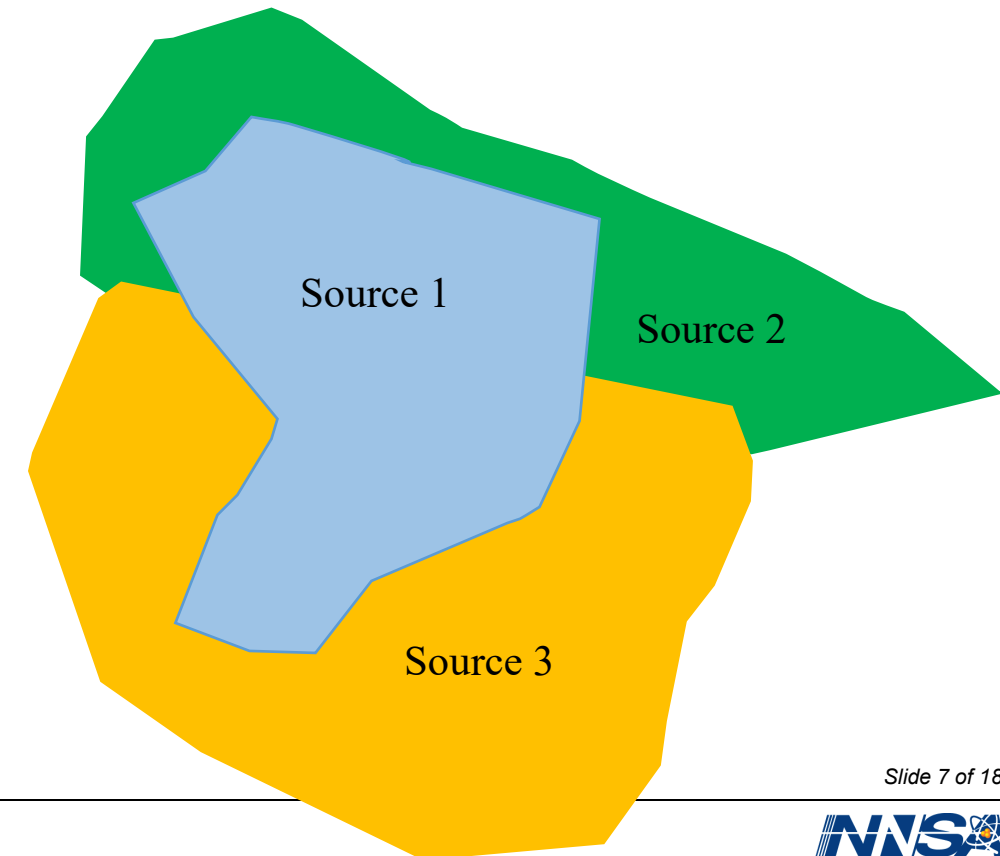


Relative Sensitivities

- The relative sensitivity of the total response R with respect to the density ρ_z of source z :

$$\begin{aligned} S_{R,\rho_z} &= \frac{\rho_z}{R} \frac{\partial R}{\partial \rho_z} \\ &= \frac{\rho_z}{R} \left(\frac{\partial R_1}{\partial \rho_z} + \frac{\partial R_2}{\partial \rho_z} + \dots + \frac{\partial R_Z}{\partial \rho_z} \right) \\ &= \frac{1}{R} \left(\frac{R_1}{R_1} \rho_z \frac{\partial R_1}{\partial \rho_z} + \frac{R_2}{R_2} \rho_z \frac{\partial R_2}{\partial \rho_z} + \dots + \frac{R_Z}{R_Z} \rho_z \frac{\partial R_Z}{\partial \rho_z} \right) \\ &= \frac{R_1}{R} S_{R_1,\rho_z} + \frac{R_2}{R} S_{R_2,\rho_z} + \dots + \frac{R_Z}{R} S_{R_Z,\rho_z} \end{aligned}$$

- $S_{R_i,\rho_z} = \frac{\rho_z}{R_i} \frac{\partial R_i}{\partial \rho_z}$ is the relative sensitivity of the response due to source region i with respect to the density of source region z .



