LA-UR-17-23453
Approved for public release; distribution is unlimited.

Title: (U) Analytic First and Second Derivatives of the Uncollided Leakage for a Homogeneous Sphere

Author(s): Favorite, Jeffrey A.

Intended for: Report

Issued: 2017-04-26

Los Alamos
NATIONAL LABORATORY

memorandum

X-Computational Physics Division
Monte Carlo Codes, Methods, and Applications Group

Group XCP-3, MS F663
Los Alamos, New Mexico 87545
505/667-1920

To/MS: Distribution
From/MS: Jeffrey A. Favorite / XCP-3, MS F663
Phone/Email: 7-7941 / fave@lanl.gov
Symbol: XCP-3:17–030(U) (LA–UR–17–?????)
Date: April 25, 2017

SUBJECT: (U) Analytic First and Second Derivatives of the Uncollided Leakage for a Homogeneous Sphere

I. Introduction

The second-order adjoint sensitivity analysis methodology (2nd-ASAM), developed by Cacuci,[1] has been applied by Cacuci[2] to derive second derivatives of a response with respect to input parameters for uncollided particles in an inhomogeneous transport problem. In this memo, we present an analytic benchmark for verifying the derivatives of the 2nd-ASAM. The problem is a homogeneous sphere, and the response is the uncollided total leakage.[3,4] This memo does not repeat the formulas given in Ref. 2. We are preparing a journal article that will include the derivation of Ref. 2 and the benchmark of this memo.

The forward and adjoint transport equations required by the 2nd-ASAM, called the 1st- and 2nd-level adjoint sensitivity system (1st- and 2nd-LASS), have been solved using the PARTISN multigroup discrete-ordinates code.[5] In this paper, the PARTISN results are compared with the analytic results.

In Sec. II, the benchmark problem is presented and the various derivatives, up to second order, are derived analytically. In Sec. III, the problem is specified with quantified parameters, numerical results are given, and results from the PARTISN implementation are compared with the analytic results. A summary and discussion of future work is in Sec. IV.

II. Problem Setup and Derivatives

Consider a homogeneous sphere of radius a. The material consists of two isotopes with number densities N_1 and N_2. The microscopic cross sections for the two isotopes are σ_1 and σ_2. Isotope 1 is a decay gamma-ray source; the line emission rate (per atom of isotope 1) is q_1. Isotope 2 may emit gamma rays, but not in the same line as isotope 1; q_2 is zero. Gamma rays are emitted isotropically.

The macroscopic cross section Σ of the material is

$$\Sigma = \sigma_1 N_1 + \sigma_2 N_2 . \tag{1}$$

The line source rate density q is

$$q = q_1 N_1. \tag{2}$$

The isotopic number densities are related to the material mass density ρ via

$$N_i = \frac{\rho\, w_i N_A}{A_i}, \quad i = 1,2, \tag{3}$$

where w_i and A_i are the weight fraction and atomic weight of isotope i and N_A is Avogadro's number. The weight fractions satisfy the normalization $w_1 + w_2 = 1$. Whenever the mass density is perturbed in this problem, both number densities are perturbed, according to Eq. (3). Weight fraction perturbations are not considered in this problem.

The uncollided escape probability P is[3]

$$P = \frac{3}{8(\Sigma a)^3}\left[2(\Sigma a)^2 - 1 + (1 + 2\Sigma a)e^{-2\Sigma a}\right]. \tag{4}$$

The uncollided leakage from the sphere is the escape probability multiplied by the total source rate.[4] The total source rate Q is the source rate density q of Eq. (2) multiplied by the volume of the sphere, V:

$$Q = qV = q_1 N_1 V. \tag{5}$$

The uncollided leakage L is

$$L = QP. \tag{6}$$

We will need derivatives of P with respect to Σ. The first derivative is

$$\begin{aligned} \frac{\partial P}{\partial \Sigma} &= \frac{3(-3)}{8(\Sigma a)^3 \Sigma}\left[2(\Sigma a)^2 - 1 + (1 + 2\Sigma a)e^{-2\Sigma a}\right] + \frac{3}{8(\Sigma a)^3}\left[4\Sigma a^2 + 2ae^{-2\Sigma a} - 2a(1 + 2\Sigma a)e^{-2\Sigma a}\right] \\ &= -\frac{3}{\Sigma}\left\{P - \frac{1}{2\Sigma a}\left(1 - e^{-2\Sigma a}\right)\right\}. \end{aligned} \tag{7}$$

The second derivative of P with respect to Σ is

$$\begin{aligned} \frac{\partial^2 P}{\partial \Sigma^2} &= \frac{3}{\Sigma^2}P - \frac{3}{\Sigma}\frac{\partial P}{\partial \Sigma} - \frac{3}{\Sigma^3 a}\left(1 - e^{-2\Sigma a}\right) + \frac{3}{\Sigma^2}e^{-2\Sigma a} \\ &= \frac{3}{\Sigma^2}P - \frac{3}{\Sigma}\frac{\partial P}{\partial \Sigma} - \frac{3}{\Sigma^3 a}\left(1 - e^{-2\Sigma a} - \Sigma a e^{-2\Sigma a}\right) \\ &= \frac{3}{\Sigma^2}\left\{P - \Sigma\frac{\partial P}{\partial \Sigma} - \frac{1}{\Sigma a}\left[1 - \left(1 + \Sigma a\right)e^{-2\Sigma a}\right]\right\}. \end{aligned} \tag{8}$$

II.A. Derivatives with Respect to Atom Densities

The first derivative of the leakage with respect to N_1 is

$$\begin{aligned} \frac{\partial L}{\partial N_1} &= \frac{\partial Q}{\partial N_1}P + Q\frac{\partial P}{\partial N_1} \\ &= q_1 V P + Q\frac{\partial P}{\partial \Sigma}\frac{\partial \Sigma}{\partial N_1} \\ &= q_1 V P + Q\sigma_1\frac{\partial P}{\partial \Sigma}. \end{aligned} \tag{9}$$

