ESTIMATION METHODS IN MONTE CARLO PARTICLE TRANSPORT SIMULATIONS

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INTRODUCTION

In Monte Carlo transport calculations, we normally wish to estimate reaction rates of interest. We start by summing up the particle statistical weights in regions of interest and use primary estimators for the collision density. Then secondary estimators are used to estimate the quantities of interest needed in the dosimetry, materials, heat transfer, shielding, criticality, and other aspects of design.

PRIMARY ESTIMATORS

1. THE COLLISION ESTIMATOR

The ingoing collision density ψ particle transport equation can be written in its operator form as:

$$\psi = S_c + (TC)\psi \tag{1}$$

where: T is the transport kernel,
C is the collision kernel,
S_c=TC is the first event source, or the uncollided particle contribution to each phase space point from the physical source S.

A Monte Carlo simulation proceeds by alternatively transporting and then colliding the source particles to yield the Neumann series solution to Eq. 1 as:

$$\begin{aligned} \psi &= S_c + \sum_{i=1}^{\infty} \psi_i \\ &= TS + (TC)TS + (TC)^2 TS + \ldots \\ &= S_c + (TC)S_c + (TC)^2 S_c + \ldots \end{aligned} \tag{2}$$

so that the i-th term corresponds to a particle that collided I times, and the zero-th term represents the first event source. Rather than carry out an analog simulation, the absorption-weighting method is normally used. When a normalized transport kernel T is used, a statistical weight is assigned to the particle and is adjusted at each collision by the nonabsorption or survival probability:

$$P_s = \frac{\Sigma_s}{\Sigma_t} \qquad (3)$$

where Σ_s is the macroscopic scattering cross section, and Σ_t is the total cross section.

Thus, for a starting particle of statistical weight ${}^{v}W_0^{\,j}$, the j-th particle's weight at the i-th collision in region v of a homogeneous medium will be:

$$\begin{aligned} {}^{v}W_i^{\,j} &= {}^{v}W_{i-1}^{\,j} \cdot \frac{\Sigma_s}{\Sigma_t} \\ &= {}^{v}W_0^{\,j} \cdot \left(\frac{\Sigma_s}{\Sigma_t} \right)^i \end{aligned} \qquad (4)$$

In the standard Monte Carlo method the collision density fluence estimator will estimate in our notation the fluence over a region v as:

$$\phi_v = \frac{\sum_{j=1}^{n} \sum_{i=0}^{\infty} {}^{v}W_i^{\,j}}{n V_v \Sigma_{tv}} \qquad (5)$$

where: ϕ is the fluence in region v in units of [interactions/(cm^2.source particle)],
${}^{v}W_i^{\,j}$ is the statistical weight of the j-th particle scattering in region v,
${}^{v}W_0^{\,j}$ = 1 for a normalized physical source,
n is the total number of histories generated,
V_v is the volume of region v.

A major difficulty of the estimator in Eq. 5 is that it assumes complete sampling of the phase space; in the sense that to obtain the Neumann series solution, the Neumann series terms must occur with uniform frequency in different volumes of interest during a given simulation. This means that Eq. 5 is assumed to be of the form:

$$\phi_v = \frac{1}{n V_v \Sigma_{tv}} [\frac{v_{n_0}}{n} . \sum_{j=1}^{n} {}^{v}W_0^{\,j} + \frac{v_{n_1}}{n} . \sum_{j=1}^{n} {}^{v}W_1^{\,j} + \ldots \;], \; with: \frac{v_{n_i}}{v} = 1. \qquad (6)$$

In the limit of complete uniform sampling of the considered phase space, when $n \to \infty$, one can expect that:

$$v_{n_0} = v_{n_1} = v_{n_2} = \ldots = n, \qquad (7)$$

and we get the right estimate for the Neumann series solution. If the conditions of Eqs. 6 and 7 are not satisfied, an effective bias in the result must be expected, and does in fact occur.

2. THE TRACK LENGTH ESTIMATOR

This is another estimator used for the estimation of the flux. In this case Eq. 5 is modified to the form:

$$\phi_v = \frac{\sum_{j=1}^{n}\sum_{i=0}^{\infty} {}^{v}W_i^{\,j}.d_{vi}^{\,j}}{nV_v} \qquad (8)$$

where: d_{vi}^{j} is the track length of the j-th particle scattering in region v in the i-th history.

Notice that in this case the distance traveled is replaced to the inverse of the total macroscopic cross section, which in turn is equal to the collision mean free path. The track length estimator performs better than the collision estimator in regions of thin optical length where the particles will definitely pass through, but not necessarily collide in a given history.

