SENSMG: A New Tool for Multigroup Discrete Ordinates Sensitivity Analysis for Criticality

Jeffrey A. Favorite

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

INTRODUCTION

SENSMG [1] is a tool for computing first-order sensitivities of neutron reaction rates, reaction-rate ratios, leakage, k_{eff}, and α using the PARTISN multigroup discrete-ordinates code [2]. Both codes are developed at Los Alamos National Laboratory (LANL). SENSMG computes sensitivities to all of the transport cross sections and data (total, fission,[a] nu, chi, and all scattering moments), two edit cross sections (absorption and capture), and the density for every isotope and energy group. It also computes sensitivities to the mass density for every material and derivatives with respect to all interface locations and outer boundaries. The tool can be used for one-dimensional spherical and slab (r) and two-dimensional cylindrical (r-z) geometries. The tool can be used for fixed-source and eigenvalue problems. The tool implements Generalized Perturbation Theory (GPT) as discussed by Williams [3] and Stacey [4]. The tool is thus limited to computing sensitivities only for GPT-allowable responses [5].

SENSMG is a combination of Python and Fortran and was developed under Linux. SENSMG is available at `https://github.com/jafavorite/SENSMG`.

SENSMG is a wrapper around PARTISN; it does not touch the PARTISN source code. In this sense SENSMG is similar to the SWANLAKE code [6] from Oak Ridge National Laboratory (1973) and the SENSIT code [7] from LANL (1980).

In this paper, we demonstrate the application of SENSMG to criticality safety problems. Sensitivities of k_{eff} to nuclear data computed using SENSMG have been compared to sensitivities from the MCNP6.2 KSEN card [8] for several high-enriched uranium problems [9, 10]. This paper applies SENSMG to sensitivities of k_{eff} to different parameters: interface locations, material mass densities, and isotopic densities. We also review the methods for computing constant-mass derivatives using adjoint-based constant-volume and -density derivatives [11] and for computing sensitivities with respect to constrained weight fractions [12].

PU-FLATTOP MODEL

The calculations of this paper use a spherical Pu-Flattop model as a test problem. Pu-Flattop is PU-MET-FAST-006 Rev. 1 [13] in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook. The materials, dimensions, mass densities, and compositions are listed in Table I.

All PARTISN calculations used the 618-group MENDF71 multigroup library, S_{128} quadrature, P_3 scattering, and 0.005-cm mesh spacing (arbitrary values). The baseline k_{eff} for this model is 0.9997577.

STANDARD SENSMG OUTPUTS

Derivative of Pu-Flattop k_{eff} with Respect to Material Interface Locations

The derivative of the quantity of interest with respect to all material interface locations, including the outer system boundary, is a standard output of SENSMG. Adjoint-based derivatives of k_{eff} with respect to material interfaces are computed using the formula derived by Favorite and Bledsoe [14]. A portion of this output is shown for the Pu-Flattop problem in Fig. 1. The summary (sums over energy groups) gives the total derivative. The contribution from each energy group is then listed for each interface.

The adjoint-based derivatives from SENSMG are compared with central-difference estimates in Table II. The central-difference estimate for the Pu/U interface (radius 1) was computed using $\pm\Delta r = 0.01$ cm (where r is the radius). The central-difference estimate for the outer boundary (radius 2) was computed using $\pm\Delta r = 0.04$ cm. (All perturbations in this paper balance the need for small enough changes for linearity but large enough changes for an effect to be computed.) It is a hard quantity to compute. The agreement between the adjoint derivatives and the central differences is excellent.

In the central differences, the mass density was not perturbed. Thus, the central difference is estimating a constant-mass derivative. The adjoint formula implemented in SENSMG is also a constant-mass derivative.

Relative Sensitivity of Pu-Flattop k_{eff} with Respect to Material Mass Densities

The relative sensitivity of the quantity of interest with respect to all material mass densities is also a standard output of SENSMG. A portion of this output is shown for the Pu-Flattop problem in Fig. 2. The summary (sums over energy groups) gives the total relative sensitivity.

