TITLE: SUPERTRACK MONTE CARLO VARIANCE REDUCTION EXPERIENCE FOR NON-BOLTZMANN TALLIES

AUTHOR(S): Guy P. Estes
            Thomas E. Booth

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This paper applies a recently developed variance reduction technique to the first-principles calculations of photon detector responses. This technique makes possible the direct comparison of pulse height calculations with measurements without the need for unfolding techniques. Comparisons are made between several experiments and the calculations to demonstrate the utility of the supertrack Monte Carlo technique for reproducing and interpreting experimental count rate spectra.

I. INTRODUCTION

Traditional (i.e., Boltzmann) Monte Carlo radiation transport codes are generally only able to rigorously calculate so-called pulse height tallies or detector responses (i.e., count rate spectra) by analog methods. The reason for this is that such tallies, or responses, often depend on the collective transport of more than one physical particle (e.g., the detection of pair production photons produced in a crystal), whereas conventional variance reduction techniques only apply to individual particles. Because variance reduction cannot be used in such cases, the class of problems that can be solved efficiently is severely limited.

Although it is theoretically possible to apply variance reduction to the individual tracks and then back-figure the effect upon the tally (see the “deconvolution approach”), it becomes extremely difficult in practice when more than one variance reduction technique is used. Furthermore, the Monte Carlo method loses the direct connection with the physical situation. That is, the tally becomes a very complicated function of the individual track weights. Although mathematically correct, the practitioner’s intuition about the physical system is essentially lost, or at least severely hindered. The essential difficulty is that nature transports collections of particles whereas standard Monte Carlo codes transport individual particles.

To return the Monte Carlo technique to a more direct simulation of nature, the supertrack method was developed. Briefly, the supertrack method applies variance reduction to physical collections of tracks (“supertracks” or simply “tracks”) and requires redefinition of standard Monte Carlo concepts. For example, a multiplying process (e.g., \((n,2n)\)) does not create a new track, but instead includes the new track in the current track. The individual particle tracks no longer carry any weight: the variance reduction is applied to the supertracks, and thus the weights are associated with the supertracks.

For example, if it is desired to increase the number of \((e^+e^-)\) annihilation gamma pairs executing interesting random walks, one may make multiple copies of the pair. That is, the pair undergoes a variance reduction split. Whereas before the split one had one pair of weight \(w_0\) with locations \((r_1, v_1, t_1)\) and \((r_2, v_2, t_2)\), after the split one...
has two pairs of weight $w_0/2$ with locations $(r_1, v_1, t_1)$ and $(r_2, v_2, t_2)$. The random walks of the two pairs are sampled independently after the split.

The purpose of this paper is to demonstrate that this technique, when implemented into the MCNP™ Monte Carlo code, is indeed able to accurately predict the energy-dependent count rate responses of photon spectrometers such as sodium iodide (NaI) for measurements of sources in simple and complicated geometries. Comparisons between analog calculations with the current version of MCNP and the non-Boltzmann patch of MCNP are also made.

II. DESCRIPTION OF COMPUTATIONAL MODELS AND EXPERIMENTS

Earlier, approximate calculations of pulse height tallies were benchmarked with experiments. It was recognized at the time that the computational methodology was not rigorously correct, but the observed agreement with experiment was good and the methodology was used successfully for a number of applications. In this earlier work, the solid angle subtended by the detector relative to the source was small, making it unlikely that other branches of the same physical event that had undergone variance reduction were able to reach the detector if another branch reached it. These same experiments are used herein for comparisons with the new supertrack calculations.

A. COMPUTATIONAL MODELS: ANALOG VS. SUPERTRACK WITH VARIANCE REDUCTION

In the NaI detector experiments described later, 3"x3" detectors were used. Therefore the same detector model was used to verify that the supertrack Monte Carlo code agreed with the standard MCNP analog calculation. Figure 1 shows a two-dimensional plot through the center of the NaI detector model. The model includes the NaI crystal, the aluminum (Al) can and MgO layer around the crystal, the photomultiplier tube, the Al flange where the crystal is connected to the light pipe, and the light pipe itself. Also in this model is a 0.5" thick cylindrical lead (Pb) shield/collimator around the active volume of the detector that was used to reduce room return in some of the experiments.

