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

Jeffrey A. Favorite
Monte Carlo Methods, Codes, and Applications Group (XCP-3)
Los Alamos National Laboratory

2018 American Nuclear Society Winter Meeting
Orlando, Florida
November 11–15, 2018

What Is It?

- SENSMG is a tool for computing first-order sensitivities of
  + neutron reaction rates,
  + neutron reaction-rate ratios,
  + neutron leakage,
  + k_{eff},
  + α

using the PARTISN multigroup discrete-ordinates code.

- 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),
  + isotope density

for every isotope and energy group.

- SENSMG also computes
  + sensitivities to mass density for every material
  + derivatives with respect to all interface locations and outer boundaries.

- One-dimensional spheres and slabs and two-dimensional (r-z) cylinders.

---

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

More About 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[b] from Oak Ridge National Laboratory (1973) and the SENSIT code[c] from LANL (1980).
  + A modern code with similar capability is SUSD3D:
    I. Kodeli, "Multidimensional Deterministic Nuclear Data Sensitivity and Uncertainty Code System, Method and Application," *Nucl. Sci. Eng.*, **138**, 45-66 (2001).
    I. A. Kodeli and S. Slavič, "SUSD3D Computer Code as Part of the XSUN-2017 Windows Interface Environment for Deterministic Radiation Transport and Cross-Section Sensitivity-Uncertainty Analysis," *Science and Technology of Nuclear Installations*, **2017** (2017).

- SEMSMG is a combination of Fortran and Python.

- SENSMG was developed under Linux.

- Available on github: `https://github.com/jafavorite/SENSMG`

- I can help you adapt SENSMG to your multigroup S_N code

[b] D. E. BARTINE, F. R. MYNATT, and E. M. OBLOW, "SWANLAKE, a Computer Code Utilizing ANISN Radiation Transport Calculations for Cross-Section Sensitivity Analysis," Oak Ridge National Laboratory report ORNL-TM-3809 (May 1973).
[c] S. A. W. GERSTL, "SENSIT: A Cross-Section and Design Sensitivity and Uncertainty Analysis Code," Los Alamos National Laboratory report LA-8498-MS (August 1980).

See My Paper in *Nuclear Science and Engineering*

ANS

NUCLEAR SCIENCE AND ENGINEERING · VOLUME 192 · 80–114 · OCTOBER 2018

DOI: https://doi.org/10.1080/00295639.2018.1471296

Computer Code Abstract

SENSMG: First-Order Sensitivities of Neutron Reaction Rates, Reaction-Rate Ratios, Leakage, k_{eff}, and α Using PARTISN

Jeffrey A. Favorite*

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

Received March 26, 2018
Accepted for Publication April 26, 2018

Abstract — *SENSMG is a tool for calculating the first-order sensitivities of reaction-rate ratios, k_{eff}, and α in*

- The paper has all the equations that are solved and defines all of the sensitivities
- It has test problems showing the application to basic nuclear data.

This Paper

- Applies SENSMG to sensitivities of k_{eff} to
  + interface locations,
  + material mass densities,
  + isotopic densities.

- Demonstrates the methods for computing constant-mass derivatives using adjoint-based constant-volume and -density derivatives

- Demonstrates the methods for computing sensitivities with respect to constrained weight fractions