[a] Technically, fission is an edit cross section in PARTISN because only the product with nu is used in the transport.

TABLE I. Pu-Flattop Geometry and Material Parameters.

Material	Density (g/cm^3)	Outer Radius (cm)	Composition (wt.%)
Pu	15.53	4.5332	Pu239 93.800; Pu240 4.79988; Pu241 0.299996; Ga69 0.653652; Ga71 0.446355
Natural U	19.00	24.142	U234 0.00540778; U235 0.710966; U238 99.2836

```
summary (sums over groups)
radius0001     1.956127E-01
radius0002     8.824943E-04
group  e_lower       e_upper       e_average     radius0001    radius0002
    1  1.987500E+01  2.000000E+01  1.999659E+01  1.074856E-07  2.567615E-10
    2  1.975000E+01  1.987500E+01  1.987117E+01  1.434754E-08  9.381421E-11
    3  1.962500E+01  1.975000E+01  1.974579E+01  1.331992E-08  5.413638E-11
    4  1.950000E+01  1.962500E+01  1.962040E+01  1.401452E-08  4.621409E-11
    5  1.937500E+01  1.950000E+01  1.949500E+01  1.506160E-08  4.689379E-11
    6  1.925000E+01  1.937500E+01  1.936960E+01  1.647619E-08  5.039975E-11
    7  1.912500E+01  1.925000E+01  1.924419E+01  1.798768E-08  5.502305E-11
    8  1.900000E+01  1.912500E+01  1.911881E+01  1.969569E-08  6.020700E-11
    9  1.887500E+01  1.900000E+01  1.899340E+01  2.161297E-08  6.637957E-11
   10  1.875000E+01  1.887500E+01  1.886801E+01  2.369504E-08  7.316204E-11
   11  1.862500E+01  1.875000E+01  1.874260E+01  2.599378E-08  8.076625E-11
   12  1.850000E+01  1.862500E+01  1.861720E+01  2.836423E-08  8.792807E-11
   13  1.837500E+01  1.850000E+01  1.849180E+01  3.094240E-08  9.694729E-11
   14  1.825000E+01  1.837500E+01  1.836641E+01  3.367993E-08  1.060540E-10
   15  1.812500E+01  1.825000E+01  1.824101E+01  3.663521E-08  1.158031E-10
   16  1.800000E+01  1.812500E+01  1.811561E+01  3.996216E-08  1.270562E-10
   17  1.787500E+01  1.800000E+01  1.799020E+01  4.356458E-08  1.392516E-10
   18  1.775000E+01  1.787500E+01  1.786482E+01  4.749847E-08  1.522318E-10
   19  1.762500E+01  1.775000E+01  1.773941E+01  5.198485E-08  1.673474E-10
   20  1.750000E+01  1.762500E+01  1.761402E+01  5.687378E-08  1.835952E-10
   21  1.737500E+01  1.750000E+01  1.748862E+01  6.225880E-08  2.004826E-10
   22  1.725000E+01  1.737500E+01  1.736321E+01  6.821384E-08  2.192589E-10
   23  1.712500E+01  1.725000E+01  1.723780E+01  7.470496E-08  2.395961E-10
   24  1.700000E+01  1.712500E+01  1.711242E+01  8.193201E-08  2.623690E-10
```

