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AUTOMATED WEIGHT-WINDOW GENERATION FOR THREAT DETECTION APPLICATIONS USING ADVANTG

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ABSTRACT

Deterministic transport codes have been used for some time to generate weight-window parameters that can improve the efficiency of Monte Carlo simulations. As the use of this hybrid computational technique is becoming more widespread, the scope of applications in which it is being applied is expanding. An active source of new applications is the field of homeland security – particularly the detection of nuclear material threats. For these problems, automated hybrid methods offer an efficient alternative to trial-and-error variance reduction techniques (e.g., geometry splitting or the stochastic weight window generator). The ADVANTG code has been developed to automate the generation of weight-window parameters for MCNP using the Consistent Adjoint Driven Importance Sampling method and employs the TORT or Denovo 3-D discrete ordinates codes to generate importance maps. In this paper, we describe the application of ADVANTG to a set of threat-detection simulations. We present numerical results for an "active-interrogation" problem in which a standard cargo container is irradiated by a deuterium-tritium fusion neutron generator. We also present results for two passive detection problems in which a cargo container holding a shielded neutron or gamma source is placed near a portal monitor. For the passive detection problems, ADVANTG obtains an $O(10^4)$ speedup and, for a detailed gamma spectrum tally, an average $O(10^2)$ speedup relative to implicit-capture-only simulations, including the deterministic calculation time. For the active-interrogation problem, an $O(10^4)$ speedup is obtained when compared to a simulation with angular source biasing and crude geometry splitting.

Key Words: hybrid transport methods, weight-window simulations, nuclear material detection

1. INTRODUCTION

For some time now, deterministic transport codes have been used to generate weight-window parameters that can improve the efficiency of Monte Carlo simulations of challenging fixed-source transport problems [1]. For many problems, this hybrid computational technique provides a significant (dramatic, in some cases) reduction of the statistical uncertainty in tally estimates when compared to analog or implicit-capture-only simulations. In addition, automated hybrid methods offer an efficient alternative to trial-and-error variance reduction techniques (e.g., geometry splitting or the stochastic weight window generator). At the Oak Ridge National Laboratory, two packages have been developed to automate this computational process: (1) the MAVRIC [2] sequence of SCALE 6 [3] and (2) the ADVANTG code [4]. As the use of these automated tools is becoming more widespread, the scope of applications in which they are being applied is expanding.

An active source of new applications of hybrid methods is the field of homeland security. A key interest in this area is the detection of nuclear material threats, for example, at ports of entry. A variety of transport simulations are being studied in order to design and develop detection systems that can identify the presence of such threats. Reference 5 proposes an anomaly detection algorithm for improving the operation of radiation portal monitors that can be deployed, for example, at truck weigh-stations. The algorithm was evaluated using implicit-capture-only Monte Carlo simulations with MCNP [6]. Reference 7 describes experiments and implicit-capture-only MCNPX [8] simulations that were performed to study a system to "actively interrogate" cargo containers with pulses of high-energy neutrons and/or photons generated by a linear accelerator. Reference 9 describes the development of a deterministic transport code system for analyzing a variety of security-driven radiation detection scenarios, such as portal monitoring.

These types of transport problems generally involve relatively small, shielded threat objects located within large containers or transport vehicles that may be separated from detection equipment by several meters. For many of these problems, analog Monte Carlo simulations are terribly inefficient and require substantial computing resources. Standard variance reduction techniques (e.g., source biasing, geometry splitting, and the stochastic weight-window generator) can be used to obtain large gains in computational time but require significant effort from the user to determine problem-specific parameters through a trial-and-error process. Deterministic transport methods offer more reasonable computational times. On the other hand, Reference 9 indicates that some significant development effort is required (with a 3-D, unstructured-mesh code) to obtain a high degree of accuracy in these sorts of problems. Automated hybrid techniques may offer an attractive alternative to all of these approaches.

In this paper, we describe the ADVANTG code, which was developed to automate the generation of weight-window parameters for MCNP using the Consistent Adjoint Driven Importance Sampling (CADIS) methodology [1] and the TORT [10] or Denovo [11] 3-D discrete ordinates codes. We present numerical results for an "active-interrogation" problem in which a standard cargo container is irradiated by a deuterium-tritium fusion neutron generator. We also present results for two passive detection problems in which a cargo container holding a shielded neutron or gamma source is placed near a portal monitor.

