Adjoint-Based Sensitivity and Uncertainty Analysis for Density and Composition: A User's Guide

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Motivation for this paper

- You are using MCNP or SCALE for benchmark modeling and uncertainty analysis.
- These codes have powerful adjoint-based sensitivity capabilities.
- *Are you using them?*

Acknowledgment

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Z. Perkó et al., "Ambiguities in the Sensitivity and Uncertainty Analysis of Reactor Physics Problems Involving Constrained Quantities," *Nucl. Sci. Eng.*, **180**, 345-377 (2015).

Why do we care about sensitivities?

- The uncertainty in variable k due to uncertainty in random variable x_1 is

$$u_k^2 = \left(\frac{\partial k}{\partial x_1} u_{x_1} \right)^2$$

- Define the *first-order sensitivity*

$$S_{k,x_1} \equiv \frac{x_{1,0}}{k_0} \frac{\partial k}{\partial x_1} \bigg|_{x_1 = x_{1,0}}$$

- The relative uncertainty in response k due to the relative uncertainty in random variable x_1 is

$$\left(\frac{u_k}{k_0} \right)^2 = S_{k,x_1}^2 \left(\frac{u_{x_1}}{x_{1,0}} \right)^2$$

- Other notation to be aware of:
  + Some papers define the derivative $\partial k / \partial x_1$ as the *absolute sensitivity* and our S_{k,x_1} as the *relative sensitivity*.

Density sensitivities

- The relative sensitivity of k to the atom density N_j of nuclide j (specified as an element or isotope) in a material is

$$S_{k,N_j} \equiv \frac{N_{j,0}}{k_0} \frac{\partial k}{\partial N_j}\bigg|_{N_j = N_{j,0}}$$

- We can write this in terms of the mass density ρ_j of nuclide j in a material as

$$S_{k,N_j} = \frac{N_{j,0}}{k_0} \frac{\partial k}{\partial \rho_j}\bigg|_{\rho_j = \rho_{j,0}} \frac{\partial \rho_j}{\partial N_j}\bigg|_{N_j = N_{j,0}}$$

$$= \frac{\rho_{j,0} N_A}{k_0 A_j} \frac{\partial k}{\partial \rho_j}\bigg|_{\rho_j = \rho_{j,0}} \frac{A_j}{N_A} = \frac{\rho_{j,0}}{k_0} \frac{\partial k}{\partial \rho_j}\bigg|_{\rho_j = \rho_{j,0}} \equiv S_{k,\rho_j},$$

Recall $N_j = \dfrac{\rho_j N_A}{A_j}$

or the sensitivity with respect to the atom density is equal to the sensitivity with respect to the mass density.

Equivalence of density sensitivities

- The total atom density N and the total mass density ρ of the material are $N = \sum_{j=1}^{J} N_j$ and $\rho = \sum_{j=1}^{J} \rho_j$, respectively (where J is the number of nuclides in the material).

- The sensitivities to individual atom or mass densities can be summed to obtain the sensitivity to the total atom or mass density:

$$S_{k,N} = \sum_{j=1}^{J} S_{k,N_j} = \sum_{j=1}^{J} S_{k,\rho_j} = S_{k,\rho}.$$

- The total macroscopic cross section Σ_t of a material is $\Sigma_t = \sum_{j=1}^{J} \Sigma_{t,j}$, where $\Sigma_{t,j} = N_j \sigma_{t,j}$ and $\sigma_{t,j}$ is the microscopic total cross section of nuclide j.

- Therefore

$$S_{k,\Sigma_t} = \sum_{j=1}^{J} S_{k,\Sigma_{t,j}} = S_{k,\rho} = S_{k,N}.$$

- Second- and higher-order sensitivities are not additive.

