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SCORING METHODS FOR IMPLICIT MONTE CARLO
RADIATION TRANSPORT

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January 1981

Lawrence
Livermore
Laboratory

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Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore Laboratory under Contract W-7405-Eng-48.

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Analytical and numerical tests were made of a number of possible methods for scoring the energy exchange between radiation and matter in the implicit Monte Carlo (IMC) radiation transport scheme of Fleck and Cummings.¹ The interactions considered were effective absorption, elastic scattering, and Compton scattering. The scoring methods tested were limited to simple combinations of analogue, linear expected value, and exponential expected value scoring. Only two scoring methods were found that produced the same results as a pure analogue method. These are a combination of exponential expected value absorption and deposition and analogue Compton scattering of the particle, with either linear expected value Compton deposition or analogue Compton deposition. In both methods, the collision distance is based on the total scattering cross section.

*Work performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

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I. INTRODUCTION

In Monte Carlo calculations, many methods may be used for determining how particle energy weights and energy deposition in the medium should be determined, or scored, as a result of energy exchange and scattering processes. In the implicit Monte Carlo (IMC) radiation transport scheme of Fleck and Cummings,¹ these processes include emission, effective absorption, effective elastic scattering, and effective Compton scattering. A scoring method must provide the correct expected values of particle energy, deposited energy, and rates of energy transport, when applied over a sufficiently large number of events, and must do so for arbitrary zone configurations, time step sizes, and variations of cross sections or reaction rates with particle frequency, position, and time.

If several scoring methods satisfy these requirements, one may be chosen on the basis of the variance in the results, the complexity of the calculations, and the requirements for computation time and memory space.

The purpose of this study was to evaluate several possible scoring methods, to verify their accuracy and suitability.

Several types of evaluation were used: (1) Various scoring methods were evaluated for a single flight with a distance limit. (2) The expected values of the number of flights, the particle energy and the energy deposition were evaluated as a function of the total flight distance, for multiple flights with constant cross sections. (3) Numerical calculations were made for a model with multiple flights, a distance limit, and variable cross sections, to find those scoring methods that agree with pure analogue scoring methods.

The results of these evaluations are described below.

II. SCORING METHODS FOR A SINGLE FLIGHT WITH A DISTANCE LIMIT

A. Model System for a Single Flight with a Distance Limit

Assume a particle of initial energy weight E_0 , having a single flight of length $x_{\text{coll}} \leq L$, with collision cross sections $\sigma_A = f\sigma$, $\sigma_S = (1-f)\sigma$, and σ_C for absorption, elastic scattering, and Compton scattering. For simplicity, assume a constant fractional energy loss (or gain) of $f\sigma_{CE}/\sigma_C$ in each Compton collision. The total collision, scattering, and energy exchange cross sections σ_T , σ_{SC} , and σ_E , respectively, are then:

$$\sigma_T = \sigma + \sigma_C = \sigma_A + \sigma_S + \sigma_C \quad (1)$$

$$\sigma_{SC} = \sigma_S + \sigma_C \quad (2)$$

$$\sigma_E = \sigma_A + f\sigma_{CE} = f(\sigma + \sigma_{CE}) \quad (3)$$

The distance to collision, x_{coll} , may be selected from a normalized probability distribution $p(x)$

$$p(x) = \sigma_1 e^{-\sigma_1 x} \quad (4)$$

where σ_1 is a collision cross section in the range from σ_{SC} (to allow sufficient scatters) to σ_T (larger is not necessary)

$$\sigma_{SC} \leq \sigma_1 \leq \sigma_T \quad (5)$$

The selection from $p(x)$ may be done randomly by use of a random number u , in the interval from 0 to 1:

$$x_{coll} = -\frac{1}{\sigma_1} \ln(u) \leq L \quad (6)$$

All values larger than L are reduced to L . The probability of x_{coll} exceeding any given value x' is given by

$$P(x_{coll} > x') = \begin{cases} e^{-\sigma_1 x'}, & x' < L \\ 0, & x' \geq L \end{cases} \quad (7)$$