The Sensitivity Has a Transport Component and a Source Component

- The total derivative of the response due to source region z with respect to the density of source region z :

$$\frac{\partial R_z}{\partial \rho_z} = \underbrace{\sum_{m=1}^M \frac{\partial R_z}{\partial A_m} \frac{\partial A_m}{\partial \rho_z}}_{\text{Transport}} + \underbrace{\frac{\partial R_z}{\partial Q_z} \frac{\partial Q_z}{\partial \rho_z}}_{\text{Source}}$$

- $\frac{\partial R_z}{\partial Q_z} = \frac{R_z}{Q_z}$

- The relative sensitivity of the response due to source region z with respect to the density of source region z :

$$\begin{aligned} S_{R_z, \rho_z} &= \frac{\rho_z}{R_z} \left(\sum_{m=1}^M \frac{\partial R_z}{\partial A_m} \frac{\partial A_m}{\partial \rho_z} + \frac{R_z}{Q_z} \frac{\partial Q_z}{\partial \rho_z} \right) \\ &= \frac{\rho_z}{R_z} \sum_{m=1}^M \frac{\partial R_z}{\partial A_m} \frac{\partial A_m}{\partial \rho_z} + \frac{\rho_z}{Q_z} \frac{\partial Q_z}{\partial \rho_z} \\ &= \underbrace{S_{R_z(A), \rho_z}}_{\text{Transport}} + \underbrace{S_{Q_z, \rho_z}}_{\text{Source}} \end{aligned}$$

- The transport part is what the PERT card is calculating.

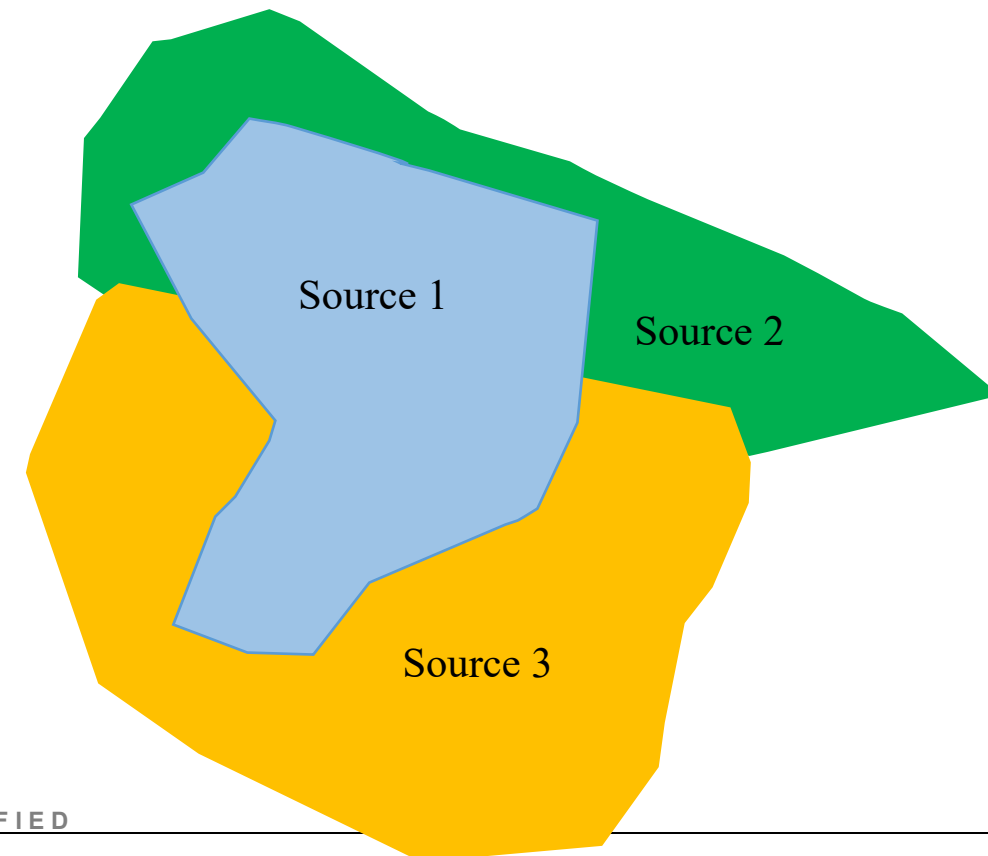
Final Equation for S_{R,ρ_Z}

- The relative sensitivity of the total response with respect to the density of one source region z :

$$S_{R,\rho_z} = \frac{R_1}{R} S_{R_1,\rho_z} + \frac{R_2}{R} S_{R_2,\rho_z} + \dots + \frac{R_Z}{R} S_{R_Z,\rho_z}$$