2. CADIS METHODOLOGY

Consider the fixed-source transport problem

$$\mathbf{H}\psi = q\,, \tag{1}$$

where $\mathbf{H}$ denotes the transport operator, q is the (known) source distribution, ψ is the (unknown) angular flux density, and boundary conditions are assumed given. It is assumed that the quantity of interest in a transport simulation of Eq. (1) can be written as the functional

$$R = \langle \sigma_d, \psi \rangle\,, \tag{2}$$

where σ_d denotes an arbitrary response function (e.g., a detector cross section) and the angle brackets denote integration over all phase-space variables. For many transport problems, *R* can be estimated with less uncertainty (in a given amount of computational time) by employing the weight-window technique (e.g., see [6]) with weights derived from an approximate solution to the adjoint transport equation

$$\mathbf{H}^{+}\psi^{+} = \sigma_d \,. \tag{3}$$

Here, $\mathbf{H}^{+}$ is the adjoint transport operator, which is related to the forward operator by

$$\left\langle \psi, \mathbf{H}^{+}\psi^{+} \right\rangle = \left\langle \psi^{+}, \mathbf{H}\psi \right\rangle . \tag{4}$$

The boundary condition for Eq. (3) is generally taken as one identical to the forward condition, though it is applied to the opposite directional half-space.

The solution to Eq. (3) can be interpreted as an importance function. This can be understood by setting $q = \delta(\mathbf{P} - \mathbf{P}_0)$, where δ is the Dirac delta function and $\mathbf{P}_0$ denotes an arbitrary location in the problem phase-space. In this case, Eq. (4) reduces to

$$\psi^{+}(\mathbf{P}_0) = \left\langle G(\mathbf{P}_0 \to \mathbf{P}), \sigma_d \right\rangle_{\mathbf{P}} , \tag{5}$$

where the forward solution is identified as the Green's function, *G*. Hence, $\psi^{+}(\mathbf{P}_0)$ is the expected contribution, to the functional *R*, from a unit-weight particle emitted at $\mathbf{P}_0$. The adjoint function, then, can be used to determine whether a particle's trajectory will carry it toward a region of higher or lower relative importance. This knowledge allows one to focus computational effort on important regions of the problem.

In the CADIS method, an importance map is generated according to Eq. (3) and appropriate boundary conditions. Weight targets are then computed in proportion to the inverse of the adjoint scalar flux

$$w(\mathbf{P}) = \frac{R}{\phi^{+}(\mathbf{P})} \,. \tag{6}$$

For the MCNP code, weight-window lower bounds are computed as

$$w_{\ell}(\mathbf{P}) = \frac{2}{(1+r)} \frac{R}{\phi^{+}(\mathbf{P})} , \tag{7}$$

where *r* is the ratio of the upper and lower weight bounds. A unique feature of the CADIS method is the use of the biased source distribution

$$\hat{q}(\mathbf{P}) = \frac{\phi^{+}(\mathbf{P}) q(\mathbf{P})}{R} , \tag{8}$$

which ensures that each source particle starts with a weight at (or near) the target value, and hence is consistent with the weights given by Eq. (6) or (7). In addition, the biased source will be preferentially sampled in regions of high importance.

3. ADVANTG CODE

The ADVANTG code was developed to automate the generation of weight-window parameters for MCNP using the CADIS method. The initial versions of ADVANTG existed as modifications to the MCNP4C3 source code and employed the TORT code for generating importance maps. In recent development work: (1) sections of code that could not be separated from the MCNP source code were split off into a separate application called MCNP-DXM, which was also updated as a modification to MCNP-5.1.40, and (2) the code was extended to use the new Denovo discrete ordinates package. Denovo offers substantial improvements with respect to efficiency and robustness due to its implementation of Krylov-subspace acceleration and an embedded first-collision source capability. In addition, Denovo can perform transport sweeps on multiple processors in parallel using the Koch-Baker-Alcouffe algorithm (see [11]). Hence, Denovo provides an obvious path forward for handling large-scale problems. Note, however, that all results presented in this paper were computed using Denovo in serial execution mode.

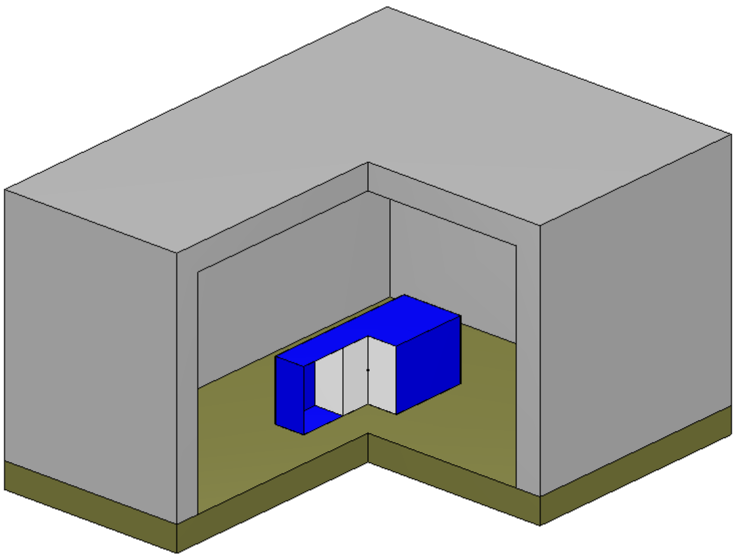
Given an MCNP input file, the ADVANTG code executes MCNP-DXM to generate (1) a material map on a user-specified, three-dimensional, structured grid and (2) material composition information, which is comprised of ZAIDs (nuclide identifiers) and number densities. The material specification is then translated into one that is appropriate for an ANISN-format multigroup library (e.g., BUGLE-96 or CASK). In some cases, the multigroup library will not have data for all of the nuclides present, and *ad hoc* substitutions are made with the understanding that extremely high fidelity is not required from the adjoint calculation. Given boundary conditions and computational parameters for the deterministic code (e.g., quadrature order, scattering expansion order, etc.), the solution to the adjoint transport problem in Eq. (3) is then estimated using Denovo. The response, R, in Eq. (2) is calculated and used to compute space- and energy-dependent weight-window lower bounds from Eq. (7) and a biased source distribution from Eq. (8). ADVANTG outputs the weight-window lower bounds and biased source distribution in a format compatible with the standard weight-window and general source (SDEF) features of both MCNP and MCNPX.