The particle is advanced to x_{coll} . Along the path, expected value scoring of particle energy weight and energy deposition in the medium may be done. A simple model for scoring the particle energy E and the deposited energy E_d follows:

$$-\frac{dE}{dx} = \sigma_2 E_0 + \sigma_3 E \quad (8a)$$

$$\frac{dE_d}{dx} = \sigma_4 E_0 + \sigma_5 E \quad (8b)$$

Integrating from 0 to x_{coll} , the energies during the flight, but before the collision, E_1 and E_{d1} , are then

$$E_1(x) = E_0 \left[\left(1 + \frac{\sigma_2}{\sigma_3}\right) e^{-\sigma_3 x} - \frac{\sigma_2}{\sigma_3} \right] \quad (9a)$$

$$E_{d1}(x) = E_0 \left[\left(\sigma_4 - \frac{\sigma_2 \sigma_5}{\sigma_3}\right) x + \frac{\sigma_5}{\sigma_3} \left(1 + \frac{\sigma_2}{\sigma_3}\right) (1 - e^{-\sigma_3 x}) \right] \quad (9b)$$

At the end of the flight, if $x_{coll} = L$, no additional change in energy occurs. However, if $x_{coll} < L$, the probabilities of absorption, elastic scattering, or Compton scattering are as follows:

If $\sigma_1 = \sigma_{SC}$:

$$P_A = 0 \quad (\text{must be done along path}) \quad (10a)$$

$$P_S = \sigma_S / \sigma_{SC} \quad (10b)$$

$$P_C = \sigma_C' / \sigma_{SC} \quad (10c)$$

If $\sigma_1 = \sigma_T$:

$$P_A = \sigma_A / \sigma_T \quad (11a)$$

$$P_S = \sigma_S / \sigma_T \quad (11b)$$

$$P_C = \sigma_C / \sigma_T \quad (11c)$$

Any events not scored along the path are scored at the collision, based on the probabilities above, and the energy effect for the event. Assume such analogue events, on the average, remove a fraction k , and deposit a fraction k_d of the particle energy. The final particle and deposited energy, E_2 and E_{d2} , are then

$$E_2 = E_1(x_{\text{coll}})(1 - k) \quad (12a)$$

$$E_{d2} = E_{d1}(x_{\text{coll}}) + E_1(x_{\text{coll}}) k_d \quad (12b)$$

B. Expected Values

The expected values of the collision distance, the final particle energy, and the final deposited energy are as follows:

$$\langle x_{\text{coll}} \rangle = \int_0^L x \sigma_1 e^{-\sigma_1 x} dx + \int_L^\infty L \sigma_1 e^{-\sigma_1 x} dx$$

$$= \frac{1}{\sigma_1} (1 - e^{-\sigma_1 L}) \quad (1)$$

$$\langle E_2 \rangle = \int_0^L E_1(x) (1 - k) \sigma_1 e^{-\sigma_1 x} dx + \int_L^\infty E_1(L) \sigma_1 e^{-\sigma_1 x} dx \quad (2a)$$

$$\langle E_{d2} \rangle = \int_0^L \left[E_{d1}(x) + E_1(x) k_d \right] \sigma_1 e^{-\sigma_1 x} dx + \int_L^\infty E_{d1}(L) \sigma_1 e^{-\sigma_1 x} dx \quad (2b)$$

