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Title: Eigenvalue Sensitivity Analysis Using the MCNP Perturbation Capability

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Eigenvalue Sensitivity Analysis Using the MCNP Perturbation Capability

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Abstract (not a viewgraph)

The MCNP perturbation capability can be used to estimate k_{eff} sensitivities to isotopic reaction cross sections. Only the first-order Taylor term is needed, and the computed sensitivities are independent of the size of the perturbation. Accuracy of the perturbation estimate can always be tested for the total cross section. Several test problem results are presented. Comparisons are made with direct estimates obtained by directly perturbing the one-group data and with TSUNAMI-3D results, respectively. The PERT card RXN keyword reaction numbers corresponding to TSUNAMI-3D reactions are given. The MCNP method becomes inaccurate when the fission source distribution is perturbed and is inaccurate for k_{eff} sensitivities to some scattering cross sections.

Introduction

- Can the MCNP PERT card be used to compute k_{eff} cross-section sensitivities?
- In this talk, I will:
  - Describe how to use the PERT card to compute cross-section sensitivities.
  - Discuss accuracy concerns, and how they can be tested.
  - Show results.
- Conclusion: The current PERT capability can be used to compute k_{eff} cross-section sensitivities, but the accuracy is extremely limited.

What is a Sensitivity?

- If a response k is linear with respect to a parameter σ, then
$$k = k_0 + m(\sigma - \sigma_0).$$
- Let σ vary with a parameter p:
$$\sigma = \sigma_0(1+p) \text{ and } p = \frac{\sigma - \sigma_0}{\sigma_0} = \frac{\Delta\sigma}{\sigma_0}.$$
- So
$$k - k_0 = m\,p\sigma_0$$

or

$$\frac{\Delta k}{k_0} = \left(\frac{\sigma_0}{k_0} m\right) p = \left(\frac{\sigma_0}{k_0} \left.\frac{dk}{d\sigma}\right|_{\sigma_0}\right) p$$
$$= S_{k,\sigma} p.$$

- Units of sensitivity are "%($\Delta k/k_0$) / %($\Delta\sigma/\sigma_0$)"
  - For a 1% change in σ ($p = 0.01$), the change in k is $S_{k,\sigma}$ PER CENT.
  - Example: $S_{k,\sigma} = 5 \times 10^{-3}$, $p = 0.01$, then $\Delta k/k_0 = 5 \times 10^{-5} = 5 \times 10^{-3}$%.
  - Example: $p = 1$ (σ doubles), then $\Delta k/k_0 = S_{k,\sigma} = S_{k,\sigma} \times 100$%.

Sensitivities and the Differential Operator Perturbation Method

- A Taylor series expansion of a response k with respect to some reaction cross section σ_x is

$$k(\sigma_x) = k_0 + \left.\frac{dk}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x + \frac{1}{2}\left.\frac{d^2k}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2 + \cdots$$

so

$$\Delta k = \left[\Delta k(\Delta\sigma_x)\right]_{1\text{st}} + \left[\Delta k(\Delta\sigma_x)\right]_{2\text{nd}} + \cdots.$$

(The MCNP perturbation method uses only two Taylor terms and no cross terms.)

- Using $p_x = \Delta\sigma_x / \sigma_{x,0}$, the first-order Taylor term is

$$\left[\Delta k(\Delta\sigma_x)\right]_{1\text{st}} = p_x \sigma_{x,0} \frac{dk}{d\sigma_x}.$$

  + The differential operator method attempts to estimate the derivative.
  + The derivative is independent of the size of p_x.

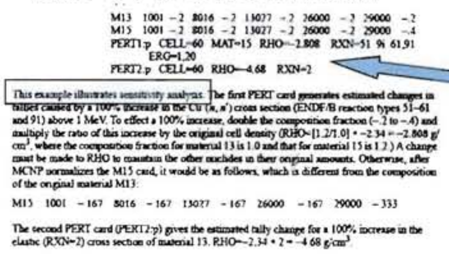
- The sensitivity of k with respect to σ_x is

$$S_{k,\sigma_x} = \frac{1}{k_0 p_x}\left[\Delta k(\Delta\sigma_x)\right]_{1\text{st}}.$$

- The first-order term is linear with p_x, with no offset. Thus p_x is *arbitrary*.

Sensitivities and MCNP – Misunderstandings

- MCNP manual, 10/3/05, p. 3-155 (cropped):



Example 4. 60 13 -2.34 105 -106 -74 73 $ mat 13 at 2.34 g/cm^3

```
M13  1001 -2  8016 -2  13027 -2  26000  -2  29000  -2
M15  1001 -2  8016 -2  13027 -2  26000  -2  29000  -4
PERT1:p  CELL=60  MAT=15  RHO=-2.808  RXN=51 9i 61,91
       ERG=1,20
PERT2:p  CELL=60  RHO=-4.68  RXN=2
```

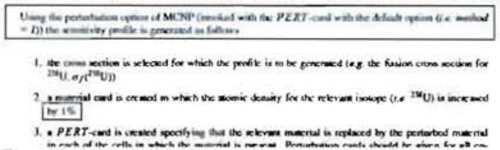
This example illustrates sensitivity analysis. The first PERT card generates estimated changes in tallies caused by a 100% increase in the Cu (n, n') cross section (ENDF/B reaction types 51–61 and 91) above 1 MeV. To effect a 100% increase, double the composition fraction (–.2 to –.4) and multiply the ratio of this increase by the original cell density (RHO=[1.2/1.0] • –2.34 = –2.808 g/cm^3, where the composition fraction for material 13 is 1.0 and that for material 15 is 1.2.) A change must be made to RHO to maintain the other nuclides in their original amounts. Otherwise, after MCNP normalizes the M15 card, it would be as follows, which is different from the composition of the original material M13:

```
M15  1001  -.167  8016  -.167  13027  -.167  26000  -.167  29000  -.333
```

The second PERT card (PERT2:p) gives the estimated tally change for a 100% increase in the elastic (RXN=2) cross section of material 13. RHO=–2.34 • 2 = –4.68 g/cm^3.

