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A FORWARD/ADJOINT TRANSPORT FORMALISM FOR SENSITIVITY STUDIES*

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ABSTRACT

We describe a formalism for efficiently estimating the sensitivity of radiative transfer solutions to perturbations in the absorption and scattering properties of the transport medium assuming a fixed material temperature distribution. This formalism is adapted from a similar formalism commonly used in the neutron transport community. It is based upon the use of solutions to both the forward (standard) and adjoint transport equations. Given any desired integral response, (any quantity expressible as an integral over phase space of the product of an arbitrary function and the radiation intensity,) one can use this formalism to obtain a first-order estimate of the change in that response as a function of any perturbation in the absorption coefficients, the scattering coefficients, and the scattering phase function. One forward transport solution and one adjoint transport solution are required for the unperturbed system. The estimate for the change in the response is expressed in terms of integrals over phase space of certain functions constructed from the forward intensity solution, the adjoint intensity solution, the absorption coefficient perturbation, the scattering coefficient perturbation, and the scattering phase function perturbation. Given a large set of perturbations, it is much less costly to use this formalism to estimate the effect of each perturbation than to solve the transport equation for each perturbed configuration. Interestingly, standard radiative transfer codes can be used to solve the adjoint transport equation, so special adjoint transport codes are not required. After describing the formalism, a simple analytic example calculation is performed to demonstrate its validity. Finally, the method is used to determine the change in the surface radiative heat flux due to changes in the multigroup (non-grey) absorption and scattering coefficients in a three-dimensional benchmark problem with anisotropic scattering.

NOMENCLATURE

$\overrightarrow{r}$	spatial position vector
dA	differential surface area, (m^2)
dV	differential spatial volume, (m^3)
$\overrightarrow{\Omega}$	direction vector
$d\Omega$	differential solid angle, $(steradians)$
E	energy, (eV)
dE	differential energy, (eV)
$\overrightarrow{p}$	phase-space vector
dP	differential phase-space volume, $(m^3 - steradians - eV)$
I	angular intensity function, $[W/(m^2 - sec - steradian - eV)]$
$I^\dagger$	adjoint intensity function, $(arbitrary\ units)$
σ_t	total extinction coefficient, (m^{-1})
σ_a	absorption coefficient, (m^{-1})
σ_s	scattering coefficient, (m^{-1})
Φ	scattering phase function, $(steradians^{-1})$

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T	material temperature, (K)
B	Planck emission function, $[W/(m^2 - sec - steradians - eV)]$
Q	emission term, $\sigma_a B$ $[W/(m^3 - sec - steradians - eV)]$
$Q^\dagger$	adjoint source function, *(arbitrary units)*
$\mathcal{R}$	integral response, *(arbitrary units)*
R	integral response function, *(arbitrary units)*

INTRODUCTION

The adjoint transport techniques have been used in the neutron transport community to efficiently estimate the effect of perturbations in material transport properties on integral transport responses, e.g., energy absorption in a volume, energy flow across a surface, etc. Such applications of adjoint transport theory are discussed in Lewis and Miller, 1993. The purpose of the present paper is to adapt these adjoint neutron transport techniques to estimate the effect of perturbations in the absorption and scattering coefficients and the scattering phase function on radiative transfer solutions assuming a fixed material temperature distribution. Given a large set of perturbations, it is much less costly to use this formalism to estimate the effect of each perturbation than to solve the transport equation for each perturbed configuration.

The remainder of this paper is organized as follows. First we define the mathematical concept of an adjoint operator. Then we define the adjoint radiative transfer equation. Next we derive an expression for the effect of coefficient and phase function perturbations upon integral responses. Finally, we give a simple analytic example that demonstrates the validity of the perturbation theory.

