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General Sensitivity Theory for Radiation Transport

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CONTENTS

Abstract

The theoretical framework of a general approach to sensitivity analysis using adjoint functions is introduced and developed for practical application. Sensitivity and the context in which it is used is defined quantitatively in terms of adjoint functionals. The physical meaning and applicability of such a definition are then discussed with reference to both analytic and predictive studies. Connections are made between the general approach and perturbation theory for predictive applications. Specific formulations useful in cross-section sensitivity work are described in detail.

I. Introduction

The goal of sensitivity analysis in its widest sense is to establish the connection between the solution of a problem and the parametric data used to obtain that solution. Two central questions are addressed in performing such an analysis, the answers to both being essential ingredients in a general sensitivity theory:

(1) How can the contribution of an input parameter to the solution of a particular problem be quantitatively measured?

(2) How will the solution change as a result of changes in such a parameter?

The answer to the first question is analytic in nature, involving a description of the role played by each parameter in determining a particular solution with an eye toward understanding the relationship between parameter and solution. An answer to the second question, in the context of a general theory, involves methods for determining the character of the new solution resulting from a change in the input data. This aspect of the theory is, therefore, predictive in nature. In the past most attempts at sensitivity analysis were based in large part on this latter approach[1-7] with little appreciation for its connection to the analytic aspect. It is hoped that a melding of the two approaches into one general theory will give impetus to the use of sensitivity analysis in a wider range of problems than is presently considered practical.

What is proposed here is a mathematical formulation of sensitivity theory, based on strong physical insights, with the aim of setting up a quantitative basis for the concept of sensitivity. The approach is sufficiently general to allow the discussion to be restricted to neutron transport problems without losing sight of its potential applicability in other areas. In this light, the problem discussed in this paper will be the solution of the time-independent Boltzmann transport equation and sensitivity questions involving basic microscopic cross-section data and the spatial transport of radiation. During the course of the developments, indications of other applications of the theory will be pointed out.

It is tacitly assumed in the present work that sensitivity questions are properly stated only after the specification of all problem data including sources, materials, geometry, and detector responses (i.e., sensitivity questions are strictly problem dependent. Generalizations to the results of a particular study are then possible only within a class of problems similar to the one specified or problems exhibiting similar sensitivity results. Also, we assume that the need for sensitivity analysis arises in part from the vast amount of data used in a calculation, and the lack of specific information about the importance of any particular data element in arriving at a result. A requirement of sensitivity theory, therefore, is that it reveals the importance of all input data without the need for prior specification of the parameters which are to be examined. Particular attention is thus focused on a methodology for analyzing the sensitivity of the result to the entire input data field.

II. Definitions

To reduce the potential size of a sensitivity study to manageable proportions and, in addition, to be able to draw from well-known mathematical formalisms, the basic nomenclature needed in any analysis must first be defined. In particular, the term "result" and the usage of the word "sensitivity" must be made mathematically precise so that they can be meaningfully discussed in the broader context of the theory.

In the first instance, the basic "result" of a solution to a problem will be assumed to be a flux integrated quantity or more simply a response. Stating this mathematically, we define:

$$R \equiv \int_{\overline{\xi}} \Sigma_R(\overline{\xi})\, N(\overline{\xi})\, d\overline{\xi} \equiv \langle \Sigma_R, N \rangle. \tag{1}$$

Here, $N(\bar{\xi})$, is the angular flux solution of the Boltzmann equation, which in operator notation can be written as:

$$LN = S \tag{2}$$

with external source S and Boltzmann operator L; $\bar{\xi}$, represents a point in phase space and is a function of the conventional independent variables $\bar{r}, \bar{\Omega}$, and E; $\Sigma_R(\bar{\xi})$, is the response function which relates the flux to the physical response desired; and R, is the flux integrated response being studied. For convenience sake, integrals over all phase space $\bar{\xi}$ will be denoted by braces as is conventionally done to connote an inner product of two functions.

While this definition appears to be somewhat restrictive, it really is not, for one is at liberty to choose $\Sigma_R(\bar{\xi})$ to fit the problem being studied. For instance, if the flux itself at a particular point in phase space were the fundamental quantity whose sensitivity one wished to examine, then $\Sigma_R(\bar{\xi})$ could be chosen to be n-dimensional delta function where n is the order of the dimensions of the phase space. That is to say, let:

$$\Sigma_R(\bar{\xi}) = \delta(\bar{\xi}-\bar{\xi}_o) \tag{3}$$

thus yielding a flux response;

$$R = \int_{\bar{\xi}} \delta(\bar{\xi}-\bar{\xi}_o)\, N(\bar{\xi})\, d\bar{\xi} = N(\bar{\xi}_o) \tag{4}$$

The freedom to choose $\Sigma_R(\bar{\xi})$ therefore increases the generality of the definition.