The first derivative of the leakage with respect to N_2 is

$$\begin{aligned}\frac{\partial L}{\partial N_2} &= \frac{\partial Q}{\partial N_2} P + Q \frac{\partial P}{\partial N_2} \\ &= Q \frac{\partial P}{\partial \Sigma} \frac{\partial \Sigma}{\partial N_2} \\ &= Q \sigma_2 \frac{\partial P}{\partial \Sigma}. \end{aligned} \tag{10}$$

The second derivative of the leakage with respect to N_1 is

$$\begin{aligned}\frac{\partial^2 L}{\partial N_1^2} &= q_1 V \frac{\partial P}{\partial N_1} + \frac{\partial Q}{\partial N_1} \sigma_1 \frac{\partial P}{\partial \Sigma} + Q \sigma_1 \frac{\partial}{\partial N_1}\left(\frac{\partial P}{\partial \Sigma}\right) \\ &= q_1 V \frac{\partial P}{\partial \Sigma} \frac{\partial \Sigma}{\partial N_1} + q_1 V \sigma_1 \frac{\partial P}{\partial \Sigma} + Q \sigma_1 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right) \frac{\partial \Sigma}{\partial N_1} \\ &= 2 q_1 V \sigma_1 \frac{\partial P}{\partial \Sigma} + Q \sigma_1^2 \frac{\partial^2 P}{\partial \Sigma^2}. \end{aligned} \tag{11}$$

The second derivative of the leakage with respect to N_2 is

$$\begin{aligned}\frac{\partial^2 L}{\partial N_2^2} &= \frac{\partial Q}{\partial N_2} \sigma_2 \frac{\partial P}{\partial \Sigma} + Q \sigma_2 \frac{\partial}{\partial N_2}\left(\frac{\partial P}{\partial \Sigma}\right) \\ &= Q \sigma_2 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right) \frac{\partial \Sigma}{\partial N_2} \\ &= Q \sigma_2^2 \frac{\partial^2 P}{\partial \Sigma^2}. \end{aligned} \tag{12}$$

The mixed partial derivative of the leakage with respect to N_1 and N_2, by differentiating Eq. (10) with respect to N_1, is

$$\begin{aligned}\frac{\partial^2 L}{\partial N_1 \partial N_2} &= \frac{\partial Q}{\partial N_1} \sigma_2 \frac{\partial P}{\partial \Sigma} + Q \sigma_2 \frac{\partial}{\partial N_1}\left(\frac{\partial P}{\partial \Sigma}\right) \\ &= q_1 V \sigma_2 \frac{\partial P}{\partial \Sigma} + Q \sigma_2 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right) \frac{\partial \Sigma}{\partial N_1} \\ &= q_1 V \sigma_2 \frac{\partial P}{\partial \Sigma} + Q \sigma_1 \sigma_2 \frac{\partial^2 P}{\partial \Sigma^2}. \end{aligned} \tag{13}$$

Differentiating Eq. (9) with respect to N_2 also gives Eq. (13).

The density derivatives here and everywhere in this paper are constant-volume partial derivatives.[6]

II.B. Derivatives with Respect to Cross Sections

The first derivative of the leakage with respect to σ_1 is

$$\frac{\partial L}{\partial \sigma_1} = \frac{\partial Q}{\partial \sigma_1} P + Q \frac{\partial P}{\partial \sigma_1}$$
$$= Q \frac{\partial P}{\partial \Sigma} \frac{\partial \Sigma}{\partial \sigma_1}$$
$$= Q N_1 \frac{\partial P}{\partial \Sigma}. \tag{14}$$

The first derivative of the leakage with respect to σ_2 is

$$\frac{\partial L}{\partial \sigma_2} = \frac{\partial Q}{\partial \sigma_2} P + Q \frac{\partial P}{\partial \sigma_2}$$
$$= Q \frac{\partial P}{\partial \Sigma} \frac{\partial \Sigma}{\partial \sigma_2}$$
$$= Q N_2 \frac{\partial P}{\partial \Sigma}. \tag{15}$$

The second derivative of the leakage with respect to σ_1 is

$$\frac{\partial^2 L}{\partial \sigma_1^2} = \frac{\partial Q}{\partial \sigma_1} N_1 \frac{\partial P}{\partial \Sigma} + Q N_1 \frac{\partial}{\partial \sigma_1}\left(\frac{\partial P}{\partial \Sigma}\right)$$
$$= Q N_1 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right) \frac{\partial \Sigma}{\partial \sigma_1}$$
$$= Q N_1^2 \frac{\partial^2 P}{\partial \Sigma^2}. \tag{16}$$

The second derivative of the leakage with respect to σ_2 is

$$\frac{\partial^2 L}{\partial \sigma_2^2} = \frac{\partial Q}{\partial \sigma_2} N_2 \frac{\partial P}{\partial \Sigma} + Q N_2 \frac{\partial}{\partial \sigma_2}\left(\frac{\partial P}{\partial \Sigma}\right)$$
$$= Q N_2 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right) \frac{\partial \Sigma}{\partial \sigma_2}$$
$$= Q N_2^2 \frac{\partial^2 P}{\partial \Sigma^2}. \tag{17}$$

The mixed partial derivative of the leakage with respect to σ_1 and σ_2, by differentiating Eq. (15) with respect to σ_1, is

$$\frac{\partial^2 L}{\partial \sigma_1 \partial \sigma_2} = \frac{\partial Q}{\partial \sigma_1} N_2 \frac{\partial P}{\partial \Sigma} + Q N_2 \frac{\partial}{\partial \sigma_1}\left(\frac{\partial P}{\partial \Sigma}\right)$$
$$= Q N_2 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right) \frac{\partial \Sigma}{\partial \sigma_1}$$
$$= Q N_1 N_2 \frac{\partial^2 P}{\partial \Sigma^2}. \tag{18}$$

Differentiating Eq. (14) with respect to σ_2 also gives Eq. (18).

