



# Differential Sampling for the Monte Carlo Practitioner

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## Abstract

One of the two methods for performing a perturbation calculation using Monte Carlo simulations is by differential sampling. The fundamental theory of differential sampling in Monte Carlo is well-presented in the literature but algorithms for implementation of the theory are not well-documented. The development of a differential sampling scheme and its implementation from the viewpoint of the Monte Carlo practitioner are presented here. Simplified examples of radiation transport and criticality of a multiplying system are used to illustrate the algorithms for implementation. Notes on applying the same schemes to more complex problems are also discussed. © Elsevier Science Ltd. All rights reserved.

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## 1 Introduction

In Monte Carlo simulation of neutral particle transport, there is often a need to calculate the difference in responses between two cases of the same problem that differ only very slightly from each other. Applying the Monte Carlo method independently to each case and calculating the difference in the two responses is not feasible because the variance of the two calculations may completely hide the actual difference. Hence, the need for Monte Carlo perturbation methods. There are two standard methods for determining the effect of small perturbations in the parameter values on the response calculated by Monte Carlo simulation: (i) correlated sampling and (ii) differential sampling. These methods permit perturbations of only material parameters and not in geometry or dimensions.

In correlated sampling, a Monte Carlo calculation is performed for one case while the transport paths and interactions are assumed to be the same for the second case. The weights of the particles for the second case are calculated at

each transport step and each interaction and are then used to calculate the response for the second case. Since the cases are fully correlated, the correct difference between responses for the two cases can be calculated so long as the second case is only a small perturbation of the first. The latter constraint is a consequence of the result that correlated sampling can have unbounded variance as shown by Rief (1986, 1996).

In differential sampling, the response for the perturbed case is calculated using a truncated Taylor series expansion around the unperturbed parameter values, outside of the Monte Carlo calculation. The required derivatives of the response with respect to the parameters are calculated during the Monte Carlo calculation of the unperturbed case and hence the name “differential sampling”.

By calculating the derivative of a response along with the response itself, differential sampling offers certain benefits over correlated sampling, including:

- Perturbation studies – instead of running the Monte Carlo code multiple times, a base response  $r$  can be calculated as a function of the set of input parameters  $\mathbf{p}$ . If this code also calculates the derivatives of the response with respect to each parameter,  $\frac{\partial r}{\partial p_i}$ , and the second derivatives,  $\frac{\partial^2 r}{\partial p_i \partial p_j}$ , and so on, then the value of the response for a small perturbation of  $\mathbf{p}$  can be found for any set of parameters by a Taylor series expansion. Thus,

$$r(\mathbf{p} + \delta\mathbf{p}) = r(\mathbf{p}) + \sum_i \left( \frac{\partial r}{\partial p_i} \right) \delta p_i + \frac{1}{2} \sum_i \sum_j \left( \frac{\partial^2 r}{\partial p_i \partial p_j} \right) \delta p_i \delta p_j + \dots (1)$$

In practice, the series has to be truncated after a few terms (usually after the second-order terms) and therefore it is only applicable for values of  $(\mathbf{p} + \delta\mathbf{p})$  close to  $\mathbf{p}$ . Correlated sampling calculates all of the perturbed cases along with the reference case – differential sampling calculates the perturbed cases outside of the Monte Carlo code. If a new perturbation case is to be investigated, no more code runs would be required once the the reference case and its derivatives had been found.

- Sensitivity studies – the derivatives  $\frac{\partial r}{\partial p_i}$  can also be used to find the sensitivity of the response to uncertainties in the input parameters. For example, which cross sections affect the response the most and need to be known with the highest accuracy? Differential sampling can reveal this.
- Total error – the uncertainty expressed in most Monte Carlo studies is only the stochastic uncertainty from the calculation. This does not represent the propagated uncertainties from any of the input parameters. With the sensitivities found by differential sampling, the total uncertainty can be stated for a Monte Carlo response.

Differential sampling can be applied to many problems, even eigenvalue problems and can also be used in conjunction with variance reduction techniques.

### 1.1 The Work of Rief

Rief (1984) showed the mathematical basis of the two methods for perturbation studies in Monte Carlo – one based on correlated sampling and the other based on a second-order Taylor series calculation. For both methods, the analysis starts out by expressing the solution to the integral form of the transport equation (where  $\mathbf{x}$  and  $\mathbf{y}$  are the position, energy and direction co-ordinates in 6-D phase space,  $K$  is the scattering kernel,  $S$  is the source term, and  $\mathbf{p}$  is the parameter vector)

$$\Psi(\mathbf{x}; \mathbf{p}) = \int_R \Psi(\mathbf{y}; \mathbf{p}) K(\mathbf{y} \rightarrow \mathbf{x}; \mathbf{p}) d\mathbf{y} + S(\mathbf{x}; \mathbf{p}) \quad (2)$$

with an infinite Neumann series solution given by

$$\begin{aligned} \Psi(\mathbf{x}; \mathbf{p}) &= \sum_{n=1}^{\infty} \int_R \cdots \int_R K(\mathbf{u}_n \rightarrow \mathbf{x}; \mathbf{p}) K(\mathbf{u}_{n-1} \rightarrow \mathbf{u}_n; \mathbf{p}) \cdots \\ &\quad K(\mathbf{u}_1 \rightarrow \mathbf{u}_2; \mathbf{p}) S(\mathbf{u}_1 \rightarrow \mathbf{u}_0; \mathbf{p}) d\mathbf{u}_n \cdots d\mathbf{u}_0 \\ &= \sum_{n=1}^{\infty} \int_R \cdots \int_R \left( \prod_{i=1}^n K_i d\mathbf{u}_i \right) S_0 d\mathbf{u}_0 \end{aligned} \quad (3)$$

The scattering kernels  $K_i$  can be expressed as a collision kernel multiplied by a transport kernel,  $C_i T_i$ . For the Taylor series approach, Rief (1984) then showed that the derivative of the solution to the transport equation with respect to one parameter  $p_j$  can be expressed as a similar infinite series.

$$\frac{\partial \Psi(\mathbf{x}; \mathbf{p})}{\partial p_j} = \sum_{n=1}^{\infty} \int_R \cdots \int_R \left\{ \sum_{i=1}^n \frac{\partial K_i}{K_i \partial p_j} \right\} \left[ \prod_{i=1}^n K_i d\mathbf{u}_i \cdot S_0 d\mathbf{u}_0 \right] \quad (4)$$

This series differs from the original solution series by a term consisting of the sum of the relative derivatives of the scattering kernels (the term in  $\{\}$ ). So, it is apparent that the derivative of a response can be tallied along with the response itself.

Rief (1984) then gave some examples of derivatives with respect to different parameters and some flow charts for the calculation of perturbed cases along with the reference case. Rief's descriptions were quite mathematical and did not easily show how one would apply the method of differential sampling to his own problem.

In a book on uncertainty analysis, Rief (1988) presented a chapter on using the differential sampling to calculate sensitivities for Monte Carlo uncertainty analysis. He showed that there are two sources of uncertainties that must be considered in a Monte Carlo calculation, the uncertainties of the data

combined with the stochastic uncertainty of the calculation itself. A Monte Carlo response set,  $\mathbf{r}$ , calculated as a function of a set of parameters  $\mathbf{p}$  with uncertainties  $\delta\mathbf{p}$  ( $\mathbf{p} = \mathbf{p}^0 + \delta\mathbf{p}$ ), can be expressed as

$$\mathbf{r} = f(\mathbf{p}^0 + \delta\mathbf{p}) + \delta\boldsymbol{\rho} \quad (5)$$

where  $\delta\boldsymbol{\rho}$  represents the stochastic error in the Monte Carlo simulation. A first order Taylor series expansion of the function  $f$  for one of the above responses  $r_i$  in the set  $\mathbf{r}$  would be

$$r_i = f_i(\mathbf{p}^0) + \sum_k \left. \frac{\partial f_i}{\partial p_k} \right|_{\mathbf{p}^0} \delta p_k + \delta\rho_i \quad (6)$$

Letting  $\mathbf{r}^0 = f(\mathbf{p}^0)$  and  $\delta\mathbf{r} = \mathbf{r} - \mathbf{r}^0$ ,

$$\delta r_i = \sum_k \left. \frac{\partial f_i}{\partial p_k} \right|_{\mathbf{p}^0} \delta p_k + \delta\rho_i \quad (7)$$

The partial derivative of the function  $f_i$  with respect to parameter  $p_k$  is the sensitivity of the response to that parameter. So to calculate the uncertainty  $\delta r_i$  in  $r_i$ , the sensitivities must be known. To compute sensitivities, differential operator sampling can be used.

Sarkar and Rief (1996) extended the differential sampling schemes to find the derivatives of the variance with respect to the biasing parameters used in a non-analog game.

### 1.2 The Work of McKinney in MCNP<sup>TM</sup>

MCNP<sup>TM</sup> Version 4B (Briesmeister, 1997) computes perturbations using a first or second order Taylor series approach. The description in the manual is brief and mathematical, which does not give the reader an understanding of how it is really applied to the code. The description follows the earlier work of McKinney (1984; McKinney and Iverson, 1996).

In this version of MCNP<sup>TM</sup>, users can calculate responses to perturbations in to material density, material composition or reaction cross section data. Many perturbations can be done at once. Limitations include the inability to work with point detectors which is expected to be remedied in the next version and a problem with tallies that are based on the parameter of interest. The solution to the second problem has been fixed by a patch first (Densmore, McKinney and Hendricks, 1997) and later as a correction to version 4C (Hess, Hendricks, McKinney and Carter, 1998).

### 1.3 Meeting the Needs of the Practitioner

The Monte Carlo practitioner needs a coherent description of a system of accumulators and tallies used to determine the derivatives of the response with respect to a parameter. The computational schemes must be described in terms of the Monte Carlo game that is being played and not described in terms of the transport equation. They must also be written out in an understandable way. This paper attempts to do this and then illustrate the implementation using two simple examples.

The notation and forms used in this article are similar to those used by Perel *et al.* (1996) in their paper on applying differential sampling to a point detector problem. Their work explained in more detail than the above references how one would implement differential sampling in a code.

A clean approach is used in this paper to explain differential sampling in general following some development by Perel *et al.* (1996). It first describes a Monte Carlo game and then adds differential sampling to it. Hopefully, this approach will serve other Monte Carlo practitioners as well as it did for us in our applications.

## 2 Monte Carlo Games and Derivatives

For the purpose of differential sampling, Monte Carlo particle transport games can be divided into two types:

- games with only one contribution to the response tally per history and
- games with multiple contributions to the response tally in one history.

Even though the first type is really a subset of the second type, it is useful to describe it separately since it is so much simpler. Games are described by a series of random walks, with each step in a history represented by a probability  $P$ .

### 2.1 Simple Games

In a simple game, where only one score to the response tally is made during a history, the response is an average over  $N$  histories of the contributions  $c_i$  from each history  $i$ , weighted by product of the probabilities for the particle

to survive to the  $J^{\text{th}}$  segment of the path, when that contribution is made.

$$\bar{r} = \frac{1}{N} \sum_{i=1}^N \left( c_i \prod_{j=1}^J P_{ij} \right) \quad (8)$$

Of course, the probabilities  $P_{ij}$  are not explicitly calculated and multiplied together to form the product but are instead the result of the various stochastic choices made during the history of  $J$  segments.

An example of this type of game is the determination of the amount of energy escaping from a certain region, where the contribution is  $E$  and the product of the  $P_{ij}$ 's is either 1 (particle escapes) or 0 (particle does not escape). Another example is the determination of the number of particles absorbed in certain region, where the contribution is 1 and the product is either 1 or 0. As each history finishes, the response from that history,  $r_i$  (the contribution multiplied by the product of segment probabilities,  $r_i = c_i \prod_{j=1}^J P_{ij}$ ) is added to a tally and the square of  $r_i$  is added to another tally, for later use in determining the variance of the response.

Most biasing schemes would not fall into this category of basic problems since they tend to make multiple contributions to tallies during one history. In the case of simple biasing games, such as implicit capture applied to the energy escaping problem above, the contribution is the same but the product of the segment probabilities,  $\prod_{j=1}^J P_{ij}$ , is now the current weight of the particle.