The second element of nomenclature requiring definition is the connotation of the term sensitivity. For our purposes the meaning of sensitivity will be derived from an explicit mathematical connection to be made between the final result and the input data used to solve a specific problem. This connection will be related to the adjoint flux $N^*(\bar{\xi})$, which is a solution to the adjoint Boltzmann equation:

$$L^*N^* = S^* \ . \tag{5}$$

Here S* is the adjoint source and L* is the adjoint Boltzmann operator, which for a suitable choice of boundary conditions[8] satisfies the following

well-known inner product relationship:

$$\langle N, L^*N^* \rangle = \langle N^*, LN \rangle . \tag{6}$$

To connect the problem input data included in the operator L to the final result the adjoint source must be chosen to be the response function of interest:

$$S^*(\bar{\xi}) = \Sigma_R(\bar{\xi}) . \tag{7}$$

Sensitivity can now be spoken of in terms of the following inner product relationship involving the adjoint flux:

$$I_x \equiv \langle N^*, L_x N \rangle . \tag{8}$$

Here L_x is some operator in the subset $\{L_x\}$ of the Boltzmann operator L, whose definition and domain determine what input parameters are being studied; the term $L_x N$ is then a source of neutrons arising from the operation denoted by L_x, and I_x, therefore, represents an adjoint weighted production rate of neutrons integrated over all space. The expression defining I_x will be denoted as the integrated sensitivity function.

It will become clearer in the next section how I_x is related to the result R and why Eq. (8) can be referred to as the sensitivity of R to the data included in the operator L_x. Specifically, the interpretation of the adjoint flux as an importance function will be used to make the connection between I_x and R. Some mathematical properties of terms of the form of I_x, in particular the functionals in perturbation theory, will also be discussed.

III. The Adjoint Flux as an Importance Function

The interpretation of the adjoint flux as a function describing the importance of particles contributing to the final result is the underlying physical basis of general sensitivity theory. While many physical arguments can be used to justify such an interpretation,[9] for the purposes of this discussion a brief mathematical explanation of the adjoint flux as a Green's function offers clear justification for its use in this context.

Following a traditional course,[8] the two alternative methods for computing the result R can be derived. The first involves a solution of the

Boltzmann equation for $N(\bar{\xi})$ [see Eq. (2)] with subsequent calculation of the result R using Eq. (1) and a suitable response function Σ_R. A second choice involves solving the adjoint Boltzmann equation for $N^*(\bar{\xi})$ [see Eq. (5)] and then computing R from the following relationship:

$$R = \int_{\bar{\xi}} S(\bar{\xi}) N^*(\bar{\xi}) d\bar{\xi} = \langle S, N^* \rangle \tag{9}$$

The fact that the R computed in this manner is entirely equivalent to that obtained using Eq. (1) is easily demonstrated by multiplying Eq. (2) by $N^*(\bar{\xi})$ and Eq. (5), with $S^* = \Sigma_R$, by $N(\bar{\xi})$, integrating over all phase space $\bar{\xi}$ and subtracting the two resulting equations. Noting that all terms other than those involving S and Σ_R cancel out as a result of the definition of the adjoint operators and suitable boundary conditions, we finally get that:

$$\langle S, N^* \rangle = \langle \Sigma_R, N \rangle \, . \tag{10}$$

From this well-known result it is possible to understand the adjoint flux as a Green's function by simply letting the problem source $S(\bar{\xi})$ be a multi-dimensional delta function. That is, let:

$$S(\bar{\xi}) = \delta(\bar{\xi} - \bar{\xi}_o) \tag{11}$$

in Eq. (9) and combine this result with Eq. (1) to get:

$$R = \int_{\bar{\xi}} \Sigma_R(\bar{\xi}) \, N(\bar{\xi}) d\bar{\xi} = N^*(\bar{\xi}_o) \tag{12}$$

This result clearly demonstrates that $N^*(\bar{\xi}_o)$ quantitatively represents the contribution of particles born at the point $\bar{\xi}_o$ in phase space to the result R. For the case above where particles are born only at $\bar{\xi}_o$, $N(\bar{\xi}_o)$ is numerically equivalent to the total result R. For a distributed source $S(\bar{\xi})$, the linear nature of the Boltzmann operator allows $N^*(\bar{\xi})$ to be used as a Green's function to sum up the contribution of particles born at all point in phase space to arrive at the result R [i.e., R can be computed from Eq. (9)].