Default METHOD is used incorrectly (1, 1st + 2nd order terms)

- A. Hogenbirk, "An Easy Way to Carry Out 3D Uncertainty Analyses," *Proc. Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)*, Monterey, California, April 15-19, 2007, on CD-ROM (2007); page 3 (cropped):



Using the perturbation option of MCNP (invoked with the *PERT*-card with the default option (*i.e.* method = *1*)) the sensitivity profile is generated as follows:

1. the cross section is selected for which the profile is to be generated (*e.g.* the fission cross section for ^{238}U, σ_f(^{238}U))
2. a material card is created in which the atomic density for the relevant isotope (*i.e.* ^{238}U) is increased by 1%
3. a *PERT*-card is created specifying that the relevant material is replaced by the perturbed material

How To: Using MCNP to Compute Sensitivities

- The sensitivity of k with respect to σ_x is

$$S_{k,\sigma_x} = \frac{1}{k_0 p_x}\left[\Delta k(\Delta\sigma_x)\right]_{1\text{st}}$$

and the first-order Taylor term is linear with p_x.

- Set up the perturbed material and the PERT card.
  + Ensure only one isotope is perturbed (next slide).
  + The sensitivity is completely independent of the size of the perturbation p_x as long as it is non-zero.
  + METHOD = 2 – use only the first-order term! In the examples of Chap. 3, the manual incorrectly implies METHOD = 1 (the default) should be used.

- Run the calculation.

- Compute S_{k,σ_x} in post-processing. Also compute the relative statistical uncertainty

$$\frac{s_{S_{k,\sigma_x}}}{S_{k,\sigma_x}} = \sqrt{\left(\frac{s_{\Delta k_1}}{\Delta k_1}\right)^2 + \left(\frac{s_{k_0}}{k_0}\right)^2},$$

where s_x^2 is the variance of quantity x and $\Delta k_1 \equiv \left[\Delta k(\Delta\sigma_x)\right]_{1\text{st}}$.

How To: Perturbed Materials and the PERT Card

- Advice: Use atom 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 = 2.

```
example input for sensitivities with PERT
1   1   N_1            -1          imp:n=1
:
c unperturbed materials
m1    I_1,1  N_1,1     I_1,2  N_1,2
c materials for sensitivities
m11   I_1,1  N_11,1    I_1,2  N_1,2
m12   I_1,1  N_1,1     I_1,2  N_12,2
pert11101:n  cell=1  rho=N_11  mat=11  rxn=R_1
             erg=E_1 E_2  method=2
pert11102:n  cell=1  rho=N_11  mat=11  rxn=R_1
             erg=E_2 E_3  method=2
:
pert11201:n  cell=1  rho=N_11  mat=11  rxn=R_2
             erg=E_1 E_2  method=2
pert11202:n  cell=1  rho=N_11  mat=11  rxn=R_2
             erg=E_2 E_3  method=2
:
pert12101:n  cell=1  rho=N_12  mat=12  rxn=R_1
             erg=E_1 E_2  method=2
pert12102:n  cell=1  rho=N_12  mat=12  rxn=R_1
             erg=E_2 E_3  method=2
:
pert12201:n  cell=1  rho=N_12  mat=12  rxn=R_2
             erg=E_1 E_2  method=2
pert12202:n  cell=1  rho=N_12  mat=12  rxn=R_2
             erg=E_2 E_3  method=2
:
```

How To: Which k_0?

- The sensitivity and its relative uncertainty are

$$S_{k,\sigma_x} = \frac{1}{k_0 p_x} \Delta k_1$$

and

$$\frac{s_{S_{k,\sigma_x}}}{S_{k,\sigma_x}} = \sqrt{\left(\frac{s_{\Delta k_1}}{\Delta k_1}\right)^2 + \left(\frac{s_{k_0}}{k_0}\right)^2}.$$

- Which k_0 should be used – track-length, combined, other?
  - + Track-length?
    - ☐ The PERT estimate Δk_1 is a track-length quantity only, so using the track-length k_0 is consistent.
    - ☐ There might be correlations between Δk_1 and k_0, invalidating the relative uncertainty equation.
  - + Combined?
    - ☐ It's supposed to be the most accurate, but it is also correlated with Δk_1.
  - + Other?
    - ☐ Not correlated with Δk_1.

Results: Analytic One-Group Two-Isotope k_∞ Test Problem (σ_t)

- In a homogenous system from which there is no neutron leakage, the energy-integrated or one-group k-eigenvalue is

$$k_\infty = \frac{\nu\Sigma_f}{\Sigma_f + \Sigma_c} = \frac{N_1\nu_1\sigma_{f,1} + N_2\nu_2\sigma_{f,2}}{N_1(\sigma_{f,1} + \sigma_{c,1}) + N_2(\sigma_{f,2} + \sigma_{c,2})}$$

when there are two isotopes.