- All of these sensitivities have only transport effects except for one that also has a source effect:

$$\begin{aligned} S_{R,\rho_z} &= \left(\frac{R_1}{R} S_{R_1(A),\rho_z} + \frac{R_2}{R} S_{R_2(A),\rho_z} + \dots + \frac{R_Z}{R} S_{R_Z(A),\rho_z} \right) + \frac{R_z}{R} S_{Q_z,\rho_z} \\ &= S_{R(A),\rho_z} + \frac{R_z}{R} S_{Q_z,\rho_z} \end{aligned}$$



Final Equation for S_{R,ρ_z}

- The relative sensitivity of the total response with respect to the density of one source region z :

$$S_{R,\rho_z} = \frac{R_1}{R} S_{R_1,\rho_z} + \frac{R_2}{R} S_{R_2,\rho_z} + \dots + \frac{R_z}{R} S_{R_z,\rho_z}$$

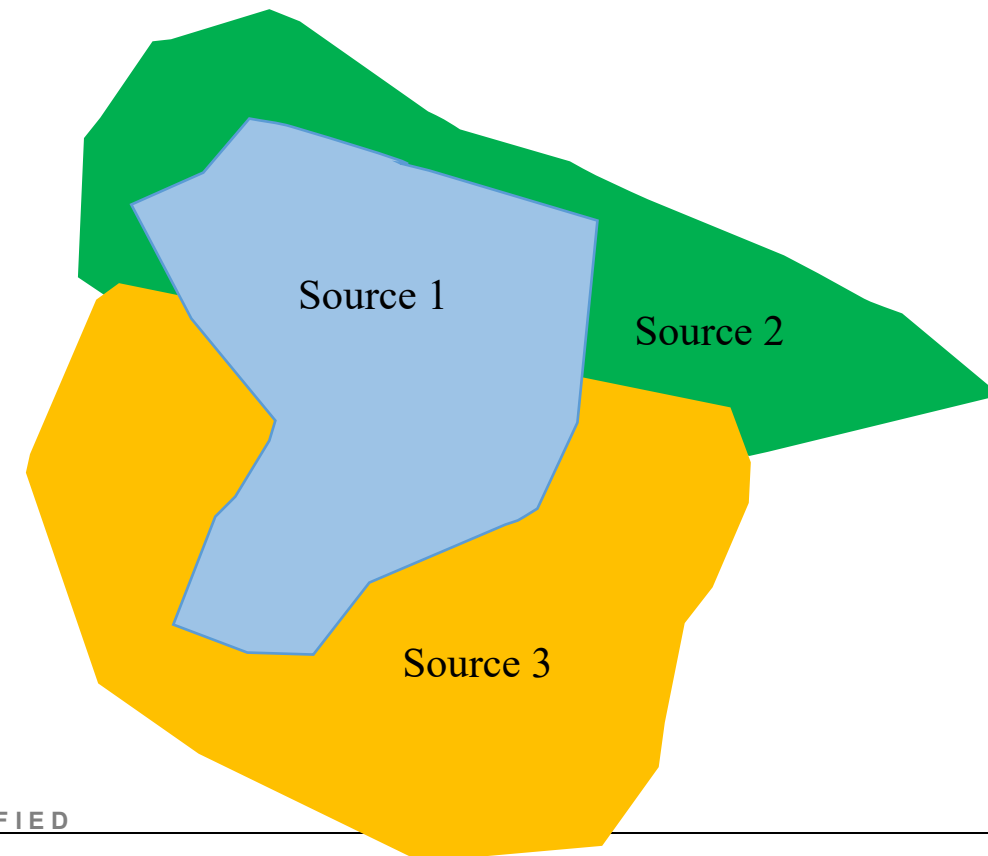
- All of these sensitivities have only transport effects except for one that also has a source effect:

$$S_{R,\rho_z} = \left(\frac{R_1}{R} S_{R_1(A),\rho_z} + \frac{R_2}{R} S_{R_2(A),\rho_z} + \dots + \frac{R_z}{R} S_{R_z(A),\rho_z} \right) + \frac{R_z}{R} S_{Q_z,\rho_z}$$

$$= \underbrace{S_{R(A),\rho_z}}_{\text{Transport}} + \underbrace{\frac{R_z}{R} S_{Q_z,\rho_z}}_{\text{Source}}$$

