Efficient $\beta/\gamma$ Monte Carlo Transport in Repetitive Structures$^1$

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Abstract

Algorithms are developed that permit the use of periodic and albedo boundary conditions in the ITS system of coupled electron/photon Monte Carlo transport codes when simulating transport in repetitive structures in satellite systems. Mutual verification is provided through the application of both algorithms to a simplified periodic geometry based on an array of microelectronics cards. The albedo algorithm is then employed to benchmark the predictions of energy deposition in silicon by a mass sectoring coupled electrodphoton Monte Carlo transport code when periodic and albedo boundary conditions in the code for this same application and to predict the shielding effectiveness of hexagonal honeycomb structures. Use of these algorithms results in a major reduction in the required problem input and significant variance reduction that could otherwise be achieved only via postprocessing that is much more problem dependent.

I. INTRODUCTION

Monte Carlo simulation of point-detector responses to an electron/photon cascade in complex satellite geometries is a difficult task because of the small solid angles that are typically involved. This difficulty should be somewhat alleviated, however, in the case of repetitive substructures, if proper advantage can be taken of the approximate spatial periodicity. By assuming that this periodicity is exact, the transport geometry can be simplified, much memory can be saved, and variance reduction can be achieved. Results obtained in this fashion correspond to an infinitely repetitive structure.

The Integrated TIGER Series (ITS) system of Monte Carlo codes [1] provides state-of-the-art simulation of the generation and transport of the electron/photon cascade. However, there is no provision in the currently available software for efficient simulation of periodic geometries. In this paper, we discuss the development and application of modified versions of the three-dimensional ACCEPT code of the ITS system that have this capability.

This developmental work was motivated by an interest in predicting silicon deposition in repetitive structures found in satellite systems, when exposed to uniform isotropic fields of electrons having either a natural or an enhanced energy spectra. We considered using both periodic (translations and/or rotations) and albedo (specular reflection) boundary conditions. Not knowing a priori which would be the most efficient, we decided to employ both approaches. Moreover, agreement between the two independent methods would provide for their mutual verification.

Two pseudo-periodic applications that permit either type of boundary conditions to some degree are considered here. The first is the deposition in a large array of microelectronics cards. The purpose here is the benchmarking of a mass sectoring (MS) code. The second is the deposition on one side of an aluminum honeycomb structure due to an electron source on the opposite side. The purpose here is the determination of the radiation shielding effectiveness of the honeycomb walls.

Calculations were carried out for the two electron source spectra. The spectra are representative of an orbit-mission-lifetime-averaged natural electron environment and a fission-enhanced electron environment. The natural spectrum had a maximum energy of 6.0 MeV and an average energy of 0.268 MeV. The enhanced spectrum had a maximum energy of 10.0 MeV and an average energy of 1.37 MeV. For the purposes of this work, the intensities of these spectra are irrelevant. A uniform isotropic flux of source electrons was assumed. It is emphasized that this is not a uniform isotropic source, but rather a uniform isotropic flux which results from sources that are effectively at infinity. A convenient method is described for simulating a source corresponding to a uniform isotropic radiation field. Finally, a method was developed for efficiently predicting the approximate non-resident silicon deposition for both applications.

II. ARRAY OF MICROELECTRONICS CARDS

In the first application, the motivation is to benchmark a less rigorous, but far more efficient, mass sectoring technique [2] that uses point kernel integration. The geometry is rectangular. The repetitive structure is that of an array of 200 geometrically similar microelectronics cards with constant void separation within a square supporting channel. For benchmarking, the MS calculation employed a stack of the all-aluminum unit cells shown in Fig. 1 that was

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repeated 200 times in the z direction. The Monte Carlo calculations assumed an infinite array. Predictions of the Monte Carlo code for the infinite array were compared with those of the MS code for a unit cell near the center of the 200-card array.

Because the high-energy tails of the spectra contributed disproportionately to the flux inside the channel, a variable power law scaling algorithm provided variance reduction by increasing the frequency of sampling from the tails.