4. NUMERICAL RESULTS

In this section, we first consider an "active-interrogation" problem in which a standard cargo container holding a shielded sphere of highly enriched uranium (HEU) is irradiated by 14.1 MeV neutrons produced by a deuterium-tritium fusion neutron generator. We also look at two passive detection problems that model a portal monitoring scenario. For these problems, ^{252}Cf and ^{133}Ba point sources are placed in a cargo container and shielded by blocks of polyethylene or low-density iron. All calculations were performed on 2 GHz Dual- or Quad-Core AMD Opteron^{TM} processors. In all cases, upscatter iterations were not performed in the Denovo calculations. However, an option was used in Denovo to ensure (a not necessarily correct) particle balance.

4.1. SEALAND-N Problem

To demonstrate the use of ADVANTG for active interrogation scenarios, we simulated a problem from Reference 7. In that work, the quantities of interest are the prompt and delayed neutron and gamma count rate response to the active interrogation of a standard cargo container (8 ft × 8 ft × 20 ft) with 11 different neutron and/or photon sources. The threat object is a 5 kg sphere of 95% enriched uranium (3.982 cm radius) placed at the center of the container and shielded by several different high-Z and/or hydrogenous materials. The interrogation is performed inside a building with 1m thick concrete walls and roof, while the floor (also 1 m thick) was modeled as soil, as shown in Figure 1. The source is located 20 cm laterally from the 20 ft side of cargo container and aligned with the center of the threat object. We selected the problem in which the threat object is embedded in a polyethylene cube (2.35 m × 2.35 m × 2.35 m) and irradiated by 14.1 MeV neutrons from a D-T generator. For convenience, we refer to this problem as the SEALAND-N problem.



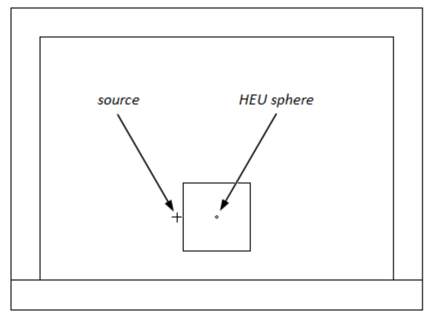


Figure 1. (left) 3-D view of the SEALAND-N problem. The front, right quarter of the building was removed to reveal the cargo container and polyethylene shielding material. (right) 2-D slice through the center of the building

An MCNPX-2.6.0 simulation was performed with continuous-energy neutron data to estimate the fission rate response in the threat object. The weight cutoffs specified on the MCNPX `cut:n` card were set to the following values: `wc1` = `-2.0e-3` and `wc2` = `-1.0e-3`, which are lower than the default values. Two additional, and more important, forms of variance reduction were used. First, the angular source distribution was biased towards the threat object. Second, the cell importance values were increased by a factor of two along the path from the source to the threat object. To obtain a relative uncertainty of less than 5%, the simulation was executed for 86.6 days.

ADVANTG was used to generate weights on a 37 × 45 × 37 mesh (61,605 cells) with a 27-group neutron cross section library (derived from ENDF/B-VII data) that is distributed as part of SCALE 6 [3]. An S_8, P_3 Denovo adjoint calculation was performed in 329 seconds of run time. The weight-window bounds and biased source distribution were then used in an MCNPX simulation for 60 minutes. The results are compared in Table I.