- The derivatives are all analytic; for example,

$$\frac{d^n k_\infty}{d\sigma_{t,1}^n} = \left(\frac{N_1}{\sigma_{t,1}}\right)^n \frac{d^n k_\infty}{dN_1^n} = \frac{(-1)^{n-1} n! \left(\nu_1\sigma_{f,1}(\sigma_{f,1} + \sigma_{c,1})^{n-1} - k_\infty(\sigma_{f,1} + \sigma_{c,1})^n\right)}{(\Sigma_f + \Sigma_c)^n} \left(\frac{N_1}{\sigma_{t,1}}\right)^n.$$

- Results for the total cross section ($p = +30\%$):

	Analytic	PERT Estimate	Difference Rel. to Analytic	 Num. Std. Devs.
Δk_∞, 1st-order term	0.02445	0.02445 ± 0.276%	0.028%	0.10
Δk_∞, 2nd-order term	-0.00484	-0.00481 ± 0.667%	0.491%	0.74
Δk_∞, Sum of terms	0.01961	0.01964 ± 0.290%	0.156%	0.54
Δk_∞, Total pert.	0.02041	0.01964 ± 0.290%	3.766%	13.48
$S_{k_\infty,\sigma_{t,1}}$	0.03273	0.03274 ± 0.276%	0.024%	0.09

- Using 12 terms, the Taylor series converges to within 10^{-6}% of the analytic result.

Results: Analytic One-Group Two-Isotope k_∞ Test Problem (σ_s)

- k_∞ does not depend on the scattering cross section:

$$k_\infty = \frac{\nu\Sigma_f}{\Sigma_f + \Sigma_c} = \frac{N_1\nu_1\sigma_{f,1} + N_2\nu_2\sigma_{f,2}}{N_1(\sigma_{f,1} + \sigma_{c,1}) + N_2(\sigma_{f,2} + \sigma_{c,2})}.$$

- The derivatives are

$$\frac{d^n k_\infty}{d\sigma_{s,1}^n} = 0.$$

- Results for the scattering cross section ($p = +30\%$):

	Analytic	PERT Estimate	Difference Rel. to Analytic	 Num. Std. Devs.
Δk_∞, 1st-order term	0.00000	0.00003 ± 233%	N/A	0.43
Δk_∞, 2nd-order term	0.00000	0.00002 ± 104%	N/A	0.97
Δk_∞, Sum of terms	0.00000	0.00005 ± 132%	N/A	0.75
Δk_∞, Total pert.	0.00000	0.00005 ± 132%	N/A	0.75
$S_{k_\infty,\sigma_{s,1}}$	0.00000	0.00003 ± 233%	N/A	0.43

- I recommended tracking the positive and negative contributions to perturbation results and printing a warning if they were too balanced:

```
the following perturbations have positive and negative contributions
that are very similar (within 0.1%):
```

Results: One-Group k_{eff} Test Problem

- A homogeneous spherical fuel region (radius 6.12745 cm) surrounded by a spherical reflector shell (thickness 3.063725 cm). Isotropic scattering.

- "Exact" derivatives were calculated with direct k_{eff} calculations using data libraries with perturbed cross sections (±10% and ±20%), and fitting the results with a line.

- Results:

		Direct	PERT Estimate	Difference Rel. to Direct
Fuel	S_{k_{eff},σ_t}	0.75801 ± 0.040%	0.73178 ± 0.088%	–3.460%
	S_{k_{eff},σ_f}	0.68296 ± 0.044%	0.67463 ± 0.024%	–1.219%
	S_{k_{eff},σ_c}	–0.06416 ± 0.461%	–0.06507 ± 0.063%	1.417%
	S_{k_{eff},σ_s}	0.13917 ± 0.213%	0.12222 ± 0.516%	–12.178%
	S_{k_{eff},σ_x}, sum	0.75797 ± 0.068%	0.73178 ± 0.089%	–3.455%
Refl.	S_{k_{eff},σ_t}	0.10891 ± 0.275%	0.12381 ± 0.165%	13.676%
	S_{k_{eff},σ_c}	–0.01825 ± 1.641%	–0.02137 ± 0.155%	17.076%
	S_{k_{eff},σ_s}	0.12742 ± 0.229%	0.14517 ± 0.150%	13.931%
	S_{k_{eff},σ_x}, sum	0.10917 ± 0.383%	0.12381 ± 0.178%	13.405%

- The PERT estimate is accurate in the fuel, except for scattering, but not accurate in the reflector.

Results: One-Group k Test Problem

- Same geometry and materials; fixed source is the fission distribution; fission is treated as capture; quantity of interest is $k = \int dV\, \nu\Sigma_f(r)\phi(r)$.
- Results:

		Direct	PERT Estimate	Difference Rel. to Direct
Fuel	S_{k,σ_t}	0.73216 ± 0.124%	0.73162 ± 0.213%	−0.381%
	S_{k,σ_f}	0.67584 ± 0.134%	0.67561 ± 0.100%	−0.318%
	S_{k,σ_c}	−0.06498 ± 1.387%	−0.06518 ± 0.161%	0.312%
	S_{k,σ_s}	0.12117 ± 0.744%	0.12119 ± 1.128%	−0.002%
	S_{k,σ_t}, sum	0.73203 ± 0.213%	0.73162 ± 0.209%	−0.321%
Refl.	S_{k,σ_t}	0.12433 ± 0.723%	0.12330 ± 0.412%	−0.866%
	S_{k,σ_c}	−0.02133 ± 4.439%	−0.02128 ± 0.354%	5.029%
	S_{k,σ_s}	0.14524 ± 0.619%	0.14458 ± 0.379%	−0.467%
	S_{k,σ_t}, sum	0.12391 ± 1.018%	0.12330 ± 0.448%	−1.358%

- Conclusion: The inability to account for the perturbed fission source distribution leads to inaccurate perturbation estimates of the sensitivities.