The three most important code modifications were (1) modifications to the tracking logic to account for the special boundary conditions, (2) modifications to the source routine to simulate the uniform isotropic radiation field, and (3) conversion of the electron-flux scoring routine into a routine for scoring deposition in non-resident silicon.

A. Periodic and Albedo Boundary Conditions

The infinite array is immersed in a uniform isotropic radiation field. Total problem symmetry of the application depends on the symmetry of both the source and the problem geometry.

No attempt was made to take maximum advantage of the symmetry of the problem geometry, either for periodic or albedo boundary conditions. Rather, the objective was to apply them both in a limited way, so as to obtain mutual verification of the two algorithms. Because neither was applied with maximum efficiency, timing comparisons are not meaningful.

The periodic and albedo geometries are shown schematically in Fig. 1. The dashed lines indicate the boundaries where the special boundary conditions are invoked. Transport across boundaries indicated by solid lines proceeds in the usual fashion without modification.

Careful study of Fig. 1 shows that neither periodicity nor reflective symmetry was fully exploited. There is an additional fourfold rotational periodicity in the X-Y projection of the periodic geometry. By considering only the axial periodicity, simple particle translation is all that is required. When a particle intersects the plane at z=0 (z=0.89), shown as a dashed line in the X-Z projection of the periodic geometry of Fig. 1, it is just translated to z=0.89 (z=0), with no change in either its direction or its x and y coordinates. This was accomplished by modifying four tracking routines in the ACCEPT code. Implementation of the rotational periodicity would only have required straightforward trajectory rotations, changing both the positions and directions of particles.

The X-Y projection of the albedo geometry shows that reflection symmetry about the channel diagonal has been ignored. Albedo boundary conditions are accounted for at the indicated boundaries through specular reflection about the local normal,

\[ \hat{\omega}' = \hat{\omega} - 2(\hat{\omega} \cdot \hat{n})\hat{n} \]  

(1)

where \( \hat{\omega} \), \( \hat{\omega}' \), and \( \hat{n} \) are the initial direction unit vector, the final direction unit vector, and the inward unit normal, respectively. Specular reflection is especially straightforward for this example where all boundaries are Cartesian planes. The same four tracking routines of the ACCEPT code must be modified as for periodic boundary conditions. For this application, the albedo boundary conditions permit transport in a smaller problem geometry. A minor disadvantage of albedo boundary conditions is that the reflective boundaries require more frequent truncation of electron random walk substeps at boundaries that are not material discontinuities. These truncations involve some approximations to the electron transport that would otherwise not be necessary.

B. Simulation of a Uniform Isotropic Radiation Field

The most common type of source in ITS, and one that is common as well in other Monte Carlo transport codes, is a surface current. Though perhaps well known to transport theorists, experience has shown that the method of using a surface-current source to simulate a uniform isotropic radiation field is much less obvious to the average user. Consequently, the method will be described briefly here.

The method is based on the fact that, for a uniform isotropic flux, the number of particles per unit area crossing an arbitrary surface in one direction (2\( \pi \) steradians) is constant in magnitude and has a cosine-law angular dependence with respect to the local normal. The procedure

\[ \hat{\omega}' = \hat{\omega} - 2(\hat{\omega} \cdot \hat{n})\hat{n} \]
then is to mound the problem geometry with a non-reentrant body, to sample a constant number of source particles per unit area over this surface, and to sample the source direction from a cosine-law distribution with respect to the inward normal at the sampled source position. The cosine-law distribution should be truncated at $\pi/2$. Source particles sampled at larger angles would be wasted because they will be directed out of the source surface.

Though the non-reentrant surface may otherwise be arbitrary, there are two practical imperatives. It should be a surface over which particles can be easily sampled uniformly in area, such as a sphere, a right circular cylinder, or a rectangular parallelepiped. Secondly, it should be as small as possible so as to minimize the number of source trajectories that miss the problem geometry.