The correct values of $\langle E_2 \rangle$ and $\langle E_{d2} \rangle$ may be obtained by using pure analogue scoring, with

$$\sigma_1 = \sigma_T \quad (3a)$$

$$\sigma_2 = \sigma_3 = \sigma_4 = \sigma_5 = 0 \quad (3b)$$

$$k = k_d = \frac{\sigma_A}{\sigma_T} + 0 \frac{\sigma_S}{\sigma_T} + \frac{\sigma_{CE}}{\sigma_C} \frac{\sigma_C}{\sigma_T} = \frac{\sigma_E}{\sigma_T} \quad (3c)$$

with the result:

$$\langle E_2 \rangle = E_0 \left[1 - \frac{\sigma_E}{\sigma_T} (1 - e^{-\sigma_T L}) \right] \quad (4a)$$

$$\langle E_{d2} \rangle = E_0 \frac{\sigma_E}{\sigma_T} (1 - e^{-\sigma_T L}) \quad (4b)$$

In addition, the expected value of the rate of energy exchange per unit path length for $0 \leq x \leq L$ is given by (using II.A.4, II.A.7, and II.B.3):

$$\left\langle \frac{dE}{dx} \right\rangle = \left\langle \frac{dE_d}{dx} \right\rangle = E_0 \left(\frac{\sigma_E}{\sigma_T} \right) (\sigma_T e^{-\sigma_T x}) = E_0 \sigma_E e^{-\sigma_T x} \quad (5)$$

C. Some Scoring Methods

Several valid scoring methods for a single flight with a distance limit may be found by carrying out the integrations in Eqs. II.B.2, equating the results to Eqs. II.B.4, and solving for σ_1 , σ_2 , σ_3 , σ_4 , σ_5 , k , and k_d . With the restriction of Eq. II.A.5, and with the simplifying restriction that each of the two energy exchange mechanisms may only be scored by one method (analogue, linear expected value, or exponential expected value), only six scoring methods remain. These are summarized in Table 1, and are all combinations of pure analogue (A), linear expected value (L), exponential expected value absorption (EA), and linear expected value Compton (LC). Method LC is always combined with method EA (EALC). There are four methods in which the particle energy and energy deposition are done the same way, and thus conserve energy exactly. The other two methods for particle/deposition scoring are methods A/L and EA/EALC. These only approach conservation of energy for a large number of events.

Method A can be used in two equivalent forms: either remove fraction k of the particle energy at each collision, or remove all of the energy in fraction k of the collisions, selected randomly. Energy deposition may also be done either way, using parameter k_d . This adds 8 methods to those listed in Table 1, for a total of 14. Also, any linear combination of the methods in Table 1 will be a valid method, allowing an infinite variety of scoring methods for a single flight with a distance limit.

Table 1. Some Methods of Scoring Particle Energy and Deposition on a Single Flight with a Distance Limit.

Method	Collision	Particle			Deposition		
	σ_1	σ_2	σ_3	k	σ_4	σ_5	k_d
A/A	σ_T	0	0	σ_E/σ_T	0	0	σ_E/σ_T
L/L	σ_T	σ_E	0	0	σ_E	0	0
A/L	σ_T	0	0	σ_E/σ_T	σ_E	0	0
EA/EA	σ_{SC}	0	σ_A	$f\sigma_{CE}/\sigma_{SC}$	0	σ_A	$f\sigma_{CE}/\sigma_{SC}$
EALC/EALC	σ_{SC}	$f\sigma_{CE}$	σ_A	0	$f\sigma_{CE}$	σ_A	0
EA/EALC	σ_{SC}	0	σ_A	$f\sigma_{CE}/\sigma_{SC}$	0	σ_E	0

D. Applicability to Multiple Flights

It is not obvious that scoring methods that give the correct expected values for single flights are also correct when applied to multiple flights. A valid method must give the correct dependence of energy flux on both time and position to do transport correctly. The single-flight scoring methods discussed above only give the same expected value of energy at the end of a single flight, which may vary in average length, and therefore in elapsed time, for different scoring methods. For correct transport, the average flight length must be balanced by the probability of scattering at the end of the flight, so that all valid methods produce equivalent results.