3. THE LAST EVENT OR ANALOG ESTIMATOR

The collision and the track length estimators are the most widely used estimators for the calculation of particle fluxes. Other estimators have been suggested and widely used. As an example is the analog estimator which scores each time a particle is absorbed in the region of interest:

$$\phi_v = \frac{\sum_{j=1}^{n}\sum_{i=0}^{\infty} {}^{v}W_{i_a}^{\,j}}{nV_v\Sigma_{av}} \qquad (9)$$

where: i_a denotes the i-th collision at which absorption occurs,
Σ_{av} is the macroscopic absorption cross section in region v.

This estimator does well in highly absorbing media. Its performance deteriorates in a highly scattering medium where few absorption events are expected to occur.

4. COMPARISON OF DIFFERENT PRIMARY ESTIMATORS

Flux at a point, next-event, variational Monte Carlo estimators, and estimators depending on the adjoint method have also been devised and are used in different circumstances.

Estimators used in Monte Carlo particle transport calculations are of five basic types:

a. The collision or Wasow estimator.
b. The last-event or Forsyth Leibler, von Neumann-Ulam estimator.
c. The track length estimator and its variations as analyzed by Gelbard, Ondis and Spanier.
d. The flux at a point and next event estimators as analyzed by Kalos and Steinberg and by Albert.
e. Estimators based on Maynard's adjoint method. These in turn can be any of the previous categories.

The last event estimator differs from the collision estimator in that scoring occurs only when the particle history is terminated by absorption. This implies the use of a terminating Markov chain model for the generation of the associated random walk. This estimator is the same as the one introduced by von Neumann and Ulam, and generalized by Forsyth and Leibler to non-unit statistical weight particles.

The collision estimator scores at each collision. It can be used for either nonabsorbing (the last event estimator is not defined in this case), or absorbing Markov chain models. When an absorbing chain is used, this corresponds to the Wasow estimator. One might expect the collision estimator to yield a lower variance than the last-event estimator; this is in fact verified in some practical cases, but in others the reverse situation occurs.

Both the last event and the collision estimators tend to suffer statistically in optically thin regions since few collisions occur there. This statistical problem is improved by the use of the path length estimator as analyzed by Spanier and Gelbard. The methods proposed by Ragheb where the individual Neumann series terms of the solution are estimated are also superior in this case.

MacMillan has compared the variance of different estimators for simple problems.

All the previous estimators tend to suffer statistically as the volume of the detector region becomes small. The next event or point-detector estimator is a candidate for problems where point values are needed as well as the Albert estimator and the adjoint method.

The next-event estimator tends to require a great deal of computational effort, since the attenuation from each collision site to the point detectors is required: this is quite a burden in problems with complex geometries. When the detector point lies within a scattering medium, the theoretical second moment of its estimate may be infinite, even though the first moment is finite. Kalos proposed a once-more collided estimator to remedy this infinite variance problem. Steinberg and Kalos also proposed to bias the selection of collision points toward the point detectors.

The Albert estimator was initially applied to an adjoint integral equation, and in this sense it is an adjoint method estimator. However, as reported by Spanier and Gelbard: "Albert himself did not point that out that, and he draws attention to a particular method of estimation and not to the equation itself."

Maynard's adjoint method deals directly with the adjoint transport equation and uses the reciprocity relation explicitly. The adjoint method is an area of active research and code development, particularly whenever point cross sections or non-multigroup applications are addressed.

The most comprehensive surveys of estimators used in Monte carlo applications in particle transport have been exposed in the books by Spanier and Gelbard and by Carter and Cashwell.

SECONDARY ESTIMATORS FOR REACTION RATES ESTIMATES

1. INTRODUCTION

We consider that the collision estimator was used with some region detectors to estimate reaction per unit volume or reaction densities per source particle in the form:

$$F_v = < \Sigma_{rv}(E_k), \chi_v(E_k) > \quad \text{[interactions/(cm}^3\text{.source particle)]} \qquad (10)$$

where: $\chi_v(E_k) = \dfrac{1}{V_v \Sigma_{tv}(E_k)} . \dfrac{\sum_{i=1}^{n_{vi}} W_j(E_k)}{n_t}$ [interactions/(cm^2.source particle)],

$\Sigma_{rv}(E_k) = \sum_{i=1}^{s} N_{vi}\sigma_i(E_k),$ is a response function of interest in region v, for energy group E_k [cm^{-1}],

N_{vi} is the nuclide number density of the considered element i in a compound or alloy or mixture of s components in detector region v [atom/(barn.cm)],

$\sigma_i(E_k)$ is the microscopic cross section of the reaction of interest for element I, and energy group E_k [barns],

v designates the region detector of interest,

n_t is the total number of source particles,

n_{vi} is the number of particles of energy E_i scattering in region v,

$W_j(E_k)$ is the statistical weight of the j-th particle at energy E_k scattering in region v,

V_v is the volume of region detector v [cm^3],

$\Sigma_{tv}(E_k)$ is the total macroscopic cross section for group E_k in region v [cm^{-1}],

G is the number of groups treated,

<,> denotes an inner product over the energy groups: k=1,2,3, … ,G.