How then are absolute results to be obtained from such a calculation for a specified absolute uniform isotropic flux? Let us assume that the Monte Carlo results are normalized to one source particle. Those results must first be multiplied by the area of the non-reentrant surface, which yields the results normalized to unit inward current density. Next, they must be multiplied by $1/4$. This is necessary because the inward current density per unit uniform isotropic flux ($4\pi$ steradian) is $1/4$. The absolute prediction is then obtained by multiplying these results by the specified scalar flux.

For the special boundary conditions considered in this application, the non-reentrant surfaces over which source particles are sampled uniformly with area are defined by the external solid-line boundaries of the X-Y projections of Fig. 1.

### C. Simulation of Non-Resident Energy Deposition in Silicon

Because the location and description of the silicon components was not specified in detail, the model included a new algorithm for estimating the non-resident energy deposition. That is, the silicon detectors were not explicitly included in the transport calculations. Rather, the deposition was estimated at selected locations by folding the restricted stopping power for silicon with the electron flux obtained from the actual transport geometry,

$$D_{Si}(r) = \int_{E_{max}}^{E_{min}} \Phi(r,E) \left[ \frac{dE}{ds} \right]_{Si} dE + \text{track-end term}, \quad (2)$$

where $D_{Si}(r)$ is the estimated energy deposition in silicon at location $r$, $\Phi(r,E)$ is the energy dependent electron flux at $r$, and $\left[ \frac{dE}{ds} \right]_{Si}$ is the collisional stopping power for Si restricted to energy losses less than $\Delta$. Though the algorithm for simulating silicon deposition using electron flux may not be the most sophisticated, we believe one-dimensional verifications described below show it to be adequate for our present purposes. The folding is accomplished on a continuous energy basis by scoring contributions to the deposition while the Monte Carlo is in progress, rather than via the less-accurate post-processing procedure of folding a histogram approximation to the flux with the stopping power.

Perhaps the greatest uncertainty in predictions by an algorithm based on Eq. (2) lies in how to define the track-end contribution. We have chosen to use the number of electrons that fall below $\Delta$ times $\Delta$ for that contribution. This means that the silicon detector should be small enough that it does not perturb the electron flux, yet large enough to absorb electrons with energies less than $\Delta$. Unfortunately, these criteria are somewhat contradictory. Another difficulty is that our choice always vanishes for void regions. Fortunately, so long as the silicon detector is small enough not to perturb the flux, $\Delta$ can be chosen low enough that the track-end term is small.

Development of this algorithm required substantial effort, quite apart from the periodicity and albedo modifications. When using a track-length estimator for volume-averaged electron flux, electron track segments from the random walk were apportioned among subzones of the same material in order to obtain additional variance reduction. This track-length apportioning in multi-dimensional geometries is quite complex relative to the default scoring of electron flux in the ACCEPT code. The latter only requires locating and scoring at a single point along each random walk segment. Apportioning, however, depends on the direction of the electron as well and requires logic of a complexity analogous to that needed in the tracking of the cascade particles. At the moment, apportioning has been implemented only for input zones that consist entirely of either a rectangular parallelepiped or a right-angle wedge, as these are the only ones required in the present applications. As an independent verification of the algorithm, we compared results from a one-dimensional version (modified TIGER code of ITS) with predictions of the discrete ordinates (DO) code, CEPXS/ONEILD [3], and with direct Monte Carlo deposition. Figure 2 compares the spatial profile of the scalar flux in aluminum for normally incident 1.0-MeV electrons as predicted by the unmodified TIGER code with that predicted by a 100-group DO code calculation. Agreement is good. Now, all quantities predicted by a DO code are explicitly flux based. Indeed, apart from the track-end term, the DO code uses Eq. (2) to predict deposition in the transport material, as well as non-resident deposition in any other material that can be assumed not to perturb the flux. In Fig. 3, the two flux-based energy depositions obtained according to Eq. (2) with $\Delta$ = 10 keV are compared with each other and with direct Monte Carlo deposition. The track-end term employed in the Monte Carlo was just the number of electrons falling below $\Delta$ in each subzone times $\Delta$ divided by the areal density of the subzone. The track-end term used in the DO calculation is not easily interpretable. Figure 4 compares the energy deposition due to electron flux above a given energy for a
subzone near the peak of Fig. 3. This result suggests that much of the difference between the two flux-based predictions may be due primarily to the differences at low energy.