Because of this property of the adjoint flux, it can physically be interpreted as an importance function. That is, it is a quantitative

measure of the importance of particles born at any point in phase space in contributing to the final result. This interpretation is quite general in that it can be applied to any problem whose results can be stated in the form of Eq. (1) and whose solution is described by a linear equation with a real-valued adjoint function. In this regard sensitivity analysis, as developed in the next section, has wide ranging applicability in other fields.

IV. Sensitivity Analysis of the Boltzmann Operator

Using the above formalism, we can begin now to answer the first of the two questions central to sensitivity theory--how do we measure the importance of an input parameter in the solution of the Boltzmann equation? To make this determination, the result, as defined in Eq. (9), is rewritten in terms of the Boltzmann operator L defined in Eq. (2). That is:

$$R = \langle N^*, LN \rangle \quad . \tag{13}$$

This alternate formulation of the definition of the result is fundamental to the general approach. From the previous developments on interpreting the adjoint flux as an importance function, it should be clear now that a quantitative assessment of the sensitivity of the result to the data specifying the problem is completely determinable from Eq. (13). The term LN here represents a birth rate for particles in phase space and N*LN their importance in contributing to the final result. Treating the integrand of the inner product in Eq. (12) as a density function describing the birth rate importance per unit volume in phase space, we can define $R(\bar{\xi})$, the differential sensitivity function as follows:

$$R(\bar{\xi}) = N^*LN \tag{14}$$

To answer any specific sensitivity question, therefore, the Boltzmann operator L can be broken down into a subset of operators $\{L_x\}$ and the sensitivity of the result to the parameters contained in any L_x can be determined in integral fashion from Eq. (8) or as a function of phase space position using Eq. (14) with L replaced by L_x. It should be understood here that there is great freedom available in choosing the L_x's for any sensitivity study. It is only the domain of definition of L_x in phase space that limits

the study to a particular set of input data. Thus spatial and angular effects as well as energy-dependent cross-section sensitivity can easily be incorporated into the theory.

To be a bit more specific, a number of important terms in the Boltzmann equation can be used to define the L_x's with an eye toward practical sensitivity applications. Only the analytic aspect of the theory will be discussed here, practical applications of the predictive possibilities being reserved for the discussion in Section V.

A. External Sources.

Clearly, before any use is made of the Boltzmann operator itself, the sensitivity of the result to the external source, S, is readily available from an inspection of Eq. (9). Defining a differential sensitivity function for this term:

$$R_S(\bar{\xi}) = N^*(\bar{\xi})\ S(\bar{\xi}) \tag{15}$$

allows the spatial, angular, and energy dependent specifications of the source to be checked for their importance in arriving at the result R. Here $R_S(\bar{\xi})$ represents the sensitivity of R per unit volume in phase space to the source neutrons born at $\bar{\xi}$. Such a sensitivity function is quite useful in trying to understand the physical mechanisms by which particles go from their point of birth to the point at which they contribute to the result. $R_S(\bar{\xi})$ will clearly define the most important energy, angular, and spatial regions from which source particles emerge and should allow simpler models for specifying the problem to be evaluated. Also worth noting here is the form of Eq. (15) normalized per source particle [i.e., divided by $S(\bar{\xi})$]; the sensitivity function here is simply $N^*(\bar{\xi})$ itself. Since no specific source specification is involved here, $N^*(\bar{\xi})$ is useful for evaluation of the importance of any source spectrum in calculating the result R. This latter application is a familiar motivation for solving the adjoint Boltzmann equation for $N^*(\bar{\xi})$ when faced with a series of problems in which only the source specifications change.

