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PULSE-HEIGHT TALLIES WITH VARIANCE REDUCTION

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ABSTRACT

Most energy deposition detectors that are used in physics, such as multichannel analyzers, are pulse-height detectors. Monte Carlo pulse-height tallies (PHTs) are difficult to model because most energy-dependent tallies score events at the energy of the projectile particle rather than score the number of events that deposit different amounts of energy. In particular, PHTs usually require that the entire Monte Carlo simulation be performed in an analog mode without variance reduction. Thus, the benefits of variance reduction, which may speed a calculation by orders of magnitude, are unavailable.

A new recursion method has been developed to enable efficient use of PHTs with variance reduction based on T. E. Booth's deconvolution method. The new method differs from other Monte Carlo deconvolution attempts because it is minimally invasive to the infrastructure of the Monte Carlo code: a single subroutine is called in a few places, and only a single line of initialization is required in a few other places. Data-storage requirements are localized, and calculations that are not using the new algorithm are unaffected. Testing has demonstrated that the new method reproduces analog PHTs to within statistical uncertainty (1%–3%) and can be faster by orders of magnitude.

Key Words: Monte Carlo, Radiation Transport, Pulse-Height Detectors, Variance Reduction

1 INTRODUCTION

A new recursion method has been developed to enable the efficient use of pulse-height tallies (PHTs) with variance reduction and has been implemented into MCNPX [1]. The new method is based on T. E. Booth's deconvolution method [2]. The new method differs from other Monte Carlo deconvolution attempts [3] because it is minimally invasive to the infrastructure of the Monte Carlo code: a single subroutine is called, and only a single line of initialization is required in a few places. Data-storage requirements are localized, and calculations that are not using the new algorithm are unaffected. Results are presented for photon, photon/thick-target bremsstrahlung (TTB), and coupled electron-photon problems, demonstrating a significant improvement in efficiency over analog-only Monte Carlo in a production Monte Carlo computer code.

1.1 Pulse-Height Detectors

Pulse-height detectors count the number of pulses of differing amounts of energy deposited in a crystal.

Because electrons and photons scattering through a material have signatures characteristic of the material, pulse-height detectors, which precisely identify the energy of the incident particle, can identify the materials through which the radiation scatters. Consequently, pulse-height detectors are used widely in many applications, from outer space (where they are used on satellites to determine the composition of nearby planets and moons) to deep underground (where they are used on oil-well logging tools to determine the location of oil and gas deposits). Pulse-height detectors also are used for nondestructive analysis, nuclear safeguards, homeland security, and many other applications.

1.2 Pulse-Height Tallies

Radiation transport codes are used to model nuclear detectors because radiation is dangerous and because detectors often are needed in hostile and remote environments such as outer space or underground. Deterministic transport codes cannot simulate PHTs accurately, but the Monte Carlo method can. Pulse-height detectors are modeled with PHTs. Monte Carlo methods simulate contributions from multiple particle segments, which are combined to produce a signal. A typical PHT spectrum for 10-MeV photons passing through limestone is illustrated in Fig. 1. The ordinate (x-axis) is the size of various energy pulse bins. The abscissa (y-axis) is the number of pulses counted for each of these bins normalized by bin width. The peak at 10 MeV corresponds to photons entering the pulse-height detector and depositing all their energy. The peak at 9.5 MeV is the first escape peak corresponding to 10-MeV photons entering the detector, with only a single pair-production photon escaping. At 9 MeV is a smaller double escape peak corresponding to both pair-production photons escaping. At 0.5 MeV is a peak from pair-production photons in the limestone entering the detector and depositing all of their energy there.

PHTs are very different from standard Monte Carlo tallies. A Monte Carlo current tally is illustrated in Fig. 2. The current tally counts the number of particles entering into the same PHT region. The total PHT pulse, summed over all PHT energy bins, is the same as the net current of the current tally (number of particles entering less those leaving). However, the energy distributions are very different. The PHT bins represent different amounts of energy deposited, as in a pulse-height detector. The current tally energy bins are merely the energies at which particles enter (or leave) the outer surface of the pulse-height detector region. The PHT and current tally are superimposed upon each other in Fig. 3 to show their dissimilarity. The escape peaks, and much of the other energy deposition information from the PHT is lost. Track-length or collision-estimator energy deposition tallies (not illustrated) are even more dissimilar to PHTs because the tally energies are those at which the tally is made; the tally is not the actual energy deposited.