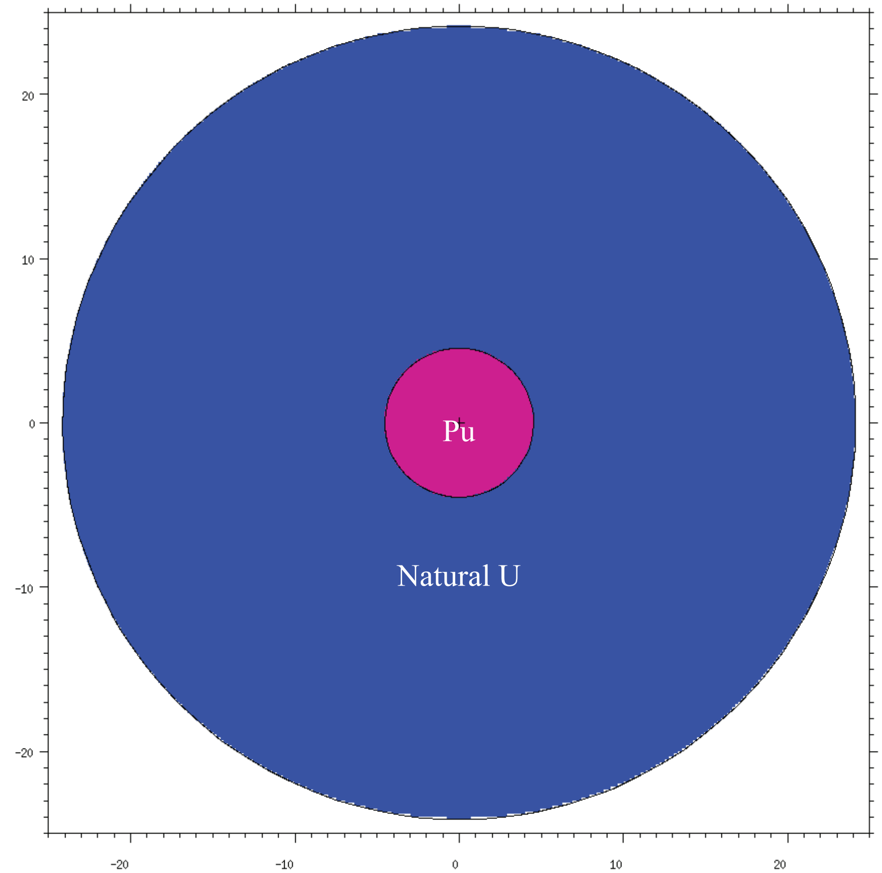
Test Problem

- Spherical Pu-Flattop, PU-MET-FAST-006 Rev. 1

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

- All PARTISN calculations used
  + the 618-group MENDF71 multigroup library,
  + S_{128} quadrature,
  + P_3 scattering,
  + 0.005-cm mesh spacing.

- The baseline k_{eff} for this model is 0.9997577.



User Interface

- Input file:

```
Pu-Flattop (PU-MET-FAST-006)
keff sphere
mendf71x
2 / no of materials
1 94239 9.38001E-01 94240 4.79988E-02 94241 2.99996E-03 31069 6.53652E-03 31071 4.46355E-03 / Pu-alloy
2 92234 5.40778E-05 92235 7.10966E-03 92238 9.92836E-01 / Flattop natural U
15.53 19.00 / densities
2 / no of shells
 4.5332 24.142  / outer radii
  1      2       / material nos
 1          / index of coarse mesh to use for reaction rates
 0          / number of reaction-rate ratios

~
~
```

- Command line:

```
sn.master% ${SENSMG_DIR}/sensmg.py -i pmf006 -ngroup 618 -isn 128 -np 32 -srcacc_no for+adj
```

- Output is in text files.

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

- A standard SENSMG output

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

```
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
```

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

- A standard SENSMG output

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

```
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
```

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

- A standard SENSMG output

- Not the same as the relative sensitivity with respect to total cross section!
  - + SENSMG does not follow the MCNP convention
  - + In SENSMG, $S^g_{R,N_i} = S^g_{R,\nu_i} + S^g_{R,\sigma_{t,i}} + S^g_{R,\sigma_{s,i}}$
  - + In SENSMG, the total cross section can vary independently

```
Pu-Flattop (PU-MET-FAST-006)
relative sensitivities (%/%), first order

 keff sensitivities          keff=  0.99975768

 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
@
```

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

- 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:

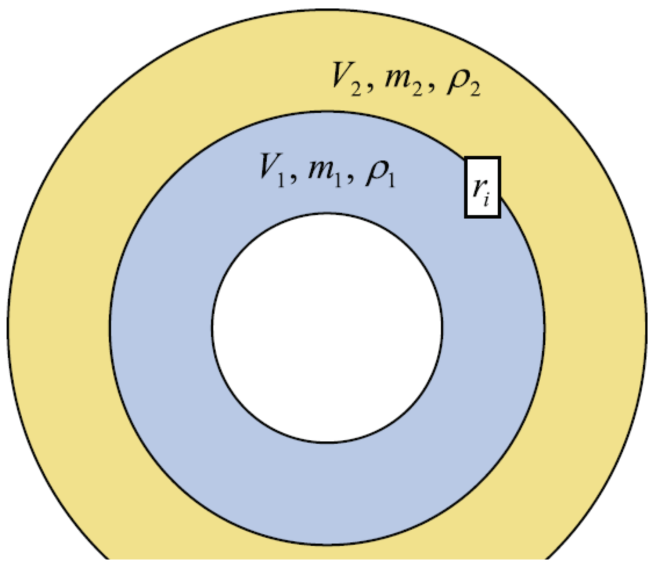
- For a sphere, the constant-mass derivative of k_{eff} with respect to interface location i is $\left(\frac{\partial k_{eff}}{\partial r_i}\right)_m = k_{eff} A_i \left(\frac{S_{k,\rho_{j+1}}}{V_{j+1}} - \frac{S_{k,\rho_j}}{V_j}\right) + \left(\frac{\partial k_{eff}}{\partial r_i}\right)_\rho$