If particles also have variable frequencies and cross sections, the scoring method must also produce the correct frequency distribution in space and time. This is most simply determined by numerical tests, to find out which of the simple methods described above are also appropriate for multiple flights with variable parameters. It is also possible that scoring methods exist which do not give the correct expected value for a single flight, but do give the correct expected value for a given flight time or total flight distance.

III. SCORING METHODS FOR MULTIPLE FLIGHTS WITH CONSTANT CROSS SECTIONS

A. The Number of Flights

For a given collision cross section σ and total distance L , the probability $P_n(\sigma, L)$ of n collisions may be calculated for all n :

$$P_0(\sigma, L) = \int_L^{\infty} \sigma e^{-\sigma x} dx = e^{-\sigma L}$$

$$P_1(\sigma, L) = \int_0^L \sigma e^{-\sigma x_1} e^{-\sigma(L-x_1)} dx_1 = \sigma L e^{-\sigma L}$$

$$P_2(\sigma, L) = \int_0^L \left[\sigma e^{-\sigma x_1} \int_0^{L-x_1} \sigma e^{-\sigma x_2} e^{-\sigma(L-x_1-x_2)} dx_2 \right] dx_1$$

$$= \frac{1}{2} (\sigma L)^2 e^{-\sigma L}$$

⋮

$$P_n(\sigma, L) = \frac{1}{n!} (\sigma L)^n e^{-\sigma L} \quad (1)$$

The total probability for all values of n is 1, as required:

$$\sum_{n=0}^{\infty} P_n(\sigma, L) = e^{-\sigma L} \sum_{n=0}^{\infty} \frac{1}{n!} (\sigma L)^n = e^{-\sigma L} e^{\sigma L} = 1 \quad (2)$$

The expected value of the number of collisions required to reach total distance L , $\langle n(\sigma, L) \rangle$, is calculated as follows:

$$\begin{aligned} \langle n(\sigma, L) \rangle &= \sum_{n=0}^{\infty} n P_n(\sigma, L) = e^{-\sigma L} \sum_{n=0}^{\infty} \frac{n}{n!} (\sigma L)^n \\ &= e^{-\sigma L} \sigma L e^{\sigma L} = \sigma L \end{aligned} \quad (3)$$

The average distance of flight per collision $\langle \Delta x_{\text{coll}}(\sigma, L) \rangle$, is given by

$$\langle \Delta x_{\text{coll}}(\sigma, L) \rangle = \frac{L}{\langle n(\sigma, L) \rangle} = \frac{L}{\sigma L} = \frac{1}{\sigma} \quad (4)$$

as expected.

B. Expected Values of the Final Particle Energy and Deposition

The probability of the particle surviving n collisions, or equivalently, the average fraction of the particle energy remaining after n collisions, in the analogue scoring method described above for the single-flight model system, is

$$\langle E_n \rangle = E_0 \left(1 - \frac{\sigma_E}{\sigma_T}\right)^n \quad (1)$$

where σ_T is the total collision cross section, and σ_E is the total energy exchange cross section. For the case of all possible number of flights for which the total distance is L , the expected value of the final energy may be calculated as follows:

$$\begin{aligned} \langle E(L) \rangle &= \sum_{n=0}^{\infty} P_n(\sigma_T, L) \langle E_n \rangle \\ &= E_0 e^{-\sigma_T L} \sum_{n=0}^{\infty} \frac{1}{n!} (\sigma_T L)^n \left(1 - \frac{\sigma_E}{\sigma_T}\right)^n \\ &= E_0 e^{-\sigma_T L} e^{\sigma_T L (1 - \frac{\sigma_E}{\sigma_T})} = E_0 e^{-\sigma_E L} \end{aligned} \quad (2)$$

The expected value of the total deposition is given by:

$$\langle E_d(L) \rangle = E_0 - \langle E(L) \rangle = E_0 (1 - e^{-\sigma_E L}) \quad (3)$$

C. Possible Scoring Methods

The generalization from a single flight to multiple flights, retaining the distance limit and constant cross sections, imposes additional constraints

on the choice of a scoring method. Not only must the scoring method provide the correct expected values of particle energy and energy deposition in the material for any arbitrary distance limit L , but the scattering of the particle must be done in a way that provides the correct transport.