B. Leakage.

Following the example above the sensitivity of the result to streaming leakage from phase space can be investigated with the sensitivity function

$$R_{ST}(\bar{\xi}) = N^*(\bar{\xi})\ \bar{\Omega}\cdot\nabla N(\bar{\xi}) \tag{16}$$

Since this term involves the spatial and angular problem specification data explicitly in the $\bar{\Omega}.\nabla$ operator, it is quite useful for sensitivity studies involving the spatial mesh and angular quadrature and should also shed some light on the mechanisms of transport and slowing down. Certainly, the regions of high leakage will appear as maxima in a plot of Eq. (16) and will indicate streaming paths in space, energy, and angle. The minima, on the other hand, should indicate regions in which slowing down dominates. Particularly useful here are the integrals of $R_{ST}(\bar{\xi})$ over angle, $R_{ST}(\bar{r},E)$, and over space, $R_{ST}(E,\bar{\Omega})$. Both of these latter functions contain valuable information about the importance of each element of the space mesh and angular quadrature as a function of energy. This information can be used to correlate streaming mechanisms with cross section behavior as a function of energy. Improvements in specifying the spatial and angular meshes as well as the cross-section data might well result from studying the sensitivity of the result reflected in these functions

C. Collisions.

In dealing with the collision processes in the Boltzmann equation, two terms are available for sensitivity analysis, one involving the loss of particles from a point in phase space as a result of particle interactions and the other involving double differential cross-section data representing the scattering of particles into a point in phase space. Determining the importance of collision losses is straightforward with the use of the following total cross-section sensitivity function:

$$R_{\Sigma_T,LOSS}(\bar{\xi}) \equiv N^*(\bar{\xi})\ \Sigma_T(\bar{\xi})\ N(\bar{\xi}) \tag{17}$$

The total cross section is used to define the loss function, since any collision at $\bar{\xi}$ removes the particle from that point in phase space.

An integration over all angles in a region of space represented by $\bar{r}_o$ (specifically a spatial region which is homogeneous in material composition), yields an energy-dependent sensitivity function for losses:

$$R_{\Sigma_T,\mathrm{LOSS}}(E) = \int_{\bar{r}_o} \int_{\bar{\Omega}} N^*(\bar{\xi})\ \Sigma_T(\bar{\xi})\ N(\bar{\xi})\ d\bar{\Omega}\ d\bar{r} \tag{18}$$

representing the importance of all collision losses as a function of energy. This latter function is quite useful in pointing out regions in energy where collision processes are very important and, therefore, should aid in selecting energy grids for solving particular problems.

The problem of defining useful sensitivity functions for double differential cross-section data is more difficult to do generally, since particular applications can lead to quite different functions. For instance, the importance of all particles scattering into a point in phase space can be represented by:

$$R_{\Sigma_S,\mathrm{IN}}(\bar{\xi}) \equiv N^*(\bar{\xi}) \int_{\bar{\xi}'} \Sigma_S(\bar{\xi}'\rightarrow\bar{\xi})\ N(\bar{\xi}')\ d\bar{\xi}' \tag{19}$$

where $\bar{\xi}$ represents $\bar{r},E,\bar{\Omega}$ and $\bar{\xi}'$ represents $\bar{r},E',\bar{\Omega}'$ (i.e., different energies and angles at the same spatial position $\bar{r}$). Since most solutions of the transport equation involve an expansion of the scattering transfer cross section, $\Sigma_S(\bar{\xi}'\rightarrow\bar{\xi})$, in Legendre polynomials in $\bar{\Omega}'\cdot\bar{\Omega}$, and the data are taken to be constant over homogeneous material zones, a more useful function is:

$$R^{\ell}_{\Sigma_S,\mathrm{IN}}(E) \equiv \int_{\bar{r}_o} N^*_{\ell}(\bar{r},E) \int_{E'} \Sigma^{\ell}_S(\bar{r},E'\rightarrow E)\ N_{\ell}(\bar{r},E')\ dE'\ d\bar{r} \tag{20}$$

where the ℓ subscripts represent the expansion of the flux and its adjoint in terms of Legendre polynomials $P_{\ell}(\mu)$ in polar angle cosine $\mu = \bar{r}\cdot\bar{\Omega}$. That is

$$N_{\ell}(\bar{r},E) = \int_{\bar{\Omega}} P_{\ell}(\mu)\ N(\bar{r},E,\bar{\Omega})\ d\bar{\Omega} \tag{21}$$

The two functions given in Eqs. (19) and (20), specifically the latter, are ideal for determining the mechanisns of particle slowing down in shielding problems. When either of these functions is broken down into separate terms

for each partial cross section (i.e., elastic, inelastic, etc.), the important mechanisms by which particles lose energy in collision and then contribute to a response should be quite apparent.