Results: 30-Group k_{eff} Test Problem (1 of 3)

- Same spherical fuel/reflector problem as before. Isotropic scattering.
- Scattering and total were the cross sections of interest.
  - + Groupwise sensitivities were estimated.
  - + For this purpose the scattering cross section for group g, Σ_s^g, is defined as self-scattering plus all outscattering.
- 30-group MCNP libraries for fuel and reflector were made using the same data used by PARTISN (690nm for fuel and 601nm for water).
- "Exact" derivatives were calculated with direct k_{eff} calculations using data libraries with perturbed cross sections (±10% and ±20% or other values), and fitting the results with a line.
  - + It was very difficult to use MCNP to compute the exact derivatives for many of the groups.
  - + The k_{eff} differences and therefore the slopes are simply too small to be accurately estimated with reasonable computing resources.
  - + Of course, this problem highlights the very need for a Monte Carlo perturbation theory!
  - + PARTISN with S_{64} quadrature and 10^{-12} convergence was used with exactly the same cross sections.

Results: 30-Group k_{eff} Test Problem (2 of 3)

- Direct (PARTISN) results and differences with PERT results:

Group Index	S_{k,σ_s} in Fuel	Diff. in Fuel	S_{k,σ_s} in Refl.	Diff. in Refl.
30	−7.910E-05	24.94%	−1.219E-03	53.88%
29	−2.716E-05	19.84%	−7.477E-05	−74.77%
28	−1.067E-04	−5.94%	−6.000E-04	−31.87%
27	−2.240E-04	−48.22%	5.962E-04	180.81%
26	−3.042E-05	−202.20%	3.373E-03	49.20%
25	−4.513E-05	−9.40%	2.268E-03	44.91%
24	−1.068E-04	−17.99%	1.681E-03	54.17%
23	−2.948E-04	−34.63%	1.584E-03	86.54%
22	−5.407E-04	−35.95%	1.049E-03	147.08%
21	−9.224E-04	−41.28%	1.238E-03	173.94%
20	−1.382E-03	−44.50%	1.914E-03	148.11%
19	−1.888E-03	−38.90%	2.405E-03	139.31%
18	−1.676E-03	−38.89%	5.024E-03	76.02%
17	−2.537E-04	−13.25%	1.028E-02	45.79%
16	5.579E-03	−30.39%	2.328E-02	28.92%
15	8.682E-03	−22.38%	2.246E-02	22.67%
14	1.313E-02	−20.63%	3.120E-02	19.57%
13	2.036E-02	−12.96%	4.089E-02	18.33%
12	2.194E-02	−10.47%	4.097E-02	16.07%
11	1.304E-02	−6.09%	1.931E-02	14.94%
10	1.367E-02	−4.85%	1.694E-02	14.03%
9	1.406E-02	−3.54%	1.371E-02	13.63%
8	1.194E-02	−3.24%	1.120E-02	12.11%
7	1.469E-02	−2.56%	1.049E-02	10.99%
6	1.675E-03	−1.44%	1.232E-03	9.70%
5	2.956E-04	2.38%	3.411E-04	8.96%
4	3.671E-05	5.86%	5.851E-05	8.20%
3	5.542E-06	−20.13%	1.107E-05	9.25%
2	1.470E-06	18.33%	3.471E-06	10.22%
1	3.251E-07	7.90%	1.475E-06	6.12%
	1.312E-01	−8.23%	2.565E-01	27.66%

Results: 30-Group k_{eff} Test Problem (3 of 3)

- Energy-integrated total cross section results:

Material	Direct	PERT Estimate	Difference Rel. to Direct
S_{k,σ_t}, Fuel	0.6102 ± 0.052%	0.5594 ± 0.020%	−8.33%
S_{k,σ_t}, Ref.	0.2485 ± 0.125%	0.3157 ± 0.041%	27.05%

- Recall the difference in energy-integrated scattering results: −8.23% in fuel, 27.66% in reflector (previous slide).
- Because there is no FM multiplier for multigroup scattering, the scattering cross-section sensitivity in group g is $S_{k_{eff},\sigma_s^g} = S_{k_{eff},\sigma_t^g} - S_{k_{eff},\sigma_c^g} - S_{k_{eff},\sigma_f^g}$, so scattering and total results are not independent.
- Nevertheless, I claim (based also on upcoming results) that the large error in the scattering sensitivity leads to the large error in the total sensitivity.

Results: 30-Group k_{eff} Test Problem with Reflector Isotopics (1 of 3)

- Same spherical fuel/reflector problem as before. Isotropic scattering.

- The elemental composition of the water reflector was explicitly represented and ^{1}H and ^{16}O sensitivities were calculated.

- 30-group MCNP libraries for fuel and reflector were made using the same data used by PARTISN (601nm).

- "Exact" derivatives were calculated with direct k_{eff} calculations using data libraries with perturbed cross sections (±10% and ±20% or other values), and fitting the results with a line.
  - + It was very difficult to use MCNP to compute the exact derivatives for many of the groups.
  - + The k_{eff} differences and therefore the slopes are simply too small to be accurately estimated with reasonable computing resources.
  - + Of course, this problem highlights the very need for a Monte Carlo perturbation theory!
  - + PARTISN with S_{64} quadrature and 10^{-12} convergence was used with exactly the same cross sections.