The DXTRAN and cell importance splitting variance reduction options of MCNP are usually necessary in order to do pulse height tally calculations efficiently, so these options were used in the non-Boltzmann calculations. In order to make the test of importance splitting more realistic, three shells of Pb, each about 1 mean free path thick, were placed around the source. For these computational comparisons, no extraneous scattering materials such as room walls, detector holding fixtures, etc. were included.

The methodology for the calculations presented here has been described previously. Since the calculational comparison has to be made with a standard MCNP analog calculation, it was necessary to move the source closer to the detector (20 cm in front) than was done in the actual experiments.

B. DESCRIPTION OF EXPERIMENTS AND COMPUTATIONAL MODELS

The experiments were designed to provide insight into the effect that nearby scattering media (e.g., walls, floors, holding fixtures, etc.) can have on detector response. The ability to accurately calculate such effects highlights the value Monte Carlo calculations can have in the understanding of the physics of detector response, thereby improving the interpretation of measured data and the design of experiments and detector systems. The measurements were made by C. E. Moss of Los Alamos in a large room with concrete walls and floor. The detectors were located near one corner of the room with the front face of the detectors about 6 ft. away from the wall behind the detector. Both the closest wall to the side of the detectors and the floor were about 5 ft. away. The source was placed 1 m in front of the detector faces. Although not shown in Fig. 1, the two nearest walls and floor of the room were modeled in all calculations in order to accurately calculate the so-called backscatter peak as discussed later.

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MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory.
Since MCNP is a continuous-energy code, individual photons are tracked and tallied with specific energies, whereas in practice, detector systems are less precise in that a beam of monoenergetic photons losing all of their energy in the active volume will be detected in an approximate Gaussian distribution about the average energy due to detector and electronic effects such as charge collection statistics, electronic noise, spatial variation in the crystal response, and drifts in operating parameters. This effect is accounted for in MCNP by introducing a "Gaussian broadening" function that in effect broadens the detector response to photons as a function of energy.

In these calculations, it has been assumed that the scintillation light pulse from a photon detection event is proportional to the energy deposited by the photon in the scintillator. In practice there is some (up to ~ 10%-15%) non-linearity with deposited photon energy, but this effect was not included in this work.

III. RESULTS

A. COMPUTATIONAL VERIFICATION OF SUPERTRACK TECHNIQUE TO ANALOG MCNP

As noted earlier, the DXTRAN and cell importance splitting variance reduction options of MCNP are usually necessary in order to do pulse height tally calculations efficiently. Therefore, both options were tested in the computational comparison of the supertrack technique to the analog calculation with the standard MCNP. First, DXTRAN was used alone on a problem without the Pb layers around the source. Next, the three mean free path layers of Pb were added around the source and importance splitting performed in addition to DXTRAN.

The spectral results for the DXTRAN-only problems are shown in Fig. 2. There is no statistically significant difference between the two count rate spectra over any energy range in the spectrum. Table I gives the MCNP figure-of-merits (FOM) for these calculations. As can be seen, the FOM for the supertrack problem is about five times better than for the analog problem.

For the DXTRAN plus splitting problem, the cell importance was increased by a factor of four whenever a particle went outward from one layer of Pb to another, or escaped from the Pb. Obviously, the analog calculation was quite inefficient, and it required several days of computation on a SUN IPX. Again, the spectral results in Fig. 3 show excellent agreement between the analog and supertrack methods. Table I indicates the the figure-of-merit is increased by about a factor of 11 for the supertrack variance reduction technique.

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<th>Mean</th>
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B. EXPERIMENTAL VERIFICATION OF SUPERTRACK APPROACH

The measured and calculated $^{137}$Cs spectra with the NaI detector plus Pb collimator are shown in Fig. 4. The agreement is excellent in the full-energy photopeak region as well as in the low-energy continuum region. Some of this low-energy continuum is caused by full-energy source photons entering the detector active volume and losing only part of their energy in it before escaping. Other contributions to this region occur when source photons first lose part of their energy outside of the active volume and then scatter into the active volume where some or all of the rest of the energy is lost. With a collimator/shield around the sides of the active volume, this continuum region is as low, relative to the height of the full energy photopeak, as possible for the particular detector and shield. Even
if a perfect collimator/shield could be designed that would prevent any previously scattered photon from entering the crystal, there would still be a low-energy continuum from scattering from inert detector components. Therefore, Fig. 4 probably represents nearly the best “peak/noise” ratio (full energy photopeak height to maximum low-energy continuum) that one can attain without going to extraordinary measures to reduce the continuum. It should be noted in the figures that follow that the magnitude of the different count rate spectra are different due to different counting times and attenuation. The peak-to-noise ratio is the significant indicator of the “noisiness” of the spectra.