ADJOINT OPERATORS

Central to the concept of an adjoint operator is the concept of an inner product. The inner product of two functions, f and h, is denoted by $\langle f, h \rangle$, and is defined as follows:

$$\langle f, g \rangle = \int f(\vec{P})\, h(\vec{P})\, dP \quad , \tag{1}$$

where f and h are any two square-integrable functions and the integral is taken over some prescribed volume (possibly unbounded) of phase-space. An operator, $A^\dagger$, is the adjoint of the operator, A, if

$$\langle Af, h \rangle = \langle f, A^\dagger h \rangle \quad , \tag{2}$$

where f and h are any two square-integrable functions defined within the prescribed phase-space volume. Different inner products yield different adjoint operators. The adjoint operator does not always exist, but if it does exist, it is unique for a given inner product. The adjoint operator may formally exist only for functions which satisfy certain conditions on the outer boundary of a prescribed phase-space volume.

THE ADJOINT RADIATIVE TRANSFER EQUATION

The radiative transfer equation with a prescribed material temperature distribution can be written as follows:

$$\vec{\Omega} \cdot \vec{\nabla} I + \sigma_t I = \int_{4\pi} \sigma_s \Phi(\vec{\Omega}' \cdot \vec{\Omega}) I(\vec{\Omega}')\, d\Omega + Q \quad , \tag{3}$$

where Q is a fixed inhomogeneous source equal to the Planck emission function. Note that the notation relating to spatial and spectral dependencies has been supressed for simplicity in Eq. (3). The corresponding adjoint equation is

$$-\vec{\Omega} \cdot \vec{\nabla} I^\dagger + \sigma_t I^\dagger = \int_{4\pi} \sigma_s \Phi(\vec{\Omega}' \cdot \vec{\Omega}) I^\dagger(\vec{\Omega}')\, d\Omega + Q^\dagger \quad , \tag{4}$$

where $I^\dagger$ denotes the adjoint intensity and $Q^\dagger$ denotes the adjoint source function. The adjoint intensity is simply the solution to Eq. (4). It is not "adjoint" to the forward intensity, I, in any sense. We assume that the desired integral response, $\mathcal{R}$, can be expressed as follows:

$$\mathcal{R} = \int_J R(\vec{P})\, I(\vec{P})\, dP \quad , \tag{5}$$

where the phase-space integral is taken over the problem domain, and R is an arbitrary function referred to as the integral response function. For reasons which will later become clear, the adjoint source function is set equal to the response function:

$$Q^\dagger = R \quad . \tag{6}$$

Note from Eq. (3) and Eq. (4) that the transport operator is almost self-adjoint. The only constituent operator that is not self-adjoint is the gradient operator, which is skew-adjoint:

$$[\vec{\Omega} \cdot \vec{\nabla}]^\dagger = -\vec{\Omega} \cdot \vec{\nabla} \tag{7}$$

This means that "adjoint photons" behave exactly like real photons except that they travel backwards. Thus

while a vacumm boundary condition for the forward intensity is

$$I(\overrightarrow{\Omega}) = 0 \quad , \text{for } \overrightarrow{\Omega} \cdot \overrightarrow{n} < 0, \tag{8}$$

the corresponding condition for the adjoint intensity is

$$I^{\dagger}(\overrightarrow{\Omega}) = 0 \quad , \text{for } \overrightarrow{\Omega} \cdot \overrightarrow{n} > 0, \tag{9}$$

where Eq. (8) and Eq. (9) are satisfied on the outer boundary of the spatial domain, and $\overrightarrow{n}$ denotes the outward-directed boundary surface normal.

The adjoint relationship, Eq. (2), is not necessarily satisfied by the gradient operator and its adjoint within a finite spatial domain. Rather, the following relationship is satisfied:

$$\langle \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} f, h \rangle = \langle f, -\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} h \rangle + \int_0^{\infty} \int_{4\pi} \oint_{\Gamma} I I^{\dagger} \overrightarrow{\Omega} \cdot \overrightarrow{n} \, dA \, d\Omega \, dE \quad , \tag{10}$$

where Γ denotes the outer boundary of the transport domain. However, if the forward and adjoint intensities satisfy certain boundary conditions (e.g., the vacuum condition,) the boundary integral will be zero and the adjoint relationship will be satisfied. The adjoint formalism remains useful whether or not the adjoint relationship is satisfied.