The difference between PHTs and other tallies can be illustrated by the Monte Carlo random walk of Fig. 4 (taken from T. E. Booth [1]). The P's represent physical events (nodes 1, 4, 6, and 7), and the V's represent variance reduction splits (nodes 2, 3, 5, and 8). Suppose the initial particle energy is E0 and that the other energies, E1, E2, …, along each branch are the energies lost along those segments. Further, suppose that segments 7, 8, 12, and 13 are totally

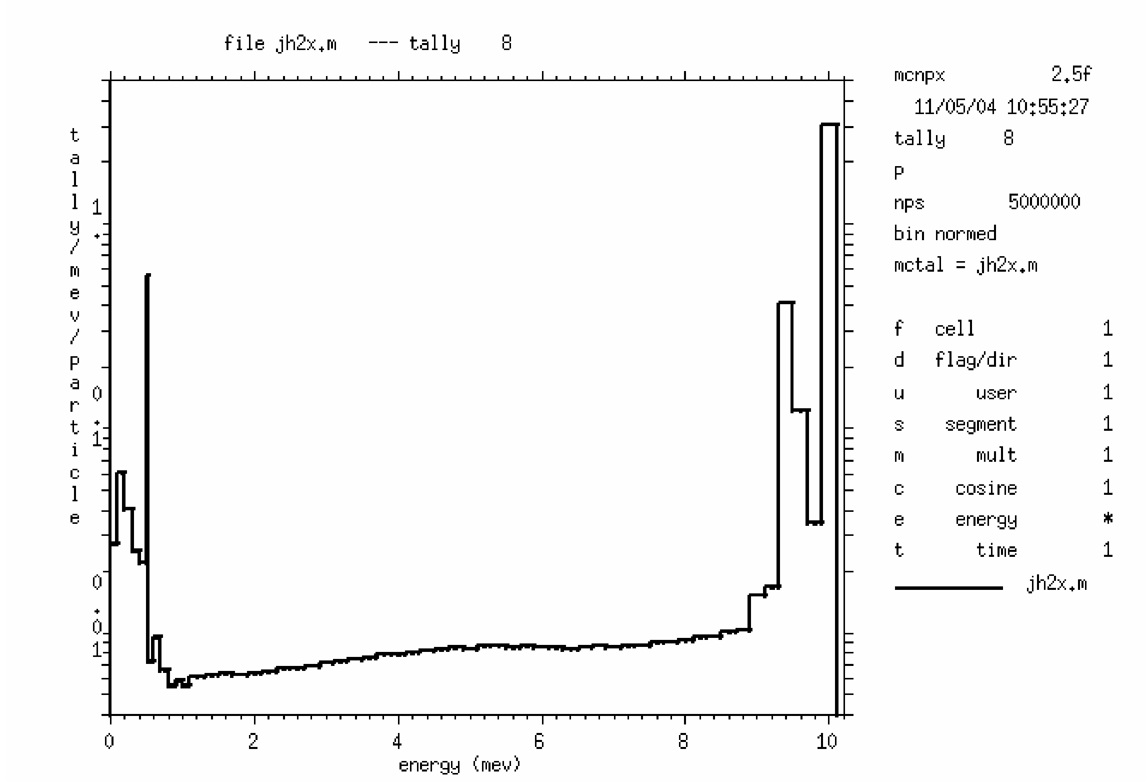

Figure 1. Pulse-height spectrum of 10-MeV photons in limestone.

