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

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Motivation for this paper

- MCNP has a powerful feature for perturbation and sensitivity theory in shielding problems:
  the PERT card

- The PERT card has been in MCNP for ~20 years

- The PERT card is misunderstood (and the manual doesn't help)

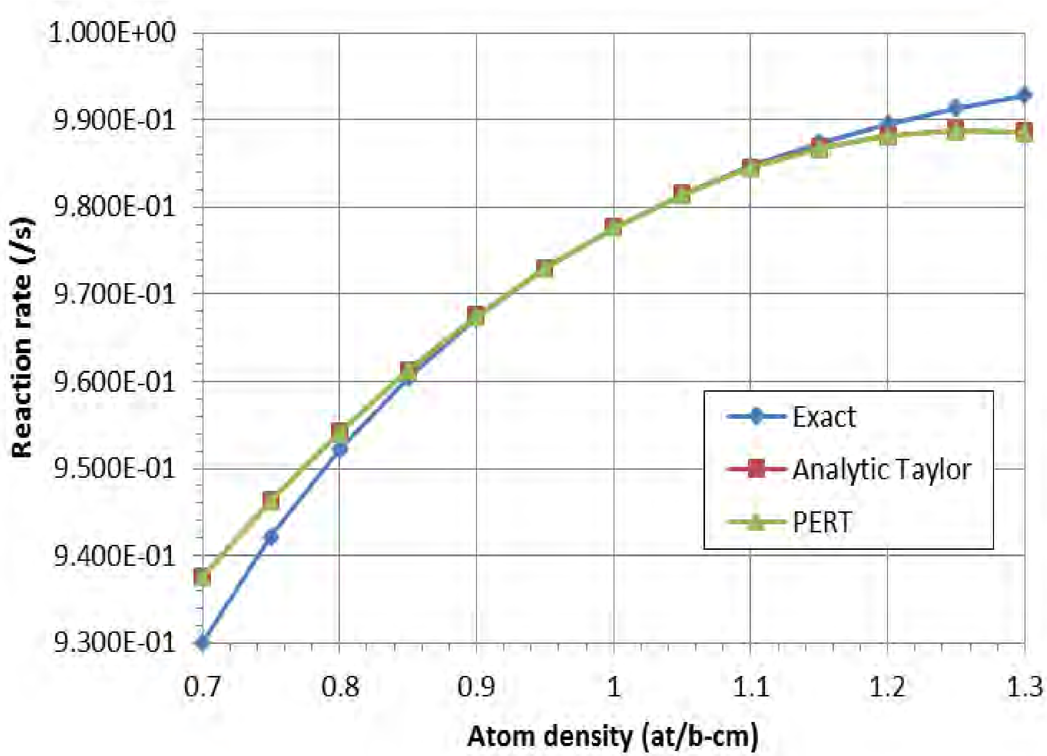
- The goal of this paper is to help you understand it and use it efficiently!

What it does

- The PERT card estimates the terms in a Taylor series expansion of a response *c* that is a function of some reaction cross section σ_x:

$$c(\sigma_x) = c(\sigma_{x,0}) + \left.\frac{dc}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x + \frac{1}{2}\left.\frac{d^2c}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2 + \cdots,$$

where $\Delta\sigma_x \equiv \sigma_x - \sigma_{x,0}$.



Calculating the different terms

$$c_{\mathrm{PERT}}(\sigma_x) = c(\sigma_{x,0}) + \left.\frac{dc}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x + \left.\frac{1}{2}\frac{d^2c}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2$$

Regular tally | 1^{st}-order term | 2^{nd}-order term

- METHOD = 2 ⇨ 1^{st}-order term
- METHOD = 3 ⇨ 2^{nd}-order term
- METHOD = 1 ⇨ 1^{st}- + 2^{nd}-order term

- METHOD = + ⇨ print 1^{st}- or 2^{nd}-order term or sum (estimate Δc)
- METHOD = – ⇨ print unperturbed tally plus 1^{st}- or 2^{nd}-order term or sum (estimate $c(\sigma_x)$)