Table I. Comparison of analog MCNPX and ADVANTG results for the SEALAND-N problem

	MCNPX[1]	ADVANTG
Mean[2]	3.402×10^{-7}	3.224×10^{-7}
Relative Error	4.13%	1.17%
VOV[3]	0.0582	0.0009
PDF Slope[4]	4.4	8.1
FOM[5]	0.0047	122 (112)[7]
Tracks Entering[6]	72,138	1,236,947
Histories	1.800×10^{9}	5.528×10^{5}
Run Time (min)	124,709	60 (65.5)[7]

[1] With implicit capture, lowered weight cutoffs, angular source biasing, and crude cell importances
[2] Fission rate per source particle
[3] Estimated variance of the variance (≤ 0.1 is desirable)
[4] Estimated slope of the empirical PDF high-score tail (max = 10.0; ≥ 3 is desirable)
[5] Figure of Merit (= $1/(R^2T)$, where R = relative error and T = time in minutes)
[6] Number of tracks entering the tally cell
[7] Including Denovo run time

The difference in the tallied fission rate between the two simulations is 5.23%, which is well-within two standard deviations of the less-certain result. In both cases, the tallies passed all 10 statistical checks that are performed in MCNPX. The number of tracks entering the tally cell per source particle is roughly 56,000 times larger when using the ADVANTG-generated weight windows. It is not surprising, then, that the figure of merit (FOM) is increased by a factor of about 24,000 (including the Denovo run time). In addition, the variance of the variance, which is sensitive to low-frequency, high-score events, is substantially lower with the ADVANTG-generated weight windows, providing confidence in the statistical convergence.

4.2. PGASP-N and PGASP-P Passive Detection Problems

To demonstrate the use of ADVANTG for passive detection scenarios, we simulated two portal monitoring problems. A model of the PNNL Generic Advanced Spectroscopy Panel (PGASP) [12], which is illustrated in Figure 2, was used for this purpose. The panel consists of a Neutron Detection Module (NDM) and a Gamma Detection Module (GDM). The NDM consists of two tubes filled with ^{3}He located within a polyethylene box that is thinnest on the front side. The GDM consists of four large NaI detectors, which are shielded laterally and on the side opposite the photomultiplier tube by 0.635 cm of lead.

The portal monitoring scenario was constructed by placing a standard 20 ft cargo container at the center of a 14 ft lane extending laterally from the front surface of the PGASP, as shown in Figure 3. The cargo container and panel were located 76.2 and 15.24 cm above the 1 ft thick concrete pavement, respectively. An equally spaced 5 × 2 array of 1 m × 1 m × 2m blocks of

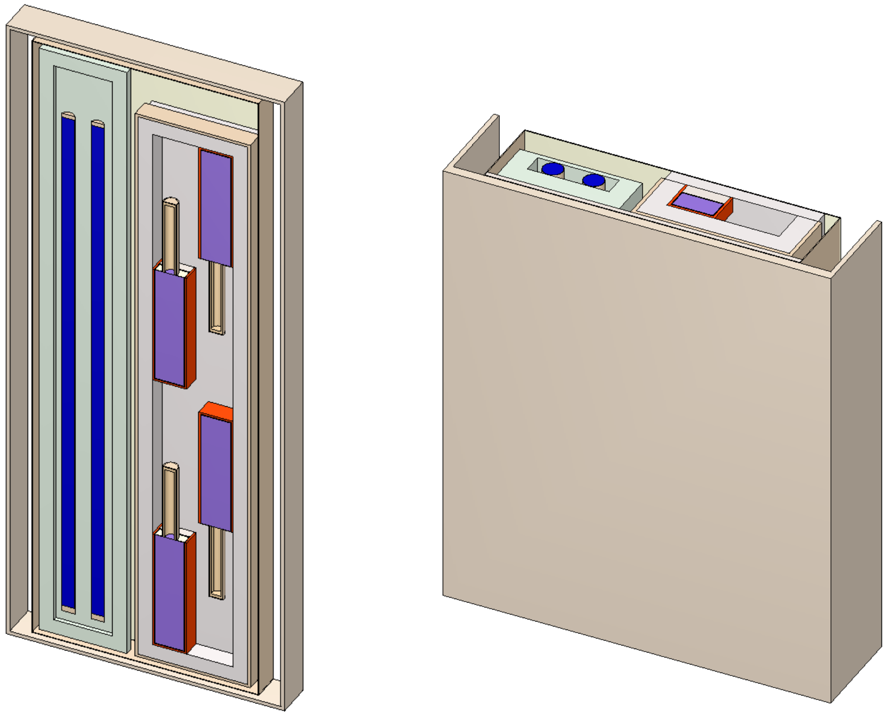


Figure 2. (left) PNNL Generic Advanced Spectroscopy Panel with the back half removed; (right) PGASP with the top half removed.