![Figure 2: Comparison of the spatial profile of the scalar flux in aluminum for normally incident 1.0-MeV electrons as predicted by the TIGER Monte Carlo code with that predicted by the CEPXS/ONELD discrete ordinates code.](image1)

![Figure 3: Comparison of the two flux-based energy deposition profiles in aluminum for normally incident 1.0-MeV electrons as predicted by the TIGER and CEPXS/ONELD codes with each other and with direct Monte Carlo deposition.](image2)

![Figure 4: Comparison of the flux-based energy deposition due to electron flux above the abscissa energy as predicted by the TIGER Monte Carlo code with that predicted by the CEPXS/ONELD discrete ordinates code, for a subzone near the peak of Fig. 3.](image3)

Nevertheless, these one-dimensional comparisons confirm the accuracy of our algorithm to a degree that is adequate for our present purposes.

**D. Results**

Figure 5 compares volume-averaged non-resident silicon deposition as predicted using the algorithm for periodic boundary conditions (Fig. 1, left) with that predicted using the algorithm for albedo boundary conditions (Fig. 1, right). The source spectrum is that of the enhanced environment. Figure 5 shows the z dependence of the deposition for two (x,y) locations inside the channel — one near the corner of the channel and the other near the center of the channel. Here and in subsequent plots, z=0 corresponds to the plane midway between a pair of cards (not the same as in Fig. 1), so that z=0.3 cm is the surface of a card. To the left of this value is the void region between the cards, and to the right is the region within a card. Also, the lines are not fits to the simulated results, but are employed simply to connect predicted values for each type of calculation defined in the legends. Predictions of the two approaches are in excellent agreement. The two corner results, where the statistical uncertainties are about 1%, are indistinguishable. Stochastic differences are observable near the center where the uncertainties rise to near 5%. As a consequence of this agreement, we will henceforth show predictions from only the albedo method. Moreover, at least for the two applications simulated in this work, the albedo algorithm can be written with much less problem dependence.

![Figure 5: Comparison of the silicon energy deposition in the microelectronics card array due to the enhanced electron spectrum as predicted by the ACCEPT code modified for periodic and albedo boundary conditions.](image4)
Figure 6: Comparison of predictions due to the natural and enhanced environments with the silicon deposition from the modified ACCEPT code (MC) near the corner and near the center of the channel. For predictions of the MS code, again, it shows the significant drop in the deposition as the detector is moved away from the channel wall.

Figure 6 compares volume-averaged predictions of the silicon deposition from the modified ACCEPT code (MC) due to the natural and enhanced environments with predictions of the MS code. Again, it shows the $z$ dependence near the corner and near the center of the channel. For the natural environment, the MS code overpredicts in the void and underpredicts within the card. Differences reach approximately a factor of five. Both models predict a significant drop in the deposition as the detector is moved away from the channel wall.

It should be emphasized, however, that these predictions are somewhat qualitative. This is because, while the MC depositions are derived from volume-averaged fluxes and are plotted at the geometric center of the volumes, the MS results are point predictions. Indeed, the MC results are sensitive to the requested spatial resolution, especially near the channel walls (corner) where the flux is changing rapidly. This is easily seen by comparing the upper MC curves in Figs. 5 with the MC results for the enhanced spectrum in Fig. 6. Because of the lower spatial resolution requested in Fig. 5, the corner results are averaged over flux contributions farther from the walls, and thus are lower than those of Fig. 6. Agreement between the MS and MC results for the enhanced spectrum is much better between the cards than for the natural spectrum, but the discrepancy rapidly increases with depth within the wall.