In a similar fashion, an alternate double differential sensitivity function can be defined to study the importance of transfer reactions out of any energy region. Using the Legendre polynomial expansion form, we can define an outscattering sensitivity function

$$R^{\ell}_{\Sigma_{S,OUT}}(E) \equiv \int_{\bar{r}_o} \int_{E'} N_{\ell}(E)\ \Sigma^{\ell}_{S}(\bar{r},E\to E')\ N^{*}_{\ell}(E')\ dE' \qquad (22)$$

Here $R^{\ell}_{\Sigma_{S,OUT}}(E)$ represents the cumulative importance of the ℓ^{th} harmonic of all particles scattering out of phase space at energy E; the term, $N_{\ell}(E)\,\Sigma^{\ell}_{S}(\bar{r},E\to E')$ represents a reaction rate for the transfer; and $N^{*}_{\ell}(E')$, the importance of the particle at its final energy E'. This latter form, while equally useful as Eq. (21) for studying slowing down mechanisms, has a more important use in cross section sensitivity analysis as spelled out in the next section. It should be noted that $R^{\ell}_{\Sigma_{S,OUT}}(E)$ is simply an adjoint formulation of $R^{\ell}_{\Sigma_{S,IN}}(E)$, since the adjoint of the Legendre moment of the transfer cross section is simply its transpose in energy. Also, noteworthy is the potential usefulness of both Eqs. (20) and (22) in determining the importance of higher order expansion terms in specifying the scattering transfer cross section in particular applications.

D. Cross-Section Sensitivity Profile.

For specific analysis of the sensitivity of the result to cross-section behavior as a function of energy a combination of previously defined sensitivity functions is needed. Since cross-section data are usually specified in a number of homogeneous regions in any problem and the energy dependence of the data is of paramount concern, a spatial and angular integrated function is of interest. In this light, we can define a sensitivity function for a particular reaction type by combining the functions defined in Eqs. (18) and (22) for handling total cross section losses and

outscattering double differential data, respectively.

If we first define $R_{\Sigma_X}(E)$ as:

$$R_{\Sigma_X}(E) \equiv - \frac{\Sigma_X(E)}{\Sigma_T(E)} R_{\Sigma_T,LOSS}(E) + \sum_{\ell} \left[\frac{2\ell+1}{4\pi} \right] R^{\ell}_{\Sigma_X,OUT}(E) \qquad (23)$$

where the first term represents the total importance of $\Sigma_X(E)$ type collisions in removing a particle from energy E and the second term is the collective gain in importance after emerging from collisions at other energies and angles. The positive and negative signs in front of the terms reflect the effect of such losses or gains of importance on the result. $R_{\Sigma_X}(E)$ then denotes the energy dependence of the total result R for reactions of type $\Sigma_X(E)$ at energy E. A "sensitivity profile" can now be simply defined as a normalized probability density for the sensitivity function given in Eq. (23). That is:

$$P_{\Sigma_X}(E) \equiv R_{\Sigma_X}(E)/R \qquad (24)$$

The normalization allows $P_{\Sigma_X}(E)$ to reflect the fractional sensitivity of the result R to reactions of type $\Sigma_X(E)$ at energy E. If this function is summed over reaction types and spatial zones and a leakage sensitivity profile added to it [i.e., Eq. (16) integrated over $\bar{r}$ and $\bar{\Omega}$ and normalized to R], the integral of the combination over energy will be unity.

Writing out the explicit functional form of $P_{\Sigma_X}(E)$ for a particular reaction type, we get the following:

$$P_{\Sigma_X}(E) = \left[- \int_{\bar{r}_o} \int_{\bar{\Omega}} N^*(\bar{r},E,\bar{\Omega})\, \Sigma_X(\bar{r},E)\, N(\bar{r},E,\bar{\Omega})\, d\bar{r}\, d\bar{\Omega} \right. \qquad (25)$$

$$\left. + \sum_{\ell} \left| \frac{2\ell+1}{4\pi} \right| \int_{\bar{r}_o} \int_{E'} N_{\ell}(\bar{r},E)\, \Sigma^{\ell}_X(\bar{r},E\to E')\, N^*_{\ell}(\bar{r},E')\, dE'\, d\bar{r} \right] \Big/ R$$

Since $\Sigma_X(\bar{r},E)$ is independent of any of the integration variables in this equation and the first term in Eq. (25) is also expandable in Legendre

polynomials, we finally get:

$$P_{\Sigma_x}(E) = \frac{\Sigma_x(E)}{R} \sum_{\ell} \left[\frac{2\ell+1}{4\pi}\right] \int_{\bar{r}_o} d\bar{r} \left[- N_\ell(\bar{r},E)\, N^*{}_\ell(\bar{r},E) + \int_{E'} N_\ell(\bar{r},E)\, f_x^\ell(E\to E')\, N_\ell^*(\bar{r},E')\, dE' \right] \quad (26)$$