A convenient transformation

- Define p_x as the relative cross-section change, $p_x \equiv \frac{\Delta\sigma_x}{\sigma_{x,0}} = \frac{\sigma_x}{\sigma_{x,0}} - 1.$
- Define

$$\Delta c_1 \equiv \left.\frac{dc}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x = \left.\frac{dc}{dp_x}\right|_{p_x=0} \left.\frac{dp_x}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x = \left.\frac{dc}{dp_x}\right|_{p_x=0} \frac{\Delta\sigma_x}{\sigma_{x.0}} = \left.\frac{dc}{dp_x}\right|_{p_x=0} p_x$$

$$\Delta c_2 \equiv \frac{1}{2}\left.\frac{d^2c}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2 = \frac{1}{2}\frac{d}{d\sigma_x}\left(\left.\frac{dc}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x\right)\Delta\sigma_x = \frac{1}{2}\frac{d}{d\sigma_x}\left(\left.\frac{dc}{dp_x}\right|_{p_x=0} p_x\right)\Delta\sigma_x = \frac{1}{2}\frac{d}{dp_x}\left(\left.\frac{dc}{dp_x}\right|_{p_x=0} p_x\right)\left.\frac{dp_x}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x = \frac{1}{2}\left.\frac{d^2c}{dp_x^2}\right|_{p_x=0} (p_x)^2$$

- Define $c_0 \equiv c(\sigma_{x,0})$
- The Taylor series is now $c_{\text{PERT}}(\sigma_x) = c_0 + \left.\frac{dc}{dp_x}\right|_{p_x=0} p_x + \frac{1}{2}\left.\frac{d^2c}{dp_x^2}\right|_{p_x=0} (p_x)^2$

The usefulness of PERT outputs

- The output of the PERT card is

METHOD = +2: $\Delta c_1 \equiv \left.\frac{dc}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x = \left.\frac{dc}{dp_x}\right|_{p_x=0} p_x$ and $s_{\Delta c_1}$

METHOD = +3: $\Delta c_2 \equiv \frac{1}{2}\left.\frac{d^2c}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2 = \frac{1}{2}\left.\frac{d^2c}{dp_x^2}\right|_{p_x=0} (p_x)^2$ and $s_{\Delta c_2}$

- p_x is a user input.

- If you divide Δc_1 by p_x, you get the first derivative, $\left.\frac{dc}{dp_x}\right|_{p_x=0}$

- If you divide Δc_2 by $(p_x)^2/2$, you get the second derivative, $\left.\frac{d^2c}{dp_x^2}\right|_{p_x=0}$

- If you know the first and second derivative, you can do a two-term Taylor series estimate for any perturbed point you want!

Prescription to do your own Taylor series expansion

- Choose a reference perturbation $p_{x,r}$; a convenient choice is $p_{x,r} = 1$.

- Set up two PERT cards with the density equal to $d_r = d_{x,0}(1 + p_{x,r})$. Obviously, if $p_{x,r} = 1$, then $d_r = 2d_0$. One PERT card uses METHOD=2 and the other uses METHOD=3.

- Run the problem using MCNP.

- In the output:
  + The METHOD = 2 perturbation result is $\Delta c_1(p_{x,r}) \pm s_{\Delta c_1}$; $c_1 = \dfrac{\Delta c_1(p_{x,r})}{p_{x,r}}$, $s_{c_1} = \dfrac{s_{\Delta c_1}}{|p_{x,r}|}$.
  + The METHOD = 3 perturbation result is $\Delta c_2(p_{x,r}) \pm s_{\Delta c_2}$; $c_2 = \dfrac{\Delta c_2(p_{x,r})}{p_{x,r}^2}$, $s_{c_2} = \dfrac{s_{\Delta c_2}}{p_{x,r}^2}$.