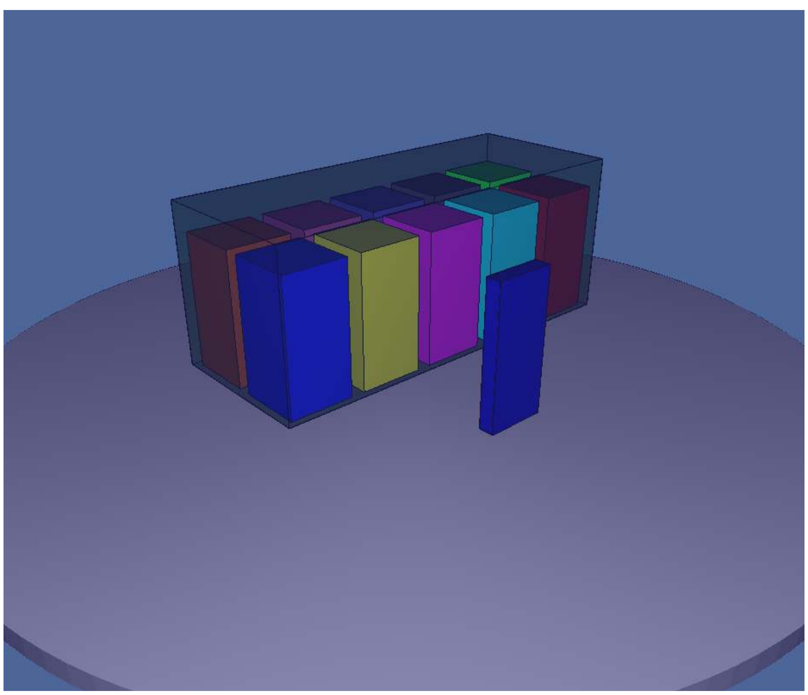


Figure 3. 3-D view of the PGASP problem geometry. The cargo container was made transparent to reveal the pallets of material inside.

polyethylene and low-density iron were placed inside the container. Two problems were created by placing: (1) a ^{252}Cf neutron point source (modeled using a Watt fission spectrum) at the center of the block nearest the panel and (2) a ^{133}Ba gamma-emitting point source (with 19 discrete lines from 3.8 to 383.8 keV) at the center of the container. We refer to these problems as the PGASP-N and PGASP-P problems, respectively. The arrangement of the materials, as well as the density of the polyethylene, was varied between problems, as shown in Figures 4a and 4b.

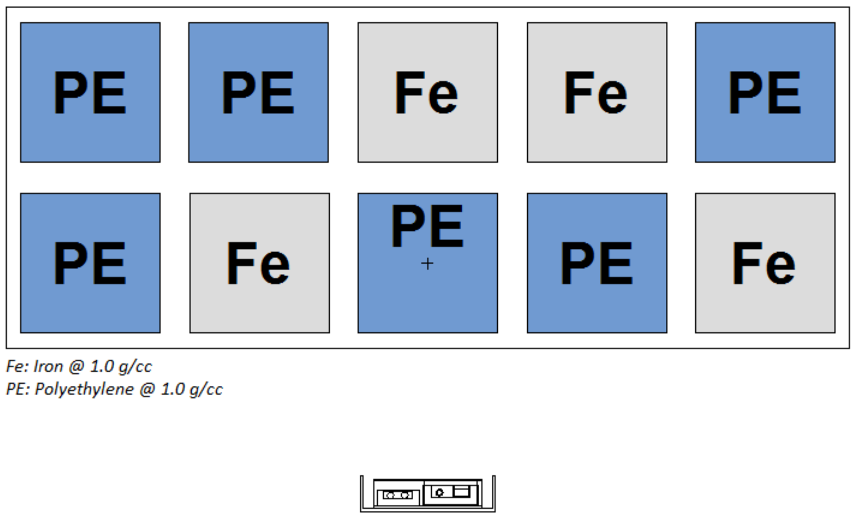


Figure 4a. Shielding materials for the PGASP-N problem. The location of the source is indicated by the cross.

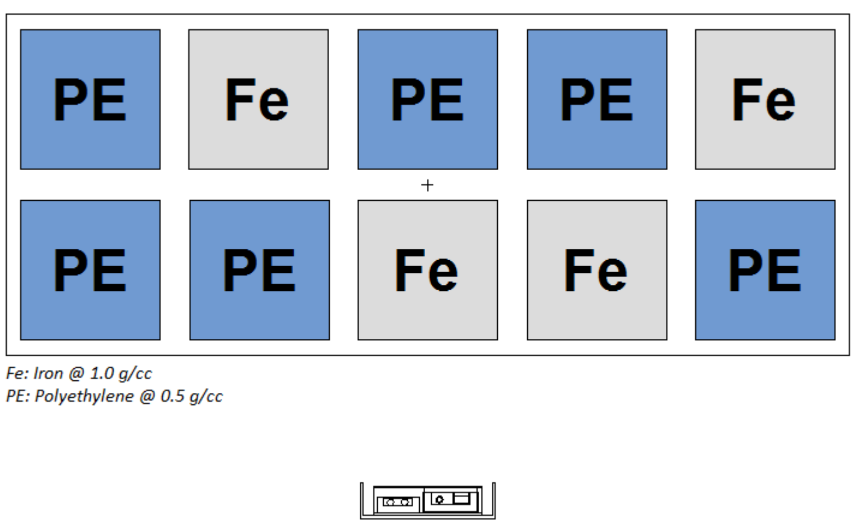


Figure 4b. Shielding materials for the PGASP-P problem. The location of the source is indicated by the cross.