Results: 30-Group k_{eff} Test Prob. w/ Refl. Iso. (2)

- Direct (PARTISN) results and differences with PERT results:

Group Index	S_{k,σ_s} in ^{1}H	Diff. in ^{1}H	S_{k,σ_s} in ^{16}O	Diff. in ^{16}O
30	−1.153E-03	54.23%	−8.417E-05	45.70%
29	−8.800E-05	−132.70%	1.132E-05	80.68%
28	−6.123E-04	−24.41%	3.791E-06	233.65%
27	5.300E-04	207.45%	5.385E-05	99.93%
26	3.216E-03	51.60%	1.412E-04	62.28%
25	2.153E-03	43.82%	9.971E-05	40.45%
24	1.567E-03	54.39%	9.697E-05	54.88%
23	1.454E-03	94.76%	1.109E-04	68.08%
22	9.119E-04	166.21%	1.138E-04	59.60%
21	1.059E-03	195.28%	1.501E-04	68.06%
20	1.664E-03	166.83%	2.134E-04	55.89%
19	2.055E-03	157.32%	3.011E-04	40.63%
18	4.455E-03	85.48%	5.031E-04	29.89%
17	9.194E-03	49.58%	9.867E-04	21.25%
16	2.055E-02	31.50%	2.576E-03	15.97%
15	1.921E-02	24.91%	3.114E-03	14.74%
14	2.204E-02	24.37%	8.907E-03	11.25%
13	3.337E-02	20.38%	7.418E-03	10.66%
12	2.904E-02	18.92%	1.181E-02	9.99%
11	1.523E-02	16.69%	4.053E-03	9.71%
10	1.363E-02	15.52%	3.294E-03	8.70%
9	1.207E-02	14.36%	1.642E-03	8.11%
8	7.990E-03	13.91%	3.205E-03	7.23%
7	7.463E-03	12.53%	3.026E-03	6.94%
6	9.257E-04	10.57%	3.064E-04	8.08%
5	2.282E-04	9.32%	1.128E-04	7.45%
4	3.348E-05	10.31%	2.504E-05	6.71%
3	5.622E-06	6.48%	5.431E-06	6.04%
2	1.600E-06	16.82%	1.850E-06	8.13%
1	1.250E-06	−52.33%	1.700E-06	−52.03%
	2.047E-01	31.52%	5.218E-02	11.91%

Results: 30-Group k_{eff} Test Problem with Reflector Isotopics (3 of 3)

- Energy-integrated total cross section results:

Material	Direct	PERT Estimate	Difference Rel. to Direct
S_{k,σ_t}, ^{1}H	0.1965 ± 0.155%	0.2575 ± 0.050%	31.05%
S_{k,σ_t}, ^{16}O	0.0516 ± 0.609%	0.0583 ± 0.076%	12.93%

- Recall the difference in energy-integrated scattering results: 31.52% for ^{1}H, 11.91% for ^{16}O (previous slide).

- The large error in the scattering sensitivity leads to the large error in the total sensitivity.

Results: Continuous-Energy k_{eff} Test Problem – Total Cross Section

- A homogeneous mixture of UF_4 and paraffin with a ^{235}U enrichment of 2% with a density of 3.863 g/cm^3 in a sphere of radius 38.5 cm.

- Continuous-energy cross sections can not be directly perturbed without special knowledge, but direct results are possible for the sensitivity of k_{eff} to isotopic total cross sections.
  - + Same as an isotopic density perturbation – use the perturbed material and the perturbed density.
  - + Use a central difference approximation:

$$S_{k,\sigma_x} \approx \frac{1}{k_0}\frac{k(p_{x+})-k(p_{x-})}{p_{x+}-p_{x-}} = \frac{k(p_{x+})-k(-p_{x+})}{2k_0 p_{x+}},$$

where $p_{x-} = -p_{x-}$ for a central difference.

  - + p_x must be small enough that the three points $(-p_x, k_-)$, $(0, k_0)$, and $(+p_x, k_+)$ are in a line, but large enough that the numerator is statistically significant.

- Energy-integrated total sensitivities from MCNP:

Isotope	Direct	PERT	Difference	Ns
^{1}H	2.310E-01 ± 0.771%	2.215E-01 ± 0.811%	−4.210%	2.662
C	2.506E-02 ± 3.487%	1.981E-02 ± 2.644%	−23.401%	3.757
^{19}F	3.937E-02 ± 2.198%	3.432E-02 ± 1.931%	−13.716%	3.307
^{235}U	2.536E-01 ± 0.724%	2.559E-01 ± 0.074%	0.922%	1.159
^{238}U	−2.110E-01 ± 0.846%	−2.130E-01 ± 0.245%	0.933%	0.857

Results: Continuous-Energy k_{eff} Test Problem – H and C

- TSUNAMI-3D results for this problem were provided by B. T. Rearden (ORNL).
  - 238 energy groups, ENDF-VI cross sections, and a light water scattering kernel.
  - Some differences from previously published results.
- Energy-integrated sensitivities, hydrogen and carbon:

Isotope	Reaction	MCNP	TSUNAMI-3D	Difference	*Ns*
^{1}H	Total	2.215E-01 ± 0.81%	2.203E-01 ± 0.09%	0.527%	0.58
	Scatter	3.223E-01 ± 0.56%	3.220E-01 ± 0.06%	0.073%	0.12
	Elastic	3.223E-01 ± 0.56%	3.220E-01 ± 0.06%	0.073%	0.12
	Capture	−1.008E-01 ± 0.05%	−1.017E-01 ± 0.01%	−0.918%	13.59
	n,γ	−1.008E-01 ± 0.05%	−1.017E-01 ± 0.01%	−0.918%	13.59
C	Total	1.981E-02 ± 2.64%	2.416E-02 ± 0.06%	−19.760%	8.07
	Scatter	2.048E-02 ± 2.56%	2.484E-02 ± 0.06%	−19.248%	8.11
	Elastic	2.028E-02 ± 2.59%	2.462E-02 ± 0.06%	−19.301%	8.04
	n,n′	1.963E-04 ± 6.87%	2.250E-04 ± 0.07%	−13.618%	2.10
	n,2n	−5.743E-10 ± 68.56%	N/A^{a} ± N/A^{a}	200%	1.46
	Capture	−6.681E-04 ± 0.12%	−6.855E-04 ± 0.01%	−2.570%	18.97
	n,γ	−4.943E-04 ± 0.06%	−4.996E-04 ± 0.01%	−1.053%	15.63
	n,p	−5.963E-08 ± 9.41%	−2.975E-08 ± 0.83%	66.877%	5.10
	n,d	−1.595E-07 ± 11.19%	−5.932E-08 ± 1.17%	91.542%	5.40
	n,α	−1.735E-04 ± 0.45%	−1.858E-04 ± 0.03%	−6.843%	14.75

[a] Not reported in TSUNAMI-3D output file

- Note agreement for hydrogen! In carbon, Capture agrees, but Scatter does not.