- The response at any perturbed point p_x is estimated using

$$c_{\mathrm{PERT}}(p_x) = c_0 + c_1 p_x + c_2 p_x^2,$$

and the variance is approximately

$$s^2_{c_{\mathrm{PERT},unc.}} = s^2_{c_0} + s^2_{c_1} p_x^2 + s^2_{c_2} p_x^4.$$

(The exact variance is derived in the paper)

Doesn't a 100% perturbation violate the assumption of "small"?

- $p_{x,r} = 1$?

- We distinguish between

Estimating the coefficients of a Taylor expansion

and

Using the Taylor expansion to estimate a perturbed response

- The PERT value of the coefficients (derivatives) is independent of the size of the perturbation.

First-order sensitivity theory

- Frequently used in uncertainty quantification:

$$\left(\frac{s_c}{c_0}\right)^2 = S_{c,\sigma_x}^2 \left(\frac{s_{\sigma_x}}{x_0}\right)^2.$$

- S_{c,σ_x} is the relative sensitivity:

$$S_{c,\sigma_x} \equiv \frac{\sigma_{x,0}}{c_0} \frac{dc}{d\sigma_x}\bigg|_{\sigma_{x,0}} = \frac{1}{c_0} \frac{dc}{dp_x}\bigg|_{p_x=0} = \frac{c_1}{c_0}$$

Prescription for first-order sensitivity analysis

- Choose a reference perturbation $p_{x,r}$; a convenient choice is $p_{x,r} = 1$.
- Set up a PERT card with the density equal to $d_r = d_{x,0}(1 + p_{x,r})$. Obviously, if $p_{x,r} = 1$, then $d_r = 2d_0$. The PERT card uses METHOD=2.
- Run the problem using MCNP.
- In the output:
  - \+ The METHOD = 2 perturbation result is $\Delta c_1(p_{x,r}) \pm s_{\Delta c_1}$; $c_1 = \dfrac{\Delta c_1(p_{x,r})}{p_{x,r}}$, $s_{c_1} = \dfrac{s_{\Delta c_1}}{|p_{x,r}|}$.
  - \+ The variance of the sensitivity is approximately

$$s_{S_{unc.}}^2 = S_{c,\sigma_x}^2 \left[\left(\frac{s_{c_0}}{c_0}\right)^2 + \left(\frac{s_{c_1}}{c_1}\right)^2\right].$$

The PERT card

- ```
  PERTi:[n|p]  CELL= cell1 cell2 cell3… MAT=m RHO=d
          ERG=e1 e2 e3…
          RXN = r1 r2 r3…
          METHOD = [+|-][1|2|3]
  ```

- The combination of MAT and RHO is used to perturb isotope densities.
  + Then the relative density change is transferred to the reaction cross sections.
  + This is how the relative cross-section change p_x is a user input.

- It is very important that you only perturb either
  + ONE isotope density, or
  + ALL of them the SAME relative amount.
  + Otherwise, the Taylor expansion has second-order cross terms that MCNP does not calculate. See Favorite and Parsons, M&C2001.

- How to perturb one isotope density is shown on the next slide.
- You perturb ALL of them the SAME amount by using RHO but not MAT.