In the PGASP-N problem, the quantity of interest is the (n, p) count rate in the two ^{3}He tubes in the NDM. The problem was first simulated using MCNP-5.1.40 with continuous-energy data for about 19.7 days. Implicit capture was the only variance reduction technique that was used. ADVANTG was then executed to generate weights on a 119 × 74 × 98 mesh (862,988 cells). This mesh resolves all material boundaries within the panel and has a relatively fine grid in the polyethylene (in the NDM, as well as in the pallets). A mesh optimization study was not performed, so it is not known if this scale of mesh was actually required for this problem. The 27-group neutron cross section library was initially used. In the weight-window simulation however, the variance of the variance was found to behave erratically. In addition, the high-score contributions to the empirical probability density function (PDF) did not appear to be well sampled. We believe that this is due to the fact that the true importance varies significantly within the highest energy group, which extends from 6.3763 to 20 MeV. The 47-group BUGLE-96 neutron cross section library [13] was then selected, since it contains six groups between 6.0653 and 17.332 MeV (the upper limit), and was found to provide excellent results. An S_8, P_1 Denovo adjoint calculation was performed in 101.3 minutes of run time. The weight-window bounds and biased source distribution were then used in an MCNP simulation for 60 minutes. The results are compared in Table II.

Table II. Comparison of analog MCNP and ADVANTG
(n, p) count-rate per source particle results for the PGASP-N problem

	Analog[1]		**ADVANTG**	
	-x ^{3}He Tube	+x ^{3}He Tube	-x ^{3}He Tube	+x ^{3}He Tube
Mean	$8.359{\times}10^{-11}$	$8.254{\times}10^{-11}$	$7.961{\times}10^{-11}$	$8.366{\times}10^{-11}$
Relative Error	4.14%	3.93%	0.51%	0.50%
VOV[2]	0.0058	–	0.0004	0.0003
PDF Slope[3]	10.0	–	5.8	6.0
FOM[4]	0.021	0.023	633 (238)[6]	672 (248)[6]
Tracks Entering[5]	3,295	3,383	1,921,186	2,011,772
Histories	$1.924{\times}10^9$		$37.87{\times}10^6$	
Run Time (min)	28,355		60 (161.3)[6]	

[1] With implicit capture
[2] Estimated variance of the variance (≤ 0.1 is desirable)
[3] Estimated slope of the empirical PDF high-score tail (max = 10.0; ≥ 3 is desirable)
[4] Figure of Merit (= $1/(R^2T)$, where R = relative error and T = time in minutes)
[5] Number of tracks entering the tally cell
[6] Including Denovo run time

The difference in the tallied count rates between the two simulations is 4.76% and 1.36%, which are well within two standard deviations of the less-certain results. In the analog simulation, tally fluctuation charts (TFCs) were saved for only the left-side ^{3}He tube (an oversight). In the ADVANTG weight-window simulation, TFC information was saved for both tallies. In all three cases, the tallies passed all 10 statistical checks that are performed in MCNP. The number of tracks entering the tally cell per source particle is roughly 30,000 times larger when the ADVANTG-generated weight windows are used. The FOM is increased by a factor of about 11,000 (including the Denovo calculation time).

For the PGASP-P problem, the quantity of interest is the energy-dependent average scalar flux (over 1 keV energy bins) in the four NaI detectors in the GDM. The problem was simulated using MCNP-5.1.40 for 8 hours and then again for 5 days using only implicit capture. ADVANTG was then used to generate weights on a 111 × 68 × 96 mesh (724,608 cells). This mesh resolves all material boundaries within the panel. As with the PGASP-N problem, it is not known if this size of mesh was actually required for this problem. The 19-group photon cross section library (based on ENDF/B-VII data) that is distributed with SCALE 6 was used. Initially, an S_8, P_3 Denovo adjoint calculation was performed in 11.3 minutes of run time over the five active energy groups. A second Denovo calculation with an S_{16} quadrature set was performed (in 41.5 minutes of run time) and found to provide substantially better results. We believe that the higher-order quadrature set more accurately represents the impact of the streaming pathways that exist between the material blocks. The weight-window bounds and biased source distribution were then used in an MCNP simulation for 8 hours.