Transport

Source



Final Equation for S_{R,ρ_z}

- The relative sensitivity of the total response with respect to the density of one source region z :

$$S_{R,\rho_z} = \frac{R_1}{R} S_{R_1,\rho_z} + \frac{R_2}{R} S_{R_2,\rho_z} + \dots + \frac{R_z}{R} S_{R_z,\rho_z}$$

- All of these sensitivities have only transport effects except for one that also has a source effect:

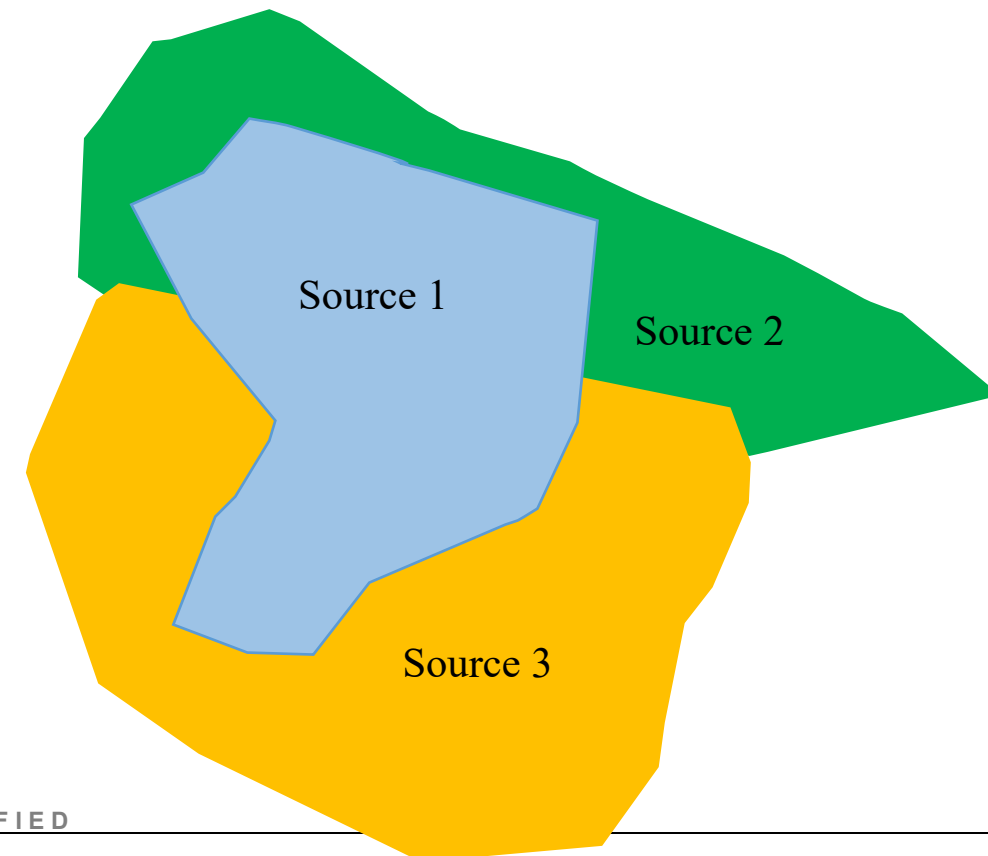
$$S_{R,\rho_z} = \left(\frac{R_1}{R} S_{R_1(A),\rho_z} + \frac{R_2}{R} S_{R_2(A),\rho_z} + \dots + \frac{R_z}{R} S_{R_z(A),\rho_z} \right) + \frac{R_z}{R} S_{Q_z,\rho_z}$$

$$= \underbrace{S_{R(A),\rho_z}}_{\text{Transport}} + \underbrace{\frac{R_z}{R} S_{Q_z,\rho_z}}_{\text{Source}}$$

Transport

Source

- The transport part is computed using the PERT card.
- We still need R_z and S_{Q_z,ρ_z} .