### 2.1.1 First Derivatives

For Monte Carlo games of the simple type, the derivative of the final response with respect to any problem parameter  $a$  is

$$\frac{\partial}{\partial a} \bar{r} = \frac{\partial}{\partial a} \left[ \frac{1}{N} \sum_{i=1}^N c_i \prod_{j=1}^J P_{ij} \right] \quad (9)$$

$$= \frac{1}{N} \sum_{i=1}^N c_i \frac{\partial}{\partial a} \prod_{j=1}^J P_{ij} \quad (10)$$

$$= \frac{1}{N} \sum_{i=1}^N \left( c_i \prod_{j=1}^J P_{ij} \right) \left\{ \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial}{\partial a} P_{ij} \right\} \quad (11)$$

which is just the average of each score of the histories,  $r_i$ , multiplied by the sum of the relative derivatives from each segment. As pointed out by Rief (1984), these probabilities are either transport,  $T$ , or collision,  $C$ , probabilities.

Thus,

$$\prod_{j=1}^J P_{ij} = T_{i1} C_{i1} T_{i2} C_{i2} \cdots \quad (12)$$

where the series is terminated in the  $J^{\text{th}}$  segment by either an escape or an absorption. The relative derivatives of the kernels with respect to parameter  $a$  can be easily found. Here it is assumed that for simple games of this type, the contribution  $c_i$  does not depend on the parameter  $a$ . Examples of this type of contribution are counting particles that leave a region or finding the energy incident on a purely absorbing region. If the parameter of interest was density then finding the derivative of dose would not fall into this simple category, since the contribution of dose is related to  $E/\rho V$ , which depends on the parameter of interest.

As the history progresses, an accumulator for the derivative of the segment probabilities with respect to each parameter is kept

$$t_a^i = \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial}{\partial a} P_{ij} \quad (13)$$

At the end of the history, when the history score  $r_i = c_i \prod_{j=1}^J P_{ij}$  (which is just  $r_i = w c_i$ , where  $w$  is the weight) is added to the response tally, the  $t_a^i$  accumulator is multiplied by the history score to get the derivative score,  $q_a^i = r_i t_a^i$ . This derivative score is added to the derivative tally and the square of the derivative score is added the derivative variance tally.

$$A_a = \sum_{i=1}^N q_a^i \quad (14)$$

$$B_a = \sum_{i=1}^N (q_a^i)^2 \quad (15)$$

At the end of the game, just like the response, the final value of the derivative of the response with respect to  $a$  and its standard deviation can be found

$$\frac{\partial}{\partial a} \bar{r} = \frac{1}{N} A_a \quad (16)$$

$$\sigma_{\partial \bar{r} / \partial a} = \sqrt{\frac{1}{N} \left[ \frac{1}{N} B_a - \left( \frac{\partial}{\partial a} \bar{r} \right)^2 \right]} \quad (17)$$

The real key to differential sampling is then finding the expressions for relative derivatives  $\frac{1}{P_{ij}} \frac{\partial}{\partial a} P_{ij}$  for both the collision and transport kernels for every parameter  $a$ .

### 2.1.2 Double Derivatives

Derivatives with respect to any combination of two parameters (including second derivatives) of the Monte Carlo response  $\bar{r}$  can also be calculated. For the simple Monte Carlo game, the double partial derivative of the response with respect to parameters  $a$  and  $b$  is

$$\frac{\partial}{\partial b} \frac{\partial}{\partial a} \bar{r} = \frac{1}{N} \sum_{i=1}^N c_i \frac{\partial}{\partial b} \frac{\partial}{\partial a} \prod_{j=1}^J P_{ij} \quad (18)$$

$$= \frac{1}{N} \sum_{i=1}^N \left( c_i \prod_{j=1}^J P_{ij} \right) \left\{ \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial^2}{\partial a \partial b} P_{ij} - \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial P_{ij}}{\partial a} \frac{1}{P_{ij}} \frac{\partial P_{ij}}{\partial b} + \left( \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial}{\partial a} P_{ij} \right) \left( \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial}{\partial b} P_{ij} \right) \right\} \quad (19)$$

From above, it appears that four accumulators are needed for the history:

$$t_{1,a,b}^i = \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial^2 P_{ij}}{\partial a \partial b} \quad (20)$$

$$t_{2,a,b}^i = \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial P_{ij}}{\partial a} \frac{1}{P_{ij}} \frac{\partial P_{ij}}{\partial b} \quad (21)$$

$$t_a^i = \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial P_{ij}}{\partial a} \quad (22)$$

$$t_b^i = \sum_{j=1}^J \frac{1}{P_{ij}} \frac{\partial P_{ij}}{\partial b} \quad (23)$$

Notice that  $t_a^i$  and  $t_b^i$  are already being kept for the first derivative calculation, so there are really only two additional accumulators that are needed for each second derivative. The notation  $t_{1,a,b}^i$  and  $t_{2,a,b}^i$  is to indicate that two types of sums need to be totaled in order to calculate a double derivative.

At the end of each history, these accumulators and the history score,  $r_i = c_i \prod_{j=1}^J P_{ij}$  (computed as  $r_i = wc_i$ ), are used to find the double derivative score for this history as

$$q_{a,b}^i = (r_i) \left\{ t_{1,a,b}^i - t_{2,a,b}^i + t_a^i t_b^i \right\} \quad (24)$$

When the response scores for the history are added to their tallies and the derivative scores are added to theirs, each double derivative score is then added to its two tallies,

$$A_{a,b} = \sum_{i=1}^N q_{a,b}^i \quad (25)$$

$$B_{a,b} = \sum_{i=1}^N (q_{a,b}^i)^2 \quad (26)$$

where the first tally is for the double derivative and the second tally is for the variance of the double derivative. In addition to the relative derivative expressions for the  $T$  and  $C$  kernels, the relative double derivatives must also be found.

## 2.2 Multi-Contribution Games

The second type of Monte Carlo game is where multiple contributions to the response tally are made during a history. Each segment  $j$  of history  $i$  makes some contribution,  $c_{ij}$ , weighted by the product of segment probabilities up to that point.

$$\bar{r} = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J c_{ij} \prod_{k=1}^j P_{ik} \quad (27)$$

where  $J$  is the total number of segments in the history. Unlike the simple Monte Carlo game strategy we have so far discussed, the contribution  $c_{ij}$  here is treated as being dependent on the parameter of interest. As the history progresses, the contributions are added not to the main response tally, but to a subtally. At the end of the history, the subtally value is added to the main tally and the square of the subtally value is added to the variance tally.

An example of a game like this would be the calculation of flux by the path-length estimator. Each time the particle crosses a region, the path length (the contribution  $c_{ij}$ ) multiplied by the product of the segment probabilities up to this point,  $\prod_{k=1}^j P_{ik}$ , is added to some subtally. The product is equal to  $w$ , the current weight of the particle (or 1 if no variance reduction methods have been employed). As the history continues, if the particle again crosses the same region, the new path length multiplied by the current weight is added to the subtally. At the end of the history, the subtally value is added to the main response tally and the square of the subtally is added to the variance tally.

The game description above can also be used for games where splitting or point detectors are being used. When a particle is at a given point in the history, the contribution to a point detector or a last flight estimation is made, and then the history continues on. The methods to calculate derivatives for these biased Monte Carlo games are the same as for the basic games.

### 2.2.1 First Derivatives

For a multi-contribution Monte Carlo game, the derivative of a response with respect to parameter  $a$  is

$$\frac{\partial}{\partial a} \bar{r} = \frac{\partial}{\partial a} \left[ \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J c_{ij} \prod_{k=1}^j P_{ik} \right] \quad (28)$$

$$= \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J \left( c_{ij} \prod_{k=1}^j P_{ik} \right) \left\{ \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial}{\partial a} P_{ik} \right\} \quad (29)$$

As mentioned earlier, the values of  $P_{ik}$  are not necessarily calculated but are the result of the events that happen during the history. With each path segment, the response for the segment  $r_{ij} = c_{ij} \prod_{k=1}^j P_{ik}$  is calculated in the code as  $r_{ij} = w c_{ij}$  and is added to the response sub tally. At the same time, a sub tally  $q_a^i$  for the derivative is also updated with the derivative score for that segment

$$q_a^i = \sum_{j=1}^J (r_{ij}) \left\{ \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t_a^{ij} \right\} \quad (30)$$

where  $t_a^{ij}$  is the current value of the relative segment probability derivative accumulator up to this segment,

$$t_a^{ij} = \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial}{\partial a} P_{ik} \quad (31)$$

In addition to the relative derivative of the kernels, the relative derivative of the contribution  $c_{ij}$  needs to be found.

At the end of the history, the response sub tally is added to the main response tally and its square is added to its associated variance tally. Also, each derivative sub tally is added to the main derivative tally and its square is added to a variance tally by calculating

$$A_a = \sum_{i=1}^N q_a^i \quad (32)$$

$$B_a = \sum_{i=1}^N (q_a^i)^2 \quad (33)$$

At the end of the game,  $A_a$  is used for finding the first derivative (the sensitivity) with respect to parameter  $a$  and  $B_a$  is used for finding the variance of the first derivative.

### 2.2.2 Double Derivatives

The double partial derivative with respect to parameters  $a$  and  $b$  of the response of a multi-contribution game is

$$\frac{\partial}{\partial b} \frac{\partial}{\partial a} \bar{r} = \frac{\partial}{\partial b} \frac{\partial}{\partial a} \left[ \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J c_{ij} \prod_{k=1}^j P_{ik} \right] \quad (34)$$

$$\begin{aligned} &= \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J \left[ \left( c_{ij} \prod_{k=1}^j P_{ik} \right) \left\{ \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial^2}{\partial a \partial b} P_{ik} \right. \right. \\ &\quad - \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial P_{ik}}{\partial a} \frac{1}{P_{ik}} \frac{\partial P_{ik}}{\partial b} \\ &\quad + \left( \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial}{\partial a} P_{ik} \right) \left( \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial}{\partial b} P_{ik} \right) + \frac{1}{c_{ij}} \frac{\partial^2}{\partial a \partial b} c_{ij} \\ &\quad + \left( \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} \right) \left( \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial}{\partial b} P_{ik} \right) + \\ &\quad \left. \left. + \left( \frac{1}{c_{ij}} \frac{\partial}{\partial b} c_{ij} \right) \left( \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial}{\partial a} P_{ik} \right) \right\} \right] \quad (35) \end{aligned}$$

which can be more conveniently expressed as

$$\begin{aligned} \frac{\partial}{\partial b} \frac{\partial}{\partial a} \bar{r} &= \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J \left[ (r_{ij}) \left\{ t_{1,a,b}^{ij} - t_{2,a,b}^{ij} + t_a^{ij} t_b^{ij} + \frac{1}{c_{ij}} \frac{\partial^2}{\partial a \partial b} c_{ij} \right. \right. \\ &\quad \left. \left. + t_a^{ij} \frac{1}{c_{ij}} \frac{\partial}{\partial b} c_{ij} + t_b^{ij} \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} \right\} \right] \quad (36) \end{aligned}$$

where the two new accumulators (type 1 and type 2) are

$$t_{1,a,b}^{ij} = \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial^2}{\partial a \partial b} P_{ik} \quad (37)$$

$$t_{2,a,b}^{ij} = \sum_{k=1}^j \frac{1}{P_{ik}} \frac{\partial P_{ik}}{\partial a} \frac{1}{P_{ik}} \frac{\partial P_{ik}}{\partial b} \quad (38)$$

and are used with their values up to the current segment. During the history, every time the response subally is updated with the response score, the subally for each double partial derivative is updated with the double derivative score

$$\begin{aligned} q_{a,b}^i &= \sum_{j=1}^J (r_{ij}) \left\{ t_{1,a,b}^{ij} - t_{2,a,b}^{ij} + t_a^{ij} t_b^{ij} \right. \\ &\quad \left. + \frac{1}{c_{ij}} \frac{\partial^2}{\partial a \partial b} c_{ij} + t_a^{ij} \frac{1}{c_{ij}} \frac{\partial}{\partial b} c_{ij} + t_b^{ij} \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} \right\} \quad (39) \end{aligned}$$

using the current values of the  $t_{1,a,b}^{ij}$ ,  $t_{2,a,b}^{ij}$ ,  $t_a^{ij}$ , and  $t_b^{ij}$  accumulators. The relative double partial derivatives of the contributions must also be found.