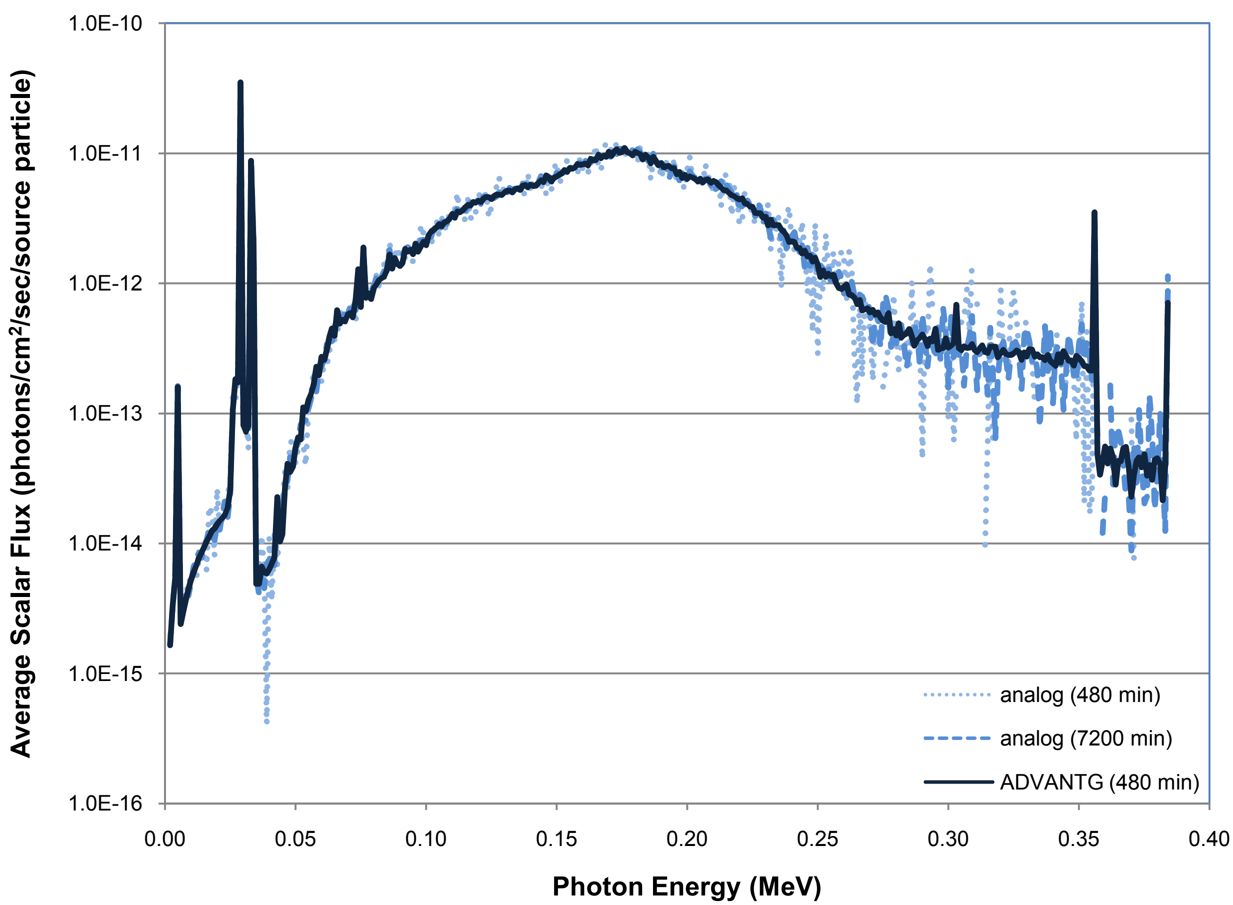


Figure 5. Energy-dependent average scalar flux results for the PGASP-P problem.

The energy-dependent average scalar flux results are plotted in Figure 5. It can be seen that the mean values agree well over the full energy range. The relative errors are compared in Figure 6, which plots the fraction of tally bins that have less than the amount of relative error given on the horizontal axis. For convenience, this data are summarized in Table III. It is clear that the results based on the ADVANTG-generated weight-windows have significantly smaller uncertainties than the implicit-capture-only case that ran 15 times longer. The FOMs for the 383 tally bins ranged from 0 to 5.5 in the analog simulation (2 bins received no contributions), and from 0.0052 to 91.1 with the ADVANTG-generated weight-windows. The average speedup factor was 258 (including the Denovo calculation time).