An integral response can be expressed either as an inner product of the forward intensity and the adjoint source or an inner product of the adjoint intensity and the forward source. To demonstrate this, we take the inner product of Eq. (3) with $I^{\dagger}$, take the inner product of Eq. (4) with I, and subtract the two resulting equations to obtain

$$\langle I, Q^{\dagger} \rangle = \langle I^{\dagger}, Q \rangle + \int_0^{\infty} \int_{4\pi} \oint_{\Gamma} I^{\dagger} \, I \, \overrightarrow{\Omega} \cdot \overrightarrow{n} \, dA \, d\Omega \, dE \quad . \tag{11}$$

Substituting from Eq. (6) into Eq. (11), we obtain

$$\mathcal{R} = \langle I^{\dagger}, Q \rangle + \int_0^{\infty} \int_{4\pi} \oint_{\Gamma} I^{\dagger} \, I \, \overrightarrow{\Omega} \cdot \overrightarrow{n} \, dA \, d\Omega \, dE \quad . \tag{12}$$

The standard method for evaluating the response corresponds to Eq. (5). One solves the forward transport equation and then takes the inner product of the forward intensity and the response function (adjoint source.) The adjoint technique for evaluating the response function corresponds to Eq. (12). One solves the adjoint transport equation and then takes the inner product of the adjoint intensity and the forward source. The adjoint approach is superior if one wants to evaluate the response for several different sources. Using the forward approach, a new forward transport solution is required for each new forward source, but using the adjoint approach, one uses the same adjoint tranport solution for all forward sources.

In general, the boundary conditions for the adjoint intensity are chosen so that one of the following conditions is met:

1. The surface integral term in Eq. (12) is identically zero.
2. The only non-zero contributions from the forward intensity to the surface integral term come from those directions for which the forward intensity is known from boundary conditions.

If the adjoint boundary conditions are not chosen in this way, a full forward intensity solution will be required to evaluate the surface integral term, thereby eliminating the fundamental advantage of the adjoint approach.

We close this section by noting that the adjoint equation can be solved using standard forward codes. We begin a demonstration of this fact by evaluating Eq. (4) at $-\overrightarrow{\Omega}$:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I^{\dagger} + \sigma_t I^{\dagger} = \int_{4\pi} \sigma_s \Phi(\overrightarrow{\Omega}' \cdot \overrightarrow{\Omega}) I^{\dagger}(-\overrightarrow{\Omega}') \, d\Omega + Q^{\dagger} \quad , \tag{13}$$

Next we make the following definitions:

$$I_o^{\dagger}(\overrightarrow{\Omega}) = I^{\dagger}(-\overrightarrow{\Omega}) \quad , \tag{14}$$

$$Q_o^{\dagger}(\overrightarrow{\Omega}) = Q^{\dagger}(-\overrightarrow{\Omega}) \quad . \tag{15}$$

Substituting from Eqs. (14) and (15) into Eq. (13), we obtain an equation which is equivalent to the adjoint transport operator, but has the same form as the forward transport operator:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_o^{\dagger} + \sigma_t I_o^{\dagger} = \int_{4\pi} \sigma_s \Phi(\overrightarrow{\Omega}' \cdot \overrightarrow{\Omega}) I_o^{\dagger}(-\overrightarrow{\Omega}') \, d\Omega + Q_o^{\dagger} \quad , \tag{16}$$

