

AN ADJOINT CHARGED PARTICLE TRANSPORT METHOD

Thomas M. Jordan
 Experimental and Mathematical Physics Consultants
 Box 66331 Los Angeles, Ca 90066 (213)398-0431

Abstract

A numerical method has been developed for accurate and efficient calculations of charged particle flux-at-a-point in complex geometries. Accuracy is obtained using the "condensed history" Monte Carlo technique. Efficiency is obtained by first sampling particle energy and direction at the point of interest and then tracking the particle backwards (particles speed up) to the source.

Introduction

The original impetus for this method was a requirement to verify approximate dose predictions for satellites and deep space probes exposed to trapped radiation belts. Typically, these dose predictions involve a material geometry described by tens to hundreds of regions of different shape and material composition. The usual method of approximating dose is to perform a 4π integration of the dose per steradian at a point representing a component¹.

The dose per steradian is determined by an interpolation--using an equivalent mass thickness for each direction in the solid angle integration--of tabulated or curve-fit dose attenuation data from one-dimensional calculations. This approximate method can be made to yield exact results for spherical shell and semi-infinite slab geometries². However, the effect of the discrete geometry and differing materials can be determined only by a Monte Carlo integration.

Since the requirement is for the dose at a point (or averaged over a small volume) Monte Carlo electron codes are usually rejected as an analysis method because of their relative inefficiency. Even neglecting charged particle range effects, the relative efficiency (histories scoring per history tracked) is approximately $(r/R)^2$ where r is a typical detector or component dimension and R is a typical spacecraft dimension, e.g. $r = 1$ and $R = 100$ cm give a relative scoring efficiency of 10^{-4} .

Flux-at-a-point estimators and/or importance sampling could be used. This requires remodeling the usual condensed history charged particle methods, which can be done^{3,4,5}. However, the remodeling produces total and scattering cross sections that, by way of comparison, make neutral particle flux-at-a-point look trivial.

A trapped radiation belt implies a particle source defined with a continuous energy spectrum for all inward directions on any surface enclosing a spacecraft. This source makes the flux-at-a-point problem an obvious candidate for the backward-integration method, i.e. the adjoint method.

In the backward integration method, the phase space coordinates (position, direction, and energy) of a particle arriving at the detector are sampled at random. The particle is then backtracked along one of its possible forward paths, speeding up as it goes, using weight factors when one of several possible interactions must be selected at random, until the particle reaches the originating source. The phase space coordinates of the particle at the source (the source distribution evaluated for the position, direction, and energy obtained for the backtracked particle) and the particle weight (flux per source particle) are then combined to give the correct flux at the detector.

Since for trapped radiation belts, every history terminates at the point detector and, in backtracking, must sooner or later start at the surface source, the relative efficiency (probability of getting a score) approaches unity. The only worthless histories are those which speedup above the maximum energy of the source spectrum. Conversely, no time is wasted on particles which range out before reaching the detector.

The backward integration has a basic difficulty in obtaining solutions for sources with discrete position, direction, and energy, just as the forward integration has difficulty giving fluxes at discrete points, directions, and energies. For some problems, discrete coordinate results are characterized as averages over corresponding coordinate intervals. For other problems, the first collision forward source can remove a discrete coordinate difficulty.

The backward integration method has been compared with a limited amount of experimental data for both simple and complicated geometries. Excellent (for the simple geometries) to good (for the complicated geometries) agreement has been obtained. Comparisons with forward Monte Carlo and numerical integrations for the same continuous source distributions are always in excellent agreement.

Assuming these comparisons constitute method verification, the backward integration method has, in turn, verified one approximate space radiation analysis method and invalidated others⁶.

Numerical Methods

The backward integration of the transport equation (starting at the detector) has several unique interpretations and difficulties not encountered in forward integrations (starting at the source). The understanding of the backward integrations, particularly the optimal sampling of precursor branching probabilities (answering the question of how an electron or photon starts a step), requires a detailed examination of minimum variance transformations of integration variables.

The backward integration formalism and numerical methods are developed in the references⁷⁻¹⁰. The significant information obtained from the formal development is:

- 1) "adjoint" kernels are not needed or used,
- 2) the solutions of problems having the same source domain can be obtained simultaneously by appropriate bookkeeping,
- 3) solutions can be obtained for point, line, surface, and/or volume sources with flux estimators analogous to the flux-at-a-point, uncollided track length, and collision density estimators used in forward integrations, and
- 4) a forward solution guess must be used to provide a reasonable estimate of optimal variable transformations prior to integration by random sampling.