Results: Continuous-Energy k_{eff} Test Problem – Uranium

- Energy-integrated sensitivities, uranium:

Isotope	Reaction	MCNP	TSUNAMI-3D	Difference	*Ns*
^{235}U	Total	2.559E-01 ± 0.07%	2.504E-01 ± 0.02%	2.165%	23.43
	Scatter	5.524E-04 ± 10.91%	4.421E-04 ± 0.03%	22.188%	1.83
	Elastic	3.255E-04 ± 17.42%	2.052E-04 ± 0.05%	45.351%	2.12
	n,n′	2.118E-04 ± 7.96%	2.196E-04 ± 0.02%	−3.607%	0.46
	n,2n	1.506E-05 ± 11.37%	1.727E-05 ± 0.03%	−13.664%	1.29
	Fission	3.657E-01 ± 0.05%	3.629E-01 ± 0.01%	0.777%	12.82
	Capture	−1.103E-01 ± 0.05%	−1.129E-01 ± 0.01%	−2.274%	35.22
	n,γ	−1.103E-01 ± 0.05%	−1.129E-01 ± 0.01%	−2.274%	35.22
^{238}U	Total	−2.130E-01 ± 0.25%	−2.049E-01 ± 0.01%	3.859%	14.75
	Scatter	3.522E-02 ± 1.39%	4.885E-02 ± 0.01%	−32.422%	27.46
	Elastic	2.315E-02 ± 2.00%	3.488E-02 ± 0.01%	−40.424%	25.02
	n,n′	1.109E-02 ± 1.25%	1.293E-02 ± 0.02%	−15.318%	12.98
	n,2n	9.833E-04 ± 1.48%	1.032E-03 ± 0.03%	−4.806%	3.25
	Fission	3.441E-02 ± 0.05%	3.350E-02 ± 0.02%	2.685%	40.44
	Capture	−2.826E-01 ± 0.05%	−2.873E-01 ± 0.01%	−1.625%	28.50
	n,γ	−2.826E-01 ± 0.05%	−2.873E-01 ± 0.01%	−1.625%	28.50

- Total is Scatter + Fission + Capture. In U isotopes, Fission and Capture agree, but Scatter does not.

Results: Continuous-Energy k_{eff} Test Problem – Fluorine

- Energy-integrated sensitivities, fluorine:

Isotope	Reaction	MCNP	TSUNAMI-3D	Difference	*Ns*
^{19}F	Total	3.432E-02 ± 1.93%	4.139E-02 ± 0.05%	−18.680%	10.36
	Scatter	3.983E-02 ± 1.67%	4.698E-02 ± 0.04%	−16.472%	10.45
	Elastic	2.564E-02 ± 2.43%	2.980E-02 ± 0.06%	−15.002%	6.49
	n,n′	1.419E-02 ± 1.35%	1.612E-02 ± 0.03%	−12.699%	9.76
	n,2n	0.000E+00 ± 0.00%	2.779E-06 ± 0.13%	−200%	771.95
	Capture	−5.609E-03 ± 0.08%	−5.592E-03 ± 0.01%	0.298%	3.13
	n,γ	−2.361E-03 ± 0.05%	−2.391E-03 ± 0.01%	−1.274%	19.65
	n,p	−2.332E-04 ± 0.22%	−2.380E-04 ± 0.03%	−2.018%	8.41
	n,d	−1.114E-05 ± 0.58%	−1.256E-05 ± 0.04%	−12.056%	20.67
	n,t	−2.052E-06 ± 1.27%	−2.625E-06 ± 0.06%	−24.514%	20.80
	n,α	−3.002E-03 ± 0.13%	−2.948E-03 ± 0.02%	1.804%	12.06

- Total is Scatter + Capture. In ^{19}F, Capture agrees, but Scatter does not.

Results: Other

- A. Hogenbirk, "An Easy Way to Carry Out 3D Uncertainty Analyses," *Proc. Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)*, Monterey, California, April 15-19, 2007, on CD-ROM (2007).
  - Two-dimensional cylindrical Gas Cooled Fast Reactor (GCFR) problem; 2400 MWth.
  - "The core regions consist of mixtures of MOX with SiC structure material; the reflectors are made of Zr_3Si_2."
  - Continuous-energy vs. 33 groups, but the same evaluations were used.
  - Page 6 (cropped):

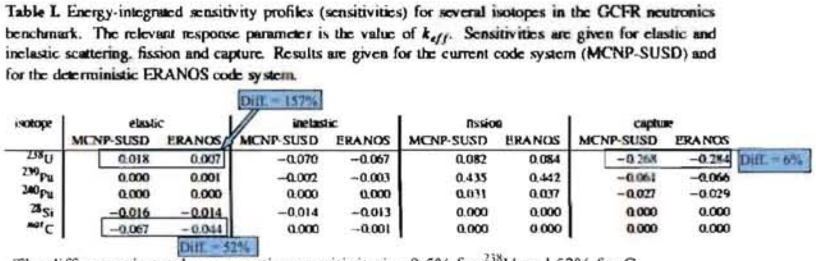


Table I. Energy-integrated sensitivity profiles (sensitivities) for several isotopes in the GCFR neutronics benchmark. The relevant response parameter is the value of k_{eff}. Sensitivities are given for elastic and inelastic scattering, fission and capture. Results are given for the current code system (MCNP-SUSD) and for the deterministic ERANOS code system.