PERTURBATION THEORY

The adjoint equation can be used to efficiently estimate perturbations in an integral response due to perturbations in the material transport coefficients. In particular, let us assume that the unperturbed forward and adjoint equations have been solved. It is convenient to write these respective equations in operator form:

$$LI = Q \quad , \tag{17}$$

and

$$L^{\dagger} I^{\dagger} = Q^{\dagger} \quad . \tag{18}$$

where L denotes the forward transport operator, $L^{\dagger}$ denotes the adjoint transport operator, and Q denotes the Planck emission term. The forward equation for the perturbed system can be written as follows:

$$(L + \delta L)(I + \delta I) = Q + \delta Q \quad , \tag{19}$$

where δL denotes the perturbation to the transport operator, $\delta L^{\dagger}$ denotes the perturbation to the adjoint transport operator, and δQ denotes the perturbation to the Planck emission term. We begin the derivation of an expression for the perturbed response by expanding Eq. (19) to first-order in the perturbations:

$$L I + \delta L\, I + L\, \delta I = Q + \delta Q \quad . \tag{20}$$

Taking the inner product of I and Eq. (18), and taking the inner product of $I^{\dagger}$ with Eq. (20), and then subtracting the resulting equations, we obtain:

$$\langle \delta I, Q^{\dagger} \rangle = \langle I^{\dagger}, \delta Q \rangle - \langle I^{\dagger}, \delta L\, I \rangle, \quad . \tag{21}$$

The inner product on the left of Eq. (21) represents the response perturbation. Thus the desired expression for the response perturbation is

$$\delta \mathcal{R} = \langle I^{\dagger}, \delta Q \rangle - \langle I^{\dagger}, \delta L\, I \rangle, \quad . \tag{22}$$

Equation (22) is first-order accurate because the only approximation made in deriving it was neglecting of the second-order term in Eq. (20). Note that the effect of any perturbation can be estimated in terms of an inner product of the unperturbed adjoint intensity with the perturbed forward source and an inner product of the unperturbed adjoint intensity with the perturbed forward transport operator acting upon the unperturbed forward intensity. Evaluating these inner products is much less expensive than solving the perturbed transport equation.

It is useful for purposes of sensitivity analysis to recognize that the adjoint formalism allows one to exactly calculate the derivative of the response with respect to any parameter. In particular, given an arbitrary transport parameter, α, we re-express Eq. (22) as follows:

$$\delta \mathcal{R} = \langle I^{\dagger}, \frac{\delta Q}{\delta \alpha} \delta \alpha \rangle - \langle I^{\dagger}, \frac{\delta L}{\delta \alpha} \delta \alpha\, I \rangle, \quad . \tag{23}$$

Assuming that $\delta \alpha$ is independent of the phase-space variables, we can move it outside of the inner product in Eq. (23) and divide both sides of the equation by $\delta \alpha$:

$$\frac{\delta \mathcal{R}}{\delta \alpha} = \langle I^{\dagger}, \frac{\delta Q}{\delta \alpha} \rangle - \langle I^{\dagger}, \frac{\delta L}{\delta \alpha} I \rangle, \quad . \tag{24}$$

Taking the limit of Eq. (24) as $\delta \alpha \rightarrow 0$, we obtain the desired expression for the derivative of the response with respect to α:

$$\frac{\partial \mathcal{R}}{\partial \alpha} = \langle I^{\dagger}, \frac{\partial Q}{\partial \alpha} \rangle - \langle I^{\dagger}, \frac{\partial L}{\partial \alpha} I \rangle, \quad . \tag{25}$$

We stress that this derivative expression is exact. Its exactness is a direct result of the first-order accuracy of the perturbation theory.