- The next release of MCNP will warn you if a perturbation violates these rules, but it won't stop you from doing it.
  ```

How to perturb a single isotope density by p_x

- Advice: Consistently use atom or mass densities on material, cell, and PERT cards:

$$N_1 = N_{1,1} + N_{1,2}$$

- Define a perturbed material for each isotope such that

$$N_{11,1} = N_{1,1} \times (1+p_x) \text{ and}$$
$$N_{12,2} = N_{1,2} \times (1+p_x)$$

p_x is arbitrary!

- The perturbed cell densities are

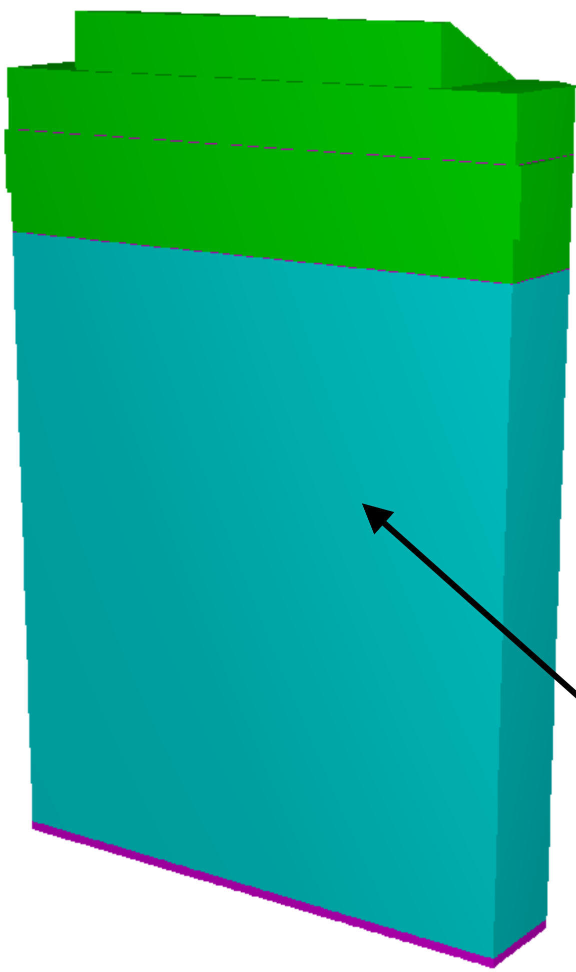
$$N_{11} = N_{11,1} + N_{1,2} \text{ and}$$
$$N_{12} = N_{1,1} + N_{12,2}$$

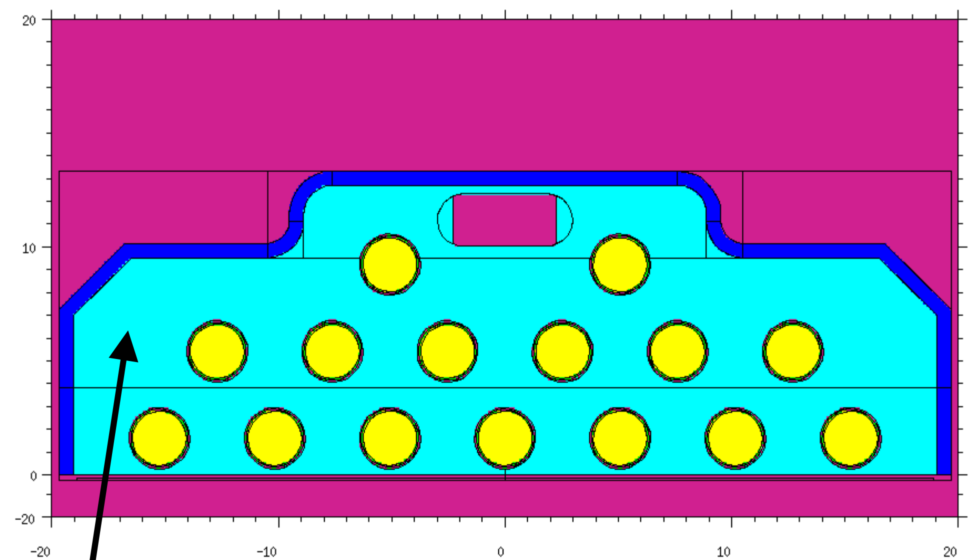
- The PERT card specifies the perturbed cell and its perturbed density, the new material, reaction x, an energy range, and METHOD.

