Title: MCNP6.1 k-Eigenvalue Sensitivity Capability: A User's Guide

Author(s):   Kiedrowski, Brian C.

Intended for: MCNP Documentation & Website

MCNP6.1 *k*-Eigenvalue Sensitivity Capability: A User's Guide

Brian C. Kiedrowski
bckiedro@lanl.gov

I. Introduction

MCNP6.1 is the first production version of MCNP to include the ability to compute sensitivity coefficients of the effective multiplication *k* for nuclear data. These types of calculations are useful for code validation and the development of benchmark suites applicable to specific set of applications, for the design of critical (integral) experiments, and uncertainty quantification.

The methods employed are based upon linear-perturbation theory using adjoint weighting, the same as those used by TSUNAMI-3D for this purpose. The adjoint weighting is performed in a single forward calculation using the Iterated Fission Probability method. The capability is specifically designed for use in continuous-energy calculations, and while it is possible to use this option in multigroup calculations, MCNP does not compute the effect of the cross section self shielding on the sensitivity coefficients.

This user's guide is structured as follows: First, a very brief overview of sensitivity theory and how to interpret the results is given. Next, the code options for calculating sensitivity coefficients in MCNP are discussed. Third, the code output formats and plotting results are discussed. Finally, there is a discussion of known issues, limitations, and future development plans.

II. Sensitivity Theory

The sensitivity coefficient is the ratio of the resulting relative change in a response (multiplication *k*) to the relative change in a system parameter *x* (cross section, fission nu, etc. over some small energy range E to $E + dE$). Assuming that the change in parameter *x* is small enough such that *k* changes linearly with respect the parameter, the following relationship holds:

$$S_{k,x} = \frac{\Delta k/k}{\Delta x/x} = \frac{x}{k}\frac{dk}{dx}. \tag{1}$$

An integral expression (more precisely one that is a ratio of integrals) may be obtained using linear-perturbation theory. The derivation involves differentiating the *k*-eigenvalue form of the neutron transport equation with respect to parameter *x* and multiplying by *x*, and then multiplying and applying the properties of adjoint functions. The end result of this derivation yields

$$S_{k,x} = -\frac{\langle \psi^{\dagger}, (\Sigma_x - S_x - k^{-1}F_x)\psi \rangle}{\langle \psi^{\dagger}, F\psi \rangle}. \tag{2}$$

The brackets denote integration over all space, direction, and energies. The term ψ is the neutron angular flux and $\psi^{\dagger}$ is its adjoint or importance function. Σ_x is the cross section for parameter *x*, and is zero if it is not a cross section. S_x is the integral scattering operator only for *x*, F_x is the integral fission operator only for *x*, and F is the integral fission operator for the entire system.

These two integrals are evaluated using the Iterated Fission Probability method. The method involves taking the neutron cycles or iterations and creating an outer iteration block. In the first cycle in the iterations, the terms to the right of the comma are estimated and the contributions are associated with

particular neutron histories. Each neutron remembers its contributions by way of a set of tags tracked within MCNP. The tags are inherited by neutron fission progeny until the final cycle in the outer iteration where the adjoint or importance weight is estimated and multiplied by the corresponding contributions. The adjoint weight is determined by way of a track-length estimate of the number of fission neutrons each descendent neutron causes in the last cycle, which is the physical interpretation of the adjoint function.

The sensitivity coefficient has the property of being additive. To illustrate with an example, the sensitivity to the total cross section of an isotope is the sum of the sensitivities of all the individual reaction cross sections of that isotope. Note that the total cross section sensitivity is equivalent to the sensitivity of the atomic or number density of that isotope globally throughout the system independent of changes to other parameters.

The same reasoning of additivity applies to the energy portion of phase space as well: the sensitivity to a particular cross section over all energies is the sum of the sensitivities of that cross section over any partitioning of the energy space.

The magnitude of a sensitivity coefficient is proportional to its impact on the system's effective multiplication. Those with relatively high magnitudes can be said to be very important in determining k, whereas those with lower magnitudes are not as important. The sign of the sensitivity coefficient gives the direction that k would change should x increase; a positive sensitivity coefficient for x implies that there would be an increase in k if x were increased, whereas a negative sensitivity coefficient for x implies that there would be a decrease in k if x were increased.

A couple examples illustrate these concepts:

Suppose a critical solution assembly contains ^{1}H and ^{235}U. The total cross section sensitivities for each are respectively 0.40 and 0.05. In this case, the hydrogen density is the most important of these parameters for determining criticality of this system. By these results, it can be said that the ^{1}H is eight times more important than ^{235}U. In other words, it is more important to control the amount of hydrogen in the system than it is to control the amount of uranium. This is often the case in undermoderated solutions of fissile material.

Suppose a system has a k of 0.95500 and the capture cross section for ^{238}U has a sensitivity coefficient of -0.14. Now suppose that this cross section is suspected to be 1% too high, i.e., it should be decreased by 1%. The effect on k can be estimated by way of the sensitivity coefficient and Eq. (1). For this situation, k can be expected to increase by 0.00134 or k would become 0.95634. Again, this calculation is only an estimate based upon the assumption of linearity with respect to the system parameter (i.e., the change is small enough).