Maximizing this peak/noise ratio can be important if photons in the 0.1–0.5 MeV range are being measured, especially if higher energy source photons are also being measured. The so called “backscatter” effect tends to populate this region preferentially as can be seen by solving the Compton scattering equation for various energies at angles between 90 and 180 degrees. Therefore, if one is looking to measure photon lines in the range 0.1–0.5 MeV, it is to one’s advantage to minimize room return, thereby maximizing the peak/noise ratio. The peak/noise ratio in Fig. 4 is about 8/1.

If the Pb collimator/shield is removed, the results in Fig. 5 are obtained. Note the change in the relative magnitude and the shape of the low-energy continuum. A prominent backscatter peak exists at about 0.2 MeV, and the entire continuum region magnitude is raised. The peak/noise ratio is now about 3/1 at the backscatter peak and about 4/1 at lower energies. The room walls and floors effected the spectral changes observed since they are the only non-detector features modeled. Note that the agreement between calculation and experiment is still excellent. The small undercalculation that seems prevalent is undoubtedly caused by the many other objects (electronics, chairs, cabinets, etc.) in the room that were not modeled in the calculations.

Next, a high-scatter environment (a 1/2" thick Al box) was placed around the detector. The photons from the source must now pass through 1/2" of Al, enabling low-angle scattered photons from the source to reach the detector in addition to the scattered radiation from the remainder of the box, floor, and walls. This geometry accentuates the large-angle backscatter component of the spectrum, making this a more difficult test of the calculational model. The measured and calculated results are shown in Fig. 6, with good agreement demonstrated, especially in shape. The slight undercalculation in the continuum region is again presumably because of the scattering contributions from unmodeled features. Note that the sharp backscatter peak of Fig. 5 has been replaced with a much broader one, generally from 0.1–0.2 MeV, and that the continuum from about 0.2–0.5 MeV is higher. Now the worst peak/noise ratio, at about 0.2 MeV, is about 2/1.

IV. DISCUSSION OF RESULTS

The results of this study clearly show that the new supertrack technique accurately predicts NaI detector responses. In addition, it has been shown that approximate (but careful) modeling of the scattering environment around the detector is crucial to predictions of accurate responses and to understanding of the responses. This capability should enhance the information content extractable from a particular set of measured data. For example, this computational capability could be used to “recalibrate” an inaccessible detector whose nearby scattering environment has changed or to perform “what if” studies in trying to explain data that is different than expected.

V. ACKNOWLEDGMENTS

The authors gratefully acknowledge the assistance of Calvin E. Moss who performed the experiments that provided the basis for comparisons with calculations and who provided much valuable insight into the workings of detectors. Funding for this project was provided through the Los Alamos National Laboratory Laboratory Directed Research and Development (LDRD) program.

VI. REFERENCES


Fig. 2. Calculations of the NaI detector with a) standard analog Monte Carlo and b) non-Boltzmann Monte Carlo with DXTRAN.
Fig. 3. Calculations of the NaI detector with a) standard analog Monte Carlo and b) non-Boltzmann Monte Carlo with DXTRAN and cell importance sampling in three 0.8 cm thick Pb shells around the source.
Fig. 4. $^{137}\text{Cs}$ response functions for the NaI detector measured and calculated (with 1σ precision bars) with 1/2" Pb shielding around the cylindrical side.
Fig. 5. $^{137}$Cs response functions for the NaI detector of Fig. 1 measured and calculated (with 1σ precision bars) without Pb shielding; room floor and wall scattering contribute significantly to the low-energy continuum.
Fig. 6. Measured and calculated (with 1σ precision bars) response of the NaI detector in a 1/2" thick Al box.