The long run times that would be required for carrying out simulations with the unmodified ACCEPT code for the 200-card geometry used in the mass sectoring calculations are prohibitive. However, the mutual verification of the algorithms for the special boundary conditions in Fig. 5 and the verification of the algorithm for flux-based energy deposition in Fig. 3 give us confidence in the results obtained from the modified ACCEPT code in Fig. 6. Consequently, we conclude that the discrepancies between the results of the two models in Fig. 6 are due to limitations of the less rigorous mass sectoring code. In particular, most of the discrepancies are probably a result of deficiencies in the precalculated one-dimensional kernels employed in the mass sectoring code.

### III. HONEYCOMB STRUCTURE

Honeycomb-like structures are often employed for light-weight mechanical support in satellite systems. It is useful to know how much radiation shielding is afforded by such structures. As a second application of the modified ACCEPT code, we studied the shielding effect of an infinite array of thin-walled, hexagonal aluminum cells sandwiched between thin layers of aluminum and exposed on one side to the same uniform isotropic radiation fields that were defined for the microelectronics-card array. This single-sided irradiation is equivalent to assuming that other satellite components have reduced the radiation exposure from the other side to a negligible value.

As illustrated in Fig. 7, it is only necessary to simulate transport in one twelfth of a single hexagonal cell, with maximum advantage taken of albedo boundary conditions. Maximum exploitation of periodic boundary conditions would have required transport in $1/6$ of a cell, but they were not employed for this application. The top layer is exposed to the uniform isotropic radiation field, and the silicon deposition is calculated at the bottom surface of the bottom layer.

There is a significant change in the albedo model employed here as compared to that used for the first application. Instead of defining explicit reflection surfaces as in Fig. 1, here we define an albedo zone. This can be accomplished via the standard execution input so that the algorithm remains problem independent. The algorithm simply requires that the second to last input zone that is specified in the input to the ACCEPT code (the one before the escape zone) be the albedo zone. With the method implied in Fig. 1, it is necessary to have explicit conditions in the algorithm that define which boundaries of which input zones are albedo boundaries. With the albedo zone of Fig. 7, on the other hand, all particles are simply specularly reflected at the point where they enter the albedo zone.
Of special note is the flatness of the results, with no evidence of honeycomb structures. The honeycomb results are obtained for the configuration shown in Fig. 7 when the top layer, bottom layer, and hex wall are all aluminum. When the hex wall is replaced by a void, results correspond to deposition behind 0.36 mm of aluminum, the sum of the equal thicknesses of the top and bottom layers. The difference between these two calculations is the shielding effectiveness of the aluminum walls. The shielding effectiveness is expressed as that of an equivalent thickness of aluminum by increasing the sum of the top and bottom layers (with void hex walls) until the deposition decreases to the honeycomb result. Thus, the shielding effectiveness of the aluminum honeycomb walls is approximately 0.48 (i.e., 0.84-0.36) and 0.63 mm of aluminum for the natural and enhanced spectra, respectively. For comparison, if the walls were replaced by a layer of aluminum having the same mass as that of the walls, the thickness of that layer would be 0.72 mm.

Another change that was made to the model for this second application was a change in the method of estimating the electron flux. The volume-averaged flux estimator worked well for the application to the microelectronics-card array. However, difficulties were encountered when we attempted to employ it for this second application. Results were obtained by adding a thin void layer subzoned in x below the bottom layer shown in Fig. 7 and extending the albedo zone a distance equal to this thickness. Unbounded variance was encountered due to high angle of emission (with respect to the z axis) from the bottom layer. Flux estimates are not incorrect, but convergence is very slow. Apportioning the very long multiply reflected track lengths among the subzones not only slows the convergence but is also quite expensive. Consequently, the volume-averaged flux was abandoned in favor of a surface estimator for the electron flux. The variance of this estimator is also unbounded, but this was avoided by limiting the value of the cosine with respect to the z axis (CTFL) according to the condition:

\[
\text{if } \text{CTFL} < 0.1, \text{CTFL} = 0.05.
\]  