III. MCNP Input Specifications

Invoking the sensitivity coefficient capability in MCNP requires that: (1) the calculation be an eigenvalue (KCODE) problem, and (2) that the user specifies KSEN card to generate sensitivity profiles. Here a sensitivity profile is taken to be the information produced by one KSEN card, of which there may be an arbitrary number.

The basic KSEN card has the following format:

KSEN*n*   XS   ISO = *ZAID1 ZAID2 …*   RXN = *MT1 MT2 …*   ERG = *E0 E1 E2 …*

The options in normal text indicate literal text of the card, and the italicized text indicates that it is to be replaced with user data. The number n is an arbitrary positive user index that must be unique for each instance of the KSEN card. The XS denotes that it is a cross section sensitivity. The other entries are as follows:

ISO   list of ZAIDs for which sensitivities are desired (default is all data tables in the problem).

RXN   list of reaction MT numbers or special reaction numbers (if not present, defaults to the total cross section without $S(\alpha, \beta)$). Note that MT is also an acceptable substitute for RXN. See Table I for a list of acceptable entries.

ERG   List of energy bin boundaries in MeV. For cross sections and fission nu, the energy is taken to be incident energy. For fission chi and scattering laws, the energy is taken to be outgoing. Unlike tallies, there is no implied zero lower bound, so the minimum number of entries that must be specified is two (if not present, defaults to an energy range of zero to infinity).

Table I: Allowed MT Numbers for KSEN with Continuous-Energy Physics

Nuclear Data	MT Number
Total	1
Total + $S(\alpha, \beta)$	-1
Capture	-2
Elastic	2
Total Inelastic	4
Elastic + $S(\alpha, \beta)$	-3
Total Fission	18, -6
First-Chance Fission	19
Second-Chance Fission	20
Third-Chance Fission	21
Fourth-Chance Fission	38
Total Fission Nu	452, -7
Prompt Fission Nu	456
Delayed Fission Nu	455
n,2n	16
n,3n	17
n,4n	37
n,γ	102
n,p	103
n,d	104
n,t	105
n,^{3}He	106
n,α	107
Inelastic Levels (1-40)	51, 52, …, 90
Inelastic Continuum	91
Total Fission Chi	-1018
Prompt Fission Chi	-1456
Delayed Fission Chi	-1455
Total Scatter Law	-1001
Elastic Scatter Law	-1002
Inelastic Scatter Law	-1004

Note that for cross sections and fission nu, the energies listed on ERG are taken to be those entering the collision, whereas for secondary distributions of fission chi and scattering laws they are taken to be energies exiting the collision.

There are additional options available should fission chi (-1018) or scattering law distributions (-1002 or -1004) be included in the list of reaction MTs.

EIN	Only used for fission-chi or scattering law sensitivities, and is used to specify a range of incident energy bins. Like with ERG, if not specified, the default is zero to infinity.
COS	Only used for scattering law sensitivities. Specifies a range of direction change cosines for the scattering events. The default range if not specified is -1 to 1.
CONSTRAIN	Increasing a distribution in one region of energy (or cosine) space would need to be offset by decreases elsewhere to preserve the condition that the distribution be normalized to a constant value, typically one. The arguments are YES or NO, with the default being YES. For most applications users should use the default.

Examples to illustrate the use of the KSEN card:

```
KSEN3   XS
```

Default behavior. Gives the total cross section sensitivities (integrated over all energies) to all isotopes and $S(\alpha, \beta)$ laws in the problem.

```
KSEN14   XS   ISO=92235.70c  92238.70c  MT=-1  2  4  -6
```

Gives total, elastic, inelastic, and fission cross section sensitivities for ^{235}U and ^{238}U.

```
KSEN8   XS   ISO=1001.70c lwtr.10t  MT=2 4  ERG=0  0.625e-6   0.1   20
```

Gives ^{1}H elastic scattering and the light-water $S(\alpha, \beta)$ inelastic scattering kernel sensitivities as a function of energy with bins between 0 and 0.625 eV, 0.625 eV to 100 keV, and 100 keV to 20 MeV.

```
KSEN99  XS   ISO=94239.70c   MT=-1018   ERG=0 0.1 1.0 2.0 5.0 10.0 20.0
             EIN=0 2.5 8.0 20.0   CONSTRAIN = NO
```

Gives ^{239}Pu fission-chi sensitivities as a function of outgoing and incident energy. The incident energy bins are 0 to 2.5 MeV, 2.5 to 8 MeV, and 8 to 20 MeV. For each of these, a fission-chi sensitivity is given for the energy range specified by the ERG keyword (see previous example). The sensitivity is also not renormalized, which is usually not recommended.

```
KSEN8016  XS  ISO=8016.70c   MT=-1002  ERG=0  19i  20  COS=-1 0  1
```

Gives ^{16}O elastic scattering law sensitivities for 1 MeV (outgoing) energy bins from 0 to 20 MeV. Each outgoing energy bin is subdivided into two cosine bins for forward and back scattering. The sensitivity includes neutrons scattering at all possible incident energies.