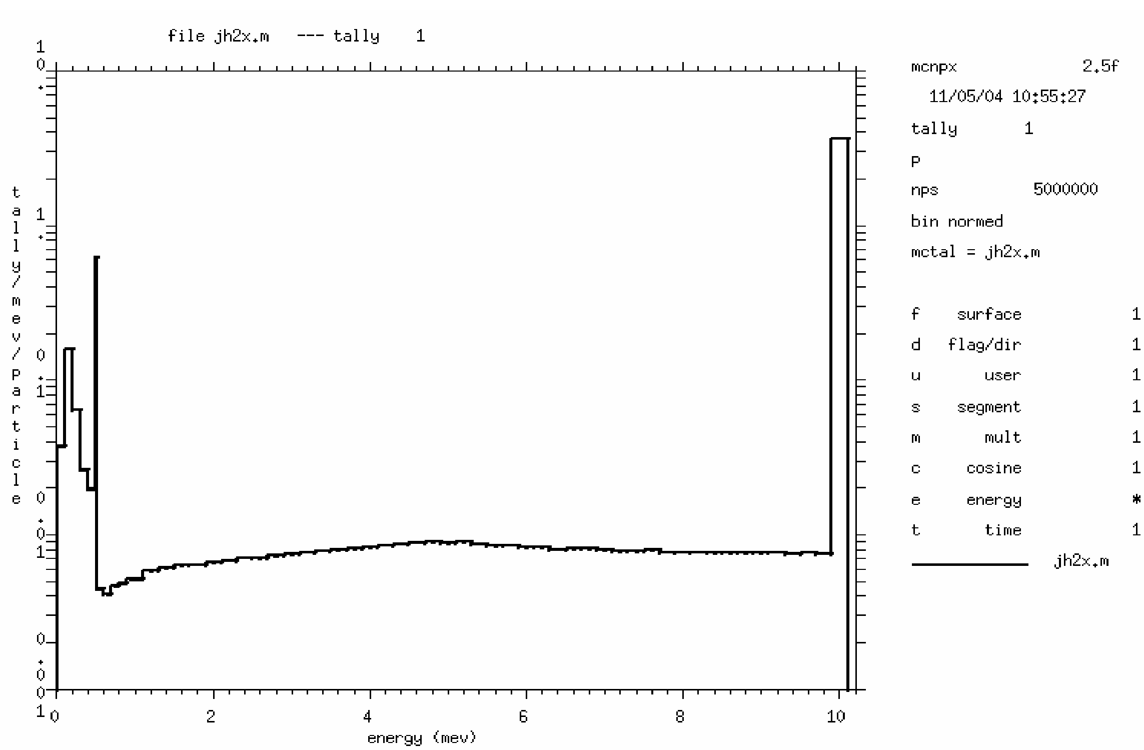

Figure 2. Current tally of 10-MeV photons in limestone.

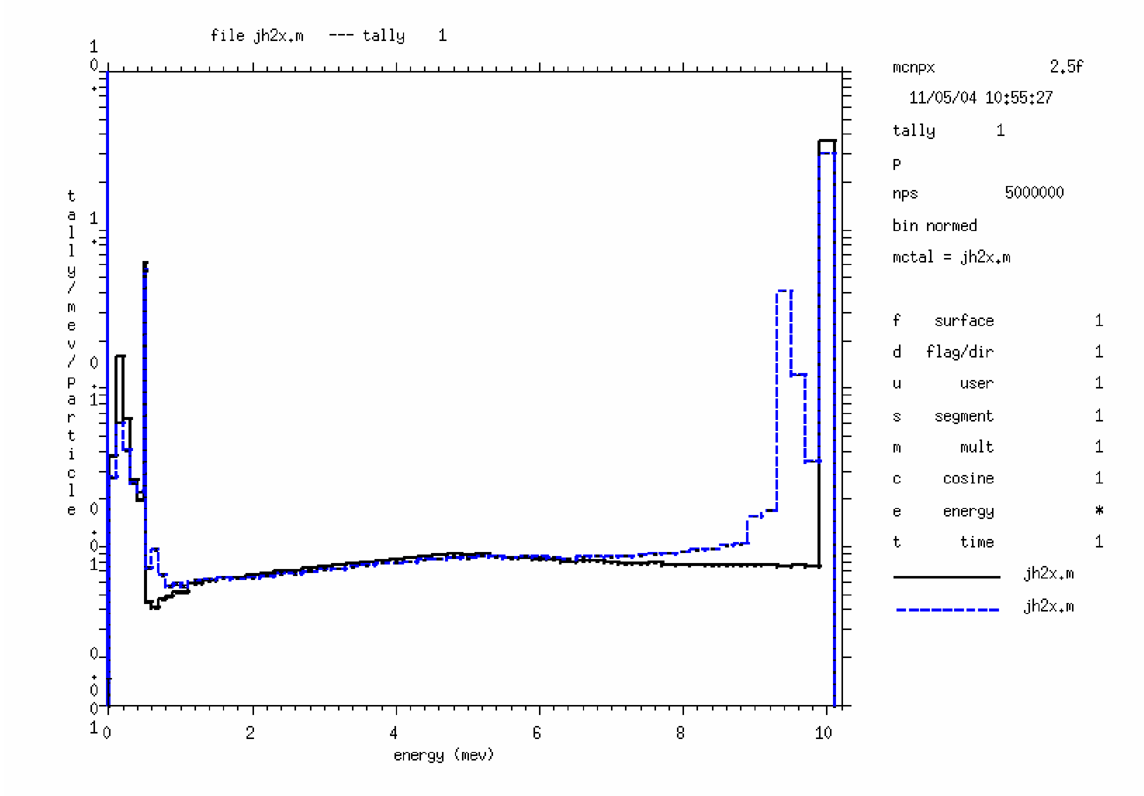

Figure 3. Comparison of PHT and current tally of 10-MeV photons in limestone.