II.C. Derivatives with Respect to Source Emission Rates

The first derivative of the leakage with respect to q_1 is

$$\begin{aligned}\frac{\partial L}{\partial q_1} &= \frac{\partial Q}{\partial q_1} P + Q \frac{\partial P}{\partial q_1} \\ &= N_1 V P.\end{aligned} \tag{19}$$

The first derivative of the leakage with respect to q_2 is 0.

The second derivative of the leakage with respect to q_1 is

$$\frac{\partial^2 L}{\partial q_1^2} = N_1 V \frac{\partial P}{\partial q_1} = 0. \tag{20}$$

The second derivative of the leakage with respect to q_2 is 0.

The mixed partial derivative of the leakage with respect to q_1 and q_2 is zero.

II.D. Derivatives with Respect to Material Mass Density

The material mass density ρ is also a quantity of interest. Using Eq. (3) in Eqs. (1) and (5), the cross section and total source rate can be written

$$\Sigma = \frac{\rho}{\rho_0} \Sigma_0 \tag{21}$$

and

$$Q = \frac{\rho}{\rho_0} Q_0, \tag{22}$$

respectively, where subscript 0 represents the initial, unperturbed configuration.

The first derivative of the leakage with respect to ρ is

$$\begin{aligned}\frac{\partial L}{\partial \rho} &= \frac{\partial Q}{\partial \rho} P + Q \frac{\partial P}{\partial \rho} \\ &= \frac{\partial Q}{\partial \rho} P + Q \frac{\partial P}{\partial \Sigma} \frac{\partial \Sigma}{\partial \rho}.\end{aligned} \tag{23}$$

Using Eqs. (21) and (22) yields

$$\frac{\partial L}{\partial \rho} = \frac{Q_0}{\rho_0} P + Q \frac{\Sigma_0}{\rho_0} \frac{\partial P}{\partial \Sigma}. \tag{24}$$

Rearranging Eqs. (21) and (22), Eq. (24) can be written in the notation of the rest of this paper:

$$\frac{\partial L}{\partial \rho} = \frac{Q}{\rho} \left(P + \Sigma \frac{\partial P}{\partial \Sigma} \right). \tag{25}$$

From Eq. (24), the second derivative of the leakage with respect to ρ is

$$
\begin{aligned}
\frac{\partial^2 L}{\partial \rho^2} &= \frac{Q_0}{\rho_0}\frac{\partial P}{\partial \rho} + \frac{\partial Q}{\partial \rho}\frac{\Sigma_0}{\rho_0}\frac{\partial P}{\partial \Sigma} + Q\frac{\Sigma_0}{\rho_0}\frac{\partial}{\partial \rho}\left(\frac{\partial P}{\partial \Sigma}\right) \\
&= \frac{Q_0}{\rho_0}\frac{\partial P}{\partial \Sigma}\frac{\partial \Sigma}{\partial \rho} + \frac{\partial Q}{\partial \rho}\frac{\Sigma_0}{\rho_0}\frac{\partial P}{\partial \Sigma} + Q\frac{\Sigma_0}{\rho_0}\frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right)\frac{\partial \Sigma}{\partial \rho} \\
&= 2\frac{Q_0}{\rho_0}\frac{\Sigma_0}{\rho_0}\frac{\partial P}{\partial \Sigma} + Q\left(\frac{\Sigma_0}{\rho_0}\right)^2\frac{\partial^2 P}{\partial \Sigma^2}.
\end{aligned}
\tag{26}
$$

Again rearranging Eqs. (21) and (22), Eq. (26) can be written in the notation of the rest of this paper:

$$
\begin{aligned}
\frac{\partial^2 L}{\partial \rho^2} &= 2\frac{Q}{\rho}\frac{\Sigma}{\rho}\frac{\partial P}{\partial \Sigma} + Q\left(\frac{\Sigma}{\rho}\right)^2\frac{\partial^2 P}{\partial \Sigma^2} \\
&= \frac{Q}{\rho^2}\left(2\Sigma\frac{\partial P}{\partial \Sigma} + \Sigma^2\frac{\partial^2 P}{\partial \Sigma^2}\right).
\end{aligned}
\tag{27}
$$

These density derivatives are constant-volume partial derivatives.[6]

II.E. Mixed Derivatives: Atom Densities and Cross Sections

The mixed partial derivative of the leakage with respect to N_1 and σ_1, by differentiating Eq. (14) with respect to N_1, is

$$
\begin{aligned}
\frac{\partial^2 L}{\partial N_1 \partial \sigma_1} &= \frac{\partial Q}{\partial N_1}N_1\frac{\partial P}{\partial \Sigma} + Q\frac{\partial P}{\partial \Sigma} + QN_1\frac{\partial}{\partial N_1}\left(\frac{\partial P}{\partial \Sigma}\right) \\
&= q_1VN_1\frac{\partial P}{\partial \Sigma} + Q\frac{\partial P}{\partial \Sigma} + QN_1\frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right)\frac{\partial \Sigma}{\partial N_1} \\
&= 2Q\frac{\partial P}{\partial \Sigma} + QN_1\sigma_1\frac{\partial^2 P}{\partial \Sigma^2}.
\end{aligned}
\tag{28}
$$

The mixed partial derivative of the leakage with respect to N_1 and σ_2, by differentiating Eq. (15) with respect to N_1, is

$$
\begin{aligned}
\frac{\partial^2 L}{\partial N_1 \partial \sigma_2} &= \frac{\partial Q}{\partial N_1}N_2\frac{\partial P}{\partial \Sigma} + QN_2\frac{\partial}{\partial N_1}\left(\frac{\partial P}{\partial \Sigma}\right) \\
&= q_1VN_2\frac{\partial P}{\partial \Sigma} + QN_2\frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right)\frac{\partial \Sigma}{\partial N_1} \\
&= q_1VN_2\frac{\partial P}{\partial \Sigma} + QN_2\sigma_1\frac{\partial^2 P}{\partial \Sigma^2}.
\end{aligned}
\tag{29}
$$

Differentiating Eq. (9) with respect to σ_1 and (separately) σ_2 also gives Eqs. (28) and (29).