The Relative Sensitivity S_{Q_z, ρ_z} of a Source Rate Density with Respect to a Mass Density

- For decay sources, the source rate density is proportional to the mass density.

$$+ S_{Q_z, \rho_z} = 1$$

- This is also true of (α, n) sources.

ANS RPSD 2018 - 20th Topical Meeting of the Radiation Protection & Shielding Division of ANS
Santa Fe, NM, August 26 – 31, 2018, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2018)



SENSITIVITY OF A RESPONSE TO THE COMPOSITION OF AN (α, n) NEUTRON SOURCE

Jeffrey A. Favorite¹ and Sophie L. Weidenbenner²

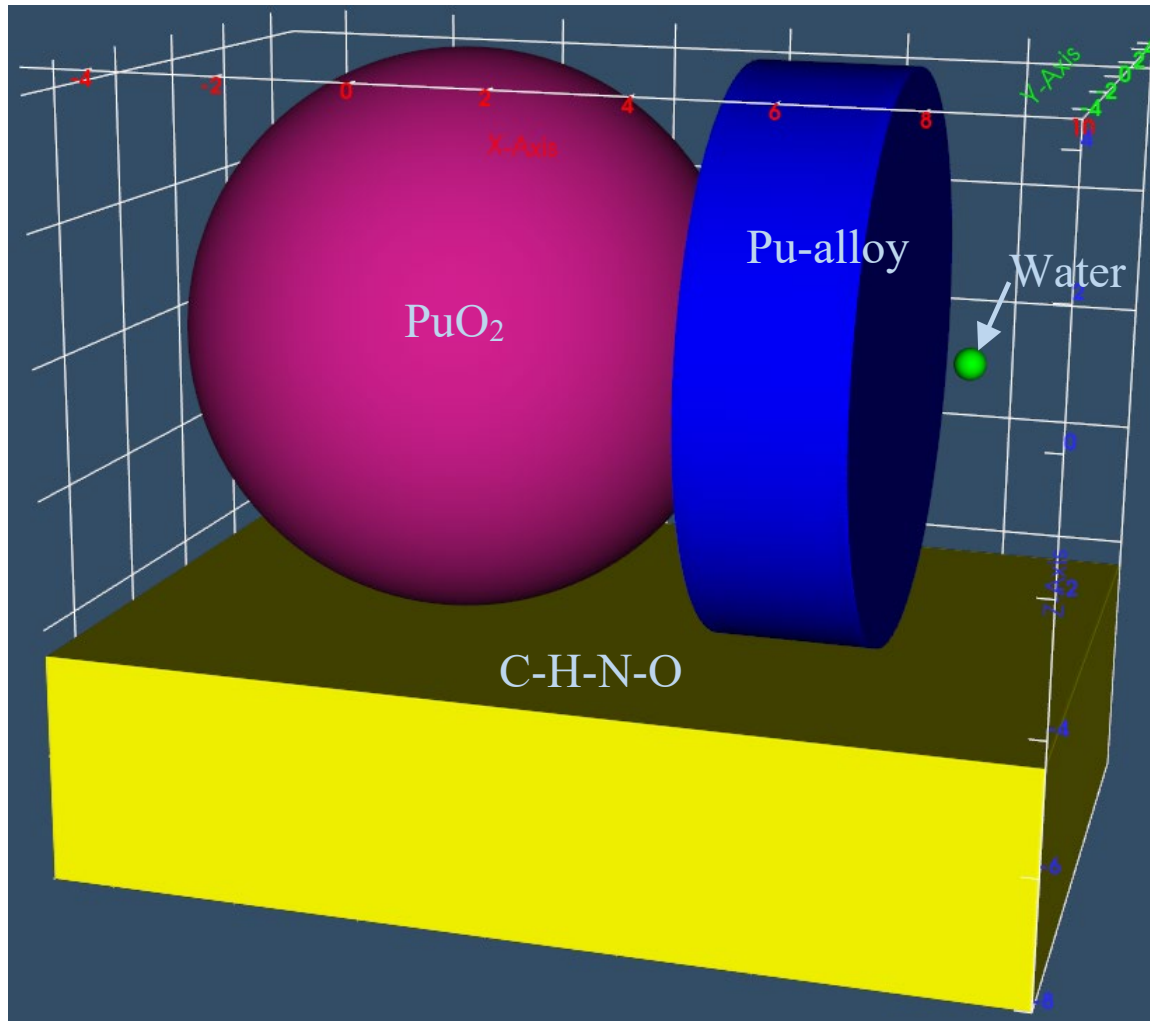
¹*Los Alamos National Laboratory, P.O. Box 1663 MS F663, Los Alamos, New Mexico, 87545, 505-667-7941, fave@lanl.gov*