```
example input for perturbations with PERT
1    1    N1          -1         imp:n=1
:
c unperturbed materials
m1    I1,1  N1,1     I1,2  N1,2
c materials for sensitivities
m11   I1,1  N11,1    I1,2  N1,2
m12   I1,1  N1,1     I1,2  N12,2
pert11101:n  cell=1  rho=N11  mat=11  rxn=R1
             erg=E1 E2  method=2
pert11102:n  cell=1  rho=N11  mat=11  rxn=R1
             erg=E1 E2  method=3
:
pert11201:n  cell=1  rho=N11  mat=11  rxn=R2
             erg=E1 E2  method=2
pert11202:n  cell=1  rho=N11  mat=11  rxn=R2
             erg=E1 E2  method=3
:
pert12101:n  cell=1  rho=N12  mat=12  rxn=R1
             erg=E1 E2  method=2
pert12102:n  cell=1  rho=N12  mat=12  rxn=R1
             erg=E1 E2  method=3
:
pert12201:n  cell=1  rho=N12  mat=12  rxn=R2
             erg=E1 E2  method=2
pert12202:n  cell=1  rho=N12  mat=12  rxn=R2
             erg=E1 E2  method=3
:
```

Example 1: Neutron detector

- A neutron detector with 15 helium-3 tubes surrounded by HDPE.
- How does the count rate change as the HDPE density changes?



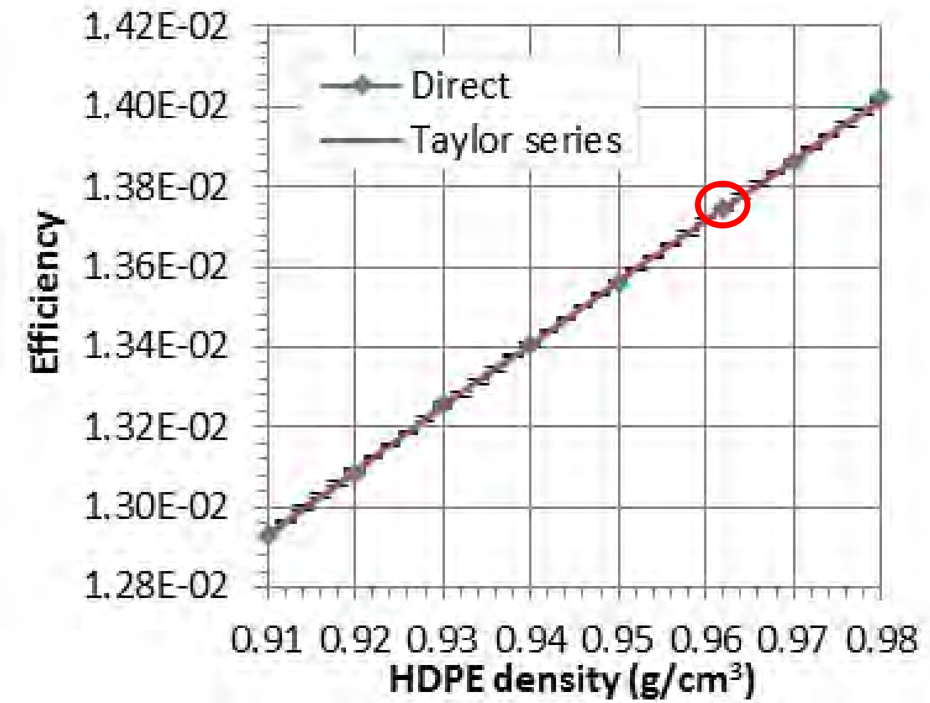


High-density polyethylene (HDPE)

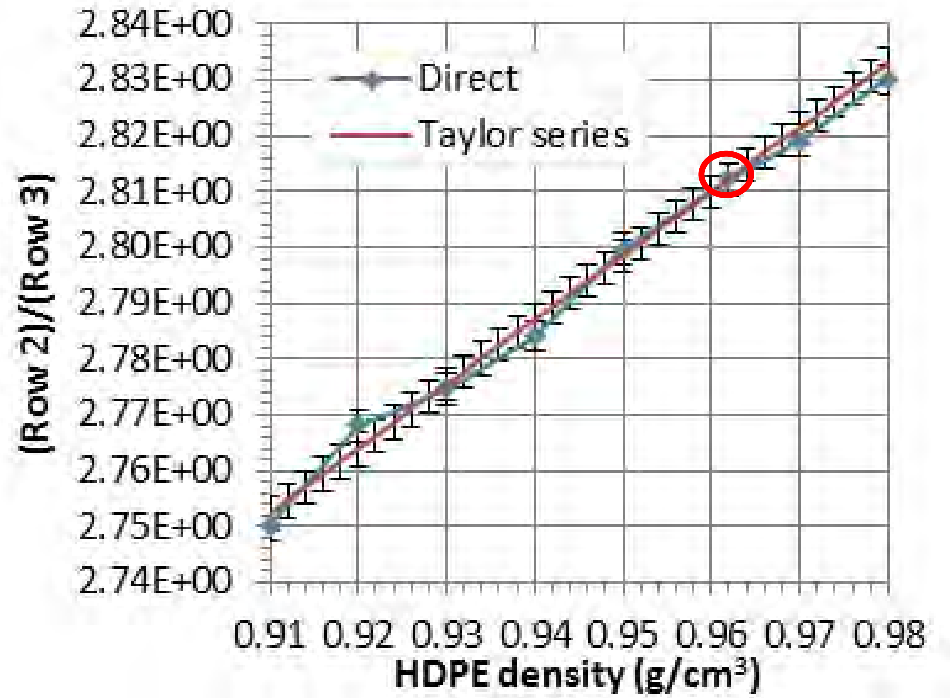
Neutron detector results

- An Am-Be neutron source was 30 cm from the front face, centered vertically
- Detector counts were modeled as captures in He-3

Efficiency = Counts per source particle



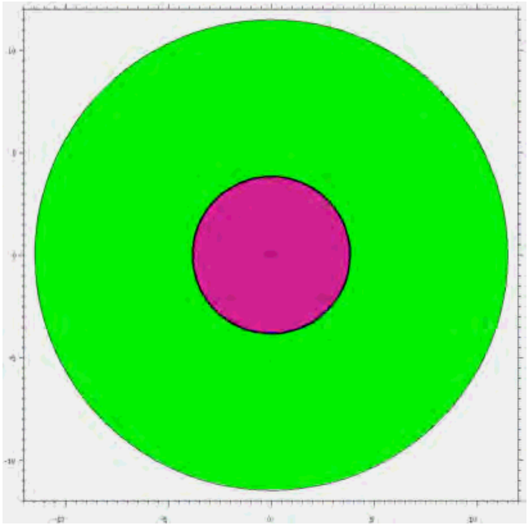
Row ratio = Ratio of counts in specified tubes

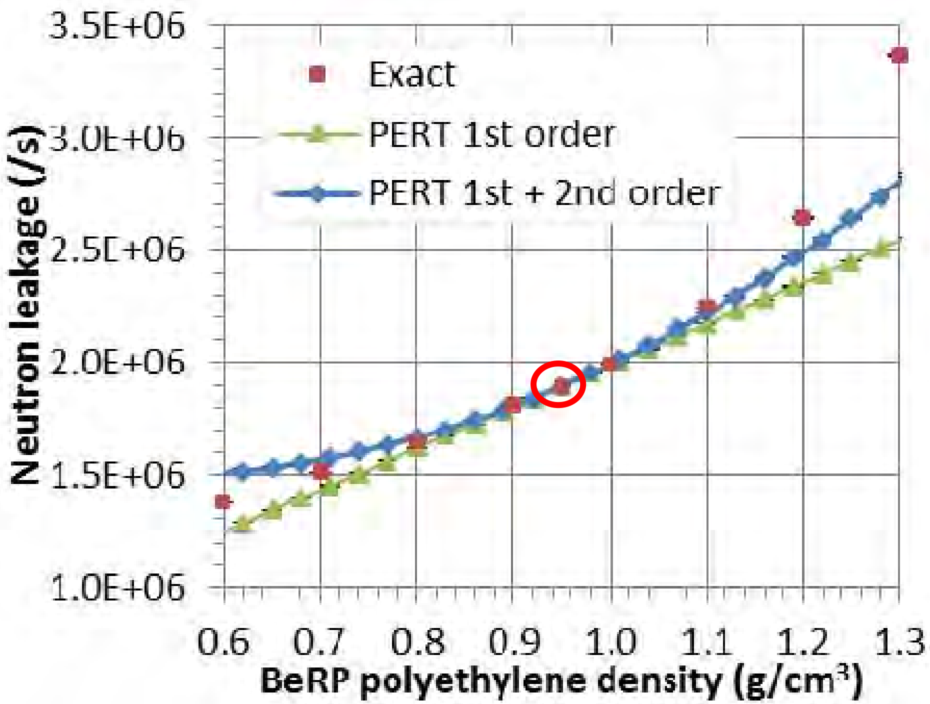


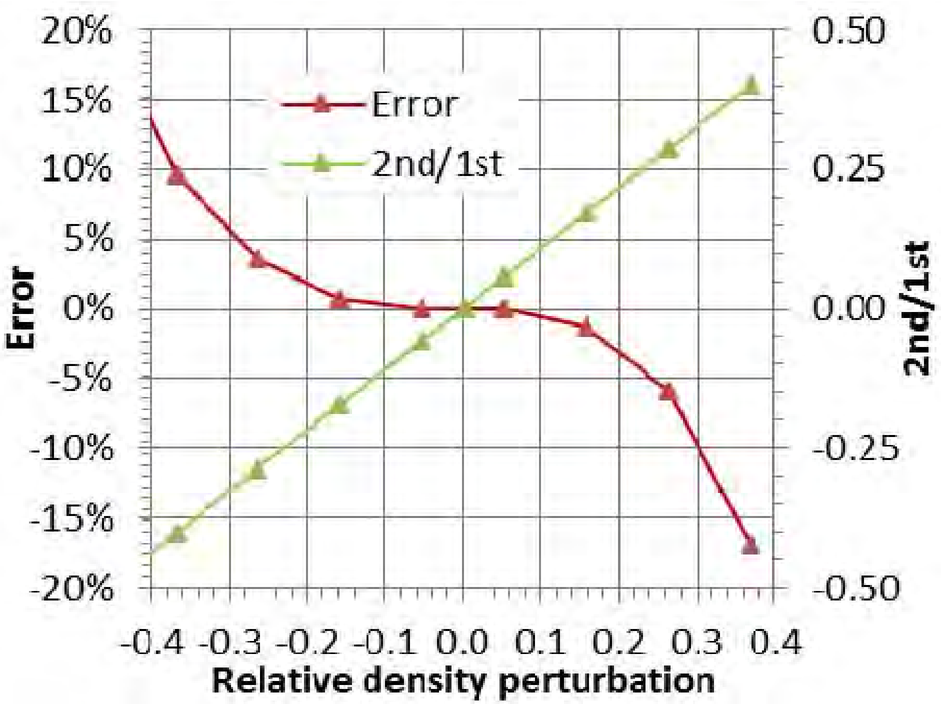
○ = Unperturbed point

Example 2: Neutron leakage from the BeRP ball

- 3-inch thick polyethylene layer surrounds a 4.484-kg sphere of α-Pu.
- The nominal polyethylene density is 0.95 g/cm^3.
- How does the neutron leakage change as the polyethylene density changes?







PERT vs. central difference for BeRP ball poly density