Other options may be controlled by use of the KOPTS card, which contains various options for KCODE calculations. The two options are BLOCKSIZE, which controls the number of cycles in every

outer iteration, and KSENTAL, which controls output printing of a results file for sensitivity profiles. The format for these is as follows:

KOPTS BLOCKSIZE = *NCY* KSENTAL = *FILEOPT*

The NCY argument denotes the number of cycles. A greater number leads to better accuracy of the answer, but the results will be less statistically resolved. The default is 10 cycles, which has been shown to be conservative for almost all cases and still preserves a reasonable about of statistical precision. For small, leakage dominated systems, this can often be reduced to 5.

The FILEOPT argument gives a file format for printing the sensitivity profiles. The default is to print no file. The only allowed argument in MCNP6.1 is MCTAL, which prints the sensitivity profiles in a special file called ksental which is similar to an mctal file for tallies, and can be plotted by MCPLOT. A description of the MCTAL file format is given in Section IV.

An example illustrating these concepts:

```
KOPTS   BLOCKSIZE = 5    KSENTAL = MCTAL
```

IV. MCNP Output Formats

By default MCNP prints the sensitivity profiles to the output file. These are located below "the box" with the *k* results with the heading "nuclear data sensitivity profiles". The ordering of results changes depending upon the requested information. Regardless, the sensitivities are presented as the sensitivity result (integrated over an energy bin) and its associated relative uncertainty. Note that because sensitivities may either be positive or negative, those near zero may have a very large (greater than one) relative uncertainty, but the absolute uncertainty may be quite small.

If no energy bins are requested, then the sensitivities will be presented as:

```
ZAID        REACTION        SENS        REL UNC
```

If energy bins are requested, then the sensitivities will be presented as a function of energy for each isotope and reaction:

```
ELOW        EHIGH           SENS        REL UNC
```

Here ELOW and EHIGH denote the energy bin boundaries. These energy-resolved results may be plotted for visualization in various plotting programs (GNUPLOT, MS Excel, etc.). When doing so, it is usually recommended to plot the profiles per unit lethargy (divide each sensitivity by the logarithm of the ratio of EHIGH to ELOW) on a semilog-x scale. Doing so makes it visually accurate in that areas under curves are visually representative of magnitudes of sensitivity coefficients integrated over energy ranges.

If incident energy grids for secondary distributions are requested, then an energy-resolved profile in the above format is given for each incident energy bin. For cosine bins, if an ERG card is specified, then additional grids in the above format is given for each cosine bin. If no ERG card is specified, but COS bins are, then the following results are given for all outgoing energies:

```
CLOW        CHIGH           SENS        REL UNC
```

Here CLOW and CHIGH are the lower and upper cosine bounds.

It is also possible to have the results printed to a special MCTAL-formatted file called "ksental". This is done with the KOPTS keyword and a discussion of its use may be found in Section III. The file is very much like the MCTAL file except that the symbols for bins have different meanings. These are:

F = cells (0 denoting all cells)
D = unused
U = unused
S = isotopes
M = reaction MTs
C = cosine bins
E = energy bins
T = incident energy bins (for fission chi or scattering laws)

The MCNP tally plotter, MCPLOT may be loaded to plot these results. Again, the results should be normalized to be per unit lethargy with the "lethargy" option and plotted on a semilog-x scale for visually accurate area plots.

V. Known Issues & Future Development

The sensitivity coefficient capability is new to MCNP6 and changes are indeed likely depending upon issues uncovered and other user feedback. Therefore, changes to various user options are possible forward in future versions of MCNP6.

For now, the MTs listed in Table I are the only ones tested and supported. There are other more exotic MTs (e.g., n,nα) that are possible, but will not yield correct results because it does not yet account for neutron production of those reactions yet. This will be addressed in MCNP6.2.

Also, the KSEN card does not allow for breaking the sensitivities down by region or cell. Such a capability would not only tell what nuclear data is important, but also what are the most important regions. The plan is to implement this feature in MCNP6.2.

Development of this feature will also continue, especially in the area of secondary distributions. At the moment, sensitivities that are normalized on different incident energy grids are not strictly additive except when the incident energy grid resolution is acceptably small. Also, for scattering laws, the current format may not be the most useful for other applications, and the handling of Legendre moments is a desirable feature going forward.

Also, there is work to extend this capability for arbitrary responses in fixed-source problems and the hope is to extend the capability for other responses than k in eigenvalue calculations. Also, there is a current effort to generate covariance data and the capability for MCNP to automatically generate the needed sensitivities and convolve those results with the covariance data to obtain uncertainty estimation.

Feedback and suggestions for this capability and this document are welcome. Please contact the author(s) with any comments, criticisms, or suggestions.

Acknowledgments