AN ANALYTIC EXAMPLE

To demonstrate the validity of Eq. (22) we consider a simple 1-D slab problem defined on the interval $(0, 1)$. The temperature is assumed to be constant throughout the slab. The scattering coefficient is assumed to be zero. The equation to be soived is

$$\mu \frac{\partial I}{\partial z} + \sigma_a I = \sigma_a B \quad , \tag{26}$$

with vacuum boundary conditions:

$$I(0, \mu, E) = 0 \quad , \text{for } \mu > 0, \tag{27}$$

and

$$I(1, \mu, E) = 0 \quad , \text{for } \mu < 0. \tag{28}$$

The solution to Eq. (26) is

$$I = B \left[1 - exp\left(-\frac{\sigma_a z}{\mu} \right) \right] \quad , \text{for } \mu > 0, \tag{29}$$

and

$$I = B \left\{ 1 - exp\left[\frac{\sigma_a (1 - z)}{\mu} \right] \right\} \quad , \text{for } \mu < 0. \tag{30}$$

The response we choose to calculate is the value of the intensity at $z = 1$, $\mu = 1$, $E = E_0$, where E_0 is an arbitrary energy. The corresponding response function is

$$R = \delta(z - 1) \frac{1}{2\pi} \delta(\mu - 1)\, \delta(E - E_0) \quad , \tag{31}$$

where $\delta(x)$ is the dirac delta function. The corresponding adjoint transport equation is

$$-\mu \frac{\partial I^{\dagger}}{\partial z} + \sigma_a I^{\dagger} = Q^{\dagger} \quad , \tag{32}$$

with vacuum boundary conditions:

$$I^{\dagger}(0, \mu, E) = 0 \quad , \text{for } \mu < 0, \tag{33}$$

and

$$I^{\dagger}(1, \mu, E) = 0 \quad , \text{for } \mu > 0, \tag{34}$$

where $Q^\dagger = R$ in accordance with Eq. (6). The solution to Eq. (32) is

$$I^\dagger = exp[\sigma_a(z-1)]\ \frac{1}{2\pi}\delta(\mu-1)\,\delta(E-E_0)\,, \quad \text{for } \mu > 0, \tag{35}$$

and

$$I^\dagger = 0 \quad , \text{for } \mu < 0. \tag{36}$$

The unperturbed response, which can be calculated either according to Eq. (6) (the forward approach) or Eq. (12) (the adjoint approach,) is given by

$$\mathcal{R} = B\,[1 - exp(-\sigma_a)] \quad , \tag{37}$$

We next define the perturbed system by replacing σ_a with $\sigma_a + \delta\sigma_a$ in Eq. (26):

$$\mu\frac{\partial I}{\partial z} + (\sigma_a + \delta\sigma_a)\,I = (\sigma_a + \delta\sigma_a)\,B \quad , \tag{38}$$

The exact perturbed response is

$$\mathcal{R} + \delta\mathcal{R} = B\,\{1 - exp[-(\sigma_a + \delta\sigma_a)]\} \quad , \tag{39}$$

Subtracting Eq. (37) from Eq. (39), we obtain the exact response perturbation:

$$\delta\mathcal{R} = B\,exp(-\sigma_a)\,[1 - exp(-\delta\sigma_a)] \tag{40}$$

Using Eq. (22) to evaluate the response perturbation, we get

$$\delta\mathcal{R} = \delta\sigma_a\,B\,exp(-\sigma_a) + O\left(\delta{\sigma_a}^2\right) \quad . \tag{41}$$

Expanding Eq. (40) in a Taylor series about $\delta\sigma_a = 0$, we get

$$\delta\mathcal{R} = \delta\sigma_a\,B\,exp(-\sigma_a) + O\left(\delta{\sigma_a}^2\right) \quad . \tag{42}$$

Comparing Eqs. (41) and (42), we find that the perturbation theory is indeed first-order accurate.