Results obtained for the shielding effectiveness of the honeycomb walls are shown in Fig. 8 for the two electron environments. Contributions to the predicted deposition in silicon at the bottom surface of the bottom layer are averaged over all possible y values for each of eight equal x increments of this surface. Of special note is the flatness of the results, with no evidence of honeycomb structures. The honeycomb results are obtained for the configuration shown in Fig. 7 when the top layer, bottom layer, and hex wall are all aluminum. When the hex wall is replaced by a void, results correspond to deposition behind 0.36 mm of aluminum, the sum of the equal thicknesses of the top and bottom layers. The difference between these two calculations is the shielding effectiveness of the aluminum walls. The shielding effectiveness is expressed as that of an equivalent thickness of aluminum by increasing the sum of the top and bottom layers (with void hex walls) until the deposition decreases to the honeycomb result. Thus, the shielding effectiveness of the aluminum honeycomb walls is approximately 0.48 (i.e., 0.84-0.36) and 0.63 mm of aluminum for the natural and enhanced spectra, respectively. For comparison, if the walls were replaced by a layer of aluminum having the same mass as that of the walls, the thickness of that layer would be 0.72 mm.

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decreases from 0.1 to 0.001. However, the convergence of the predictions decrease. For the limits at 0.1, 0.01, and 0.001, the estimated one-sigma statistical uncertainties are 4.3, 6.3, and 8.9 percent, respectively.

Figure 9: Illustration of the trade-off between the accuracy and convergence of the predicted silicon deposition based on a surface estimator of electron flux, depending on the magnitude of the limitation on the cosine of the angle of the particle trajectory with respect to the surface normal. Results are for the 0.84-mm-Al case of Fig. 8.

IV. DISCUSSION AND CONCLUSIONS

An implementation of periodic and albedo boundary conditions in the ACCEPT code of the ITS system has been employed to demonstrate the accuracy of a less accurate mass sectoring model used to predict energy deposition in satellite systems and to quantify the shielding effectiveness of a hexagonal honeycomb material used for structural support in satellites.

Using these boundary conditions to approximate the electron-photon transport in complex quasi-periodic structures can lead to major reductions in the memory that would otherwise be required. However, assessment of the effect on run time is not straightforward. Much the same run time reduction could be achieved by averaging the results from the full geometry through postprocessing. However, postprocessing algorithms will be very problem dependent. Unless one is willing to put the effort into postprocessing, run times for obtaining sufficiently accurate Monte Carlo predictions for some applications could be prohibitive without the variance reduction available from methods of the kind discussed here. For example, we estimate that in the first of our two applications, taking advantage of the approximate axial periodicity alone reduced the run time by an order of magnitude and reduced the memory required for geometry by more than two orders of magnitude.

It must be emphasized that only the special cases of two particular applications have been treated here. The two types of symmetry are quite different, and, while the geometry may sometimes permit a choice of either, other geometries may demand one or the other. In the first application, for example, a small asymmetric feature in one of the eight corners of the cards (Fig. 1) would preclude the use of albedo boundary conditions, but the geometry would still be quasi-periodic. On the other hand, reflective symmetry permits a greater reduction in the transport region of the second application than is possible with periodic boundary conditions alone. Formulation of a general set of rules on the optimal choice of boundary conditions should be possible, but is beyond the scope of this paper.

An important objective in the development of modifications to the Monte Carlo transport that take advantage of symmetries of the application geometry should be the minimization of problem dependent coding. Otherwise, one might find it just as easy to average symmetric regions of the full geometry via post processing. We have found here that, where applicable, using an albedo zone to implement albedo boundary conditions results in a less problem dependent algorithm.

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VI. REFERENCES