²*Purdue University, 400 Central Drive, West Lafayette, Indiana, 47907, 765-494-5739, sweidenb@purdue.edu*

We derive the sensitivity of a response to the composition of an (α, n) neutron source. Section VI discusses the

The Contribution R_z of Source z to a Response

- Use MCNP6's "special tally feature" FT to tally by source distribution number.



- Example

c Source

```
sdef par=n cel=d31 pos=fcel d32 rad=fcel d33  
erg=fcel d34 ext=fcel d35 axs=fcel d36  
wgt=2.772222664E+05
```

```
si31 1 1 ← 2 ← Either cell 1 or 2  
sp31 d 1.647950612E+05 1.124272052E+05
```

...

c Tallies

```
f1004:n 4
```

```
ft1004 scx 31 ← Tally by bin of  
f2004:p 4 source dist. 31
```

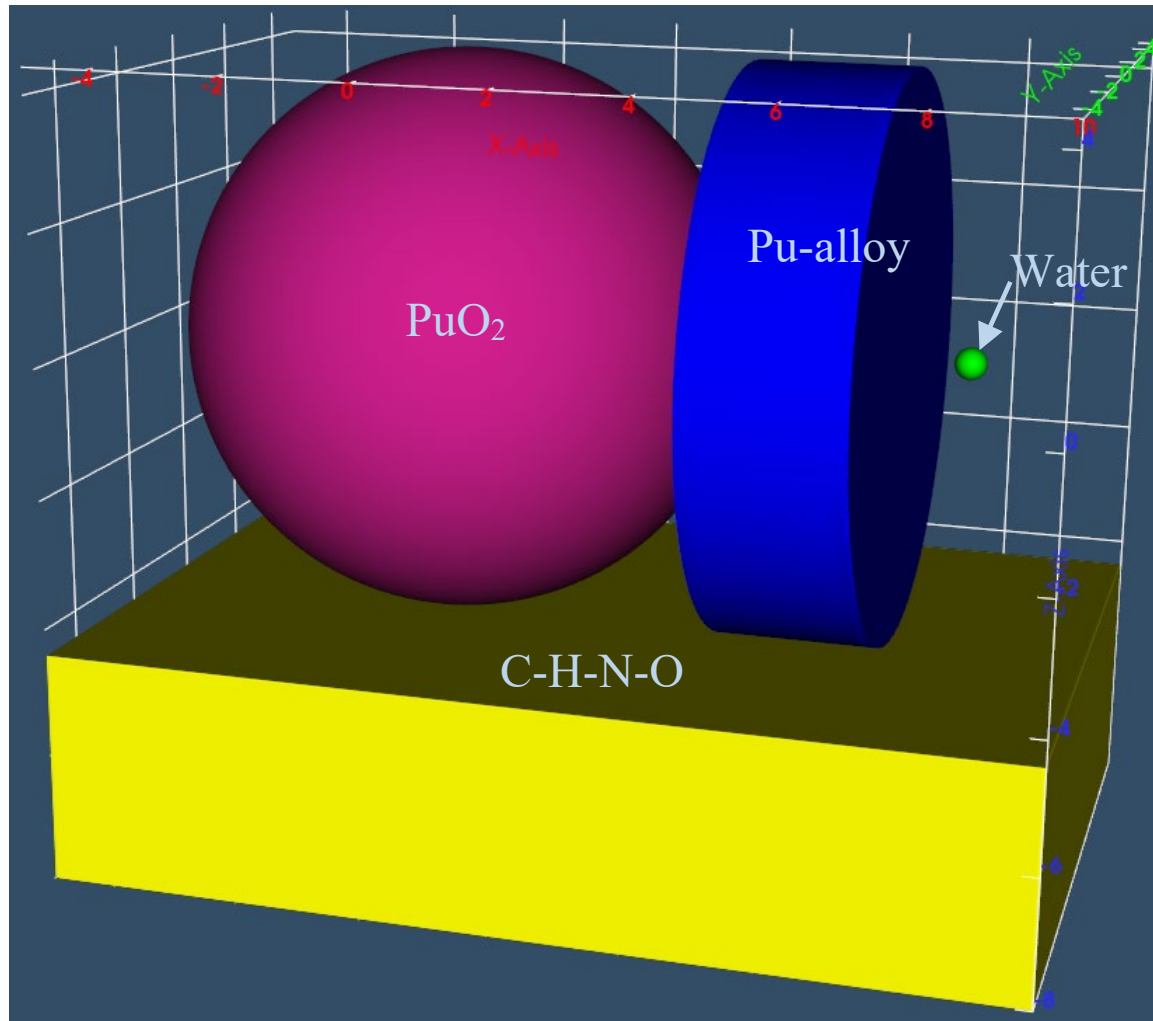
```
ft2004 scx 31
```

...

- The output will include three entries:

- + The contribution from the 1st item in distribution 31
- + The contribution from the 2nd item in distribution 31
- + The total

Test Problem



- The PuO₂ has 4 Pu isotopes and 3 oxygen isotopes
 - + $\rho_1 = 9.533052 \text{ g/cm}^3$
 - + $Q_1 = 1.647950612\text{E}+05 \text{ neutrons/s}$
- The Pu-alloy has 3 Pu isotopes and 2 Ga isotopes
 - + $\rho_2 = 15.82 \text{ g/cm}^3$