These requirements seem to be satisfied by either of the two analogue methods A1 and A2, in which the collision distance is based on the total cross section σ_T . In method A1, at the collision, absorption, elastic scattering, Compton scattering are selected randomly according to their relative probabilities σ_A/σ_T , σ_S/σ_T and σ_C/σ_T . In method A2, at the collision, fraction σ_A/σ_T of the energy is absorbed, and then either elastic scattering or Compton scattering is selected randomly according to their relative probabilities $\sigma_S/(\sigma_S + \sigma_C)$ and $\sigma_C/(\sigma_S + \sigma_C)$, for the particle with fraction $(1 - \sigma_A/\sigma_T)$ of its initial energy.

The scoring and transport requirements would also seem to be satisfied by a scoring method which uses exponential expected value energy exchange along the path, based on σ_E , since this would satisfy Eqs. III.B.2 and III.B.3, for all values of x and L . The transport requirements would be satisfied by basing collisions on the total scattering cross section σ_{SC} .

Various combinations of analogue and expected value particle energy scoring might also work. For each such combination, various energy deposition scoring methods might work. In principle, each such scoring method could be evaluated by finding the sum of the expected values for all possible numbers of collisions. In practice, if it is required that cross sections be arbitrary functions of particle frequency and position, and that Compton scattering be done more realistically, then rigorous mathematical analysis becomes impractical, except for the pure analogue methods.

IV. SCORING METHODS FOR MULTIPLE FLIGHTS WITH VARIABLE CROSS SECTIONS

A. Model System for Multiple Flights with Variable Cross Sections

Assume a group of particles with various energy weights and frequencies, with collision cross sections σ_A , σ_S , and σ_C for effective absorption, effective elastic scattering, and effective Compton scattering, all functions of frequency ν :

$$\sigma_A = f\sigma(\nu) \quad (1)$$

$$\sigma_S = (1 - f) \sigma(\nu) \quad (2)$$

$$\sigma_C = \sigma_C(\nu) \quad (3)$$

Where f is the Fleck factor, representing the ratio of the net average rate of energy exchange over a time step, to the initial rate, and $\sigma(\nu)$ and $\sigma_C(\nu)$ are arbitrary functions of frequency. Assume that effective elastic scattering scatters the particle frequency to a new value ν_S' with a distribution $p_S(\nu_S')$, while Compton scattering produces a new frequency ν_C' with a distribution $p_C(\nu, \nu_C')$. An explicit Compton scatter also preserves the number of photons, and therefore the ratio of energy weight to frequency, so that an initial energy weight E is changed to E_C' as follows:

$$E_C' = \frac{\nu_C'}{\nu} E \quad (4)$$

$$\langle E_C' \rangle = \langle \frac{\nu_C'}{\nu} \rangle E \quad (5)$$

The expected value of the energy exchange cross section for Compton scattering is then given by:

$$\langle \sigma_{CE} \rangle = \sigma_C \left(1 - \frac{\langle E_C' \rangle}{E} \right) = \sigma_C \left(1 - \langle \frac{\nu_C'}{\nu} \rangle \right) \quad (6)$$

Effective Compton scattering is obtained by multiplying $\langle \sigma_{CE} \rangle$ by f .