isotope	elastic		inelastic		fission		capture	
	MCNP-SUSD	ERANOS	MCNP-SUSD	ERANOS	MCNP-SUSD	ERANOS	MCNP-SUSD	ERANOS
^{238}U	0.018	0.007	−0.070	−0.067	0.082	0.084	−0.268	−0.284
^{239}Pu	0.000	0.001	−0.002	−0.003	0.435	0.442	−0.061	−0.066
^{240}Pu	0.000	0.000	0.000	0.000	0.031	0.037	−0.027	−0.029
^{28}Si	−0.016	−0.014	−0.014	−0.013	0.000	0.000	0.000	0.000
^{nat}C	−0.067	−0.044	0.000	−0.001	0.000	0.000	0.000	0.000

Diff. = 157%

Diff. = 6%

Diff. = 52%

- The difference in total cross section sensitivity is –8.5% for ^{238}U and 52% for C.
- MCNP overestimates ^{238}U elastic sensitivity; in the previous problem, it underestimated.
- If it's MOX fuel, where is the ^{235}U and oxygen? I tried to get the input file but was refused.

Testing Accuracy

- Density or composition perturbations can be tested with direct calculations.

- Unfortunately, cross-section sensitivities can only be tested in this way for the energy-integrated total cross section sensitivity.

- The second-order Taylor term might be useful for testing the assumption of linearity, but I haven't figured out a way to test the accuracy of the first-order term for arbitrary reactions.

Reaction Numbers for Comparing MCNP and TSUNAMI-3D

- In the TSUNAMI-3D output, reactions are identified with words rather than specific MT numbers.

- The corresponding reaction numbers to use on the MCNP PERT card RXN keyword are:

Reaction	SCALE Identifier	MCNP PERT RXN
Sum of scattering	scatter	2 16 51 39i 91 [and 4 for $S(\alpha,\beta)$[a]]
Total	total	1
Elastic scattering	elastic	2 [and 4 for $S(\alpha,\beta)$[a]]
Inelastic scattering	n,n'	51 39i 91
n,2n	n,2n	16
Fission	fission	–6
Neutron disappearance	capture	–2
n,γ	n,gamma	102
n,p	n,p	103
n,d	n,d	104
n,t	n,t	105
n,^{3}He	n,he-3	106
n,α	n,alpha	107

[a] Only ^{1}H has been tested.

- These were determined in some cases by trial and error, and only five isotopes have been tested.

Bugs

- Perturbed tally results depend on the presence or absence of unrelated tallies and their FM cards.
  - \+ Affects KCODE and fixed-source problems.
  - \+ First reported Dec. 9, 2008.
  - \+ For accurate perturbed tallies, need a dummy tally with the "right" FM card and a tally number smaller than the tallies of interest.

- The perturbation capability sometimes gives nonzero Δk_{eff} results for fission reactions that do not exist.
  - \+ First reported March 17, 2009.
  - \+ I reported a problem in which fission was given with MT=18, but perturbing reactions 19, 20, 21, and 38 caused nonzero Δk_{eff} results.
  - \+ RXN = –6 is recommended for fission.

Recommendations

- Fix bugs.

- Modify the manual to point out that METHOD=2 should be used.

- Print more digits for both the result and the standard deviation in the "predicted changes in keff" output (to facilitate code comparisons).

- The user number of each perturbation should be printed in the "predicted changes in keff" output as is presently done for perturbed tallies (MCNPX did this).

- Separate positive and negative contributions to perturbed quantities and report if they are too similar in magnitude.

- Add Brian's continuous-energy adjoint-based capability ASAP.
  - \+ Keep the present output style.
  - \+ Use differential operator for fixed-source problems and use adjoint for k_{eff} problems.

- Add capability to perturb ν, the number of neutrons produced per fission.

Computing Sensitivities with the PERT Card

- In cases where it is accurate, the PERT card can be used to compute energy-, isotope-, reaction-dependent sensitivity profiles:

```
example input for sensitivities with PERT
1   1   N1          -1        imp:n=1
2   2   N2          -2  1     imp:n=1
:
c unperturbed materials
m1   I1,1  N1,1    I1,2  N1,2
m2   I2,1  N2,1    I2,2  N2,2
c materials for sensitivities
m11   I1,1  N11,1    I1,2  N1,2
m12   I1,1  N1,1     I1,2  N12,2
m21   I2,1  N21,1    I2,2  N2,2
m22   I2,1  N2,1     I2,2  N22,2
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=E2 E3  method=2
:
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=E2 E3  method=2
:
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=E2 E3  method=2
:
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=E2 E3  method=2
:
pert21101:n  cell=2  rho=N21  mat=21  rxn=R1  erg=E1 E2  method=2
pert21102:n  cell=2  rho=N21  mat=21  rxn=R1  erg=E2 E3  method=2
:
pert21201:n  cell=2  rho=N21  mat=21  rxn=R2  erg=E1 E2  method=2
pert21202:n  cell=2  rho=N21  mat=21  rxn=R2  erg=E2 E3  method=2
:
pert22101:n  cell=2  rho=N22  mat=22  rxn=R1  erg=E1 E2  method=2
pert22102:n  cell=2  rho=N22  mat=22  rxn=R1  erg=E2 E3  method=2
:
pert22201:n  cell=2  rho=N22  mat=22  rxn=R2  erg=E1 E2  method=2
pert22202:n  cell=2  rho=N22  mat=22  rxn=R2  erg=E2 E3  method=2
:
```