The mixed partial derivative of the leakage with respect to N_2 and σ_1, by differentiating Eq. (14) with respect to N_2, is

$$\begin{aligned}\frac{\partial^2 L}{\partial N_2 \partial \sigma_1} &= \frac{\partial Q}{\partial N_2} N_1 \frac{\partial P}{\partial \Sigma} + Q N_1 \frac{\partial}{\partial N_2}\left(\frac{\partial P}{\partial \Sigma}\right) \\ &= Q N_1 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right)\frac{\partial \Sigma}{\partial N_2} \\ &= Q N_1 \sigma_2 \frac{\partial^2 P}{\partial \Sigma^2}. \end{aligned} \tag{30}$$

The mixed partial derivative of the leakage with respect to N_2 and σ_2, by differentiating Eq. (15) with respect to N_2, is

$$\begin{aligned}\frac{\partial^2 L}{\partial N_2 \partial \sigma_2} &= \frac{\partial Q}{\partial N_2} N_2 \frac{\partial P}{\partial \Sigma} + Q \frac{\partial P}{\partial \Sigma} + Q N_2 \frac{\partial}{\partial N_2}\left(\frac{\partial P}{\partial \Sigma}\right) \\ &= Q \frac{\partial P}{\partial \Sigma} + Q N_2 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right)\frac{\partial \Sigma}{\partial N_2} \\ &= Q \frac{\partial P}{\partial \Sigma} + Q N_2 \sigma_2 \frac{\partial^2 P}{\partial \Sigma^2}. \end{aligned} \tag{31}$$

Differentiating Eq. (10) with respect to σ_1 and (separately) σ_2 also gives Eqs. (30) and (31).

These density derivatives are constant-volume partial derivatives.[6]

II.F. Mixed Derivatives: Atom Densities and Source Emission Rates

The mixed partial derivative of the leakage with respect to N_1 and q_1, by differentiating Eq. (19) with respect to N_1, is

$$\begin{aligned}\frac{\partial^2 L}{\partial N_1 \partial q_1} &= VP + N_1 V \frac{\partial P}{\partial N_1} \\ &= VP + N_1 V \frac{\partial P}{\partial \Sigma}\frac{\partial \Sigma}{\partial N_1} \\ &= VP + N_1 V \sigma_1 \frac{\partial P}{\partial \Sigma}. \end{aligned} \tag{32}$$

The mixed partial derivative of the leakage with respect to N_1 and q_2 is zero. Differentiating Eq. (9) with respect to q_1 also gives Eq. (32).

The mixed partial derivative of the leakage with respect to N_2 and q_1, by differentiating Eq. (19) with respect to N_2, is

$$\begin{aligned}\frac{\partial^2 L}{\partial N_2 \partial q_1} &= N_1 V \frac{\partial P}{\partial N_2} \\ &= N_1 V \frac{\partial P}{\partial \Sigma}\frac{\partial \Sigma}{\partial N_2} \\ &= N_1 V \sigma_2 \frac{\partial P}{\partial \Sigma}. \end{aligned} \tag{33}$$

The mixed partial derivative of the leakage with respect to N_2 and q_2 is zero. Differentiating Eq. (10) with respect to q_1 also gives Eq. (33).

These density derivatives are constant-volume partial derivatives.[6]

II.G. Mixed Derivatives: Cross Sections and Source Emission Rates

The mixed partial derivative of the leakage with respect to σ_1 and q_1, by differentiating Eq. (19) with respect to σ_1, is

$$\begin{aligned}\frac{\partial^2 L}{\partial\sigma_1\partial q_1} &= N_1 V \frac{\partial P}{\partial\sigma_1} \\ &= N_1 V \frac{\partial P}{\partial\Sigma}\frac{\partial\Sigma}{\partial\sigma_1} \\ &= N_1^2 V \frac{\partial P}{\partial\Sigma}. \end{aligned} \tag{34}$$

The mixed partial derivative of the leakage with respect to σ_1 and q_2 is zero. Differentiating Eq. (14) with respect to q_1 also gives Eq. (34).

The mixed partial derivative of the leakage with respect to σ_2 and q_1, by differentiating Eq. (19) with respect to σ_2, is

$$\begin{aligned}\frac{\partial^2 L}{\partial\sigma_2\partial q_1} &= N_1 V \frac{\partial P}{\partial\sigma_2} \\ &= N_1 V \frac{\partial P}{\partial\Sigma}\frac{\partial\Sigma}{\partial\sigma_2} \\ &= N_1 N_2 V \frac{\partial P}{\partial\Sigma}. \end{aligned} \tag{35}$$

The mixed partial derivative of the leakage with respect to σ_2 and q_2 is zero. Differentiating Eq. (15) with respect to q_1 also gives Eq. (35).

II.H. Mixed Derivatives: Atom Densities and Material Density

The mixed partial derivative of the leakage with respect to N_1 and ρ, by differentiating Eq. (9) with respect to ρ, is

$$\begin{aligned}\frac{\partial^2 L}{\partial\rho\partial N_1} &= q_1 V \frac{\partial P}{\partial\rho} + \frac{\partial Q}{\partial\rho}\sigma_1\frac{\partial P}{\partial\Sigma} + Q\sigma_1\frac{\partial}{\partial\rho}\left(\frac{\partial P}{\partial\Sigma}\right) \\ &= q_1 V \frac{\partial P}{\partial\Sigma}\frac{\partial\Sigma}{\partial\rho} + \frac{Q_0}{\rho_0}\sigma_1\frac{\partial P}{\partial\Sigma} + Q\sigma_1\frac{\partial}{\partial\Sigma}\left(\frac{\partial P}{\partial\Sigma}\right)\frac{\partial\Sigma}{\partial\rho} \\ &= \left(q_1 V\frac{\Sigma}{\rho} + \frac{Q}{\rho}\sigma_1\right)\frac{\partial P}{\partial\Sigma} + Q\sigma_1\frac{\Sigma}{\rho}\frac{\partial^2 P}{\partial\Sigma^2}. \end{aligned} \tag{36}$$