The total collision, scattering, and (expected value) energy exchange cross sections σ_T , σ_{SC} , and $\langle \sigma_E \rangle$, respectively are then

$$\sigma_T = \sigma_A + \sigma_S + \sigma_C = \sigma(\nu) + \sigma_C(\nu) \quad (7)$$

$$\sigma_{SC} = \sigma_S + \sigma_C = (1 - f) \sigma(\nu) + \sigma_C(\nu) \quad (8)$$

$$\langle \sigma_E \rangle = \sigma_A + f \langle \sigma_{CE} \rangle = f \sigma(\nu) + f \sigma_C \left(1 - \langle \frac{\nu_C'}{\nu} \rangle \right) \quad (9)$$

In order to do numerical tests, I have used the following absorption and scattering functions:

$$\sigma(\nu) = a(2 - \nu) \quad (10)$$

$$\sigma_C(\nu) = b(2 - \nu) \quad (11)$$

$$p_S(\nu') = p_C(\nu, \nu') = \begin{cases} 1, & 0.5 \leq \nu' \leq 1.5 \\ 0, & \nu' < 0.5, \nu' > 1.5 \end{cases} \quad (12)$$

where a and b are arbitrary constants. For these scattering functions:

$$\langle \frac{\nu_C'}{\nu} \rangle = \frac{1}{\nu} \quad (13)$$

$$\langle \sigma_{CE} \rangle = \sigma_C \left(1 - \frac{1}{\nu} \right) \quad (14)$$

Also, since the scattered frequency is uniformly distributed over the interval from 0.5 to 1.5, the equilibrium frequency distribution $p(x)$ is obtained by requiring that the probability of scattering from each frequency is also uniformly distributed:

$$p(\nu)\sigma_{SC} = \text{constant}, \quad 0.5 \leq \nu \leq 1.5 \quad (15)$$

Substituting from Eqs. III.A.8, III.A.10, and III.A.11 and normalizing:

$$p(\nu) = \left[(2 - \nu) \ln 3 \right]^{-1} \quad (16)$$

The number-average frequency $\bar{\nu}_N$ and the energy-average frequency $\bar{\nu}_E$ are then given by:

$$\bar{\nu}_N = \int_{0.5}^{1.5} \nu p(\nu) d\nu = 2 - \frac{1}{\ln 3} \approx 1.08976 \quad (17)$$

$$\bar{\nu}_E = \frac{1}{\bar{\nu}_N} \int_{0.5}^{1.5} \nu^2 p(\nu) d\nu = \frac{4 \ln 3 - 3}{2 \ln 3 - 1} \approx 1.16473 \quad (18)$$

For some tests, other absorption functions were also used. These included

$$\sigma(\nu) = a\nu^{-3} \quad (19)$$

and

$$\sigma(\nu) = a \quad (20)$$

B. Scoring Methods for IMC Absorption

A model for IMC absorption, without Compton scattering, is obtained by choosing the parameters $a = 1$, $b = 0$ in Eqs. IV.A.10 and IV.A.11 above.

Several scoring methods were tested numerically. For each method, several tests were made, with different values of the Fleck factor f , to vary the relative amounts of effective absorption and scattering. For each f , a maximum distance to census was selected to obtain an approximate factor of 2 attenuation.

$$d_{\text{cen}} = \min \left(100, \frac{\ln 2}{f} \right) \quad (1)$$

Other absorption functions $\sigma(v)$ were also tried ($1, v^{-3}$). Up to 50,000 particles were then generated with initial energy weights of 1, and initial frequencies in the distribution $p(v)$ (Eq III.A.16), and tracked over distance d_{cen} . Various statistics were calculated, including average energies lost by particle and deposited, energy-weighted average path length, number-average and energy-average frequencies, and average number of photons.

The following methods for particle/deposition all agreed (see Table 1): A/A, A/L, and EA/EA. In addition, the analogue method A was tried in two forms: method A1, in which the particle was killed with probability f , and scattered with probability $1-f$ at each collision, and method A2, in which fraction f of the particle energy is removed and fraction $1-f$ scattered at each collision. Both forms agreed in the combinations above, replacing A with either A1 or A2, for a total of seven valid methods.

The following methods did not agree with the analogue results: EA/EA (modified, $\sigma_1 = \sigma_T$), L/L, L/L (modified, $\sigma_1 = \sigma_{SC}$). The failure of method L/L shows that satisfying the single-flight expected value criterion is

insufficient proof of satisfying the multiple-flight criteria, even when all cross sections are constant.