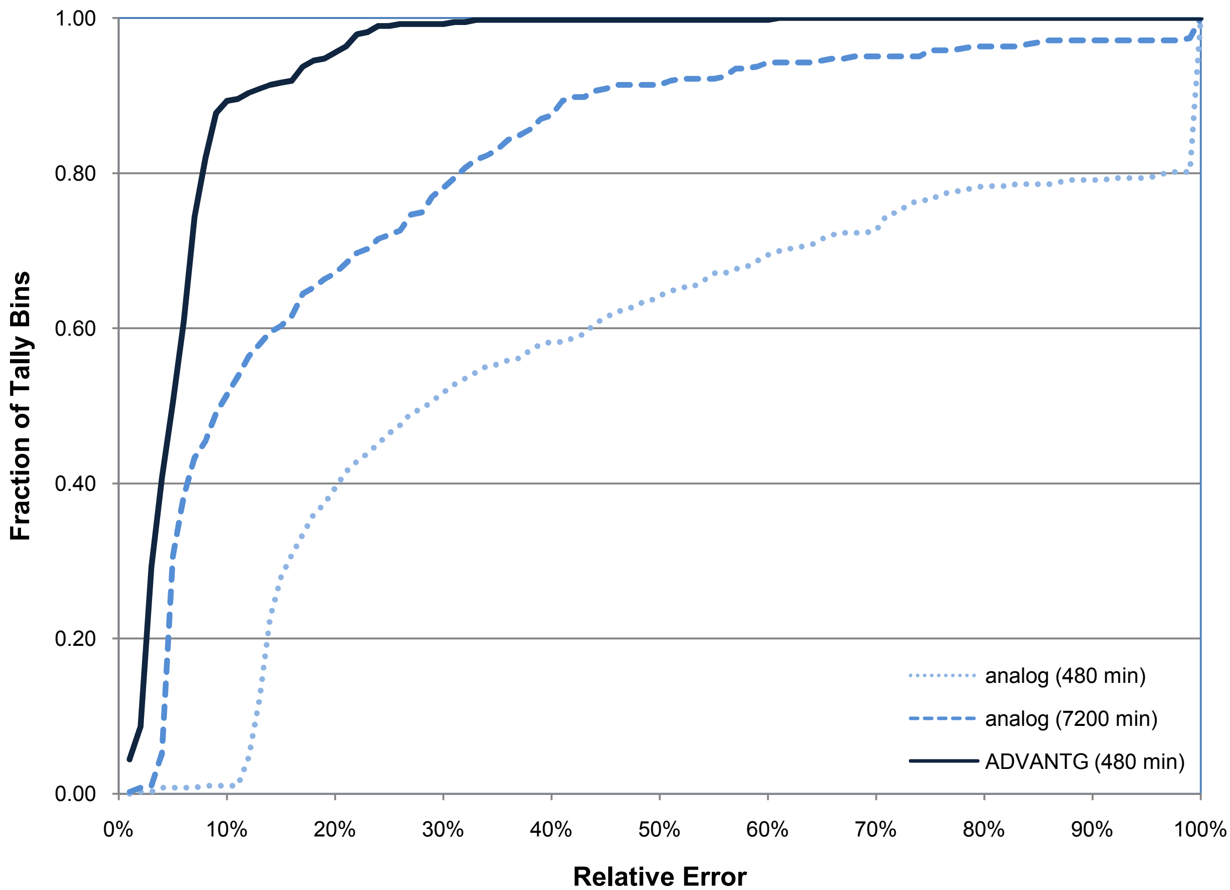


Figure 6. Fraction of tally bins with less than the given relative error for the PGASP-P problem.

Table III. Fraction of tally bins with less than a given relative error for the PGASP-P problem

Rel. Error	Analog[1]	Analog[2]	ADVANTG[3]
1%	0%	0.26%	4.44%
5%	0.78%	30.55%	50.39%
10%	1.04%	51.44%	89.30%
25%	46.48%	72.06%	98.96%
50%	64.23%	91.38%	99.74%

[1] With implicit capture, 480 minute run time
[2] With implicit capture, 7200 minute run time
[3] 480 minute run time

5. CONCLUSIONS

The ADVANTG code has been developed to automate the generation of weight-window parameters for MCNP using the CADIS method. In this paper, we described the application of ADVANTG to a set of three realistic threat-detection simulations. For the passive detection problems, ADVANTG obtains an $O(10^4)$ speedup and, for a detailed gamma spectrum tally, an average $O(10^2)$ speedup relative to implicit-capture-only simulations, including the deterministic calculation time. For the active-interrogation problem, an $O(10^4)$ speedup is obtained compared to a simulation with angular source biasing and crude geometry splitting. In addition, the automated weight-window generation capability in ADVANTG allows one to avoid the labor-intensive trial-and-error process required to implement geometry splitting or use the stochastic weight window generator. Hence, our experience indicates that ADVANTG is a very effective tool for efficiently estimating quantities of interest in difficult shielding problems.

Some challenges remain, however. We have observed difficulties in problems with sources that emit particles into a small cone of directions (i.e., a beam) in thin materials (e.g., air). We believe that this is caused by the strongly anisotropic distribution of the importance function (in the thin medium) that is not represented in the scalar adjoint flux. Hence, future work is planned to investigate the use of angular-dependent information.

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