At the end of the history, when the main tally is updated by adding the response subtally, each double partial derivative subtally is added to the main double partial derivative tally and its square is added to the variance tally.

$$A_{a,b} = \sum_{i=1}^N q_{a,b}^i \quad (40)$$

$$B_{a,b} = \sum_{i=1}^N (q_{a,b}^i)^2 \quad (41)$$

$A_{a,b}$  is then used for finding the double derivative and  $B_{a,b}$  is used for calculating the variance of the double derivative.

The relative derivatives of the contributions and of the transport/collision kernels have not been discussed yet since they are problem-dependent. The easiest way to understand these is through an example. Most problems will have similar  $T$  and  $C$  kernels and the contributions depend on what responses (tallies) one is trying to determine.

### 3 An Example Problem

We shall now implement the above procedure on a simple problem. Consider a sphere with a point source of monoenergetic photons at its center. The sphere is made of a material of density  $\rho$ , with mass attenuation coefficient for scatter  $\mu_s$ , and mass attenuation coefficient for absorption  $\mu_a$ . The total mass attenuation coefficient is  $\mu = \mu_s + \mu_a$ . For simplicity, we assume that the mass attenuation coefficients are not energy-dependent and that scattering is isotropic. We will also assume that a scatter reduces the energy of the photon by 10%. None of these simplifications detract from the methodology we wish to illustrate. For this problem, five responses will be investigated:

- (i) the energy deposited in the sphere
- (ii) the energy escaping the sphere
- (iii) the average flux in the sphere, using the path-length estimator
- (iv) the average flux in the sphere, using the collision density estimator
- (v) the energy arriving at a point detector outside of the sphere

In addition to these five responses, their first derivatives with respect to  $\mu_s$ ,  $\mu_a$  and  $\rho$  will be calculated ( $5 \times 3$  of them), as well as every combination of double derivative ( $5 \times 6$  of them). (Note: For  $n$  parameters, there are  $n(1 + (n - 1)/2)$  unique double derivatives.)

### 3.1 Derivatives of the Kernels

The first step in finding all the derivatives for the above quantities is finding the relative derivatives for the transport,  $T$ , and collision kernels,  $C$ , for each parameter. The kernels for this problem are defined as

$$T = \begin{cases} \rho\mu e^{-\rho\mu s} & \text{interacts within sphere} \\ e^{-\rho\mu s} & \text{escapes from sphere} \end{cases} \quad (42)$$

$$C_s = \frac{1}{4\pi} \frac{\mu_s}{\mu} \quad \text{isotropic scatter to any direction} \quad (43)$$

$$C_a = \frac{\mu_a}{\mu} \quad \text{absorption} \quad (44)$$

where  $s$  is the distance traveled in the sphere material. These are not explicitly calculated in the Monte Carlo code but are integrated into the sampling routines.

The relative derivatives of the transport kernel are

$$\frac{1}{T} \frac{\partial}{\partial \mu_f} T = \begin{cases} 1/\mu - \rho s & \text{interacts within sphere} \\ -\rho s & \text{escapes from sphere} \end{cases} \quad (45)$$

$$\frac{1}{T} \frac{\partial}{\partial \rho} T = \begin{cases} 1/\rho - \mu s & \text{interacts within sphere} \\ -\mu s & \text{escapes from sphere} \end{cases} \quad (46)$$

where  $\mu_f$  is either absorption or scatter. The relative derivative of the collision kernel of type  $g$  with respect to mass attenuation of type  $f$  is

$$\frac{1}{C_g} \frac{\partial}{\partial \mu_f} C_g = \begin{cases} 1/\mu_g - 1/\mu & f = g \\ -1/\mu & f \neq g \end{cases} \quad (47)$$

The relative derivative of either collision kernel with respect to density is zero ( $\frac{1}{C_g} \frac{\partial}{\partial \rho} C_g = 0$ ) since neither collision kernel depends on the density.

The relative double partial derivatives of the transport kernel are

$$\frac{1}{T} \frac{\partial^2}{\partial \mu_f \partial \mu_g} T = \begin{cases} -2\rho s/\mu + \rho^2 s^2 & \text{interacts within sphere} \\ +\rho^2 s^2 & \text{escapes from sphere} \end{cases} \quad (48)$$

$$\frac{1}{T} \frac{\partial^2}{\partial \mu_f \partial \rho} T = \begin{cases} 1/\rho\mu - 3s + \rho\mu s^2 & \text{interacts within sphere} \\ \rho\mu s^2 - s & \text{escapes from sphere} \end{cases} \quad (49)$$

$$\frac{1}{T} \frac{\partial^2}{\partial \rho^2} T = \begin{cases} -2s\mu/\rho + \mu^2 s^2 & \text{interacts within sphere} \\ \mu^2 s^2 & \text{escapes from sphere} \end{cases} \quad (50)$$

The relative double partial derivatives of the collision kernel of type  $h$  with respect to the mass attenuation coefficients of type  $f$  and  $g$  are

$$\frac{1}{C_h} \frac{\partial}{\partial \mu_f \partial \mu_g} C_h = \begin{cases} \frac{2}{\mu^2} - \frac{2}{\mu\mu_h} & f = g = h \\ \frac{2}{\mu^2} - \frac{1}{\mu\mu_h} & f = h \text{ xor } g = h \\ \frac{2}{\mu^2} & f \neq h \text{ and } g \neq h \end{cases} \quad (51)$$

### 3.2 Derivatives of the Contributions

Even though the second response of the five responses in this example problem can be calculated as a Monte Carlo problem of the basic type, all of the responses in this example will be treated as problems of the multi-contribution type. Each response has to be cast into the form of

$$\bar{r} = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J c_{ij} \prod_{k=1}^j P_{ik} \quad (52)$$

For the five responses of this problem, the contributions,  $c_{ij}$ , are

- (i) energy being deposited (current energy  $E$  if absorption, 10% of current energy  $E$  if a scatter reaction).
- (ii) current energy  $E$  that escapes
- (iii) length of track,  $s$ , in the sphere, for each motion
- (iv) 1, for every collision
- (v) for the point detector, where  $D$  is the total distance to the point detector from the current location,  $\hat{\Omega}$  is the direction of travel to the point detector from the current location and  $\hat{n}$  is the unit vector normal to the surface containing the point detector

$$c_{ij} = \begin{cases} E \frac{1}{4\pi D^2} e^{-\rho\mu s} \hat{\Omega} \cdot \hat{n} & \text{source photons} \\ E \frac{\mu_s}{\mu} \frac{1}{4\pi D^2} e^{-\rho\mu s} \hat{\Omega} \cdot \hat{n} & \text{non-source photons} \end{cases} \quad (53)$$

where  $E$  is the energy at the current interaction site.

### 3.3 Algorithm

Implementing the differential sampling scheme for the five responses of this sphere problem is fairly simple. For every response  $r$ , a subtally  $q(r)$  is kept. At the end of each history, the subtallies are added to the main tallies and the squares of the subtallies are added to the main variance tallies. For each combination of response and parameter, a derivative subtally  $q(r, a)$  is kept. Similarly, for every combination of response, parameter  $a$  and parameter  $b$ , a second derivative subtally  $q(r, a, b)$  is kept. At the end of each history, these subtallies are added to the main derivative tallies and their squares are added to the derivative variance tallies.

Independent of the responses, other accumulators are kept. For every parameter  $a$ , the accumulator  $t_a$  is kept as an element of an array  $t(a)$  for the relative derivative of the kernels. For every pair of parameters, the two types of second derivative accumulators  $t_{1,a,b}$  and  $t_{2,a,b}$  are kept in two other arrays,  $t_1(a, b)$  and  $t_2(a, b)$ . These accumulators follow the photon path, similar to the weight of the photon. (Here we have dropped the  $i$  superscript denoting the  $i^{\text{th}}$  history. It is clear that the same accumulators can be cleared and reused with each history.)

During a history, the accumulators  $t_a$ ,  $t_{1,a,b}$  and  $t_{2,a,b}$  are updated at every transport step and collision for every parameter  $a$  and  $b$ . The subtally for a particular response derivative is updated only when the subtally for that response is updated. In general, whenever a subtally for a response is about to be updated, the following also occurs:

- Calculate the segment contribution to the tally (tally number  $Z$ ) as  $c_{ij}$  and set the tally score as the photon weight multiplied by the segment contribution,  $score = wc_{ij}$ .
- Calculate all relative derivatives and double derivatives of  $c_{ij}$ .
- Update the response subtally,  $q(Z) = q(Z) + score$ .
- Update every derivative subtally with respect to every parameter  $a$   $q(Z, a) = q(Z, a) + score * \left( \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \right)$ .
- Update every second derivative subtally,  $q(Z, a, b) = q(Z, a, b) + score * \left( t_1(a, b) - t_2(a, b) + t(a)t(b) + \frac{1}{c_{ij}} \frac{\partial^2}{\partial a \partial b} c_{ij} + t(b) \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \frac{1}{c_{ij}} \frac{\partial}{\partial b} c_{ij} \right)$ .

Note that the current values up to this segment of  $w$ ,  $t(a)$ ,  $t(b)$ ,  $t_1(a, b)$ , and  $t_2(a, b)$  are used here.

A short code was written to demonstrate the implementation of differential sampling for this example problem. Two common variance reduction techniques, implicit capture and the last flight estimator, were also included to show that differential sampling can be compatible with variance reduction

methods if implemented correctly. The full algorithm for one history of the code is given at the end of this article as an appendix.

At the end of a history, the response subtallies are added to the main tallies and the squares of the subtallies are added to the variance tallies. The same procedure is used for the first derivative subtallies and the double derivative subtallies.

After all  $N$  histories of the simulation are complete, the final calculations can be performed. First, the final responses are found by dividing the tally by the number of histories and the associated standard deviation is found. Then the derivatives of the responses are found by dividing the derivative tallies by the number of histories and their standard deviations are calculated.

### 3.4 Final Responses

The above algorithm calculated five quantities, the first derivatives with respect to three variables and every combination of double derivative. The five responses calculated were (per source photon):

- (i) the energy deposited in the sphere
- (ii) the energy escaping the sphere
- (iii) the average path-length through the sphere
- (iv) the average number of collisions in the sphere
- (v) the energy arriving at a point detector

The third and fourth items are now used to calculate the average flux in the sphere by the path-length and collision estimators.

For the path-length estimator, the flux is simply found by dividing by the volume of the sphere. This is also done for its associated variance and for each derivative with respect to any of the parameters.

Calculating the flux from the average number of collisions [ $A(4)$  in the algorithm] is a little more complex since the flux is equal to

$$\phi = \frac{1}{\rho\mu V} A(4) \quad (54)$$

The derivatives can not be simply divided by  $\rho\mu V$ . The derivative of flux with respect to density is really

$$\frac{\partial}{\partial \rho} \phi = \frac{1}{\rho\mu V} \frac{\partial}{\partial \rho} A(4) - \frac{1}{\rho^2\mu V} A(4) \quad (55)$$

$$= \frac{1}{\rho\mu V} A(4, \rho) - \frac{1}{\rho^2\mu V} A(4) \quad (56)$$

and simply dividing the average number of collisions by  $\rho\mu V$  (eq. (54)) would leave out the second term of eq. (56). The expression for the variance of this derivative would also have multiple terms, as would the derivatives (and their associated variances) with respect to the cross section parameters.