C. Scoring Methods for Explicit Monte Carlo Compton Scattering

A model for explicit Monte Carlo Compton scattering is obtained by choosing the parameters $a = 0$, $b = 1$, and $f = 1$ in Eqs. IV.A.10, IV.A.11, and IV.A.9 above.

Several scoring methods were tested numerically. In each test, a particle was given an initial energy weight and frequency of 1, and tracked through a large number (10^5 to 10^6) of Compton scattering events. Various statistics were calculated, including the net energy loss or gain by the particle and by the medium, energy-weighted average path length, number-average and energy-average frequency, and average number of photons.

In the model system, the particle energy is bounded, in the range from 0.5 to 1.5, and the deposition is therefore also bounded, in the range from -0.5 to 0.5. All scoring methods tried which used expected values for either particle energy or frequency failed, either due to distortion of the average spectrum to a singularity, or due to a growing error in particle energy. All scoring methods tried which used an exponential form of expected value deposition failed, due to exponentially growing errors in deposition.

Only two scoring methods were found that worked: pure analogue scoring, method EA/EA, and method EA/EALC, in which the particle energy was scored by analogue, and the deposition scored by linear expected value along the path. In method EA/EALC the average error in deposition per scatter was 0.3% for 10^5 scatters and 0.04% for 10^6 scatters, in agreement with an expected error of about $1/N$ for N scatters.

D. Scoring Methods for IMC Compton Scattering

The scoring methods that work for explicit Monte Carlo Compton scattering, methods EA/EA and EA/EALC, also work for IMC Compton scattering ($f < 1$ in Eq. IV.A.6), when modified to reduce the average energy exchange by the Fleck factor f , while still conserving photons ($E/\nu = \text{constant}$).

In method EA/EA, no particle energy change or energy deposition is done along a flight path. At a collision, based on cross section σ_C (Eqs. IV.A.3 and IV.A.11), one of two cases is chosen randomly. With probability $1 - f$, geometric scattering occurs, but with no change in E or ν . With probability f , a Compton scatter is done, which changes the frequency from ν to ν' , the energy from E to $E\nu'/\nu$, and deposits energy $E(1 - \nu'/\nu)$. For this test, frequency ν' was chosen randomly from the distribution $p_C(\nu, \nu')$ (Eq. IV.A.12).

In method EA/EALC, the particle energy is scored as in method A/A, but energy $fE <\sigma_C>\Delta x$ is deposited along each flight path of length Δx , whether to collision or to distance limit L . Method EA/EALC had an average error of less than 0.16% per collision for 10^5 collisions, with $f = 0.1$.

Methods EA/EA and EA/EALC both reduce the rate at which the radiation spectrum approaches a spectrum in equilibrium with the matter, by the factor f . This is not quite correct, but may be acceptable in systems that remain near spectral equilibrium, or in which Compton scattering is not the predominate process. Other systems may have to be calculated explicitly.

E. Scoring Methods for IMC Absorption and Compton Scattering

A valid method for combined IMC absorption and Compton scattering can be obtained by combining one or more of the acceptable methods for scoring IMC absorption described in Section IV.B. above, with either of the acceptable

methods for scoring IMC Compton scattering, described in Section IV.D, above. Methods EA/EA and EA/EALC (see Table 1) combine the exponential expected value particle and deposition scoring of implicit absorption with either pure analogue, or analogue particle and linear expected value deposition scoring of implicit Compton scattering.