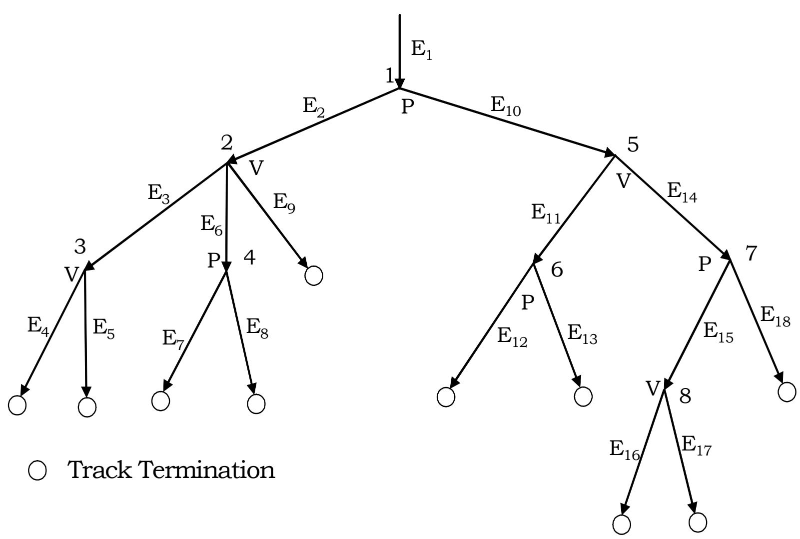

Figure 4. PHT "tree"—Monte Carlo random walk.

within the pulse-height detector. Then the current tally would have two bins, where W and EB indicate scoring weight and energy bin as

$$W1 = 1/3 \; ; \; EB1 = E0 - E1 - E2 - E6 = E7 + E8$$
$$W2 = 1/2 \; ; \; EB2 = E0 - E1 - E10 - E11 = E12 + E13. \quad (1)$$

The PHT would have one bin:

$$W7 = 1/6 \; ; \; EB7 = E7 + E8 + E12 + E13. \quad (2)$$

It is evident that the current tally [Eq. (1)] is very different from the PHT tally [Eq. (2)]. Further, the current tally is easy to compute. W1 and W2, and EB1 and EB2 are simply the weights and energies of the particles crossing into the pulse-height-detector tally region. However, for the PHT, the tally can be made only after the entire history is complete and the entire random walk, or PHT tree, can be deconvolved. The full deconvolution of the tree (assuming that all segments are within the PHT) in Fig. 4 is

$$W1 = 1/12 \; ; \; EB1 = E1 + E2 + E3 + E4 + E10 + E11 + E12 + E13$$
$$W2 = 1/24 \; ; \; EB2 = E1 + E2 + E3 + E4 + E10 + E14 + E15 + E16 + E18$$
$$W3 = 1/24 \; ; \; EB3 = E1 + E2 + E3 + E4 + E10 + E14 + E15 + E17 + E18$$
$$W4 = 1/12 \; ; \; EB4 = E1 + E2 + E3 + E5 + E10 + E11 + E12 + E13$$
$$W5 = 1/24 \; ; \; EB5 = E1 + E2 + E3 + E5 + E10 + E14 + E15 + E16 + E18$$
$$W6 = 1/24 \; ; \; EB6 = E1 + E2 + E3 + E5 + E10 + E14 + E15 + E17 + E18$$
$$W7 = 1/6 \; ; \; EB7 = E1 + E2 + E6 + E7 + E8 + E10 + E11 + E12 + E13$$
$$W8 = 1/12 \; ; \; EB8 = E1 + E2 + E6 + E7 + E8 + E10 + E14 + E15 + E16 + E18$$
$$W9 = 1/12 \; ; \; EB9 = E1 + E2 + E6 + E7 + E8 + E10 + E14 + E15 + E17 + E18$$
$$W10 = 1/6 \; ; \; EB10 = E1 + E2 + E9 + E10 + E11 + E12 + E13$$
$$W11 = 1/12 \; ; \; EB11 = E1 + E2 + E9 + E10 + E14 + E15 + E16 + E18$$
$$W12 = 1/12 \; ; \; EB12 = E1 + E2 + E9 + E10 + E14 + E15 + E17 + E18$$

If branches 7, 8, 12, and 13 are the only branches in the pulse-height detector, then all of the other energies are not counted and the result is EB7 = E7 + E8 + E12 + E13, as provided in Eq. (2).