For trapped radiation belts in the absence of photon-electron cascade modeling, method implementation is straight forward. The differences relative to a forward solution are

- 1) particles speed up on each condensed history step,
- 2) the usual multiple scattering distribution applies,
- 3) the usual energy-loss straggling distribution can be used with negligible error, and
- 4) it is necessary to account for the change in particles/Mev on each step (the "particle weight" has different properties than forward solution "weights").

For the more general problems involving high energy knock-ons and electron bremsstrahlung cascades, it is essential that a reasonable estimate of the forward solution spectrum be available. Without this estimated spectrum it is impossible to efficiently sample precursor branching modes (photon to electron, electron to photon, photon to photon, and electron to electron interactions).

In practice, it has proven sufficient to use a spatially independent, material dependent, slowing-down spectrum for weighting precursor branching probabilities. For electrons, an infinite medium slowing-down spectrum is assumed. For photons, the slowing-down spectrum is an approximation of the slowing down in a cell of dimensions on the order of the maximum-energy electron range.

Precursor sampling in the backward integration must use importance sampling, i.e. weighting of scattering cross sections by the assumed slowing-down spectrum. The transformation Jacobian ensures the value of the integral is unchanged. Transformations do have a large effect on the variance integrals. Energy transformations involving the estimated forward slowing-down spectrum produce very good convergence (small variances).

Other Techniques

The preceding discussion summarized unique aspects of the backward integration of the electron transport equation. Other modeling implied by the discussion is usually the same as in the forward Monte Carlo program BETA-II¹¹. Pertinent models are summarized here.

Electron cross section models include the Mott-to-Rutherford cross section with screening angle (processed into the angular straggling distribution), Møller electron-electron cross section for high energy secondary electron production and energy-loss straggling effects, bremsstrahlung production formulas as suggested by Koch and Motz, and stopping powers with density effect and restricted energy loss corrections. Options are available to perform positron or heavy charged particle transport calculations.

Photon cross sections are obtained from ENDF/B data files and account explicitly for Compton, pair, and photoelectric interactions. The corresponding secondary electrons (pair positrons are tracked as electrons) are produced and explicitly followed.

Material geometries are generally described by quadric surfaces with regular surfaces and region shapes having simple descriptions.

Source spectra are accepted in various forms including discrete lines, differential or integral tabulations, and analytic formulae. Spatial and angular source distributions implemented in the backward method are either exterior to all geometry and uniform over solid angle intervals (or 4π) and uniform per unit projected area (trapped radiation belts or beams with a finite angular spread), or volume electron sources, isotropic (e.g. activation beta decay) or angular (first collision photon electron source).

Detectors are either volumes in rectangular, cylindrical or spherical coordinates (with arbitrary limits on each of the three orthogonal coordinates) or any limiting point, line, or surface. Alternatively, the detector volume can have arbitrary shape (quadric surface boundaries) by rejecting those regular geometry points outside specific geometric regions.

Basic outputs include detector fluxes by source group and spectrum. In addition, sensitivities of the basic output can be selected to any multiplicity from source volume, source direction, scoring volume, scoring direction, cascade generation, material geometry correlation set, and coincident counting in other sensitive volumes.

In practice, sensitivity arrays can get very large and sparse. Therefore, some many-dimensional sensitivities are obtained by post processing a history file. A restart procedure is used to get the effect of additional histories.

Applications

The initial verification of the method involved comparisons with forward Monte Carlo calculations (BETA-II). Figure 1 demonstrates the agreement for the 1-D depth dose profile in aluminum with a cosine source (isotropic flux) and a particular Jovian electron spectrum. (The SHIELD curve was generated by a 1-D numerical integration procedure which uses the BETA-II cross section formulation.)

Figure 2 indicates the agreement between forward and adjoint methods for a simple two-dimensional detector mockup (cylindrical geometry with mirror symmetry at the midplane), with an isotropic external electron source.

The agreement in calculated deposition versus electron source energy is very good. (This detector was also modeled in three dimensions, including the Pioneer F/G spacecraft and the in situ calibration curve obtained¹².)