For convenience, the two methods are summarized below, with arbitrary parameter $g = 0$ for method EA/EA, and $g = 1$ for method EA/EALC. The distance to collision, d_{coll} , is based on the total scattering cross section $\sigma_{SC} = \sigma_S + \sigma_C$, and is selected randomly from the probability distribution

$$p(x) = \sigma_{SC} e^{-\sigma_{SC}x} \quad (1)$$

by use of a random number $0 < u < 1$:

$$d_{coll} = -\frac{1}{\sigma_{SC}} \ln(u) \quad (2)$$

The actual flight distance, x , is the minimum of d_{coll} , the distance to census d_{cen} , or the distance to a zone boundary d_{edge} .

$$x = \min(d_{coll}, d_{cen}, d_{edge}) \quad (3)$$

The particle energy weight, initially E , is attenuated to E' along the path, and the energy change $E_{d,A}$ deposited.

$$E' = E e^{-\sigma_A x} \quad (4)$$

$$E_{d,A} = E - E' = E(1 - e^{-\sigma_A x}) \quad (5)$$

The energy deposition along the path, due to Compton scattering, $E_{d,C}$, is obtained by integrating

$$E_{d,C} = g \int_0^x \langle \sigma_{CE} \rangle E \, dx = E \frac{g \langle \sigma_{CE} \rangle}{\sigma_A} (1 - e^{-\sigma_A x}) \quad (6)$$

where $\langle \sigma_{CE} \rangle$ is given by Eq. IV.A.6. The total energy deposition is then:

$$E_d(x) = E_{d,A} + E_{d,C} = E \left[1 + \frac{g \langle \sigma_{CE} \rangle}{\sigma_A} (1 - e^{-\sigma_A x}) \right] \quad (7)$$

In the case of $\sigma_A x \ll 1$, the exponential term may be expanded and truncated to three terms, and the expressions rearranged to avoid numerical error.

At a scatter, a random selection is made between an effective scatter, with probability σ_S/σ_{SC} , or a Compton scatter with probability σ_C/σ_{SC} . If an effective scatter is done, the particle energy is not changed and no energy is deposited, but a new direction is selected randomly from an isotropic distribution, and a new frequency is selected from a $\sigma(\nu)b(\nu)$ distribution, where $\sigma(\nu) = \sigma_A(\nu) + \sigma_S(\nu)$ and $b(\nu)$ is the Planckian distribution function. If an effective Compton scatter is done, a new direction is selected as for an actual Compton scatter. With probability $1 - f$, no energy or frequency change is made. With probability f , the new frequency ν' selected for an actual Compton scatter is given to the particle, and the new particle energy and the energy deposited are calculated as follows:

$$E'' = E' \frac{\nu'}{\nu} \quad (8)$$

$$E_d = E_d(x) + (1 - g)(E' - E'') \quad (9)$$

These two methods were extensively tested, with various values of the Fleck factor f , other absorption and scattering functions, and with various relative amounts of absorption and Compton scattering, and agreed within expected limits with pure analogue scoring.

V. SUMMARY AND CONCLUSIONS

Various energy scoring methods for IMC radiation transport were tested. The tests included mathematical analyses of single-flight and multiple-flight models with a distance limit and constant cross sections, and numerical analyses of a multiple-flight model with a distance limit and variable cross sections. The latter tests included tests of pure absorption, implicit absorption with effective scattering, explicit Compton scattering, implicit Compton scattering, and a combination of implicit absorption and implicit Compton scattering. Several different forms of frequency-dependent cross sections were used.

Several different scoring methods were found that give results in agreement with pure analogue scoring methods. These include the methods: (a) particle energy scoring based on an exponential expected value model of absorption along each path, with collision distance based on the total scattering cross section, and an analogue form of Compton energy exchange, and (b) energy deposition scoring either complementary to the particle energy scoring, or with Compton energy deposition along each path based on a linear expected value model. Method (a) has the advantage of an explicit energy balance, and method (b) has the advantage of distributing the Compton energy deposition smoothly over time and position. There appears to be no significant advantage in other models tested.

Although an infinite number of valid scoring methods may exist, any particular scoring method should be tested carefully to insure its validity.

VI. BIBLIOGRAPHY

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