Equivalence of weight fraction and density sensitivities

- Consider the sensitivity S_{k,w_j} of k to the weight fraction of nuclide j, $w_j \equiv \rho_j / \rho$:

$$S_{k,w_j} \equiv \frac{w_{j,0}}{k_0} \left.\frac{\partial k}{\partial w_j}\right|_{w_j = w_{j,0}} = \frac{w_{j,0}}{k_0} \left.\frac{\partial k}{\partial \rho_j}\right|_{\rho_j = \rho_{j,0}} \left.\frac{\partial \rho_j}{\partial w_j}\right|_{w_j = w_{j,0}}$$

$$= \frac{\rho_{j,0}}{k_0 \rho_0} \left.\frac{\partial k}{\partial \rho_j}\right|_{w_j = w_{j,0}} \rho_0 = \frac{\rho_{j,0}}{k_0} \left.\frac{\partial k}{\partial \rho_j}\right|_{\rho_j = \rho_{j,0}} = S_{k,\rho_j},$$

demonstrating that the sensitivity to the weight fraction of nuclide j is also equal to the sensitivity to the mass density of nuclide j, i.e.,

$$S_{k,N_j} = S_{k,\rho_j} = S_{k,w_j}.$$

- Although the weight fractions are constrained, the sensitivity S_{k,w_j} is unconstrained!

How to compute density sensitivities: MCNP 6.1.1

- Uses iterated fission probability.
- Automatically calculates sensitivity coefficients for all nuclides.

```
KOPTS   blocksize = 5
KSENn   xs   cell = c1 c2 ... MT=-1
```

(• Sensitivities by cell are new in MCNP 6.1.1.)

- Energy bins can be specified.
- MCNP treats an $S(\alpha,\beta)$ table as a separate nuclide.
  + Using `MT=-1` on the `KSEN` card causes the $S(\alpha,\beta)$ contribution to be added to the total reaction sensitivity for the associated nuclide.
  + For isotopes and materials with no $S(\alpha,\beta)$ component, using `MT=-1` will give the same result as `MT=1` (or no specified reaction).
- Brian Kiedrowski's experience has been that a blocksize of 5 is almost always adequate and more efficient than the default of 10.

How to compute density sensitivities: SCALE 6.2

- Uses the TSUNAMI-3D sequence.
- Automatically calculates energy-dependent sensitivity coefficients for all materials, nuclides, and reactions in a system.
- Automatically accounts for any $S(\alpha,\beta)$ effects present for materials in the model.
- User chooses iterated fission probability (`cet=2`) or CLUTCH (`cet=1`).
- Example of TSUNAMI-3D input cards for CLUTCH:

```
read parameter
cet=1  cfp=10  cgd=2
...
read gridGeometry 2
    title="Mesh for CLUTCH calc."
    xLinear  60.  -60.  60.
    yLinear  60.  -60.  60.
    zLinear 120. -120. 120.
end gridGeometry
```

`cfp` is the number of latent generations; it is MCNP's blocksize plus 2.

How to compute density sensitivities: Central difference

- You can always use a central difference:

$$S_{k,N_j} \approx \frac{N_{j,0}}{k_0}\left(\frac{k(N_{j,+})-k(N_{j,-})}{N_{j,+}-N_{j,-}}\right)$$

$$= \frac{N_{j,0}}{k_0}\left(\frac{k(N_{j,0}+\Delta N_j)-k(N_{j,0}-\Delta N_j)}{2\Delta N_j}\right),$$

where $N_{j,\pm} = N_{j,0} \pm \Delta N_j$.

- It is important to choose the perturbation ΔN_j carefully!
  - + Small enough that the points $k(N_{j,-})$, $k(N_{j,0})$, and $k(N_{j,+})$ lie approximately on the $\left(\partial k/\partial N_j\right)\big|_{N_j=N_{j,0}}$ tangent line.
  - + Large enough that the difference $k(N_{j,+})-k(N_{j,-})$ can be calculated accurately, and, if a Monte Carlo code is used, with a small uncertainty.

- This method estimates the same S_{k,N_j} that the adjoint methods do.
  - + Therefore, there is no reason to do it!

Using the sensitivities: Mass density

- Recall $S_{k,\rho} = \sum_{j=1}^{J} S_{k,N_j}$.

- The relative uncertainty in k is

$$\left(\frac{u_k}{k_0}\right)^2 = \frac{1}{k_0^2}\left(\frac{\partial k}{\partial \rho} u_\rho\right)^2 = S_{k,\rho}^2 \left(\frac{u_\rho}{\rho_0}\right)^2,$$

not accounting for correlations among mass, density, and volume.