The mixed partial derivative of the leakage with respect to N_2 and ρ, by differentiating Eq. (10) with respect to ρ, is

$$\frac{\partial^2 L}{\partial \rho \partial N_2} = \frac{\partial Q}{\partial \rho}\sigma_2 \frac{\partial P}{\partial \Sigma} + Q\sigma_2 \frac{\partial}{\partial \rho}\left(\frac{\partial P}{\partial \Sigma}\right)$$
$$= \frac{Q_0}{\rho_0}\sigma_2 \frac{\partial P}{\partial \Sigma} + Q\sigma_2 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right)\frac{\partial \Sigma}{\partial \rho}$$
$$= \frac{Q}{\rho}\sigma_2 \frac{\partial P}{\partial \Sigma} + Q\sigma_2 \frac{\Sigma}{\rho}\frac{\partial^2 P}{\partial \Sigma^2}. \tag{37}$$

Differentiating Eq. (24) or (25) with respect to N_1 and (separately) N_2 also yields Eqs. (36) and (37).

Another way to do this that recognizes that atom densities and material density are not independent is to apply the chain rule:

$$\frac{\partial^2 L}{\partial \rho \partial \alpha} = \sum_{i=1}^{2} \frac{\partial}{\partial N_i}\left(\frac{\partial L}{\partial \alpha}\right)\frac{\partial N_i}{\partial \rho}. \tag{38}$$

The atom density of Eq. (3) can be written

$$N_i = \frac{\rho N_{i,0}}{\rho_0}, \quad i = 1,2. \tag{39}$$

Using Eq. (39) and $\alpha = N_1$ yields

$$\frac{\partial^2 L}{\partial \rho \partial N_1} = \frac{\partial^2 L}{\partial N_1^2}\frac{\partial N_1}{\partial \rho} + \frac{\partial^2 L}{\partial N_1 \partial N_2}\frac{\partial N_2}{\partial \rho}$$
$$= \frac{N_{1,0}}{\rho_0}\frac{\partial^2 L}{\partial N_1^2} + \frac{N_{2,0}}{\rho_0}\frac{\partial^2 L}{\partial N_1 \partial N_2}. \tag{40}$$

Using Eq. (39) and $\alpha = N_2$ yields

$$\frac{\partial^2 L}{\partial \rho \partial N_2} = \frac{\partial^2 L}{\partial N_1 \partial N_2}\frac{\partial N_1}{\partial \rho} + \frac{\partial^2 L}{\partial N_2^2}\frac{\partial N_2}{\partial \rho}$$
$$= \frac{N_{1,0}}{\rho_0}\frac{\partial^2 L}{\partial N_1 \partial N_2} + \frac{N_{2,0}}{\rho_0}\frac{\partial^2 L}{\partial N_2^2}. \tag{41}$$

Rearranging Eq. (39) and using Eqs. (11) through (13), it can be shown that Eqs. (40) and (41) are equal to Eqs. (36) and (37), respectively.

These density derivatives are constant-volume partial derivatives.[6]

II.I. Mixed Derivatives: Cross Sections and Material Density

Using Eq. (39), the mixed partial derivative of the leakage with respect to σ_1 and ρ, by differentiating Eq. (14) with respect to ρ, is

$$\frac{\partial^2 L}{\partial \rho \partial \sigma_1} = \frac{\partial Q}{\partial \rho}N_1 \frac{\partial P}{\partial \Sigma} + Q\frac{\partial N_1}{\partial \rho}\frac{\partial P}{\partial \Sigma} + QN_1 \frac{\partial}{\partial \rho}\left(\frac{\partial P}{\partial \Sigma}\right)$$
$$= \frac{Q_0}{\rho_0}N_1 \frac{\partial P}{\partial \Sigma} + Q\frac{N_{1,0}}{\rho_0}\frac{\partial P}{\partial \Sigma} + QN_1 \frac{\partial}{\partial \Sigma}\left(\frac{\partial P}{\partial \Sigma}\right)\frac{\partial \Sigma}{\partial \rho}$$
$$= \frac{QN_1}{\rho}\left(2\frac{\partial P}{\partial \Sigma} + \Sigma\frac{\partial^2 P}{\partial \Sigma^2}\right). \tag{42}$$

The mixed partial derivative of the leakage with respect to σ_2 and ρ, by differentiating Eq. (15) with respect to ρ, is

$$\begin{aligned}\frac{\partial^2 L}{\partial\rho\partial\sigma_2} &= \frac{\partial Q}{\partial\rho} N_2 \frac{\partial P}{\partial\Sigma} + Q\frac{\partial N_2}{\partial\rho}\frac{\partial P}{\partial\Sigma} + QN_2 \frac{\partial}{\partial\rho}\left(\frac{\partial P}{\partial\Sigma}\right) \\ &= \frac{Q_0}{\rho_0} N_2 \frac{\partial P}{\partial\Sigma} + Q\frac{N_{2,0}}{\rho_0}\frac{\partial P}{\partial\Sigma} + QN_2 \frac{\partial}{\partial\Sigma}\left(\frac{\partial P}{\partial\Sigma}\right)\frac{\partial\Sigma}{\partial\rho} \\ &= \frac{QN_2}{\rho}\left(2\frac{\partial P}{\partial\Sigma} + \Sigma\frac{\partial^2 P}{\partial\Sigma^2}\right). \end{aligned} \tag{43}$$

Differentiating Eq. (24) or (25) with respect to σ_1 and (separately) σ_2 also yields Eqs. (42) and (43).