The extra term in eq. (56) is not taken into account in the MCNP<sup>TM</sup>4B differential sampling routines and must be added by the user outside of the code, as explained in a report by Densmore *et al.* (1997). The patch must be used for every derivative of a response that depends on a parameter that is in the contribution to that derivative. Version 4C is expected to include the extra term automatically (Hess *et al.*, 1998), if the user indicates that the tally is dependent on the parameter.

### 3.5 A Better Way

With a slight change in the definitions of the segment contributions  $c_{ij}$  for the two flux tallies, the Los Alamos-style correction can be avoided – removing the possibility of an error caused by the user forgetting to set a flag, as he will have to in the next version of MCNP<sup>TM</sup>. This can be done by using definitions for the third and fourth contributions of

- (iii)  $s/V$ , length of track in the sphere divided by the volume
- (iv)  $1/\rho\mu V$ , the ratio of the flux to the collision density

The derivatives of  $c_{ij}$  would then be found and added to every update of the first and double derivatives in the algorithm. For flux from the path-length estimator, only the score changes, since the derivative of  $c_{ij}$  with respect to any of the three parameters is zero. This changed score is then used in the derivative calculations.

For the collision estimator, the derivatives of  $c_{ij}$  are non-zero and must be added into the calculations each time the derivatives are updated. In the algorithm shown in the appendix, this response is only scored once, at the point of an interaction. The new steps of the collision density tally would then be

- New collision tally routine:
  - Calculate the contribution to the collision density tally (tally 4) as  $c_{ij} = 1/(\rho\mu V)$  and set  $score = wc_{ij}$ .
  - Calculate all relative derivatives and relative double derivatives of  $c_{ij}$ .
  - Update the response sub tally,  $q(4) = q(4) + score$ .

- Update every derivative subtotally,  
 $q(4, a) = q(4, a) + score * \left( \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \right)$ .
- Update every second derivative subtotally,  
 $q(4, a, b) = q(4, a, b) + score * \left( t_1(a, b) - t_2(a, b) + t(a)t(b) + \frac{1}{c_{ij}} \frac{\partial^2}{\partial a \partial b} c_{ij} + t(b) \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \frac{1}{c_{ij}} \frac{\partial}{\partial b} c_{ij} \right)$ .

When this strategy is implemented, the variance of the flux is lower than that of calculating an average collision density first and then calculating a flux outside of the history loop. This will be illustrated in the following section.

### 3.6 Results

For the sphere problem, the base case values of  $\rho = 1 \text{ g/cm}^3$ ,  $\mu_s = 1 \text{ cm}^2/\text{g}$ ,  $\mu_a = 1 \text{ cm}^2/\text{g}$ , a radius of 1 cm and an initial energy of 1 (any units) were used. Since there are five responses, fifteen first derivatives and thirty double derivatives, not all of the results can be shown; only a few representative cases are shown.

The first test is to vary one of the parameters and determine if the derivatives calculated by differential sampling correspond to derivatives calculated by using independent Monte Carlo runs with a change in that parameter. Examples are shown in Figs. 1 through 3. All of these runs were for  $10^5$  histories and both implicit capture and the last flight estimator were used. These three, as well as the others not in the figures, show that the differential sampling routine as described above calculates the derivatives with respect to these parameters quite well.

To demonstrate how useful differential sampling can be in perturbation studies, the Monte Carlo code was run independently for cases where the three parameters took on values of  $\rho \in [0.85 \ 1.0 \ 1.15] \text{ g/cm}^3$ ,  $\mu_s \in [0.85 \ 1.0 \ 1.15] \text{ cm}^2/\text{g}$  and  $\mu_a \in [0.85 \ 1.0 \ 1.15] \text{ cm}^2/\text{g}$ . These 27 cases were run for  $5 \times 10^5$  histories with both variance reduction techniques turned on. These were then compared to the responses calculated by a Taylor series expansion using a single run of the Monte Carlo at the base case of the parameters. The single Monte Carlo was run using  $10^6$  histories to ensure that the relative errors in all of the derivatives were small. The comparisons between the ‘true’ calculations (independent Monte Carlo calculations) against the Taylor series calculations are shown in Figs. 4 and 5. In both figures, the second order Taylor series calculations match the independent MC runs very well. The real benefit of using the Taylor series approach is that a whole suite of perturbed cases can be calculated without running another Monte Carlo game, if the response and all of derivatives were saved from the Monte Carlo single run at the base case of parameters.

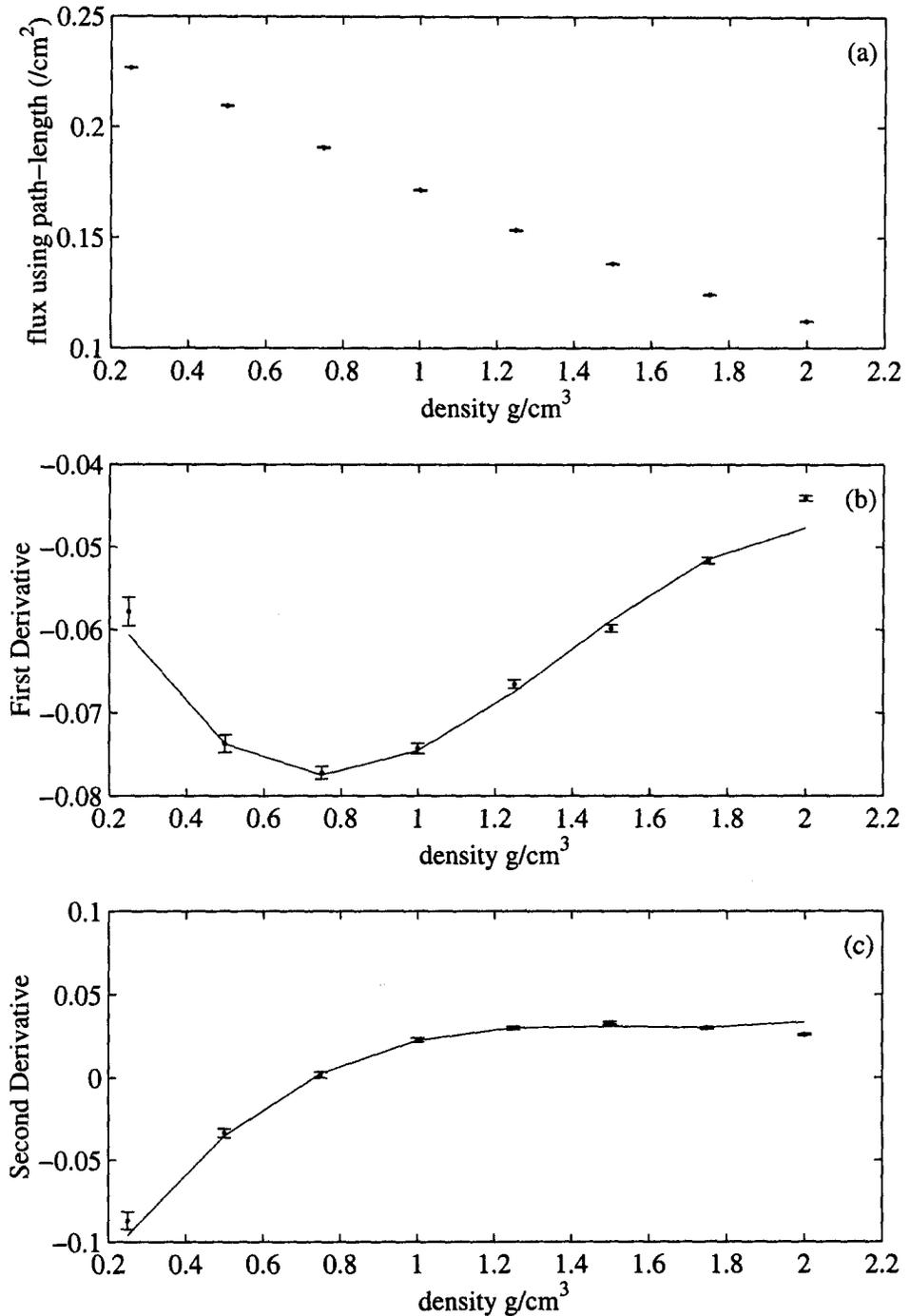


Fig. 1. (a) Flux  $\phi$  in the sphere calculated with the path-length estimator for different values of density. (b)  $\partial\phi/\partial\rho$ . (c)  $\partial^2\phi/\partial\rho^2$ . The points with error bars are from independent Monte Carlo calculations. The lines in (b) and (c) are the derivatives of the curve fit of the MC data points from graphs (a) and (b) respectively.

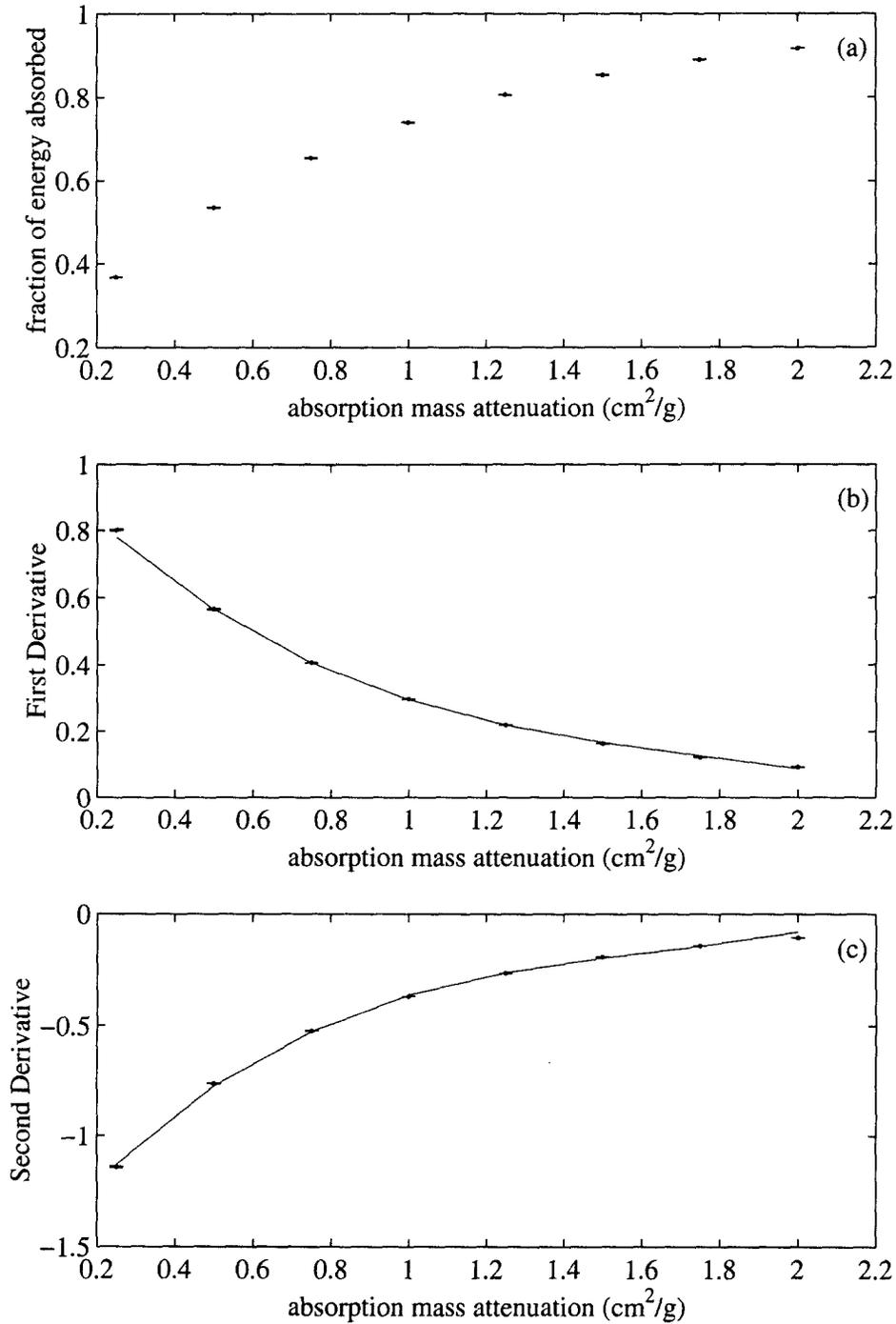


Fig. 2. (a) Energy fraction absorbed,  $E_a$ , in the sphere for different values of absorption mass attenuation. (b)  $\partial E_a / \partial \mu_a$ . (c)  $\partial^2 E_a / \partial \mu_a^2$ . The points with error bars are from independent Monte Carlo calculations. The lines in (b) and (c) are the derivatives of the curve fit of the MC data points from graphs (a) and (b) respectively.