 - + $Q_2 = 1.124272052\text{E}+05 \text{ neutrons/s}$
- The C-H-N-O material is there to create gamma rays from neutrons
 - + $\rho_3 = 1.678 \text{ g/cm}^3$
- Neutron source rates and spectra were computed using SOURCES4D
- All MCNP6 results were obtained using “DBCN 49j 2”
 - + Prints more digits in the tally and the relative uncertainty in the tally fluctuation chart (TFC) than in the regular tally output
 - + Tallies were repeated so that all bins had a TFC

```
1tally      1004      nps = 200000000000
tally type 4      track length estimate of particle flux.      units      1/cm**2
particle(s): neutrons
this tally is modified by      ft      scx

volumes
      cell:      4
              6.54498E-02

cell  4
      5.66433151E+02  0.00090

cell  4
      1.64944753E+03  0.00038

cell  4
      2.21588068E+03  0.00036
```

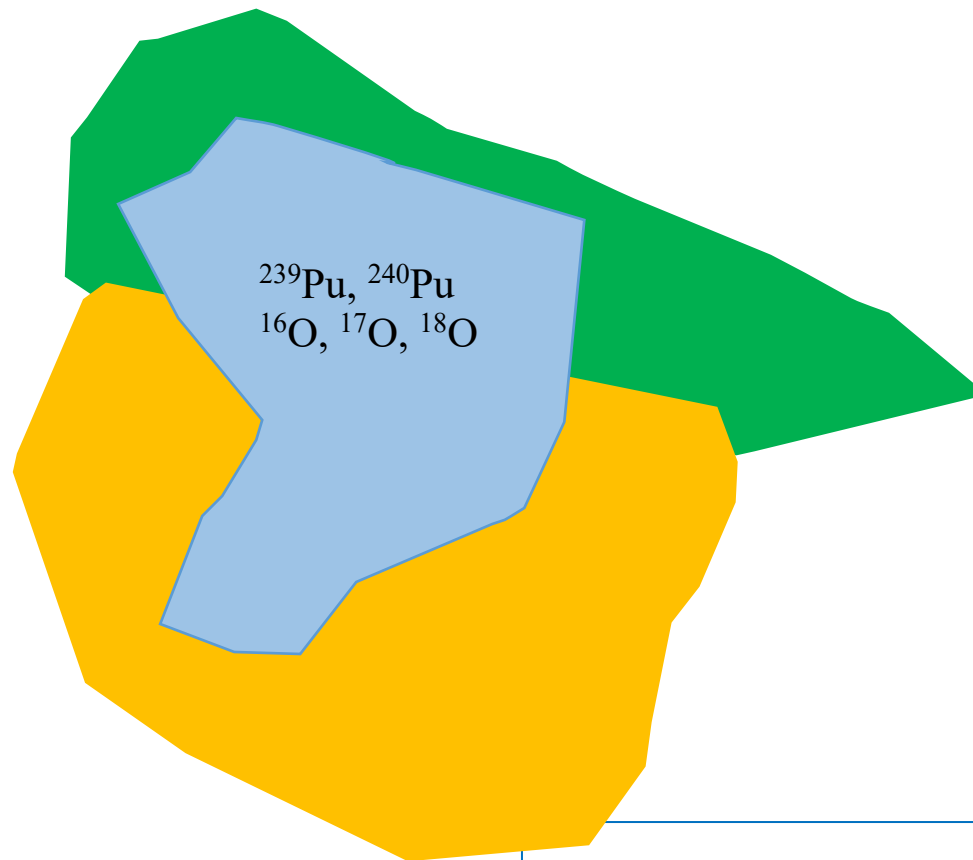
- The ratio for the Pu-alloy is
$$\frac{R_2}{R} = \frac{1.64944753E+03}{2.21588068E+03} \pm \sqrt{0.00038^2 + 0.00036^2}$$
$$= 0.74438 \pm 0.0523\%$$
- But the tallies are correlated. Taking correlations into account,
$$\frac{R_2}{R} = 0.74438 \pm 0.0311\%$$
- The code I use for this is COSUBS (ref. at end).