Additional method verification included comparisons with experimental data. The UCSD detector¹³ (Pioneer F/G) was modeled, including the spacecraft, and the response was calculated versus electron source energy for several energy-deposition (per particle) thresholds. The agreement with the experimentally determined response is shown in Figure 3.

Finally, a comparison was made for the dose from an isotropic fission electron spectrum, $n(E) = \exp(-.575E - .055E^2)$, cosine incident on one side of an eight inch cube with 60 mil aluminum walls. Figure 4 indicates the agreement between measured¹⁴ and calculated¹⁵ dose versus distance from the irradiated wall. Similar agreement was obtained for 30 and 125 mil walls.

Timing

The method was developed with parametric analysis in mind. Therefore, the number of source spectra has little effect on computer time (over 100 source spectra have been used in a single 1-D dose attenuation calculation).

Computer times for the method depend more critically on the complexity of the material geometry and the convergence required on a particular output. Assuming calculated precisions on the order of 10 per cent or less for integral response, e.g. dose, typical computer times (Univac 1108) are

1-D single material slab....	1 minute
3-D few(10) regions.....	2-3 minutes
3-D many (100) regions.....	6-12 minutes
3-D detailed (400) regions..	10-30 minutes

Sensitivity of deposition or counting rates to source energy and direction requires more time. An energy sensitivity in an isotropic flux field and a relatively simple geometry may require 8 to 10 minutes (Figure 2). An energy and direction sensitivity on a complicated geometry may require 2 to 5 hours or more (Figure 3).

Problems where material thicknesses approach or exceed the maximum range of primary electrons require more histories. However, the calculated variance--for a fixed number of histories--increases slowly with depth. In the region where bremsstrahlung dose (actually secondary electron dose in the calculation) is 90 per cent of the answer, calculated errors are typically twice as large as when the dose is dominated by the primary electrons.

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BETA II - SHIELD - ADJOINT COMPARISON

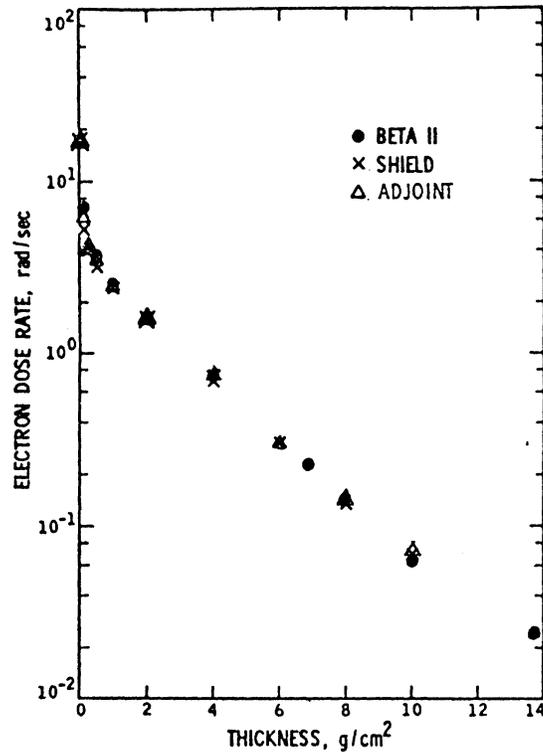


Figure 1.

COMPARISON OF BETA-II FORWARD AND ADJOINT MONTE CARLO DETECTOR RESPONSE

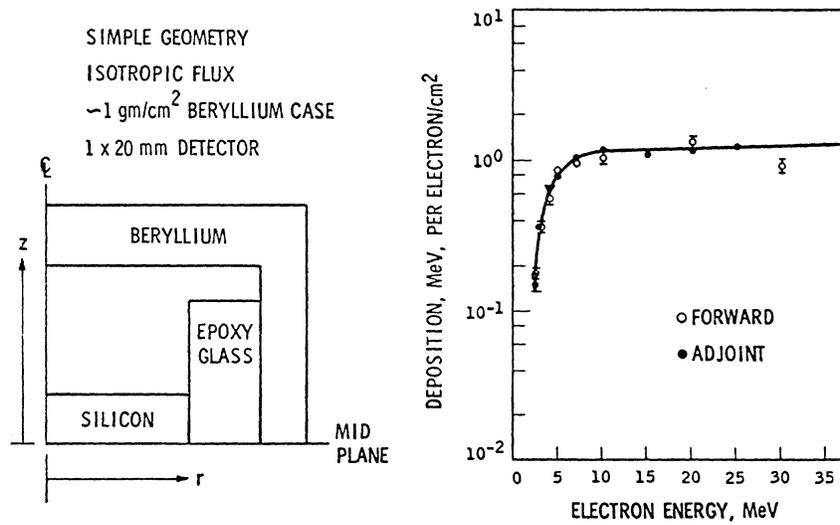


Figure 2.