Fig. 1. SENSMG output for derivatives with respect to material interface locations.

```
summary (sums over groups)
material0001   6.783584E-01
material0002   2.298951E-01
group  e_lower       e_upper       e_average     material0001  material0002
    1  1.987500E+01  2.000000E+01  1.999659E+01  1.395924E-06  6.476025E-07
    2  1.975000E+01  1.987500E+01  1.987117E+01  1.748655E-07  1.141945E-07
    3  1.962500E+01  1.975000E+01  1.974579E+01  1.659442E-07  8.694576E-08
    4  1.950000E+01  1.962500E+01  1.962040E+01  1.755756E-07  8.661363E-08
    5  1.937500E+01  1.950000E+01  1.949500E+01  1.890292E-07  9.247281E-08
    6  1.925000E+01  1.937500E+01  1.936960E+01  2.065407E-07  1.007263E-07
    7  1.912500E+01  1.925000E+01  1.924419E+01  2.252229E-07  1.097298E-07
    8  1.900000E+01  1.912500E+01  1.911881E+01  2.463935E-07  1.199220E-07
    9  1.887500E+01  1.900000E+01  1.899340E+01  2.698229E-07  1.313780E-07
   10  1.875000E+01  1.887500E+01  1.886801E+01  2.950198E-07  1.437733E-07
   11  1.862500E+01  1.875000E+01  1.874260E+01  3.232341E-07  1.575732E-07
   12  1.850000E+01  1.862500E+01  1.861720E+01  3.528723E-07  1.716550E-07
   13  1.837500E+01  1.850000E+01  1.849180E+01  3.859778E-07  1.880734E-07
   14  1.825000E+01  1.837500E+01  1.836641E+01  4.220116E-07  2.055890E-07
   15  1.812500E+01  1.825000E+01  1.824101E+01  4.607591E-07  2.244297E-07
   16  1.800000E+01  1.812500E+01  1.811561E+01  5.040249E-07  2.456056E-07
   17  1.787500E+01  1.800000E+01  1.799020E+01  5.510432E-07  2.685110E-07
   18  1.775000E+01  1.787500E+01  1.786482E+01  6.019267E-07  2.932589E-07
   19  1.762500E+01  1.775000E+01  1.773941E+01  6.590260E-07  3.211846E-07
   20  1.750000E+01  1.762500E+01  1.761402E+01  7.205020E-07  3.511166E-07
   21  1.737500E+01  1.750000E+01  1.748862E+01  7.877882E-07  3.833679E-07
   22  1.725000E+01  1.737500E+01  1.736321E+01  8.621670E-07  4.188333E-07
   23  1.712500E+01  1.725000E+01  1.723780E+01  9.422988E-07  4.572665E-07
   24  1.700000E+01  1.712500E+01  1.711242E+01  1.031503E-06  4.999891E-07
```

Fig. 2. SENSMG output for relative sensitivities with respect to material mass densities.

The contribution from each energy group is then listed for each material.

The adjoint-based derivatives from SENSMG are compared with central-difference estimates in Table III. The central-difference estimates for the Pu density (material 1) and the U density (material 2) were computed using $\pm\Delta\rho$ = 0.1 g/cm^3 (where ρ is the density). The agreement between the adjoint derivatives and the central differences is excellent.

In the central differences, the volume was not perturbed. Thus, the central difference is estimating a constant-volume derivative. The adjoint formula implemented in SENSMG is also a constant-volume derivative.

TABLE II. Constant-Density Derivative of Pu-Flattop k_{eff} with Respect to Material Interface Locations (/cm)

Radial Index	Adjoint	Central Difference	Difference (%)
1	1.95613E-01	1.95606E-01	0.0034
2	8.82494E-04	8.82625E-04	–0.0148

TABLE III. Constant-Volume Relative Sensitivity of Pu-Flattop k_{eff} with Respect to Material Mass Densities (%/%)

Material Index	Adjoint	Central Difference	Difference (%)
1	6.78358E-01	6.78359E-01	–0.0002
2	2.29895E-01	2.29941E-01	–0.0202

Relative Sensitivity of Pu-Flattop k_{eff} with Respect to Isotopic Number Densities

The relative sensitivity of the quantity of interest with respect to all isotopic number densities is also a standard output of SENSMG. A portion of this output is shown for the Pu-Flattop problem, for Pu239, in Fig. 3. The summary (sums over energy groups) gives the total relative sensitivity to the isotope density as well as all of the cross sections and data available. The contribution from each energy group is then listed for the density and all of the cross sections and data.