Computing Sensitivities with a SENS Card

- These two inputs should yield identical results (and identical to all the PERT cards on the previous slide):

```
example input for sensitivities with SENS
1   1   N1          -1        imp:n=1
2   2   N2          -2  1     imp:n=1
:
m1   I1,1  N1,1    I1,2  N1,2
m2   I2,1  N2,1    I2,2  N2,2
sens00001:n  cell=1 2  rxn=R1 R2  erg=E1 E2 E3 ...
```

```
example input for sensitivities with SENS
1   1   N1          -1        imp:n=1
2   2   N2          -2  1     imp:n=1
:
m1   I1,1  N1,1    I1,2  N1,2
m2   I2,1  N2,1    I2,2  N2,2
sens11101:n  mat=1  iso=I1,1  rxn=R1  erg=E1 E2 E3 ...
sens12101:n  mat=1  iso=I1,2  rxn=R1  erg=E1 E2 E3 ...
sens11201:n  mat=1  iso=I1,1  rxn=R2  erg=E1 E2 E3 ...
sens12201:n  mat=1  iso=I1,2  rxn=R2  erg=E1 E2 E3 ...
sens21101:n  mat=2  iso=I2,1  rxn=R1  erg=E1 E2 E3 ...
sens22101:n  mat=2  iso=I2,2  rxn=R1  erg=E1 E2 E3 ...
sens21201:n  mat=2  iso=I2,1  rxn=R2  erg=E1 E2 E3 ...
sens22201:n  mat=2  iso=I2,2  rxn=R2  erg=E1 E2 E3 ...
```

- The SENS card:

Keyword	Parameter Values	Default	Entries
CELL[a]	Integer > 0	All cells with the material on the MAT keyword[a]	Unlimited
MAT[a]	Integer > 0	The single material in the cells on the CELL list	1
ISO	ZAID	Each isotope in the material	Unlimited
RXN	Integer	1	Unlimited
ERG	Real, Integer > 0, NT	All energies (as a sum)	Unlimited
RES	K or integer	All tallies, and k_{eff} if KCODE	Unlimited

[a] Either the CELL or MAT keyword is required, but only one of them is allowed.

Aside: Computing Sensitivities with Respect to Surface Locations

- The sensitivity of k_{eff} to an interface location is the usual forward-adjoint product evaluated on the unperturbed surface.
- An F2-like tally – fluxes on surfaces – but the tally is the forward-adjoint product.
- The tally also uses the difference in cross sections across the interface.
- There is no unvoiding of voids, no divide-by-zero, etc.

```
example input for sensitivities with SENS
1   1   N1          -1        imp:n=1
2   2   N2          -2  1     imp:n=1
:
1   so    10.
2   so    20.
:
sens00001:n  surf=1 2  erg=E1 E2 E3 ...
```

Summary and Conclusions

- k_{eff} sensitivities to cross sections can be calculated using the PERT card in MCNP.
  - + METHOD=2 (first-order Taylor term).
  - + The accuracy is limited because the differential operator method does not account for the perturbation of the fission source distribution.
  - + Accuracy of the sensitivity to the total cross section S_{k,σ_t} can always be tested directly.
  - + Scattering affects the fission source spatial distribution more than capture does – so the error in S_{k,σ_s} can be large, and this affects the error in S_{k,σ_t} (this is the conclusion of a future talk). (This conclusion evidently does not apply to $S(\alpha,\beta)$ scattering.)
- It would be more accurate to compute sensitivities using an adjoint-based method, as does TSUNAMI-3D:
  - + $$\frac{dk}{du_n} = -k_0^2 \frac{\left\langle \psi_0^*, \left(\frac{dL}{du_n} - \frac{1}{k_0}\frac{dF}{du_n} \right) \psi_0 \right\rangle}{\left\langle \psi_0^*, F_0 \psi_0 \right\rangle}.$$
  - + Brian Kiedrowski's thesis.

Publications and Reports

Journal article

1. Jeffrey A. Favorite and Keith C. Bledsoe, "Eigenvalue Sensitivity to System Dimensions," *Annals of Nuclear Energy*, accepted for publication (2010).

Conference proceeding

2. Jeffrey A. Favorite, "Eigenvalue Sensitivity Analysis Using the MCNP5 Perturbation Capability," *Proceedings of the 2009 Nuclear Criticality Safety Division* (of the American Nuclear Society) *Topical Meeting on Realism, Robustness, and the Nuclear Renaissance*, Richland, Washington, September 13-17, CD-ROM (2009).

ANS Summaries

3. Jeffrey A. Favorite, "Adjoint-Based Eigenvalue Sensitivity to Geometry Perturbations," *Transactions of the American Nuclear Society*, **102**, submitted (2010).
4. Jeffrey A. Favorite, "On the Accuracy of the Differential Operator Monte Carlo Perturbation Method for Eigenvalue Problems," *Transactions of the American Nuclear Society*, **101**, 460-462 (2009).

Reports

5. Jeffrey A. Favorite, "One-Group Analytic Test Problems for MCNP5 Perturbation Verification (U)," X-1–RN(U)09–06, LA–UR–09–2440, April 16, 2009.
6. Jeffrey A. Favorite, "A Comparison of MCNP5 Perturbation Estimates of k_{eff} Sensitivities with TSUNAMI-3D Results for a Homogeneous Thermal Sphere (U)," X-1–RN(U)09–05, LA–UR–09–1724, March 17, 2009.
7. Jeffrey A. Favorite, "Thoughts on a Built-In Sensitivity Capability for MCNP (U)," X-1–RN(U)09–04, January 27, 2009.
8. Jeffrey A. Favorite, "Comparison of MCNP5 Perturbation Estimates of *k*-Eigenvalue Sensitivities with Exact Results for One-Group and 30-Group Problems (U)," X-1–RN(U)09–03, LA–UR–09–0499, January 26, 2009.