A 3-D COMPUTATIONAL EXAMPLE

Tong and Skocypec (1992) defined several transport problems which have been used to compare various numerical transport methods and codes. We consider one of these problems. It consists of a rectangular enclosure (a box) containing a mixture of carbon particles, CO_2 and N_2. The width of the box is 2 m, the height of the box is 3 m, and the length of the box is 5 m. The carbon particle density is 2×10^9 particles/m^3, and the gas pressure is 1 atm. The participating medium is held at a uniform temperature of 1000 K. The radiative heat flux (W/m^2) is calculated at a point on the exterior surface of the box having coordinates x=0.5 m, y=0.0 m, z=1.5 m. The origin of the coordinate system lies at the center of the box. The x-axis is oriented along the width of the box, the y-axis is oriented along the length of the box, and the z-axis is oriented along the height of the box. Both absorption and scattering interactions are modeled. All additional information about the problem can be obtained from Tong and Skocypec (1992).

We used a simplified P_3 method (Larsen, Morel, and McGhee, 1990) with P_3 anisotropic scattering to solve the forward and adjoint transport equations. The SP_n equations were spatially discretized using a linear finite-element technique on a tetrahedral mesh. The standard multigroup method (Lewis and Miller, 1993), was used to discretize the equations in energy. All of the calculations were performed on a Connection Machine CM-200 computer at Los Alamos National Laboratory using twelve energy groups and a spatial mesh consisting of 50,688 tetrahedra having 11,676 nodes.

Using the forward equation to calculate the radiative heat flux, we obtained 4.92×10^4 W/m^2. Using the adjoint equation to calculate the radiative heat flux (the response), we obtained the same result. This is to be expected since our numerical adjoint equations are exactly adjoint to our numerical forward equations. Each calculation took about 45 s of CPU time.

To demonstrate the utility of the adjoint approach, we have calculated the derivatives of the radiative heat flux with respect to the absorption coefficient and the scattering coefficient for each energy group These derivatives are given in Table 1. The data in this table was generated using Eq. (25) together with the solutions generated in the forward calculation and the adjoint calculation for the radiative heat flux. Evaluation of the inner products in Eq. (25) took approximately 0.7 s for *all* of the data in the table. Thus approximately 91 s of total CPU time was required to generate the table.

To validate the accuracy of the adjoint-generated response derivatives, we performed three calculations. The first was an unperturbed forward calculation for the radiative heat flux. The second was a calculation in which the absorption coefficient was changed by 10^{-3} m^{-1} in each group. The third was identical to the second except that the scattering coefficient rather than the absorption coefficient was changed. The three corresponding solutions were used to construct a numerical estimate for the response derivative. Since a uniform change in the coefficients for each group was made, the resulting derivative corresponds to the sum over groups of the derivatives in Table 1. The sum of the absorption derivatives from Table 1 is 952 W/m, and the sum of the scattering derivatives from Table 1 is -263 W/m. The forward estimates for these derivatives are identical to three digits.

The three forward calculations used to estimate the

TABLE I RESPONSE DERIVATIVES

Group Energies	$\partial R/\partial \sigma_a$	$\partial R/\partial \sigma_s$
eV	W/m	W/m
0.062 - 0.080	236	-69.2
0.080 - 0.103	218	-64.2
0.103 - 0.133	408	-119
0.133 - 0.172	697	-201
0.172 - 0.222	1071	-313
0.222 - 0.287	1484	-426
0.287 - 0.371	1816	-496
0.371 - 0.479	1693	-453
0.479 - 0.618	1184	-307
0.618 - 0.798	532	-139
0.798 - 1.031	154	-38.7
1.031 - 1.332	23.7	-5.97

derivatives each required approximately 121 s of CPU time. Because two nearly equal numbers had to be subtracted to estimate the derivative, a tighter iterative convergence tolerance was required for these calculations. This is why they required more CPU time than the initial forward and adjoint calculations required. The total CPU time required to evaluate the response derivatives using the standard forward approach was 333 s, whereas the total CPU time required using the adjoint approach was 91 s. This is a savings in CPU time of over a factor of three. However, one must remember that any *additional* response derivatives would require less than 1 s of CPU time using the adjoint approach, whereas 121 s of CPU time would be required for each additional response derivative using the forward approach. It is clear that the adjoint is vastly superior to the forward approach when a large number of response derivatives are desired.

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