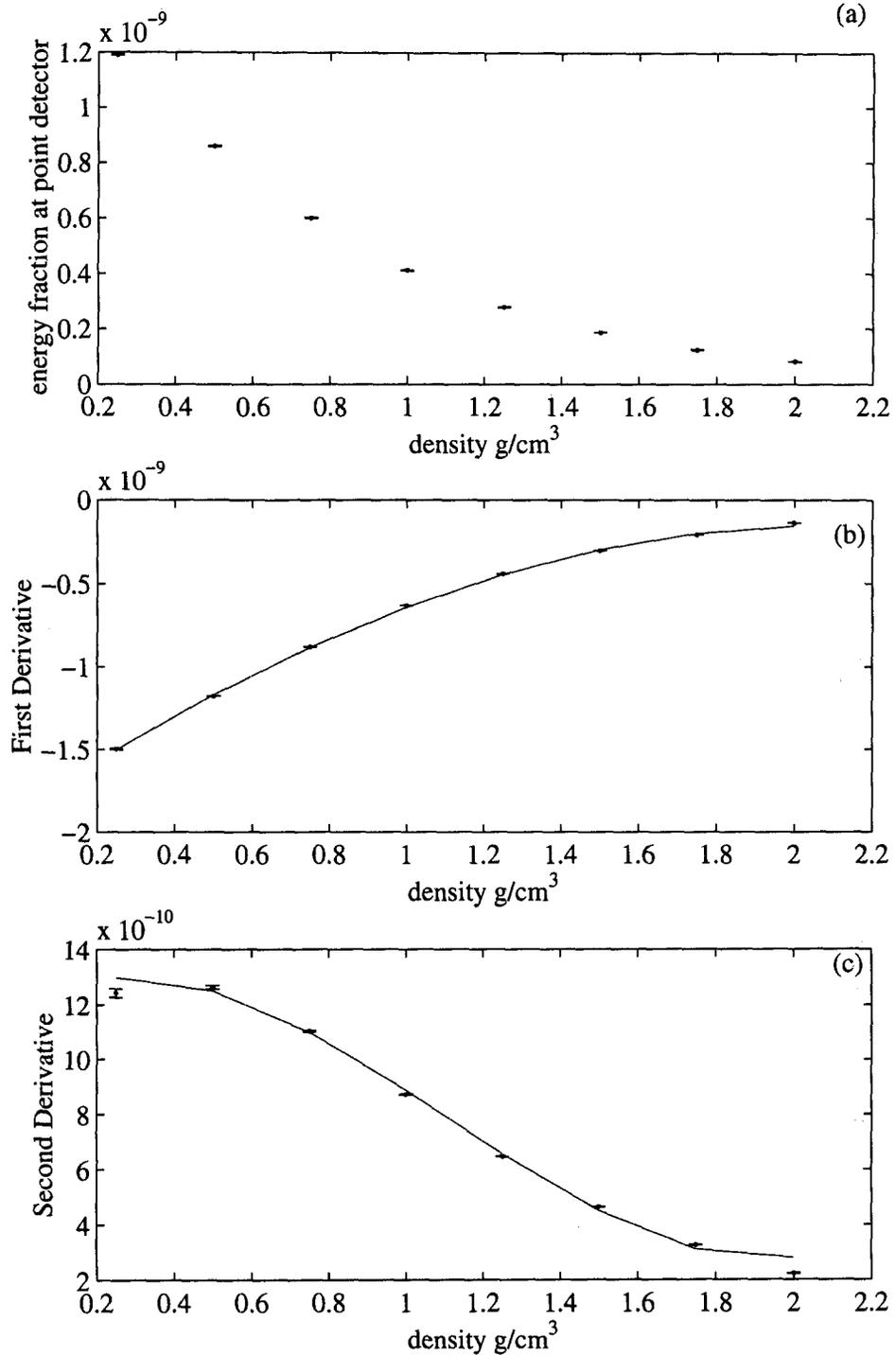


Fig. 3. (a) Energy fraction arriving at a point detector,  $E_p$ , in the sphere for different values of density. (b)  $\partial E_p / \partial \rho$ . (c)  $\partial^2 E_p / \partial \rho^2$ . The points with error bars are from independent Monte Carlo calculations. The lines in (b) and (c) are the derivatives of the curve fit of the MC data points from graphs (a) and (b) respectively.

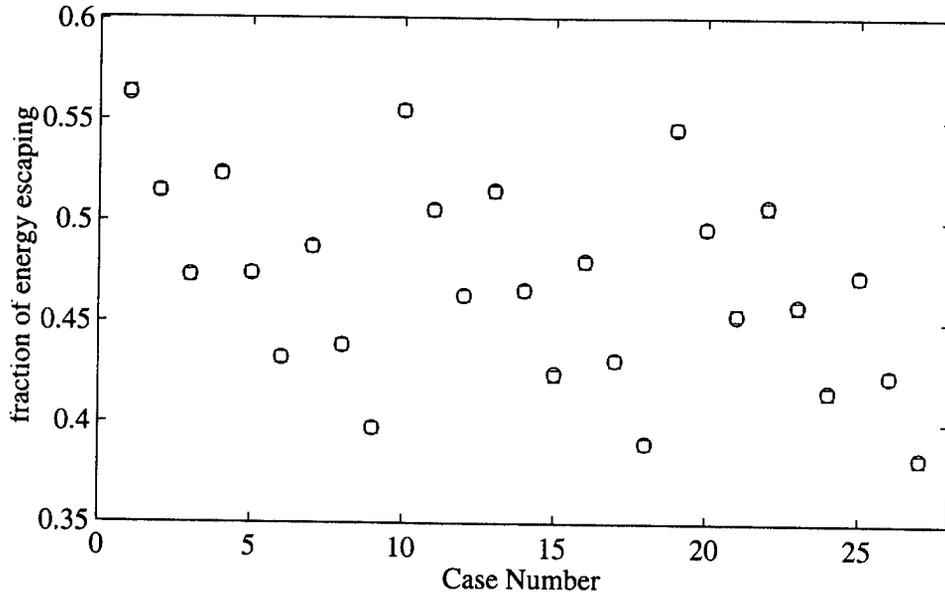


Fig. 4. Comparison of 27 independent Monte Carlo calculations (circles) and values calculated by the second order Taylor series approach (squares) for the fraction of escaping energy. The error bars for both series of points are about the size of these markers.

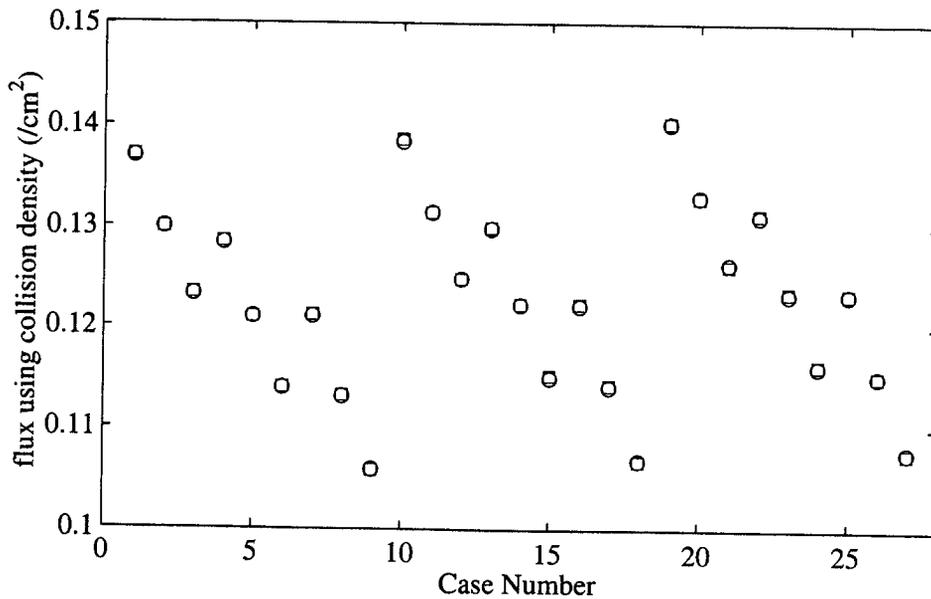


Fig. 5. Comparison of 27 independent Monte Carlo calculations (circles) and values calculated by the second order Taylor series approach (squares) for the flux calculated by the collision density. The error bars for both series of points are about the size of these markers.

One last result for this problem that is worth displaying is the comparison of the relative error in calculating the flux in the sphere by the collision density estimator. Figure 6 shows the flux (collision density estimator) calculated using the Los Alamos approach of correcting after all of the histories have been run and the approach described in this chapter where a slightly more complicated contribution derivative is scored during each segment in the history. Also shown in Fig. 6 is the relative uncertainty for each method. Here, it is assumed that the uncertainty for the Los Alamos approach is calculated by the standard propagation of errors technique, which assumes independence of the two terms. This yields a larger uncertainty value than using the approach described in this paper.

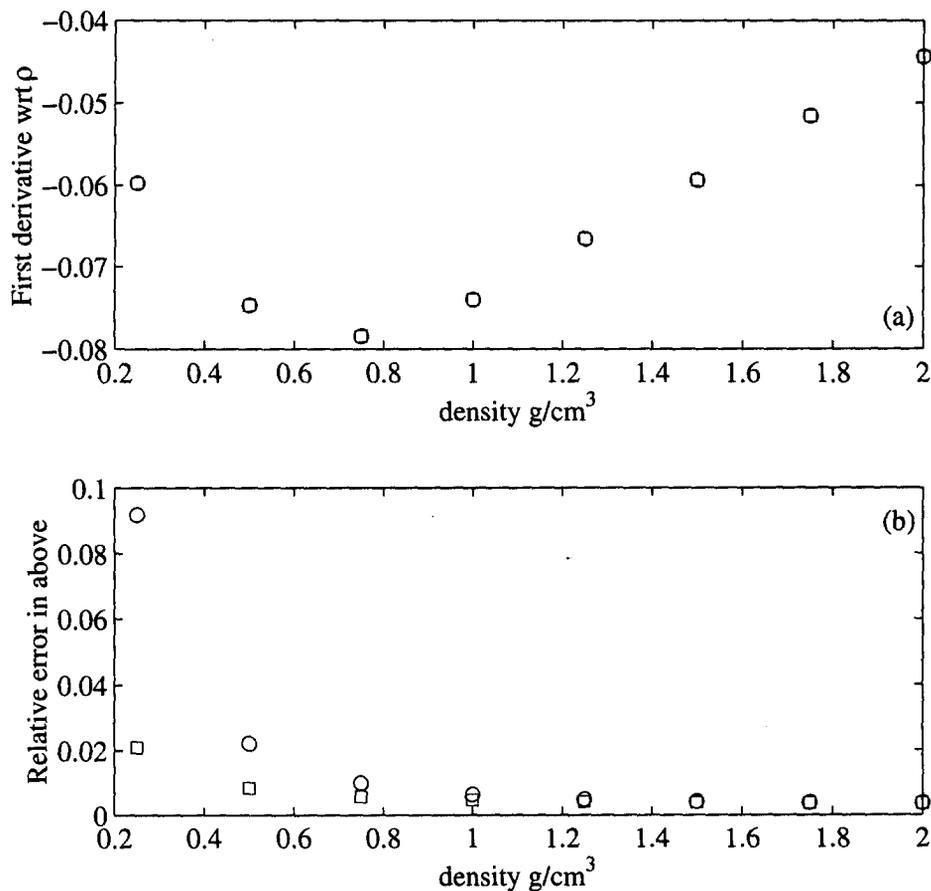


Fig. 6. (a) Comparison of the first derivative of the flux calculated by the collision density estimator. (b) The relative uncertainty by the Los Alamos approach (circles) and by the approach described in this report (squares).