UCSD DETECTOR CALIBRATION COMPARISON

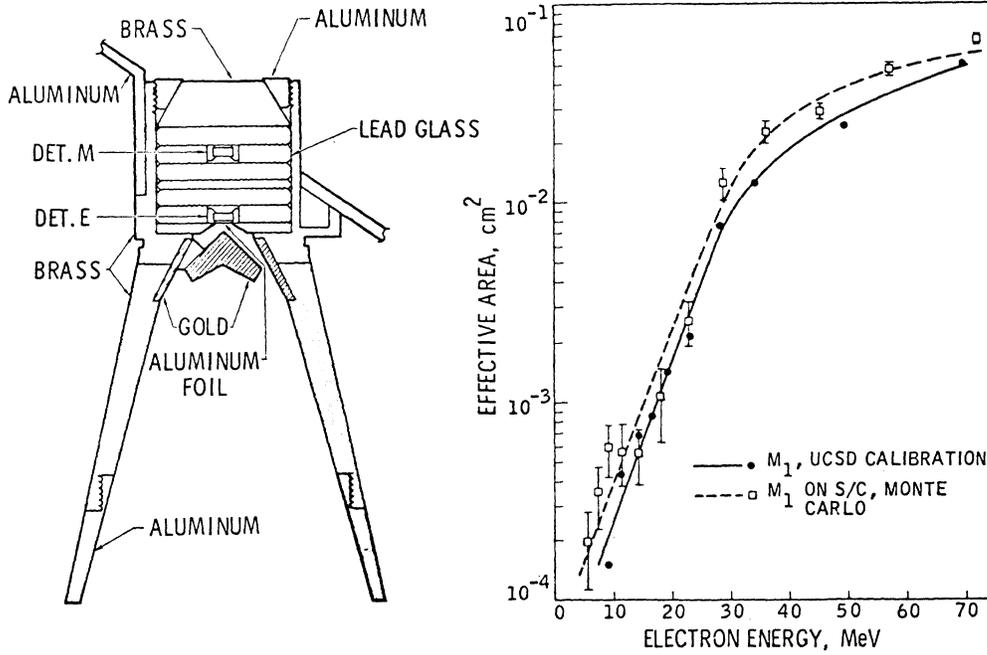


Figure 3.

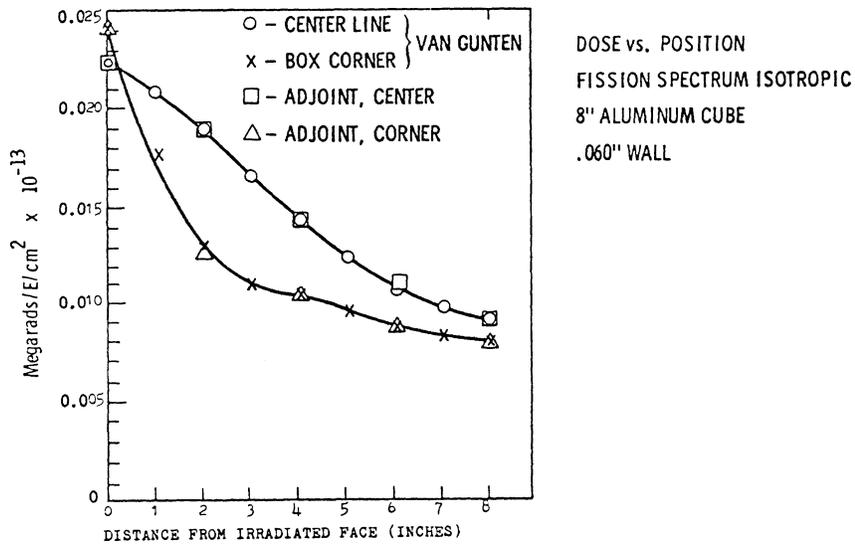


Figure 4.