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

Constant-Density Derivative o
to Material Interface Locations

Radial Index	Adjoint
1	1.95613E-01
2	8.82494E-04



Favorite, *Ann. Nucl. Energy*, **110** (2017).

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

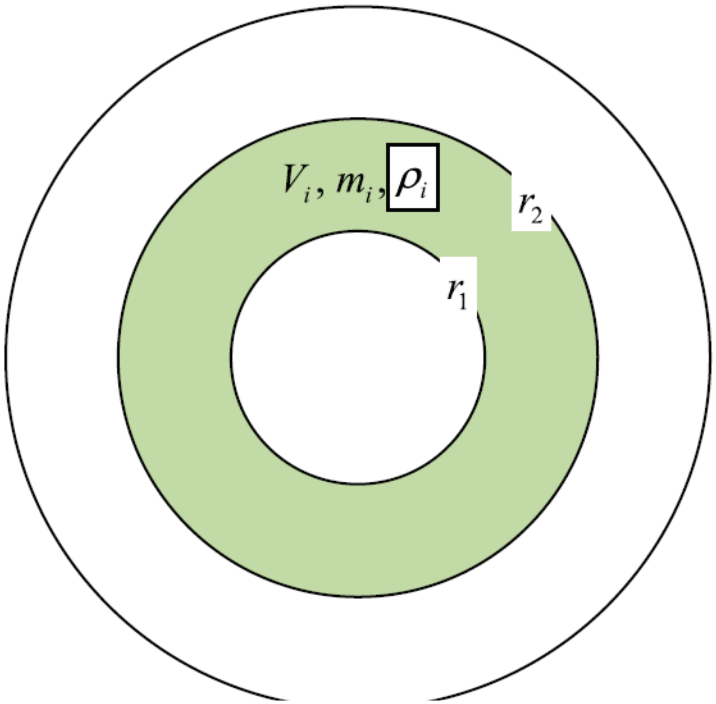
- For a sphere, the constant-mass derivative of k_{eff} with respect to the mass density of region i is $\left(\frac{\partial k_{eff}}{\partial \rho_i}\right)_m = \frac{V_i}{\rho_i} \frac{\left(\frac{\partial k_{eff}}{\partial r_j}\right)_m - \left(\frac{\partial k_{eff}}{\partial r_{j+1}}\right)_m}{A_j + A_{j+1}}$

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

Constant-Volume Relative Ser
Respect to Material Mass Dens

Material Index	Adjoint
1	6.78358E-01
2	2.29895E-01



Favorite, *Ann. Nucl. Energy*, **110** (2017).

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

- The full-normalization constrained sensitivity S_{k,w_j}^{FN} to the weight fraction of isotope *j* can be computed using the unconstrained isotopic density sensitivities output from SENSMG using

$$S_{k,w_j}^{FN} = \frac{w_I S_{k,N_j} - w_{j,0} S_{k,\rho}}{w_I}$$

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

Unconstrained Relative Sensitivity of Pu-Flattop k_{eff} with Respect to Isotopic Weight Fractions (%/%)

Isotope	Adjoint
Pu239	6.55282E-01
Pu240	1.99732E-02
Pu241	1.96701E-03
Ga69	6.50700E-04
Ga71	4.85655E-04
U234	2.73890E-05
U235	8.17756E-03
U238	2.21690E-01

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.

This work was funded by the United States National Nuclear Security Administration's Office of Defense Nuclear Nonproliferation Research & Development (NA-22).