- First-order sensitivity of the leakage to the polyethylene density

- The first-order PERT method is compared with central-difference estimates computed using

$$S_{c,\rho}^{CD} \approx \frac{\rho_0}{c_0}\left(\frac{c(\rho_0+h)-c(\rho_0-h)}{2h}\right)$$

Sensitivity of neutron leakage to polyethylene density.

Method	***h*** **(g/cm^3)**	**Sensitivity (%/%)**	**Diff. w.r.t. PERT (*Ns*)[a]**
PERT	N/A	0.9270 ± 0.23%	N/A
Central Diff.	0.05	0.9370 ± 0.32%	1.94
Central Diff.	0.15	0.9949 ± 0.11%	20.7
Central Diff.	0.25	1.136 ± 0.07%	69.4

(a) Number of standard deviations of difference.

Example 3: Analytic verification

- A slab of width X, no scattering, a monoenergetic beam source impinges on the left, the total reaction rate R within the slab is

$$R = \int_0^X dx \Sigma \phi(x)$$
$$= \int_0^X dx \Sigma q e^{-\Sigma x}$$
$$= q\left(1 - e^{-\Sigma X}\right).$$

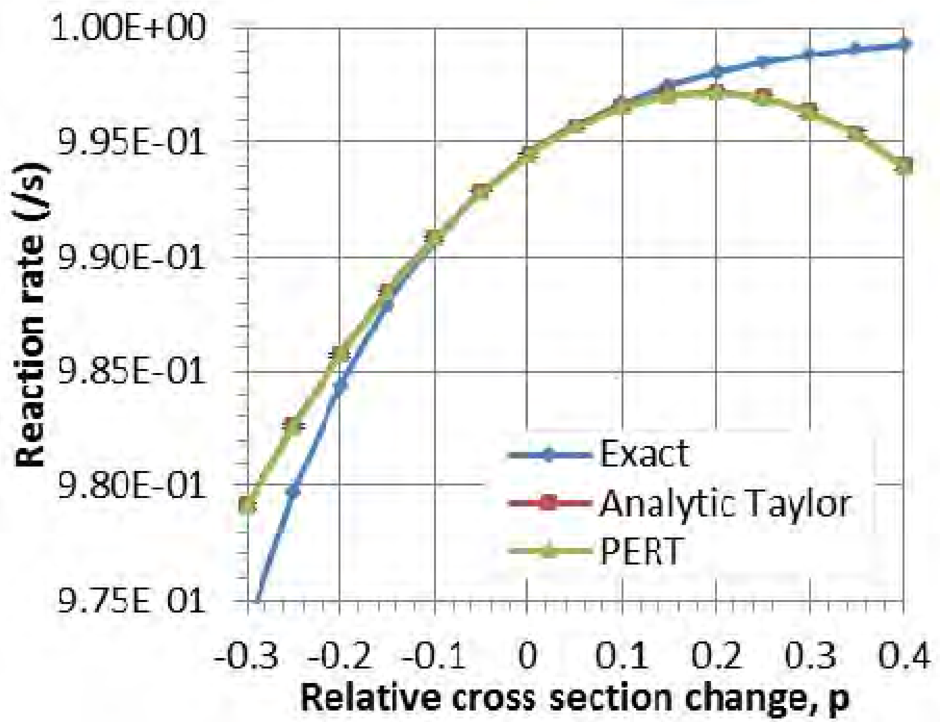
Parameters of the analytic slab problem.

Parameter	Value
q	1.0 cm^{-2}s^{-1}
X	1.0 cm
Σ_0	5.2 cm^{-1}

Coefficients of the Taylor expansion.

Coefficient	Analytic	MCNP PERT	Ns[a]
R_0 (s^{-1})	0.994483	0.994428 ± 0.01%	0.57
R_1 (s^{-1})	0.0286861	0.0287011 ± 0.83%	0.06
R_2 (s^{-1})	–0.0745840	–0.0746330 ± 0.48%	0.14

(a) Number of standard deviations of diff.



Summary and Conclusions

- Use the PERT card for sensitivity and perturbation studies of shielding problems!

  + First-order sensitivity theory → METHOD=2

  + Perturbations → METHOD=2 and METHOD=3 will get the coefficients of a Taylor expansion that can be used to estimate any perturbed point

    - Watch out for cross terms – change one thing at a time

    - Do check the relative size of the first- and second-order terms but know that it is not a foolproof accuracy indicator

- The next release of MCNP will fix a bug affecting the second-order coefficient of a density perturbation (RHO but no MAT).