## 4 An Example Criticality Problem

Differential sampling applied to criticality problems can provide some important information and make critical searches much faster. To illustrate this, we will extend the methods outlined in the previous sections to find the derivative of  $k_{\text{eff}}$  with respect to two parameters.

The example we will use is a critical slab problem taken from a series of benchmark calculations (Sood *et al.*, 1999): a slab of thickness  $t = 3.707444$  cm, the number of neutrons per fission of  $\nu = 3.24$ , and macroscopic cross sections for scatter, fission, and radiative capture of  $\Sigma_s = 0.225216$ ,  $\Sigma_f = 0.081600$  and  $\Sigma_c = 0.019584$  /cm. The total cross section is simply  $\Sigma = \Sigma_s + \Sigma_f + \Sigma_c$ .

To demonstrate differential sampling, we will assume that this is a single isotope and that the density  $\rho$  is equal to 1 g/cm<sup>3</sup>. Then  $\Sigma = \rho N_A \sigma / M$ , where  $N_A$  is Avogadro's number,  $\sigma$  is a microscopic cross section and  $M$  is the atomic mass of the isotope. The reason for this is so that the dependence on density can be shown and derivatives with respect to density may be found. This also reduces the problem to the true independent physical quantities: the density and the microscopic cross sections.

We will use this example and calculate the derivative of  $k_{\text{eff}}$  with respect to the slab density and the number of neutrons per fission. The value of  $k_{\text{eff}}$  is calculated in the traditional manner – the number of neutrons produced at each absorption event is kept as a function of space to be used as the source distribution in the next outer iteration. At each absorption the number of fission neutrons expected,  $c_{ij} = \nu \sigma_f / (\sigma_f + \sigma_c)$  is recorded in an array depending on its location in the slab. For this problem, we divided the slab into 20 regions. The number of fission neutrons produced in each of the slab regions is then used as the source term in the next iteration (spatial bins are not usually used in a criticality problem but this will not affect our demonstration). Each iteration started with  $2 \times 10^5$  neutrons and the iteration  $k_{\text{eff}}$  was calculated as the sum of all of the fission neutrons in the various slab regions divided by the number of source neutrons. Starting with a uniform source in the first iteration, about 20 iterations were required before the flux profile had converged. After that, with each iteration an average was made over the next 30 iterations to determine  $k_{\text{eff}}$ . One run of the code for 50 iterations of  $2 \times 10^5$  neutrons took about five minutes on a Sun Ultra 60.

#### 4.1 Derivatives

To apply differential sampling to this problem, the relative derivatives of the transport and collision kernels are needed as well as the relative derivatives of the contribution to the score.

The kernels for this example are defined as

$$T = \begin{cases} \Sigma e^{-\Sigma s} & \text{interacts within slab} \\ e^{-\Sigma s} & \text{escapes from slab} \end{cases} \quad (57)$$

$$C_s = \frac{1}{4\pi} \frac{\sigma_s}{\sigma} \text{ scatter (isotropic to any angle)} \quad (58)$$

$$C_a = \frac{\sigma_f + \sigma_c}{\sigma} \text{ absorption} \quad (59)$$

where  $s$  is the distance traveled in the slab material and  $\sigma = \sigma_s + \sigma_f + \sigma_c$ . Relative derivatives with respect to the two parameters of interest,  $\rho$  and  $\nu$  are

$$\frac{1}{T} \frac{\partial}{\partial \rho} T = \begin{cases} 1/\rho - \Sigma s/\rho & \text{interacts within slab} \\ -\Sigma s/\rho & \text{escapes from slab} \end{cases} \quad (60)$$

$$\frac{1}{T} \frac{\partial}{\partial \nu} T = 0 \quad (61)$$

$$\frac{1}{C_g} \frac{\partial}{\partial \rho} C_g = 0 \quad (62)$$

$$\frac{1}{C_g} \frac{\partial}{\partial \nu} C_g = 0 \quad (63)$$

where  $g$  is either absorption or scatter. The double derivatives are

$$\frac{1}{T} \frac{\partial^2}{\partial \rho^2} T = \begin{cases} -2\Sigma s/\rho^2 + (\Sigma s/\rho)^2 & \text{interacts within slab} \\ (\Sigma s/\rho)^2 & \text{escapes from slab} \end{cases} \quad (64)$$

$$\frac{1}{T} \frac{\partial^2}{\partial \nu^2} T = 0 \quad (65)$$

$$\frac{1}{T} \frac{\partial^2}{\partial \rho \partial \nu} T = 0 \quad (66)$$

$$\frac{1}{C_g} \frac{\partial^2}{\partial \rho^2} C_g = 0 \quad (67)$$

$$\frac{1}{C_g} \frac{\partial^2}{\partial \nu^2} C_g = 0 \quad (68)$$

$$\frac{1}{C_g} \frac{\partial^2}{\partial \rho \partial \nu} C_g = 0 \quad (69)$$

The relative derivatives of the contribution  $c_{ij} = \nu\sigma_f/(\sigma_f + \sigma_c)$  are also easily found to be

$$\frac{1}{c_{ij}} \frac{\partial}{\partial \rho} c_{ij} = 0 \quad (70)$$

$$\frac{1}{c_{ij}} \frac{\partial}{\partial \nu} c_{ij} = 1/\nu \quad (71)$$

and the relative double partial derivatives are

$$\frac{1}{c_{ij}} \frac{\partial^2}{\partial \rho^2} c_{ij} = 0 \quad (72)$$

$$\frac{1}{c_{ij}} \frac{\partial^2}{\partial \nu^2} c_{ij} = 0 \quad (73)$$

$$\frac{1}{c_{ij}} \frac{\partial^2}{\partial \nu \partial \rho} c_{ij} = 0 \quad (74)$$

## 4.2 Algorithm

Including differential sampling into this example criticality code was very similar to the previous example with the additional steps of averaging the Monte Carlo calculated derivatives over the many iterations of the outer loop. As fission neutrons are created in each of the regions of the slab, a score of  $c_{ij} = \nu\sigma_f/(\sigma_f + \sigma_c)$  is made to the tally for that region. At the same time, derivative scores are added to derivative tallies and double derivative scores are added to the double derivative tallies. These derivative scores include the relative derivatives of the transport/collision kernels and the relative derivatives of the contribution.

After all of the histories of one outer iteration are done, the total number of fission neutrons in all of the slabs are added together and then divided by the number of source neutrons, giving  $k_{\text{eff}}$ . In the same manner, the derivative tallies in each slab region are also added together and divided by the number of source neutrons to give the derivatives of  $k_{\text{eff}}$  with respect to the parameters.

Over the many iterations, the values of  $k_{\text{eff}}$ ,  $\partial k_{\text{eff}}/\partial \rho$ ,  $\partial k_{\text{eff}}/\partial \nu$ , etc. are then averaged to give values with smaller variances than just a single iteration alone.

### 4.3 Results

Using the values listed above which should result in an exactly critical system, a single run of the code calculated the following values:

$$k_{\text{eff}} = 0.9995 \pm 0.0028 \quad (75)$$

$$\frac{\partial}{\partial \rho} k_{\text{eff}} = 0.6760 \pm 0.0041 \text{ cm}^3/\text{g} \quad (76)$$

$$\frac{\partial}{\partial \nu} k_{\text{eff}} = 0.3085 \pm 0.0009 \quad (77)$$

$$\frac{\partial^2}{\partial \rho^2} k_{\text{eff}} = -0.3746 \pm 0.0082 \text{ cm}^6/\text{g}^2 \quad (78)$$

$$\frac{\partial^2}{\partial \nu^2} k_{\text{eff}} = 0 \quad (79)$$

$$\frac{\partial^2}{\partial \nu \partial \rho} k_{\text{eff}} = 0.2086 \pm 0.0013 \text{ cm}^3/\text{g} \quad (80)$$

To test the derivatives, the critical slab problem was run at various densities, from 40% below normal to 40% above normal. These independent Monte Carlo calculations of  $k_{\text{eff}}$  were then compared to values estimated by a truncated Taylor series using the values of  $k_{\text{eff}}$ ,  $\partial k_{\text{eff}}/\partial \rho$  and  $\partial^2 k_{\text{eff}}/\partial \rho^2$  all calculated at  $\rho = 1 \text{ g/cm}^3$ . The results are shown in Fig. 7. This figure shows two things: (i) the calculated values of the first and second derivatives are correct and (ii) a second order Taylor series approximation fits the independent calculations very well, even to  $\pm 40\%$  of the base value. The zeroth order Taylor series is shown in the figure so that one can easily see the first order change (difference between the dot-dash line and dashed line) and then the second order change (difference between the dashed line and solid line).

It is useful to take the value of the first derivatives and compute the sensitivity of  $k_{\text{eff}}$  to  $\rho$ . This is found to be

$$\frac{\rho}{k_{\text{eff}}} \frac{\partial}{\partial \rho} k_{\text{eff}} = 0.6763 \pm 0.0045 \quad (81)$$

For a 10% increase in density, there would be about a 6.8% increase in  $k_{\text{eff}}$ . It can also be interpreted to say that a 1% uncertainty in the value of density will give an uncertainty of 0.68% in  $k_{\text{eff}}$ . Combined with the 0.28% stochastic uncertainty of the Monte Carlo calculation of  $k_{\text{eff}}$ , a 1% uncertainty in  $\rho$  gives a total error of 0.73% in  $k_{\text{eff}}$ .

The accuracy of the computed first and second derivatives of  $k_{\text{eff}}$  with respect to  $\nu$  were also checked by running the code at various values of  $\nu$ . One would expect that since  $\nu$  is the same everywhere in the slab,  $k_{\text{eff}}$  ought to be directly

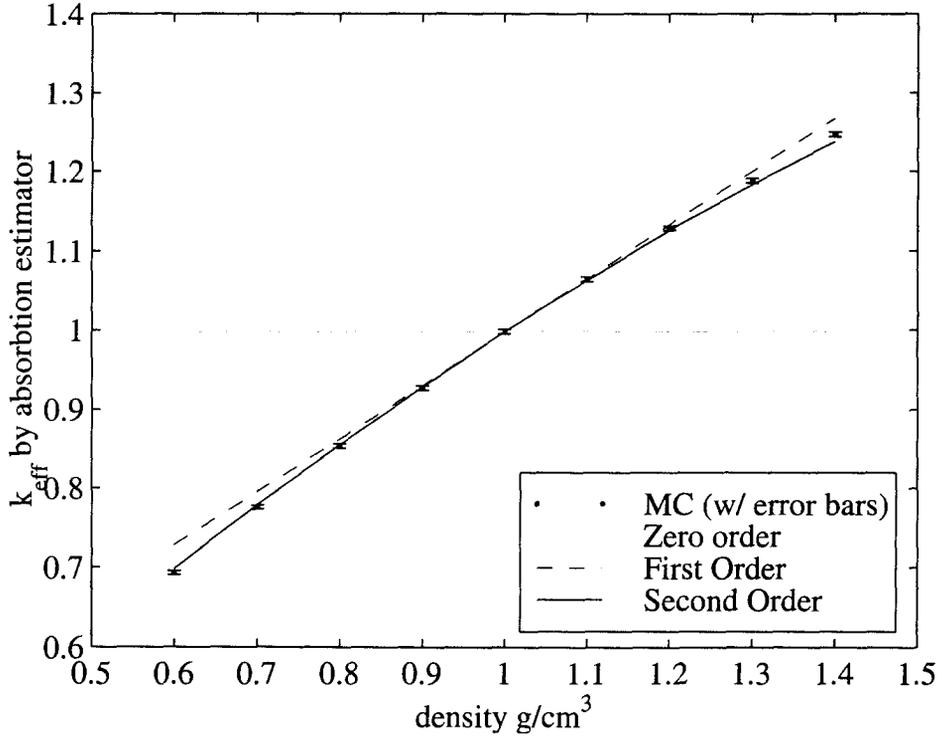


Fig. 7. Comparison of nine independent Monte Carlo calculations of  $k_{\text{eff}}$  and values using  $k_{\text{eff}}$  and its derivatives at  $\rho = 1 \text{ g/cm}^2$  in different order Taylor series calculations.

proportional to  $\nu$ . This is true, as shown in Fig. 8. Calculating the sensitivity of  $k_{\text{eff}}$  to  $\nu$  gives

$$\frac{\nu}{k_{\text{eff}}} \frac{\partial}{\partial \nu} k_{\text{eff}} = 1.000 \pm 0.0040 \quad (82)$$

which also shows that our expectation of direct proportionality was right. (The reason this example was picked, is because it is fairly obvious what the answer should be.) The second derivative found by differential sampling of  $k_{\text{eff}}$  with respect to  $\nu$  is zero, as would be expected since the second derivatives of the  $T$  and  $C$  kernels and of the score contributions with respect to  $\nu$  were all zero.