A comparison with central differences is deferred until the next section.

```
94239.711nm             isotope   1 in material   1
summary (sums over groups)
density        6.552819E-01
total         -1.245012E+00
abs           -2.611589E-01
(n,g)         -1.308094E-02
chi_(fn)      -4.398046E-17
nu             8.816547E-01
fiss           6.329931E-01
in-scat-0      1.862857E-02
self-scat-0    5.665918E-02
out-scat-0     1.862857E-02
in-scat-1     -9.218621E-04
self-scat-1   -4.137040E-02
out-scat-1    -9.218621E-04
in-scat-2     -2.507000E-05
self-scat-2    1.817221E-03
out-scat-2    -2.507000E-05
in-scat-3     -3.351141E-08
self-scat-3   -1.469475E-06
out-scat-3    -3.351141E-08
ssctt          1.018639E+00
group  e_lower       e_upper       e_average     density       total         abs
fiss           in-scat-0     self-scat-0   out-scat-0    in-scat-1     self-scat-1   out
-2    in-scat-3     self-scat-3   out-scat-3    ssctt
    1  1.987500E+01  2.000000E+01  1.999659E+01  1.324073E-06 -1.717642E-06 -4.150573E
1.256946E-06  0.000000E+00  1.439415E-07 -1.593998E-07  0.000000E+00 -1.501190E-07 -1.4
F-10  0.000000E+00 -1.112316E-10 -2.559145E-12  1.133142E-06
```

Fig. 3. SENSMG output for relative sensitivities with respect to the isotopic number density of Pu239.

SENSITIVITIES DERIVED FROM STANDARD SENSMG OUTPUTS

Constant-Mass Derivatives of Pu-Flattop k_{eff} with Respect to Material Interfaces and Mass Densities

The familiar adjoint-based formulas for density sensitivities, which are implemented in SENSMG, yield constant-volume sensitivities. The adjoint-based formulas for interface-location derivatives (less familiar but extremely useful), also implemented in SENSMG, yield constant-density derivatives. Constant-mass derivatives are sometimes needed.

Simplifying the equations in Ref. 11 to a sphere, the constant-mass derivative of k_{eff} with respect to interface location i is

$$\left(\frac{\partial k_{eff}}{\partial r_i}\right)_m = k_{eff} A_i \left(\frac{S_{k,\rho_{j+1}}}{V_{j+1}} - \frac{S_{k,\rho_j}}{V_j}\right) + \left(\frac{\partial k_{eff}}{\partial r_i}\right)_\rho , \qquad (1)$$

where A and V are surface area and volume, respectively; $S_{k,\rho}$ is the usual relative sensitivity of the response (in this case, k_{eff}) to the mass density; subscript j indicates the region inside radius i; subscript j+1 indicates the region outside radius i; and subscripts m and ρ indicate constant-mass and -volume partial derivatives, as usual. The constant-mass derivative of k_{eff} with respect to the mass density of region i is

$$\left(\frac{\partial k_{eff}}{\partial \rho_i}\right)_m = \frac{V_i}{\rho_i} \frac{\left(\frac{\partial k_{eff}}{\partial r_j}\right)_m - \left(\frac{\partial k_{eff}}{\partial r_{j+1}}\right)_m}{A_j + A_{j+1}}, \qquad (2)$$

where subscript j indicates the radius inside region i; subscript j+1 indicates the radius outside region i; and the constant-mass interface-location derivatives are computed using Eq. (1).

The constant-mass derivatives of Eqs. (1) and (2) can be computed very efficiently using adjoint-based constant-volume and -density sensitivities or derivatives. Such constant-mass derivatives, computed using the adjoint-based derivatives shown in Tables II and III, are compared with constant-mass central differences, computed by perturbing radii and densities simultaneously, in Tables IV and V. The agreement is excellent.

Equation (2) specifies that the region of interest be expanded and contracted by perturbing its boundaries by equal but opposite amounts $\pm\Delta r$ and adjusting the density of each affected region to preserve the mass. The best-fit slope of the resulting three points is the estimated derivative. It is not exactly a central difference. A different relationship among the boundaries can be used.