These density derivatives are constant-volume partial derivatives.[6]

II.J. Mixed Derivatives: Source Emission Rates and Material Density

Using Eq. (39), the mixed partial derivative of the leakage with respect to q_1 and ρ, by differentiating Eq. (19) with respect to ρ, is

$$\begin{aligned}\frac{\partial^2 L}{\partial\rho\partial q_1} &= \frac{\partial N_1}{\partial\rho} VP + N_1 V\frac{\partial P}{\partial\rho} \\ &= \frac{N_{1,0}}{\rho_0} VP + N_1 V\frac{\partial P}{\partial\Sigma}\frac{\partial\Sigma}{\partial\rho} \\ &= \frac{N_1 V}{\rho}\left(P + \Sigma\frac{\partial P}{\partial\Sigma}\right). \end{aligned} \tag{44}$$

The mixed partial derivative of the leakage with respect to q_2 and ρ is zero. Differentiating Eq. (24) or (25) with respect to q_1 also yields Eq. (44).

These density derivatives are constant-volume partial derivatives.[6]

III. Numerical Results

The material in the sphere has the parameters shown in Table I. Isotope 1 is ^{239}Pu and isotope 2 is ^{240}Pu. The total macroscopic cross section and source rate density from Eqs. (1) and (2), respectively, for the material are also shown in Table I. The cross sections and source rate correspond to the 646-keV gamma-ray line from ^{239}Pu. The cross sections were obtained from the MCPLIB04 ACE-formatted photon cross-section library, which is distributed with MCNP, and do not contain coherent scattering. The source emission rate q_1 is from Gunnick.[7]

The sphere radius is a = 3.794 cm.

Table I. Sphere and Material Parameters.

Parameter	Value
a	3.794 cm
ρ	15.8 g/cm^3
w_1	0.94
w_2	0.06
N_1	3.74142E-02 atoms/(b·cm)
N_2	2.37817E-03 atoms/(b·cm)
σ_1	5.27263E+01 b
σ_2	5.27263E+01 b
q_1	1.341E+05 γ/(10^{24} atoms·s)
q_2	0 γ/(atom·s)
Σ	2.09810E+00 /cm
q	5.01724E+03 γ/(cm^3·s)

Analytic values computed using the equations of Sec. II are presented in Sec. III.A. Results computed using PARTISN are compared with the analytic values in Sec. III.B.

III.A. Analytic Results

The escape probability, its derivatives, and the leakage are shown in Table II.

Table II. Escape Probability, Its Derivatives, and the Leakage.

Parameter	Value
P	9.34752E-02
$\partial P/\partial\Sigma$	–4.38435E-02 cm
$\partial^2 P/\partial\Sigma^2$	4.07803E-02 cm^2
L	1.07286E+05 γ/s

Derivatives of the leakage with respect to atom densities, cross sections, source emission rates, and the material density are shown in Table III, Table IV, Table V, and Table VI, respectively.

Table III. Derivatives of the Leakage with Respect to Atom Densities.

Parameter	Value
$\partial L/\partial N_1$	2.14263E+05 γ/s/[atoms/(b·cm)]
$\partial^2 L/\partial N_1^2$	–1.17096E+07 γ/s/[atoms/(b·cm)]^2
$\partial L/\partial N_2$	–2.65325E+06 γ/s/[atoms/(b·cm)]
$\partial^2 L/\partial N_2^2$	1.30122E+08 γ/s/[atoms/(b·cm)]^2
$\partial^2 L/\partial N_1 \partial N_2$	5.92062E+07 γ/s/[atoms/(b·cm)]^2

Table IV. Derivatives of the Leakage with Respect to Cross Sections.

Parameter	Value
$\partial L/\partial \sigma_1$	–1.88273E+03 γ/s/b
$\partial^2 L/\partial \sigma_1^2$	6.55191E+01 γ/s/b^2
$\partial L/\partial \sigma_2$	–1.19673E+02 γ/s/b
$\partial^2 L/\partial \sigma_2^2$	2.64718E-01 γ/s/b^2
$\partial^2 L/\partial \sigma_1 \partial \sigma_2$	4.16462E+00 γ/s/b^2

Table V. Derivatives of the Leakage with Respect to Source Emission Rates.

Parameter	Value
$\partial L/\partial q_1$	8.00043E-01 γ/s/[γ/(10^{24} atoms·s)]
$\partial^2 L/\partial q_1^2$	0 γ/s/[γ/(10^{24} atoms·s)]^2
$\partial L/\partial q_2$	0 γ/s/[γ/(10^{24} atoms·s)]
$\partial^2 L/\partial q_2^2$	0 γ/s/[γ/(10^{24} atoms·s)]^2
$\partial^2 L/\partial q_1 \partial q_2$	0 γ/s/[γ/(10^{24} atoms·s)]^2

Table VI. Derivatives of the Leakage with Respect to Material Density.

Parameter	Value
$\partial L/\partial \rho$	1.08011E+02 γ/s/(g/cm^3)
$\partial^2 L/\partial \rho^2$	–2.05068E+01 γ/s/(g/cm^3)^2

The mixed derivatives are shown in Table VII.

Table VII. Mixed Derivatives of the Leakage.[(a)]

Parameter	Value
$\partial^2 L/\partial N_1 \partial \sigma_1$	–8.30901E+03 γ/s/cm^{-1}
$\partial^2 L/\partial N_1 \partial \sigma_2$	2.67044E+03 γ/s/cm^{-1}
$\partial^2 L/\partial N_2 \partial \sigma_1$	9.23334E+04 γ/s/cm^{-1}
$\partial^2 L/\partial N_2 \partial \sigma_2$	–4.44522E+04 γ/s/cm^{-1}
$\partial^2 L/\partial N_1 \partial q_1$	1.59779E+00 γ/s/[γ/(cm^3·s)]
$\partial^2 L/\partial N_2 \partial q_1$	–1.97856E+01 γ/s/[γ/(cm^3·s)]
$\partial^2 L/\partial \sigma_1 \partial q_1$	–1.40397E-02 γ/s/[b·γ/(10^{24} atoms·s)]^2
$\partial^2 L/\partial \sigma_2 \partial q_1$	–8.92413E-04 γ/s/[b·γ/(10^{24} atoms·s)]^2
$\partial^2 L/\partial \rho \partial N_1$	–1.88165E+04 γ/s/[(g/cm^3)(atoms/{b·cm})]
$\partial^2 L/\partial \rho \partial N_2$	1.59785E+05 γ/s/[(g/cm^3)(atoms/{b·cm})]
$\partial^2 L/\partial \rho \partial \sigma_1$	–5.77782E+00 γ/s/[g/(cm^3·b)]
$\partial^2 L/\partial \rho \partial \sigma_2$	–3.67258E-01 γ/s/[g/(cm^3·b)]
$\partial^2 L/\partial \rho \partial q_1$	8.05453E-04 γ/s/[g·γ/cm^3/(10^{24} atoms·s)]

(a) All derivatives with respect to q_2 are zero.