Where $\Sigma_x(E) = \Sigma_x(\bar{r}_o,E)$ and $\Sigma_x(\bar{r},E\to E') = \Sigma_x(E)\, f_x^\ell(E\to E')$ in zone $\bar{r}_o$ and $f_x^\ell(E\to E')$ is simply the Legendre moment of the normalized probability for transferring from E to E' by reaction type x. This form is particularly convenient from a computational point of view since spatial integrals of the Legendre moments of the flux appear explicitly as separate terms in the equation. In fact, it is quite useful to define a special function for these terms in a homogeneous spatial region $\bar{r}_o$ in the form of a matrix:

$$M_\ell(E,E') \equiv \int_{\bar{r}_o} N_\ell(\bar{r},E)\, N^*{}_\ell(\bar{r},E')\, d\bar{r} \quad (27)$$

In terms of this function, we can rewrite Eq. (26) in the same homogeneous zone as:

$$P_{\Sigma_x}(E) = \frac{\Sigma_x(E)}{R} \sum_{\ell} \frac{2\ell+1}{4\pi} \left[- M_\ell(E,E) + \int_{E'} f_x^\ell(E\to E')\, M_\ell(E,E')\, dE' \right] \quad (28)$$

Eq. (28) is in a form which is easily used to study cross section sensitivity. Graphical display of $P_{\Sigma_x}(E)$ for all partial cross sections used in a given problem is a great aid in understanding particle transport.[10,11] The most important energy ranges in each partial cross section set under study are clearly identified in such a plot by the maxima in the function $P_{\Sigma_x}(E)$.

V. Predictive Aspects of the Theory

A. Connections with General Perturbation Theory.

The analytic aspects of the theory should now be apparent from both the definitions of the sensitivity functions and their application in

analyzing the Boltzmann transport operator. The other important aspect of the theory is its potential for predicting changes in R as a result of changes in the operators $\{L_x\}$. To demonstrate this capability, the connection between a general sensitivity function $R(\bar{\xi})$ and the principles of perturbation theory will be examined.

The more formal mathematical implications of the definition introduced in Eq. (8) for discussing sensitivity can most easily be developed by showing that such a mathematical form is a first-order functional in general perturbation theory. Starting from Eq. (13):

$$R = \langle N^*, LN \rangle \tag{29}$$

we can define a perturbed problem such that the perturbed flux N' and its adjoint N*', resulting from the perturbed operators L' and L*', respectively, satisfy the following equations:

$$L'N' = S \tag{30}$$

$$L^{*\prime}N^{*\prime} = S^* \tag{31}$$

A result for the perturbed problem can then be found from the expression:

$$R' = \langle N^{*\prime}, L'N' \rangle \tag{32}$$

The relationship between the perturbed result, R', and the unperturbed result, R, can easily be established by letting the perturbation be defined by a series of incremental changes, such that:

$$N' = N + \delta N \tag{33}$$

$$N^{*\prime} = N^* + \delta N^* \tag{34}$$

$$L' = L + \delta L \tag{35}$$

$$L^{*\prime} = L^* + \delta L^* \tag{36}$$

Expanding R' in terms of these quantities, we get:

$$\begin{aligned} R' &= \langle (N^* + \delta N^*), L'N' \rangle \\ &= \langle N^*, L'N' \rangle + \langle \delta N^*, L'N' \rangle \\ &= \langle N^*, L'N' \rangle + \langle \delta N^*, L'N \rangle + \langle \delta N^*, L'\delta N \rangle \end{aligned} \tag{37}$$

Noting that L'N' = LN = S, we can identify the first term in the final form of Eq. (37) simply as the unperturbed result R and rewrite this equation as:

$$R' = R + \langle \delta N^*, L'N \rangle + \langle \delta N^*, L'\delta N \rangle \tag{38}$$

Taking the adjoint of the second term in Eq. (38):

$$\langle \delta N^*, L'N \rangle = \langle N, L^{*\prime} \delta N^* \rangle \tag{39}$$

and noting that $L^{*\prime}N^{*\prime} = L^*N^* = S^*$ such that:

$$L^{*\prime}(N^* + \delta N^*) = L^*N^* \tag{40}$$

and therefore:

$$L^{*\prime}\delta N^* = -(L^{*\prime} - L^*)\, N^* = -\delta L^* N^* \tag{41}$$