One result that is not expected is the non-zero value for  $\frac{\partial^2}{\partial \nu \partial \rho} k_{\text{eff}}$ . The double derivative of the two kernels and the contribution are all zero. The derivative has a non-zero value because the score to the sub tally has six terms, only some of which are zero.

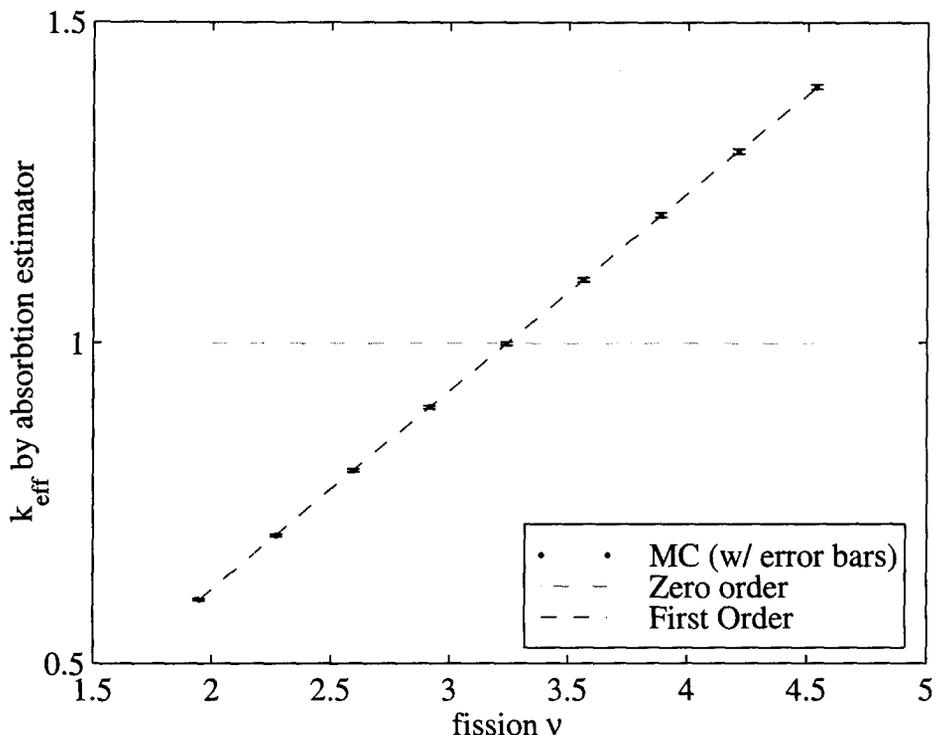


Fig. 8. Comparison of nine independent Monte Carlo calculations of  $k_{\text{eff}}$  and values using  $k_{\text{eff}}$  and its derivatives at  $\nu = 3.24$  in different order Taylor series calculations.

#### 4.4 Critical Searches

Where differential sampling really helps in criticality problems is in the critical search. For example, change the above problem to one where we are trying to find the critical density. Perhaps we guess  $0.8 \text{ g/cm}^3$  and then we calculate  $k_{\text{eff}}$  to be 0.8540. Without differential sampling we would guess a density higher, recalculate, guess again, etc. Perhaps we would use a bisection method to locate the critical density quickly.

If we would have used differential sampling, at  $\rho = 0.8 \text{ g/cm}^3$  we would have also calculated first and second derivatives with respect to density to be  $0.7534 \text{ cm}^3/\text{g}$  and  $-0.4339 \text{ cm}^6/\text{g}^2$ . From these numbers, we could find the change in density required to make the slab critical is  $\delta\rho = 0.206$ . This guess of  $\rho = 1.006$  is very close to the true critical density. With differential sampling, the outer iteration of a critical search can go from a bisection method to a Newton's method (or even better with second derivatives), speeding up the process.

## 5 Hints for More Realistic Problems

The discussion in this paper has focused on explaining differential sampling and showing its implementation on simple problems. In real problems, cross sections are not constant with energy, there is more than one region, etc. These complexities do not prevent differential sampling from being used, they only add to the number of arrays and the accounting in the Monte Carlo code. Three real-world problems will be discussed in this section.

### 5.1 Energy-Dependent Cross Sections

Because cross sections are energy-dependent, trying to find the derivative of a response, such as energy deposited in a region, with respect to a particular cross section could only be done at exactly one specific energy. Another way to look at this problem is this: suppose one did calculate the derivative of response  $r$  with respect to cross section  $p$ . In calculating a truncated Taylor series to do a perturbation study,

$$r(p + \delta p) = r(p) + \left(\frac{\partial r}{\partial p}\right) \delta p + \frac{1}{2} \left(\frac{\partial^2 r}{\partial p^2}\right) (\delta p)^2 + \dots \quad (83)$$

one would find that describing a  $\delta p$  would be difficult since it is a function of energy and the response  $r$  is only a scalar.

One way to work around this problem is by defining the total macroscopic cross section of a region as the sum of the various interaction cross sections for the different possible reactions

$$\Sigma(E) = a_1 \Sigma_1(E) + a_2 \Sigma_2(E) + \dots + a_n \Sigma_n(E) \quad (84)$$

where the constants  $a_i$  are all normally equal to 1. One could then find the derivative of the responses with respect to one of the  $a_i$  constants. This way, the energy dependence problem is avoided and perturbations can be cast in a form of one partial cross section increasing ( $a_1$  going from 1 to 1.1) and another partial cross section decreasing ( $a_2$  going from 1 to 0.9). This system is also easier for the user compared to finding derivatives with respect to relative cross sections ( $\Sigma_i/\Sigma$ ) as others have done (Rief, 1984), since there is no ambiguity about whether or not the total cross section is changing when a study of one of the interaction cross sections is changing – with the above system, eq. (84), it is obvious that the total does change. This system was implemented on a mammography image simulation code and shown to work well (Peplow, 1999).

MCNP (Briesmeister, 1997) has the ability to calculate perturbations on the weight fraction of a certain element in a compound. One should also be careful here since increasing one weight fraction implies that the others are also decreasing. It is not clear from the manual how this is taken into consideration.

## 5.2 Multiple Geometry Regions

For a low-energy photon problem involving multiple geometry regions, the transport kernel can be expressed as

$$T = \rho_M \mu_M \exp\left(-\sum \rho_m \mu_m s_m\right) \quad (85)$$

for a photon that crosses many regions  $m$  with a path length of  $s_m$  in each region and finally interacts in region  $M$ . Using the notation from the previous subsection for the energy-dependent mass attenuation coefficients, the total mass attenuation in each region is

$$\mu_m = a_m^{\text{phot}} \mu_m^{\text{phot}} + a_m^{\text{cohe}} \mu_m^{\text{cohe}} + a_m^{\text{inco}} \mu_m^{\text{inco}} \quad (86)$$

where the values of the  $a_m^i$ 's are 1.

The relative derivative of the transport kernel is then found to be

$$\frac{1}{T} \frac{\partial T}{\partial \rho_m} = \begin{cases} -\mu_m s_m & m \neq M \\ -\mu_m s_m + 1/\rho_m & m = M \end{cases} \quad (87)$$

with respect to any of the region densities. With respect to one of the cross section coefficients,  $a_m^i$ , where the interaction type  $i$  is photoelectric, coherent or incoherent, the relative derivative of the transport kernel is

$$\frac{1}{T} \frac{\partial T}{\partial a_m^i} = \begin{cases} -\rho_m \mu_m^i s_m & m \neq M \\ -\rho_m \mu_m^i s_m + \mu_m^i / \mu_m & m = M \end{cases} \quad (88)$$

The double partial derivatives of the transport kernel can be found to be

$$\frac{1}{T} \frac{\partial}{\partial \rho_m} \frac{\partial}{\partial \rho_n} T = \begin{cases} \mu_m s_m \mu_n s_n & m \neq M, n \neq M \\ \mu_m s_m \mu_n s_n - \frac{\mu_n s_n}{\rho_m} & m = M, n \neq M \\ \mu_m s_m \mu_m s_m - 2 \frac{\mu_m s_m}{\rho_m} & m = n = M \end{cases} \quad (89)$$

$$\frac{1}{T} \frac{\partial}{\partial a_m^i} \frac{\partial}{\partial a_n^j} T = \begin{cases} \rho_m \mu_m^i s_m \rho_n \mu_n^j s_n & m \neq M, n \neq M \\ \rho_m \mu_m^i s_m \rho_n \mu_n^j s_n - \frac{\mu_m^i}{\mu_m} \rho_n \mu_n^j s_n & m = M, n \neq M \\ \rho_m \mu_m^i s_m \rho_m \mu_m^j s_m - 2 \frac{\mu_m^i}{\mu_m} \rho_m \mu_m^j s_m & m = n = M \end{cases} \quad (90)$$

$$\frac{1}{T} \frac{\partial}{\partial a_m^i} \frac{\partial}{\partial \rho_n} T = \begin{cases} \rho_m s_m \mu_n s_n \mu_m^i & m \neq M, n \neq M, m \neq n \\ \rho_m s_m \mu_n s_n \mu_m^i - s_m \mu_m^i & m \neq M, n \neq M, m = n \\ \rho_m s_m \mu_n s_n \mu_m^i - \frac{\mu_n s_n}{\mu_m} \mu_m^i & m = M, n \neq M \\ \rho_m s_m \mu_n s_n \mu_m^i - \frac{\rho_m s_m}{\rho_n} \mu_m^i & m \neq M, n = M \\ \rho_m s_m \mu_m s_m \mu_m^i & \\ -3 s_m \mu_m^i + \frac{\mu_m^i}{\rho_m \mu_m} & m = n = M \end{cases} \quad (91)$$

For neutron problems, a definition similar to eq. (85) for the transport kernel can be made in terms of microscopic cross sections and densities of each region.

### 5.3 Anisotropic Scattering

Another complexity in real problems is that of anisotropic scattering. This does not present a problem for the implementation of differential sampling. Again, for a low-energy photon problem, the scattering kernels can be described as

$$C_{\text{phot}} = \frac{a^{\text{phot}} \mu^{\text{phot}}}{\mu} \quad (92)$$

$$C_{\text{cohe}} = \frac{a^{\text{cohe}} \mu^{\text{cohe}}}{\mu} P^{\text{cohe}}(\Omega \rightarrow \Omega') \quad (93)$$

$$C_{\text{inco}} = \frac{a^{\text{inco}} \mu^{\text{inco}}}{\mu} P^{\text{inco}}(\Omega, E \rightarrow \Omega', E') \quad (94)$$

where the  $P^i$  terms represent the scattering distributions for photons of direction and energy of  $\Omega, E$  to scatter to direction and energy of  $\Omega', E'$ . These probabilities can even include the scattering form factors if they are being used in the simulation.

The relative derivative of the collision kernel for reaction type  $k$  with respect to the cross section multiplier  $a^i$  is (suppressing the  $m$  subscript since collision can only happen inside one region)

$$\frac{1}{C_k} \frac{\partial C_k}{\partial a^i} = \begin{cases} -\mu^i / \mu & i \neq k \\ -\mu^i / \mu + 1/a^i & i = k \end{cases} \quad (95)$$

Since none of the collision kernels depend on the density of the material,  $\frac{1}{C_k} \frac{\partial C_k}{\partial \rho} = 0$ . Derivatives of the collision kernels in one region with respect to a parameter in another region are also 0.