- If the part mass and density are measured independently and have independent uncertainties, the relative uncertainty in k that considers constraints among mass, density, and volume by adjusting the part volume is

$$\left(\frac{u_k}{k_0}\right)^2 = \left[\frac{V_0}{k_0}\left(\frac{\partial k}{\partial V}\right)\right]^2 \left(\frac{u_m}{m_0}\right)^2 + \left[S_{k,\rho} - \frac{V_0}{k_0}\left(\frac{\partial k}{\partial V}\right)\right]^2 \left(\frac{u_\rho}{\rho_0}\right)^2$$

- The derivative of k with respect to volume is

$$\frac{\partial k}{\partial V} = \sum_{n=1}^{N}\left(\frac{\partial k}{\partial r_n}\right) \Big/ \sum_{n=1}^{N}\left(\frac{\partial V}{\partial r_n}\right)$$

Using the sensitivities: Trace elements or impurities specified by range

- Subscript *r* represents the "range" element and *b* represents the "balance" element.

- This equation can be derived in several ways, but the most straightforward is Perkó's control parameter adjustment:

$$S_{k,w_r}^{CPA} = S_{k,w_r} - \frac{w_{r,0}}{w_{b,0}} S_{k,w_b}$$

- The relative uncertainty is due to the uncertainty in the weight fraction of nuclide *r* is

$$\left(\frac{u_k}{k_0}\right)^2 = \left(S_{k,w_r}^{CPA}\right)^2 \left(\frac{u_{w_r}}{w_{r,0}}\right)^2 = \left(\frac{1}{w_{r,0}} S_{k,N_r} - \frac{1}{w_{b,0}} S_{k,N_b}\right)^2 u_{w_r}^2$$

- Note that u_{w_r} is the absolute uncertainty and u_{w_r} / w_r is the relative uncertainty.

Using the sensitivities: Part isotopics

- *Isotopics* refers to the composition of the major constituent of a part, typically the fuel.

- If there are I isotopes comprising the constituent of interest, then $w_F \equiv \sum_{i=1}^{I} w_i$ is the total weight fraction of the constituent of interest in the material.

- Assume that the mass density of the material is unchanged when the composition is perturbed.

- If the rest of the nuclides' weight fractions are renormalized to maintain the constraint when nuclide i is perturbed, the constrained sensitivity of nuclide i is

$$S^{PN}_{k,w_i} = \frac{w_{F,0} S_{k,N_i} - w_{i,0} S_{k,N_F}}{w_{F,0} - w_{i,0}} \qquad \text{(Partial Normalization)}$$

- If *all* of the nuclides' weight fractions are renormalized to maintain the constraint when nuclide i is perturbed, the constrained sensitivity of nuclide i is

$$S^{FN}_{k,w_b} = \frac{S_{k,N_b} - w_{b,0} S_{k,N}}{1 - w_{b,0}} \qquad \text{(Full Normalization)}$$

- The relative uncertainty due to the uncertainty in the weight fraction of nuclide i is

$$\left(\frac{u_k}{k_0}\right)^2 = \left(S^C_{k,w_i} \frac{u_{w_i}}{w_{i,0}}\right)^2$$

Using the sensitivities: Balance element specified by range

- If the weight fraction of the balance element is perturbed and the other weight fractions are renormalized, the constrained sensitivity is

$$S_{k,w_b}^{PN} = \frac{S_{k,N_b} - w_{b,0} S_{k,N}}{1 - w_{b,0}} \qquad \text{(Partial Normalization)}$$

- If the weight fraction of the balance element is perturbed and *all* the weight fractions are renormalized, the constrained sensitivity is

$$S_{k,w_b}^{FN} = S_{k,N_b} - w_{b,0} S_{k,N} \qquad \text{(Full Normalization)}$$

- The relative uncertainty due to the uncertainty in the weight fraction of nuclide b is

$$\left(\frac{u_k}{k_0}\right)^2 = \left(S_{k,w_b}^{C} \frac{u_{w_b}}{w_{b,0}}\right)^2$$

Using the sensitivities: Full or partial normalization?