We finally get the second term to be:

$$\langle \delta N^*, L'N \rangle = -\langle N, \delta L^* N^* \rangle \tag{42}$$

Taking the adjoint of this result again, the perturbed result can be written simply as:

$$R' = R - \langle N^*, \delta LN \rangle + \langle \delta N^*, L'\delta N \rangle \tag{43}$$

From the standpoint of linear perturbation theory where second-order effects of the form of the third term on the right hand side of Eq. (43) are ignored, we get:

$$R' - R = \delta R \tilde{=} - \langle N^*, \delta LN \rangle \tag{44}$$

It is this relationship that clearly defines the connection between the analytic and predictive aspects of the definition offered in Eq. (8) for discussing sensitivity. If L_x in that equation is defined as the perturbed operator δL, then we can formally write I_x for this case as

$$I_{\delta L} = \langle N^*, \delta LN \rangle \tilde{=} - \delta R \tag{45}$$

The integrated sensitivity function as applied to answering the second fundamental sensitivity question -- how will the solution change as a result to changes in the input data? -- can readily be interpreted as the first-order change in the result arising from the data change specified in δL.

With this formal equivalence having been established, Eqs. (15) through (28), derived in the previous section can be applied to perturbed problems to predict changes in the result. This procedure is particularly powerful when the sensitivity of the result to changes in an operator is viewed as a function of phase space position. For instance, energy-dependent cross-section uncertainties, represented by $\delta\Sigma_x(E)$, can be incorporated into the definition of the sensitivity profile $P_{\Sigma_x}(E)$ given in Eq. (28) such that a graphical display of a first-order approximation to $\delta R_{\Sigma_x}(E)/R$ can be presented. An energy-dependent assessment of the effect of these cross-section uncertainties on the final result is immediately available from such a plot. This function is as useful in determining which cross section uncertainties are important, as is the expression given in Eq. (28) for determining which cross sections are important. A similar strategy can be used to compare diffusion and transport theory calculations simply by specifying the operator in Eq. (16) to be the difference between leakage operators in the two theories (i.e., $\delta L = \bar{\Omega}\cdot\nabla - D(\bar{r},E)\nabla^2$). $D(\bar{r},E)$ here is the diffusion coefficient.

In problems where linear perturbation theory proves to be inadequate for predictive purposes, the definition of the sensitivity function can easily be shown to be compatible with generalized perturbation theory. The result for the perturbed problem, R', as given in Eq. (32), simply leads to a perturbed functional of the form:

$$R' = \langle N^{*\prime},\ L'N' \rangle \tag{46}$$

But since $L'N' = LN = S$, it is formally equivalent to:

$$R' = \langle N^{*\prime}, LN \rangle \tag{47}$$

The only differences between the unperturbed and the perturbed cases is the the use of the perturbed adjoint in computing the function. With this generalization, Eq. (43) can be recast in the following form:

$$R' = R - \langle N^{*\prime}, \delta LN \rangle \tag{48}$$

Here we can readily see that if δL is used for L_x, we can generalize the definition of I_x for a perturbed problem as follows:

$$I_{\delta L} = \langle N^{*\prime}, \delta L N \rangle = -\delta R \tag{49}$$

where $I_{\delta L}$ is exactly equal to δR now.

Thus, graphical representations of any of the sensitivity functions previously derived with suitable changes so as to reflect the behavior of $N^{*\prime}$, can be used to rigorously predict changes in the result as a function of position in phase space.

B. Interpretation in Terms of Partial Derivatives.

In many aspects of optimization theory one seeks to minimize or maximize a certain function using iterative procedures and first-order approximations to the rates of change of the function with respect to the parameters varied in the optimization process. For the purposes of optimizing the procedures for solving the Boltzmann equation with respect to specification of the input data, the rates of change of the result R with respect to the input parameters are important quantities. Within the framework of the sensitivity theory just developed, such partial derivatives are available in some special cases. Fortunately, these cases do include a number of practical problems for which optimization might to contemplated.