The double partial derivatives of the collision kernels are (again, suppressing the subscript  $m$ )

$$\frac{1}{C_k} \frac{\partial}{\partial a^i} \frac{\partial}{\partial a^j} C_k = \begin{cases} 2 \frac{\mu^i}{\mu} \frac{\mu^j}{\mu} & i \neq k, j \neq k \\ 2 \frac{\mu^i}{\mu} \frac{\mu^j}{\mu} - \frac{\mu^j}{a^i \mu} & i = k, j \neq k \\ 2 \frac{\mu^i}{\mu} \frac{\mu^j}{\mu} - 2 \frac{\mu^i}{a^i \mu} & i = j = k \end{cases} \quad (96)$$

Any double derivative of any of the collision kernels with respect to any density or with respect to  $a_m^i$  from another region are all zero.

## 6 Summary

The number of problems that Monte Carlo can solve can be expanded with the use of differential sampling. Perturbation problems can be performed to at least second-order accuracy without worrying about the large stochastic uncertainties caused by differencing two Monte Carlo solutions. Sensitivities can be accurately computed along with variances of those sensitivities. By using derivative information, criticality searches can be performed faster. With only a little extra coding, the scope of Monte Carlo simulation can be broadened considerably.

The goal of this paper is to elucidate differential sampling in a manner that allows Monte Carlo practitioners to easily implement the methods into their own problems. The computational schemes are described in a manner very similar to how the Monte Carlo game is actually played, as opposed to description in terms of the transport equation. Not every type of photon and neutron problem has been discussed here but with the detailed game descriptions, the kernels and kernel derivative expressions, the two example problems and the sample algorithm in the appendix, practitioners should be able to understand differential sampling and then implement it into their own code for their own specific problem. The methods described here can be expanded to calculate higher order derivatives. We feel that the system presented here is much easier on the code developer than the way differential sampling is presented in the previous literature.

This paper provides examples of simple problems and derivatives with respect to the parameters. Notes on extending these methods to real problems are also given.

One important parameter that is not discussed in this paper is region size. It would be useful to researchers in many fields to be able to find the derivative of responses with respect to a region size. As with correlated sampling, this appears to be a much more difficult problem than calculating responses for perturbations in material parameters.

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## 8 Appendix: Example Code Algorithm

The following is a detailed algorithm for the code in the first example (the point source in a sphere) which computes five responses, fifteen first derivatives and thirty double derivatives. This is only for one history:

- For every response  $r$  ( $r = 1$  through 5) and every parameter combination  $a$  and  $b$ , clear all subtallies:  $q(r) = 0$ ,  $q(r, a) = 0$  and  $q(r, a, b) = 0$ .
- For every parameter combination  $a$  and  $b$ , clear all accumulators:  $t(a) = 0$ ,  $t_1(a, b) = 0$  and  $t_2(a, b) = 0$ .
- Source: select direction of travel,  $\hat{\Omega}$ , set energy  $E = E_0$ , set weight  $w = 1$ .
- Point detector (tally 5) from source
  - Calculate the contribution to the point detector,  $c_{ij}$  and set  $score = wc_{ij}$ .
  - Calculate every  $\frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij}$  and every  $\frac{1}{c_{ij}} \frac{\partial^2}{\partial a \partial b} c_{ij}$ .
  - Update the response sub tally,  $q(5) = q(5) + score$ .
  - Update every derivative sub tally,  $q(5, a) = q(5, a) + score * \left( \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \right)$ .
  - Update every second derivative sub tally,  $q(5, a, b) = q(5, a, b) + score * \left( t_1(a, b) - t_2(a, b) + t(a)t(b) + \frac{1}{c_{ij}} \frac{\partial^2}{\partial a \partial b} c_{ij} + t(b) \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \frac{1}{c_{ij}} \frac{\partial}{\partial b} c_{ij} \right)$ .
- 10 Continue
- Transport - calculate distance to edge  $d$  and pick  $s$ , a distance to travel.
- If last flight estimator=.true., force a portion to leave, force a portion to interact within  $d$ .
  - Calculate the contribution to the energy escaping tally (tally 2) as  $c_{ij} = E \exp(-\rho\mu d)$  and set  $score = wc_{ij}$ .
  - Calculate all relative derivatives and double derivatives of  $c_{ij}$ .
  - Update the response sub tally,  $q(2) = q(2) + score$ .
  - Update every derivative sub tally,  $q(2, a) = q(2, a) + score * \left( \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \right)$ .
  - Update every second derivative sub tally,  $q(2, a, b) = q(2, a, b) + score * \text{(six terms)}$ .
  - Calculate the contribution to the path-length tally (tally 3) as  $c_{ij} = d \exp(-\rho\mu d)$  and set  $score = wc_{ij}$ .
  - Calculate all relative derivatives and double derivatives of  $c_{ij}$ .
  - Update the response sub tally,  $q(3) = q(3) + score$ .
  - Update every derivative sub tally,  $q(3, a) = q(3, a) + score * \left( \frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a) \right)$ .
  - Update every second derivative sub tally,  $q(3, a, b) = q(3, a, b) + score * \text{(six terms)}$ .
  - Re-pick distance  $s$  such that  $s < d$ . Set weight  $w = w(1 - e^{-\rho\mu d})$ .
- If  $s > d$  then (photon escapes)
  - Update every  $t(a)$ , all  $t_1(a, b)$  and all  $t_2(a, b)$  with  $T$  kernel, using  $d$ .
  - Calculate the contribution to the energy escaping as  $c_{ij} = E$  and set  $score = wc_{ij}$ . (Derivatives of  $c_{ij}$  are all zero.)
  - Update the response sub tally,  $q(2) = q(2) + score$ .

- Update every derivative subtotally,  $q(2, a) = q(2, a) + score * t(a)$ .
- Update every sec. der. subtotally,  $q(2, a, b) = q(2, a, b) + score * (t_1(a, b) - t_2(a, b) + t(a)t(b))$ .
- Calculate the contribution to the path-length tally as  $c_{ij} = d$  and set  $score = wc_{ij}$ . (Derivatives of  $c_{ij}$  are all zero.)
- Update the response subtotally,  $q(3) = q(3) + score$ .
- Update every derivative subtotally,  $q(3, a) = q(3, a) + score * t(a)$ .
- Update every sec. der. subtotally,  $q(3, a, b) = q(3, a, b) + score * (t_1(a, b) - t_2(a, b) + t(a)t(b))$ .
- History is over, goto the “clean-up” section.
- Move photon distance  $s$  in direction  $\hat{\Omega}$ .
- Update every  $t(a)$ , all  $t_1(a, b)$  and all  $t_2(a, b)$  with  $T$  kernel and  $s$ .
- Path-length tally:
  - Calculate the contribution to the path-length tally as  $c_{ij} = s$  and set  $score = wc_{ij}$ . (Derivatives of  $c_{ij}$  are all zero.)
  - Update the response subtotally,  $q(3) = q(3) + score$ .
  - Update every derivative subtotally,  $q(3, a) = q(3, a) + score * t(a)$ .
  - Update every sec. der. subtotally,  $q(3, a, b) = q(3, a, b) + score * (t_1(a, b) - t_2(a, b) + t(a)t(b))$ .
- Photon is now at the next interaction site.
- Point detector (PD) – similar to the above PD operations with more complicated  $c_{ij}$ .
- Collision density tally: (Replace this with the code listed in Section 3.5)
  - Calculate the contribution to the collision density tally (tally 4) as  $c_{ij} = 1$  and set  $score = wc_{ij}$ . (Derivatives of  $c_{ij}$  are all zero.)
  - Update the response subtotally,  $q(4) = q(4) + score$ .
  - Update every derivative subtotally,  $q(4, a) = q(4, a) + score * t(a)$ .
  - Update every sec. der. subtotally,  $q(4, a, b) = q(4, a, b) + score * (t_1(a, b) - t_2(a, b) + t(a)t(b))$ .
- If implicit capture=.true. (a portion gets absorbed, a portion scatters)
  - Calculate the contribution to the energy absorbed tally (tally 1) as  $c_{ij} = EC_a$  and set  $score = wc_{ij}$ .
  - Calculate all relative derivatives and double derivatives of  $c_{ij}$ .
  - Update the response subtotally,  $q(1) = q(1) + score$ .
  - Update every derivative subtotally,  $q(1, a) = q(1, a) + score * (\frac{1}{c_{ij}} \frac{\partial}{\partial a} c_{ij} + t(a))$ .
  - Update every second derivative subtotally,  $q(1, a, b) = q(1, a, b) + score * (six terms)$ .
  - Set weight  $w = w\mu_s/\mu$ . Reaction type is set to “scatter”.
- If implicit capture=.false., pick reaction type as either scatter or absorption.
- If reaction type is absorption:
  - Update every  $t(a)$ , all  $t_1(a, b)$  and all  $t_2(a, b)$  with  $C_a$  kernel.
  - Calculate the contribution to the energy absorbed tally as  $c_{ij} = E$  and set  $score = wc_{ij}$ . (Derivatives of  $c_{ij}$  are all zero.)
  - Update the response subtotally,  $q(1) = q(1) + score$ .

- Update every derivative subtally,  $q(1, a) = q(1, a) + score * t(a)$ .
- Update every sec. der. subtally,  $q(1, a, b) = q(1, a, b) + score * (t_1(a, b) - t_2(a, b) + t(a)t(b))$ .
- History is over, goto the “clean-up” section.
- Photon scatters. Update every  $t(a)$ , all  $t_1(a, b)$  and all  $t_2(a, b)$  with  $C_s$  kernel. Pick new  $\hat{\Omega}$ .
- Energy absorbed tally:
  - Calculate the contribution to the energy absorbed tally as  $c_{ij} = 0.1E$  and set  $score = wc_{ij}$ . (Derivatives of  $c_{ij}$  are all zero.)
  - Update the response subtally,  $q(1) = q(1) + score$ .
  - Update every derivative subtally,  $q(1, a) = q(1, a) + score * t(a)$ .
  - Update every sec. der. subtally,  $q(1, a, b) = q(1, a, b) + score * (t_1(a, b) - t_2(a, b) + t(a)t(b))$ .
- Set energy  $E=0.9E$ .
- Russian Roulette – perform for low weights. If history is terminated, deposit the energy in a similar manner as the photon absorption routine.
- Goto 10.

Once a history terminates, some “clean-up” is necessary.

- For every  $r$ , add the response subtally to the main response and variance tally,  $A(r) = A(r) + q(r)$  and  $B(r) = B(r) + (q(r))^2$ .
- Add first derivative subtallies to the first derivative and their variance tallies, for every response  $r$  and every parameter  $a$ ,  $A(r, a) = A(r, a) + q(r, a)$  and  $B(r, a) = B(r, a) + (q(r, a))^2$ .
- Add double derivative subtallies to the double derivative and their variance tallies, for every  $r$  and every pair of parameters  $a$  and  $b$ ,  $A(r, a, b) = A(r, a, b) + q(r, a, b)$  and  $B(r, a, b) = B(r, a, b) + (q(r, a, b))^2$ .

After all  $N$  histories of the simulation are complete, the final calculations can be performed.

- For all of the responses reset  $A(r) = A(r)/N$  and then the variances are calculated as  $\sigma_r^2 = [B(r)/N - (A(r))^2]/N$ . The standard deviation of  $A(r)$  is then  $\sigma_r$ .
- Similarly, for all of the first derivatives, reset  $A(r, a) = A(r, a)/N$  and calculate  $\sigma_{r,a}^2 = [B(r, a)/N - (A(r, a))^2]/N$ .
- Finally, for the second derivatives,  $A(r, a, b) = A(r, a, b)/N$  and calculate  $\sigma_{r,a,b}^2 = [B(r, a, b)/N - (A(r, a, b))^2]/N$ .