The equations of Sec. II and the results presented in this section were verified using numerical differences.

III.B. PARTISN Results Compared to Analytic Results

The equations of the 2nd-LASS have sources that are the angular flux solutions of the 1st-LASS (the usual forward and adjoint transport equations).[2] PARTISN is unable to accept angular fluxes as volumetric sources—only moments expansions are accepted.[5] However, when anisotropic source moments are input, an anisotropic scattering expansion of the order of the source expansion (at least) is required. Thus, to use PARTISN on this problem requires inputting anisotropic scattering cross sections where *no* scattering is desired.

To solve this problem, we used an L^{th}-order scattering expansion and set the isotropic (0^{th}-order) scattering cross section and the L^{th}-order scattering cross section to 10^{-24} times the total cross section. We set all other scattering cross section moments to zero.

The cross sections were entered in the PARTISN input file using the ODNINP format. A mesh spacing of 0.005 cm was used (759 meshes in 3.794 cm).

The results presented in this section used a P_{31} scattering expansion and S_{2048} angular quadrature. With this quadrature order, the ratio of the leakage computed in the forward and adjoint calculations in the 1st-LASS was 1.00000093.

The difference between PARTISN results and analytic results for the leakage and derivatives of the mass density are shown in Table VIII. Density derivatives are obtained from the PARTISN results using the chain rule:

$$\begin{aligned}\frac{\partial L}{\partial \rho} &= \sum_{i=1}^{2} \frac{\partial L}{\partial N_i}\frac{\partial N_i}{\partial \rho} \\ &= \frac{N_1}{\rho}\frac{\partial L}{\partial N_1} + \frac{N_2}{\rho}\frac{\partial L}{\partial N_2},\end{aligned} \tag{45}$$

$$\begin{aligned}\frac{\partial^2 L}{\partial \rho^2} &= \sum_{i=1}^{2}\sum_{j=1}^{2} \frac{\partial^2 L}{\partial N_i \partial N_j}\frac{\partial N_i}{\partial \rho}\frac{\partial N_j}{\partial \rho} \\ &= \left(\frac{N_1}{\rho}\right)^2 \frac{\partial^2 L}{\partial N_1^2} + 2\frac{N_1}{\rho}\frac{N_2}{\rho}\frac{\partial^2 L}{\partial N_1 \partial N_2} + \left(\frac{N_2}{\rho}\right)^2 \frac{\partial^2 L}{\partial N_2^2}.\end{aligned} \tag{46}$$

These density derivatives are constant-volume partial derivatives.[6]

Table VIII. Difference Between PARTISN and Analytic Results for the Leakage and Mass Density Derivatives.

L	0.000%
$\partial L/\partial \rho$	–0.012%
$\partial^2 L/\partial \rho^2$	–0.009%

The difference between PARTISN results and analytic results for isotopic first derivatives are shown in Table IX.

Table IX. Difference Between PARTISN and Analytic Results for Isotopic First Derivatives.

i	$\partial L/\partial N_i$
1 (^{239}Pu)	–0.002%
2 (^{240}Pu)	0.000%
i	$\partial L/\partial \sigma_i$
1 (^{239}Pu)	0.000%
2 (^{240}Pu)	0.000%
i	$\partial L/\partial q_i$
1 (^{239}Pu)	0.000%
2 (^{240}Pu)	N/A[(a)]

(a) All derivatives with respect to q_2 are zero.

The difference between PARTISN results and analytic results for isotopic second derivatives (including mixed derivatives) are shown in Table X.

Table X. Difference Between PARTISN and Analytic Results for Isotopic Second Derivatives.

i	j	$\partial^2 L/\partial N_i \partial N_j$	$\partial^2 L/\partial N_i \partial \sigma_j$	$\partial^2 L/\partial N_i \partial q_j$
1 (^{239}Pu)	1 (^{239}Pu)	–0.002%	–0.003%	–0.004%
	2 (^{240}Pu)	0.001%	0.001%	N/A[(a)]
2 (^{240}Pu)	1 (^{239}Pu)	0.001%	0.001%	0.001%
	2 (^{240}Pu)	0.001%	0.000%	N/A[(a)]
i	j	$\partial^2 L/\partial \sigma_i \partial N_j$	$\partial^2 L/\partial \sigma_i \partial \sigma_j$	$\partial^2 L/\partial \sigma_i \partial q_j$
1 (^{239}Pu)	1 (^{239}Pu)	–0.002%	0.001%	0.001%
	2 (^{240}Pu)	0.001%	0.001%	N/A[(a)]
2 (^{240}Pu)	1 (^{239}Pu)	0.001%	0.001%	0.001%
	2 (^{240}Pu)	0.000%	0.001%	N/A[(a)]
i	j	$\partial^2 L/\partial q_i \partial N_j$	$\partial^2 L/\partial q_i \partial \sigma_j$	$\partial^2 L/\partial q_i \partial q_j$
1 (^{239}Pu)	1 (^{239}Pu)	–0.002%	0.000%	N/A[(a)]
	2 (^{240}Pu)	0.000%	0.000%	N/A[(a)]
2 (^{240}Pu)	1 (^{239}Pu)	N/A[(a)]	N/A[(a)]	N/A[(a)]
	2 (^{240}Pu)	N/A[(a)]	N/A[(a)]	N/A[(a)]

(a) All derivatives with respect to q_2 are zero.