One important instance in which derivatives can be obtained from sensitivity theory occurs in the specific case of an operator of the form:

$$LN = \sum_i L_{\alpha_i} N = \sum_i \alpha_i(\xi)\, L_i N \tag{50}$$

where the α_i's are parameters whose sensitivity one is interested in studying, and the L_i's are operators independent of the α_i's. Using generalized perturbation theory, we can develop an expression for δR in terms of such an operator by starting with Eq. (49). Thus, let us introduce a perturbation in a specific region of phase space $\overline{\Delta\xi}$ with a δL defined as follows:

$$\delta L \equiv \begin{cases} \delta\alpha_i(\bar{\xi})\, L_i N & \bar{\xi} - \dfrac{\overline{\Delta\xi}}{2} \leq \bar{\xi} \leq \bar{\xi} + \dfrac{\overline{\Delta\xi}}{2} \\ 0 & \text{Elsewhere} \end{cases} \tag{51}$$

Here, $\bar{\xi} \pm (\overline{\Delta\xi}/2)$ is understood to be of the form $(x \pm \Delta x/2,\ y \pm \Delta y/2,$ etc.). The perturbation in the result will then be given by :

$$\delta R = \int_{\bar{\xi}-(\overline{\Delta\xi}/2)}^{\bar{\xi}+(\overline{\Delta\xi}/2)} N^{*\prime}\delta L N \, d\bar{\xi} \tag{52}$$

If we now assume that $\delta\alpha_i/\alpha_i$ is a constant in the perturbed region, we can rewrite Eq. (52), making use of the definition of the perturbation given in Eq. (51), to get:

$$\delta R = \frac{\delta\alpha_i}{\alpha_i} \int_{\bar{\xi}-(\overline{\Delta\xi}/2)}^{\bar{\xi}+(\overline{\Delta\xi}/2)} N^{*\prime}\alpha_i L_i N d\bar{\xi} \tag{53}$$

This can be rewritten as:

$$\frac{\delta R}{\delta(\ln \alpha_i)\ \overline{\Delta\xi}} = \frac{\int_{\bar{\xi}-(\overline{\Delta\xi}/2)}^{\bar{\xi}+(\overline{\Delta\xi}/2)} N^{*\prime} L_{\alpha_i} N d\bar{\xi}}{\overline{\Delta\xi}} \tag{54}$$

If the perturbed region contains no source singularities then N*LN will be a continuous, bounded function, and we can let $\overline{\Delta\xi}$ approach a differential region in phase space and $\delta\alpha_i/\alpha_i$ approach zero. In this limit, we get

$$\begin{aligned} N^{*\prime} &\to N^* \\ \overline{\Delta\xi} &\to \overline{\partial\xi} \\ \frac{\delta R}{\delta(\ln\alpha_i)} &\to \frac{\partial R}{\partial(\ln\alpha_i)} \end{aligned} \tag{55}$$

and therefore:

$$\frac{\partial R}{\partial(\ln\alpha_i)\ \overline{\partial\xi}} = N^* L_{\alpha_i} N = R_{\alpha_i}(\bar{\xi}) \tag{56}$$

Thus, in this instance the sensitivity function per unit volume in phase space, $R_{\alpha_i}(\bar{\xi})$, is related to the local rate of change of the result with respect to a change in the sensitivity parameter α_i. It is quite useful to note that the form of the sensitivity function for cross-section studies [see Eq. (28)] is included in this special case of multiplicative operators. The derivative form above should allow optimization procedures to be

implemented in the selection of the energy grid used to produce group averaged cross sections in the multigroup transport equation. The α_i's here would represent the group averaged cross section in group i and the error in the result, δR, could be minimized by an appropriate selection of group energy boundaries.

VI. Conclusions

In building a mathematical theory of sensitivity analysis and developing specific tools for analyzing the sensitivity of the Boltzmann equation to its input parameters, new areas of study will hopefully be opened up. The theory outlined in this paper includes the possibility of making analytic studies of the Boltzmann operator to understand the physical processes underlying particle transport. Such studies are made possible by the availability of procedures for analyzing all input data and regions in phase space for their contributions to the solution of a problem. Its compatibility with perturbation theory adds a predictive aspect to the theory which allows an estimation to be made of changes in the result arising from changes in the input data. Considerable progress is possible in the area of optimizing transport calculations as a result of such a combination of analytic and predictive capabilities. In the case of cross-section studies, the detailed outline of actual procedures needed to implement both capabilities, together with the interpretation of the sensitivity function as a local derivative of the result, should prove most useful in this phase of sensitivity analysis.

In summary, using a consistent mathematical basis, sensitivity theory should greatly increase the understanding of what parameters are important in the solution of a problem and what effect approximations have on the result. The physical insight gained from this understanding should enable transport calculations, cross-section measurements, and integral experiments to be made far more efficiently than they are at present.

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