Results Compared with Central Difference

	Neutrons	Gamma rays
PuO₂		
Direct	$5.1272\text{E-}01 \pm 0.84\%$	$5.2838\text{E-}01 \pm 2.59\%$
PERT	$5.1413\text{E-}01 \pm 0.09\%$	$5.0795\text{E-}01 \pm 0.19\%$
Diff.	0.27%	−3.87%
Pu-alloy		
Direct	$1.5933\text{E+}00 \pm 0.84\%$	$1.7452\text{E+}00 \pm 2.59\%$
PERT	$1.5878\text{E+}00 \pm 0.05\%$	$1.7374\text{E+}00 \pm 0.11\%$
Diff.	−0.34%	−0.45%

- Direct perturbations used central differences with density perturbations of $\pm 5\%$.
- Correlated sampling (COSUBS) was used to reduce the statistical uncertainties.

A Related Problem



- There are 4 (α, n) sources and 2 spontaneous-fission sources.
- Suppose you perturb the density of ^{239}Pu with the PERT card.
- The calculated tally perturbation will include changes in the cross sections, but not changes in the source emissions.

NUCLEAR SCIENCE AND ENGINEERING · VOLUME 198 · 287–299 · FEBRUARY 2024
© 2023 The Author(s). Published with license by Taylor & Francis Group, LLC.
DOI: <https://doi.org/10.1080/00295639.2022.2161279>



Source Nuclide Density First-Order and Second-Order Sensitivities in Monte Carlo Codes

Jeffrey A. Favorite*

Computational Physics (X-CP) Division, MS F663, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Summary and Conclusions

- To calculate the relative sensitivity S_{R,ρ_z} of a response R with respect to the density ρ_z of a source material, use this:

$$S_{R,\rho_z} = S_{R(A),\rho_z} + \frac{R_z}{R} S_{Q_z,\rho_z}$$

- For decay sources and (α ,n) sources, $S_{Q_z,\rho_z} = 1$.
- In MCNP6,
 - + $S_{R(A),\rho_z}$ is from the PERT card
 - + R_z is from the SCX special tally treatment.
- Useful tools:
 - + SOURCES4D—Jeffrey A. Favorite, “Release of SOURCES4D Featuring Sensitivity Capabilities,” *Proceedings of the 22nd Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society (RPSD 2024)*, 229–232, Orlando, Florida, November 17–21 (2024); <https://doi.org/10.13182/T131-45778>.
 - + COSUBS—Jeffrey A. Favorite, “A General-Purpose Code for Correlated Sampling Using Batch Statistics with MCNP6 for Fixed-Source Problems [version 1; peer review: 2 approved],” *Nuclear Science and Technology Open Research*, 2:33 (2024); <https://doi.org/10.12688/nuclscitechnolopenres.17496.1>.