The difference between PARTISN results and analytic results for isotopic mixed second derivatives that include the mass density are shown in Table XI. Again, these are obtained from the PARTISN results using the chain rule, Eq. (38), where α represents the isotopic density, cross section, or source emission rate for either isotope.

Table XI. Difference Between PARTISN and Analytic Results for Mixed Second Derivatives that Include Mass Density.

j	$\partial^2 L / \partial\rho\partial N_j$	$\partial^2 L / \partial\rho\partial\sigma_j$	$\partial^2 L / \partial\rho\partial q_j$
1 (^{239}Pu)	–0.003%	–0.012%	–0.022%
2 (^{240}Pu)	0.001%	–0.012%	N/A[(a)]

(a) All derivatives with respect to q_2 are zero.

When a P_3 scattering expansion was used (with an S_{2048} angular quadrature), errors in the isotopic second derivatives were up to 3%, except for $\partial^2 L / \partial q_1 \partial N_j$ and $\partial^2 L / \partial q_1 \partial \sigma_j$, which were still basically zero because the 2nd-LASS equations for those derivatives use only the physical source emission rate density, which is isotropic. Errors in the derivatives that include the mass density were larger, up to 12%.

Using many scattering moments was crucial to having PARTISN solve this problem correctly, but the choice of the scattering cross section is not important as long as it is very small. The first-order relative sensitivities of the leakage to the 0th- and Lth-order ^{239}Pu scattering cross sections is 7E-25%/% and 5E-31%/%, respectively, and the sensitivities to the ^{239}Pu scattering cross sections are an order of magnitude smaller.

IV. Summary and Future Work

This memo provides analytic benchmark results for the derivatives derived in the 2nd-ASAM for uncollided particles,[2] but it does not provide a benchmark for the 2nd-LASS. The computed results match the analytic results extremely well. This memo does not provide results for derivatives of the detector response function.

In the future, we will extend the 2nd-ASAM to include derivatives with respect to interface locations.[8,9] We will also apply the 2nd-ASAM to transport problems with scattering, including eigenvalue problems.

An off-the-shelf discrete-ordinates code, PARTISN, was used for the transport calculations, indicating the general applicability of the 2nd-ASAM. In the future, we will solve the 2nd-LASS equations in the context of ray-tracing.[10]

References

1. Dan G. Cacuci, “Second-Order Adjoint Sensitivity Analysis Methodology (2nd-ASAM) for Computing Exactly and Efficiently First- and Second-Order Sensitivities in Large-Scale Linear Systems: I. Computational Methodology,” *J. Comp. Phys.*, **284**, 687–699 (2015). DOI: 10.1016/j.jcp.2014.12.042.

2. Dan Gabriel Cacuci, “Second-Order Sensitivity Analysis of Uncollided Particle Contributions to Radiation Detector Responses,” April 25, 2017.

3. James J. Duderstadt and William R. Martin, *Transport Theory*, Chap. 2.1.6, John Wiley & Sons, New York (1979).

4. Philippe Humbert, “Application of Inverse Gamma Transport to Material Thickness Identification with SGRD Code,” *Proceedings of the 13th International Conference on Radiation Shielding (ICRS-13) & 19th Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society (RPSD-2016)*, CD-ROM <Oral/T6/T6_S3/000120_FP.pdf>, Paris, France, October 3-6 (2016).

5. R. E. Alcouffe, R. S. Baker, J. A. Dahl, E. D. Fichtl, S. A. Turner, R. C. Ward, and R. J. Zerr, “PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System,” Los Alamos National Laboratory report LA–UR–08-7258 (Revised March 2015).

6. Jeffrey A. Favorite, “Adjoint-Based Constant-Mass Partial Derivatives,” *Annals of Nuclear Energy*, submitted (2017).

7. R. Gunnick, J. E. Evans, and A. L. Prindle, “A Reevaluation of the Gamma-Ray Energies and Absolute Branching Intensities of ^{237}U, ^{238,239,240,241}Pu, and ^{241}Am,” Lawrence Livermore National Laboratory report UCRL-52139 (October 1976).

8. Keith C. Bledsoe, Jeffrey A. Favorite, and Tunc Aldemir, “Using the Levenberg-Marquardt Method for Solutions of Inverse Transport Problems in One- and Two-Dimensional Geometries,” *Nuclear Technology*, **176**, *1*, 106-126 (2011). DOI: 10.13182/NT176-106.

9. Jeffrey A. Favorite and Esteban Gonzalez, “Revisiting Boundary Perturbation Theory for Inhomogeneous Transport Problems,” *Nuclear Science and Engineering*, **185**, *3*, 445-459 (2017). DOI: 10.1080/00295639.2016.1277108.

10. Jeffrey A. Favorite, Keith C. Bledsoe, and David I. Ketcheson, “Surface and Volume Integrals of Uncollided Adjoint Fluxes and Forward-Adjoint Flux Products,” *Nuclear Science and Engineering*, **163**, *1*, 73-84 (2009). DOI: 10.13182/NSE163-73.

JAF:jaf

Distribution:
A. Sood, XCP-3, MS F663, `sooda@lanl.gov`
C. J. Werner, XCP-3, MS F663, `cwerner@lanl.gov`
D. G. Cacuci, University of South Carolina, `cacuci@cec.sc.edu`
K. C. Bledsoe, Oak Ridge National Laboratory, `bledsoekc@ornl.gov`
R. S. Baker, CCS-2, MS D409, `rsb@lanl.gov`
J. A. Dahl, CCS-2, MS D409, `dahl@lanl.gov`
E. J. D. Fichtl, CCS-2, MS D409, `efichtl@lanl.gov`
R. J. Zerr, CCS-2, MS D409, `rzerr@lanl.gov`
J. A. Favorite, XCP-3, MS F663, `fave@lanl.gov`
XCP-3 File
X-archive