2. ESTIMATION OF PARTICLE FLUXES

For the estimation of particle scalar fluxes, the response function $\Sigma_{rv}(E_k)$ in Eq. 10 is given as an input in the form of a step function in the energy groups and regions of interest, normalized by the source term, to obtain the volume averaged fluxes from the secondary estimator:

$$\varphi_v = < \Sigma_{fv}(E_k), \chi_v(E_k) > \text{ [particles/(cm}^2\text{.sec)]} \qquad (11)$$

where: $\Sigma_{fv}(E_k) = S$,

S is the source term [source particles/sec].

In a reactor calculation the source S can be estimated from the reactor power.

3. ESTIMATION OF REACTION RATES

To calculate reaction rates of interest such as tritium breeding ratios in a fusion blanket, which is the number of tritium atoms produced per source particle in each region v from neutrons reactions with Li^6 and Li^7 are estimated from:

$$T_v = < \Sigma_{tv}(E_k), \chi_v(E_k) > \qquad \text{[tritons/(source particle)]} \qquad (12)$$

where: $\Sigma_{tv}(E_k) = V_v . \sum_{i=1}^{2} N_{vi} \sigma_{Ti}(E_k)$,

V_v is the volume of region v [cm^3],

$\sigma_{T1}(E_k)$ is the macroscopic cross section for the reaction $Li^6(n,He^4)T^3$,

$\sigma_{T2}(E_k)$ is the macroscopic cross section for the reaction $Li^7(n,n'He^4)T^3$.

4. ESTIMATION OF RADIATION DAMAGE PARAMETERS

As an input to the materials calculations, the gas production rate are estimated from:

$$G_v = < \Sigma_{Gv}(E_k), \chi_v(E_k) >, \text{ [appm/year]} \qquad (15)$$

where: $$\Sigma_{Gv}(E_k) = SC_Y.10^{-18}.\frac{\sum_{i=1}^{s} N_{vi}\sigma_{Gi}(E_k)}{\sum_{i=1}^{s} N_{vi}}$$

$C_Y = 3.15x10^7$ is a conversion factor from seconds to years,

For hydrogen gas production: $\sigma_{Gi}(E_k) = \sigma_i(n, p) + \sigma_i(n, D) + \sigma_i(n,T)$

For helium gas production: $\sigma_{Gi}(E_k) = \sigma_i(n, He^3) + \sigma_i(n, He^4)$.

The atomic displacement rates are estimated from:

$$D_v =< \Sigma_{Dv}(E_k), \chi_v(E_k) > \quad \text{[displacements/(atom.year)]} \qquad (16)$$

where: $$\Sigma_{Dv}(E_k) = SC_Y.10^{-24}.\frac{\nu_D(E_k)N_v\sigma_{vpk}(E_k)}{N_v} ,$$

$\nu_D(E_k)$ is the number of displacements per primary knock-on of energy E_k,

$\sigma_{vpk}(E_k)$ is the primary knock-on cross section from radiation damage theory [barns],

N_v is the atomic density of the metal matrix, in units of [atoms/(barn.cm)].

5. ESTIMATION OF DOSE AND HEATING RATES

As an input to the dosimetry or thermal and hydraulic calculations, the neutron or gamma heating per source particle or the dose response can be estimated from:

$$H_v =< \Sigma_{Hv}(E_k), \chi_v(E_k) > \qquad \text{[MeV/source particle]} \qquad (13)$$

where: $\Sigma_{Hv} = V_v C_H \sum_{i=1}^{n} N_{vi} K_i(E_k)$ is the heating response function in region v [eV.cm^{-1}],

$C_H = 10^{-6}$, is a conversion factor from eV to MeV,

$K_i(E_k)$ is the Kerma factor in energy group k [barn.eV], for element i.

To get the average volumetric heating rates in region v one can use:

$$Q_v = \langle \Sigma_{Qv}(E_k), \chi_v(E_k) \rangle \text{ [MW/m}^3\text{]} \quad (14)$$

where: $$\Sigma_{Qv}(E_k) = \frac{S.C_Q}{V_v}.\Sigma_{Hv}(E_k),$$

$C_Q = 1.6021 \text{x} 10^{-13}$, is a conversion ratio from MeV to Joules.

For neutron dosimetry calculations, cross sections libraries of Kerma factors have been compiled, such as the one by M. Abdou.