TABLE IV. Constant-Mass Derivative of Pu-Flattop k_{eff} with Respect to Material Interface Locations (/cm)

Radial Index	Adjoint	Central Difference	Difference (%)
1	–2.52192E-01	–2.52202E-01	–0.0041
2	–2.78688E-02	–2.78682E-02	0.0020

TABLE V. Constant-Mass Relative Sensitivity of Pu-Flattop k_{eff} with Respect to Material Mass Densities (%/%)

Material Index	Adjoint	Central Difference	Difference (%)
1	3.81171E-01	3.81179E-01	–0.0022
2	–1.73260E+00	–1.73281E+00	–0.0124

Equations (1) and (2) can also be used with numerical differences for the sensitivities and derivatives on the right sides, of course.

It is noteworthy that if the uranium mass is constant, k_{eff} is much more sensitive to the outer boundary and to the uranium density than if the mass is not constant.

Relative Sensitivity of Pu-Flattop k_{eff} with Respect to Isotopic Weight Fractions

As noted earlier, the relative sensitivity of the quantity of interest with respect to all isotopic number densities is a standard output of SENSMG. Frequently, an uncertainty analysis is done for weight fractions of isotopes in a material. Then the sensitivity of the quantity of interest with respect to all isotopic weight fractions is needed. Weight fractions are constrained to sum to unity, and the sensitivities must account for this constraint. There are several ways of doing so, but full normalization [12] is generally (but not always) preferred. The full-normalization constrained sensitivity S^{FN}_{k,w_j} to the weight fraction of isotope j can be computed using the unconstrained isotopic density sensitivities output from SENSMG using [12]

$$S^{FN}_{k,w_j} = \frac{w_I S_{k,N_j} - w_{j,0} S_{k,\rho}}{w_I}, \qquad (3)$$

where S_{k,N_j} and $S_{k,\rho}$ are the usual relative sensitivity of the response (in this case, k_{eff}) to the atom density of isotope j and the mass density of the material, both of which are standard SENSMG outputs; $w_{j,0}$ is the unperturbed weight fraction of isotope j in the material; and w_I is the combined weight fractions of the I isotopes in the material whose combined weight fractions are constrained (sometimes a subset of all materials whose combined weight fraction is $w_I < 1$).

TABLE VI. Constrained Relative Sensitivity of Pu-Flattop k_{eff} with Respect to Isotopic Weight Fractions (%/%) Using Full Normalization

Isotope	Adjoint	Central Difference	Difference (%)
Pu239	1.89809E-02	1.89827E-02	–0.0095
Pu240	–1.25872E-02	–1.25715E-02	0.1248
Pu241	–6.80355E-05	–6.80406E-05	–0.0075
Ga69	–3.78340E-03	–3.78344E-03	–0.0009
Ga71	–2.54223E-03	–2.54227E-03	–0.0016
U234	1.49567E-05	1.49561E-05	0.0039
U235	6.54308E-03	6.55113E-03	–0.1228
U238	–6.55804E-03	–6.55977E-03	–0.0264

The adjoint-based sensitivities computed from Eq. (3) using adjoint-based isotopic densities from SENSMG are compared with central-difference estimates in Table VI. The central differences also used a full normalization scheme [12]. The agreement is excellent.

SUMMARY AND CONCLUSIONS

This paper has demonstrated the application of the SENSMG code to problems of interest to nuclear criticality safety. SENSMG is a wrapper for LANL's PARTISN multigroup discrete-ordinates code. SENSMG's standard output sensitivities have been compared with central differences, and the agreement is excellent.

Also, the standard output sensitivities from SENSMG have been combined using previously derived formulas to compute constrained sensitivities with respect to isotopic weight fractions and constant-mass derivatives. These have also been compared with central differences, and the agreement is excellent.

Adjoint-based sensitivities are much more accurate and efficient than central differences.

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