1.3 The Challenge of Pulse-Height Tallies

Most Monte Carlo computer codes require analog transport (no variance reduction) for PHT problems. Without variance reduction techniques (VRTs) to accelerate Monte Carlo convergence, some problems can take many times longer to run in the analog mode—even orders of magnitude longer. However, variance reduction generally has not been implemented for PHTs in Monte Carlo codes because of its difficulty. Booth suggested several possible methods years ago [4]. We believe that the best of these approaches is deconvolution, as illustrated previously. Deconvolution has not been available in a major Monte Carlo code until now because of its complexity. The deconvolution approach requires the following.

1. Reconstruction of the entire random walk into a deconvolution PHT tree. This reconstruction can require recording every event of the random walk, which clutters

up a Monte Carlo code greatly by having PHT coding spread throughout the code. Further, constructing the tree can result in huge trees requiring huge amounts of storage with constantly changing memory requirements. Also, the entire tree must be put into the "bank," with every particle split so that it can be retrieved properly by subsequent branches of a split.

2. Deconvolution of the tree. The deconvolution algorithm can be complex and time consuming. Further, the tree shown in Fig. 4 is used for splitting only. It becomes far more complex for Russian roulette and other variance reduction methods.

2 IMPLEMENTATION OF PULSE-HEIGHT TALLIES WITH VARIANCE REDUCTION TECHNIQUES

The PHT deconvolution method has been implemented into MCNPX [1] and works with most VRTs. MCNPX is a successor code to the popular general-purpose Monte Carlo MCNP4A, MCNP4B, and MCNP4C [5] codes. Indeed, MCNPX is a superset of MCNP4C3 and tracks it identically. However, MCNPX extends MCNP4C much further [6], now including the recent addition of PHTs with variance reduction.

The implementation of PHTs with VRTs in MCNPX does not congest the code with copious PHT logic to record the deconvolution tree. A single subroutine is called at seven key places. Further, the entire deconvolution tree need not go into the "bank" at each particle split. Only one bank word is required for the MCNPX implementation, and only four words total are added to the code common blocks. Thus, the PHT with VRTs has a minimal impact on Monte Carlo problems when it is not used, and it has a very isolated logic when it is used. The single routine is admittedly quite complex, with seven cases (similar to entry points) and several dynamically adjusted storage arrays that can become large. However, the complexity of the algorithm was minimized by the development of a novel regression technique: the tree is deconvolved from the bottom up using a Fortran recursion routine.

Among many innovations in the MCNPX implementation are the following.

1. The entire PHT tree need not go into the bank at every particle split. All that is necessary is an index that allows the tree to be "resumed" for particles coming out of the bank.

2. Not all tree information must be saved—only the
   a. event type at each tree branch,
   b. incoming particle weight at each tree branch,
   c. energy and weight at track termination, and
   d. energy entering and exiting the PHT. The energy deposited along each branch of the tree is not required (Booth method).

3. At physical splits, all of the energy deposited so far can be associated with the main branch of the tree and zero energy with the subsequent branches. The arbitrary allocation is possible because in the deconvolution, the energies from the branches of

a split are all added together again. In this way, all physical split particles coming out of the bank do not need to be associated with the energy deposited up to that point, thus greatly simplifying bookkeeping in constructing the deconvolution tree.

4. Branches of the deconvolution tree can undergo Russian roulette if the tree gets too large.

3 RESULTS

PHTs with variance reduction are now available in MCNPX. The following variance reduction methods are available: importance sampling (geometric splitting and Russian roulette), weight windows (both cell and mesh based), forced collisions, and exponential transform. Analog capture rather than implicit capture is required because it is more efficient and avoids rouletting of entire PHT trees. DXTRAN is under development. Currently, the PHTs may be used for photon-only problems, photon transport with the TTB approximation, and fully coupled photon-electron transport.