- Perkó showed that partial normalization may give erroneous results for uncertainties when the covariances among the measured weight fractions are known precisely and therefore the covariance matrix is properly normalized.

- However, in most cases, the difficulty is that the covariances are *not* known, and the covariance matrix is *not* properly normalized.

- In such cases, it is impossible to know which constrained sensitivities need to be used.

- You should compute uncertainties using partial *and* full normalization. Then pick one.

Sample problem: TREAT fuel

- A bare, homogeneous cylindrical reactor consisting of fuel similar to that used in the Transient Reactor Test Facility (TREAT) at Idaho National Laboratory.
- Height and radius are 240 cm and 60 cm, respectively.

There is a whole session on TREAT Thursday morning.

- The atom density and the mass density of the fuel are 0.113705 atoms/b·cm and 2.27 g/cm^3, respectively.
- Composition of the fuel:

Nuclide	Atom Density (atoms/b·cm)	Weight Fraction
^{1}H	1.13694E–4	8.38215E–5
^{10}B	5.68468E–7	4.16390E–6
C (nat.)	1.13579E–1	9.97955E–1
^{235}U	1.05735E–5	1.81803E–3
^{238}U	7.95855E–7	1.38591E–4

- In MCNP, the $S(\alpha,\beta)$ table grph.20t was associated with the fuel.
- In SCALE, the cross section table for carbon in graphite was associated with natural carbon, and the sensitivities were calculated using the CLUTCH method.

	k_{eff}
MCNP	0.99347 ± 0.00002
SCALE	0.99439 ± 0.00004

Sample problem results

- Sensitivity to constituents (S_{k,N_j}):

  + Completely different Monte Carlo codes, different cross section data processing tools, and slightly different cross section data were able to produce sensitivity coefficients that agree well!
  + Within ~3σ and within ~1% (except for C, where the difference is 2.8%).

Nuclide	MCNP	SCALE
^{1}H	4.0059E–3 ± 4.37%	4.0194E–3 ± 1.63%
^{10}B	–2.0248E–1 ± 0.02%	–2.0235E–1 ± 0.00%
C (nat.)	5.9836E–1 ± 0.46%(a)	5.8209E–1 ± 1.58%
^{235}U	3.5071E–1 ± 0.04%	3.5032E–1 ± 0.01%
^{238}U	–2.5392E–3 ± 0.50%	–2.5494E–3 ± 0.14%
$S(\alpha,\beta)$	2.3217E–1 ± 0.82%	N/A(b)

(a) Includes the $S(\alpha,\beta)$ sensitivity.
(b) Not applicable—$S(\alpha,\beta)$ scattering is not calculated separately in SCALE.

- Sensitivities to fuel density and nonfissionable composition:

S	Adjoint(a)	Central Difference(b)
$S_{k,\rho}$	7.4806E–1 ± 0.37%	7.5193E–1 ± 0.38%
S^{CPA}_{k,w_H}	3.9556E–3 ± 4.43%	4.0767E–3 ± 0.70%
S^{CPA}_{k,w_B}	–2.0248E–1 ± 0.02%	–2.0457E–1 ± 0.01%
S^{PN}_{k,w_C}	2.2517E+3 ± 1.96%	2.2503E+3 ± 0.06%
S^{FN}_{k,w_C}	1.9851E–1 ± 1.96%	1.9860E–1 ± 0.14%

(a) Using MCNP results.
(b) Using MCNP; this is a constrained central difference.

+ Adjoint uncertainties are estimated.

+ Note the large difference between partial and full normalization.

Summary and Conclusions

- We want you to perform more efficient sensitivity analyses for material compositions!
  - + Use adjoint methods to compute nuclide density sensitivities.
  - + Combine those appropriately to compute constrained weight fraction sensitivities.

- We have a forthcoming paper (with Zoltán Perkó) in *Nuclear Science and Engineering* (scheduled for February).

- For more on these issues, see

  Z. Perkó et al., "Ambiguities in the Sensitivity and Uncertainty Analysis of Reactor Physics Problems Involving Constrained Quantities," *Nucl. Sci. Eng.*, **180**, 345-377 (2015).