Figure 5 illustrates the results for a pulse-height detector embedded in limestone. Three pairs of curves can be seen. Each pair is the analog and weight window result; these curves lie on top of each other, demonstrating that the PHT provides the same results with and without

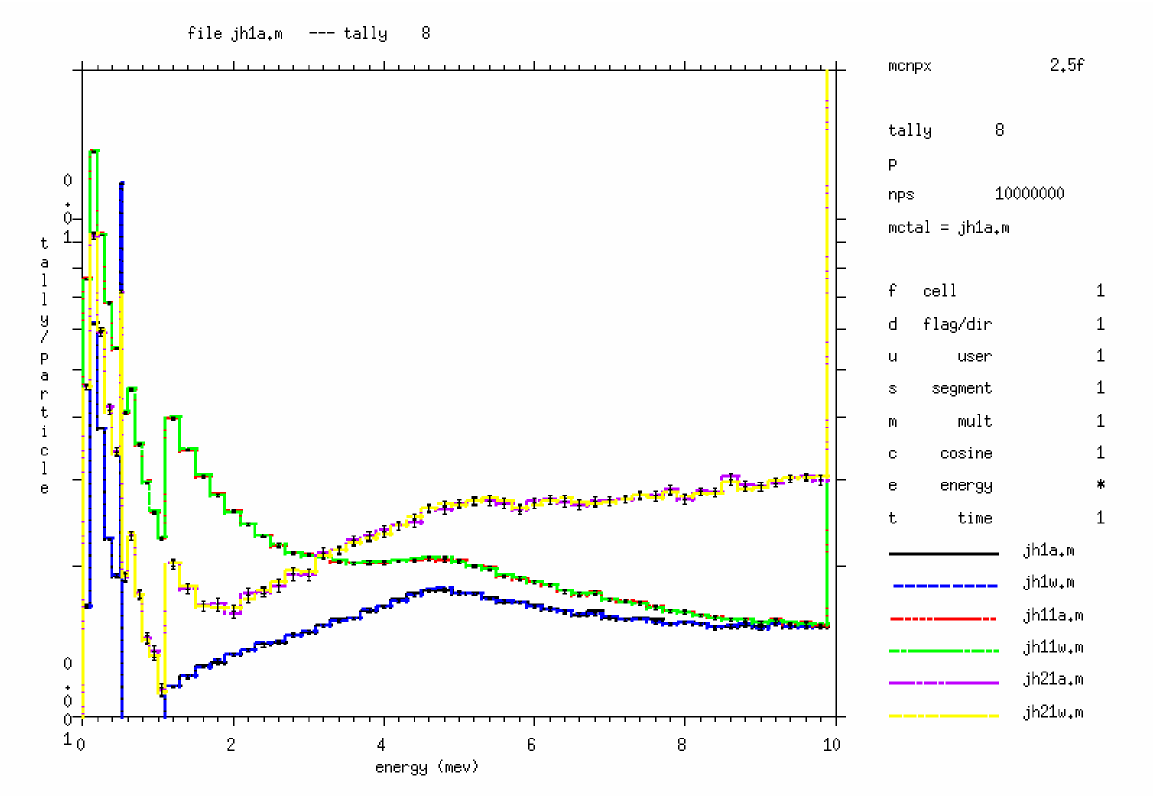

Figure 5. Comparison of analog and weight window results for photon-only, TTB, and full-electron transport.

variance reduction. The three pairs of curves are seen for photon-only transport (black-blue: bottom), photons with TTB (red-green: top on left and middle on right), and full electron-photon transport (yellow-purple: middle on left and top on right). To obtain an analog comparison result that converges in a reasonable amount of time, knock-on electrons are turned off.

The speedup resulting from variance reduction is highly problem dependent. For some problems, the analog case is faster because of the effort involved in deconvolution or because Russian rouletting of very large PHT trees causes weight fluctuations that increase the variance. However, in other problems, particularly those where variance reduction improves the efficiency of standard tallies such as the current tally, the new method is much more efficient. Improvement in factors up to 80 in the "figure-of-merit" measure of problem efficiency has been observed. Even better results are anticipated with further refinements in the method.

4 CONCLUSIONS

PHTs with variance reduction have been implemented into MCNPX using Booth's deconvolution method but have been engineered to (1) have minimal code impact on problems without PHTs; and (2) be unobtrusive, fast, and compact when used with pulse-height problems. Major variance reduction methods are available, and the method works for photon-only, photon-plus-TTB, and full photon-electron transport. The method is being extended to other particle types and variance reduction methods. Comparisons with analog transport give excellent agreement for many problems.

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