

Transport Code Simulations for Shielded Special Nuclear Material Discrimination

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ABSTRACT

Every year, millions of containers of cargo enter the United States. Radiation portal monitors based on passive emissions are used to determine if radiological threats are present. Special Nuclear Materials (SNM), which refers to certain uranium and plutonium isotopes, are of particular interest. Since even moderate shielding can prevent passive detection thereof, this thesis investigates use of an X-ray based active interrogation as an alternative. Active interrogation works by exposing the cargo container to a high energy beam which then induces gamma and neutron emissions from SNM that can be detected. Complicating matters, benign materials like lead and tungsten also emit gammas and neutrons when irradiated. In order to identify radiological threats, the active background produced by non-SNM must be estimated and subtracted from the measured data. We investigate use of the Monte Carlo N-Particle Transport Code (MCNP) developed at Los Alamos National Laboratory for generating the active background estimate given a density map of a cargo container. We show that MCNP, which is the gold standard for solving the Boltzmann transport equation, does indeed facilitate the desired material separation only not in the time required in spite of using variance reduction techniques for speeding up the computation. We also study use of Geant4, which is a Monte Carlo transport code from CERN, but find that better physics modules are needed in order for that to be a viable alternative. Finally, we look at discrete ordinates methods, namely, ADVANTG from Oak Ridge National Laboratory and Attila developed by Silver Fir Software. We conclude that the former, which is used to accelerate MCNP simulations, adds too much overhead, while the latter, which can be used to produce an approximate solution in and of itself, has potential for being a feasible platform once modeling of photo-nuclear reactions has been added.

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Chapter 1

INTRODUCTION

1.1. Problem Statement

Currently, detection of radiological and nuclear (RN) threats in cargo is achieved primarily by passively screening for gamma-ray or neutron-emissions [1]. However, even moderate shielding can prevent passive detection of special nuclear material (SNM) [2] which is defined by the U.S. Nuclear Regulatory Commission as “plutonium, uranium-233, or uranium enriched in the isotopes uranium-233 or uranium-235” [3]. Active interrogation, which refers to the induction of nuclear reactions, especially induction of fission in fissionable materials using an active source, can reduce the impacts of shielding [1]. The source energy required for this will, however, also induce emissions from benign materials in the cargo that interfere with the signal from fissionable materials.

In order to determine if the cargo contains a RN threat, the active signal, S , from the threat must be separated from the active background, B , emitted from the benign materials in the cargo. As the active background cannot be measured without the source of the active signal removed, the background signal must be estimated. In order to do so, an interlaced X-ray source can be used to generate a voxelized 3D Zeff map of the cargo [4] which, in turn, can be used to estimate the background signal, $\hat{B}$, using Monte Carlo or discrete methods as discussed later in this chapter. For the work described in this thesis, the source is an interlaced 9MV and 6MV linear accelerator. The background signal estimate can be used to estimate the active signal, $\hat{S}$, needed to detect and identify any SNM. Our ultimate goal is to develop a method to rapidly estimate the active background signal to facilitate real-time detection of special nuclear material. Figure 1.1 shows the process. The 3D Zeff map will be assumed to be available either from reconstruction of the in-beam detector data or from another system such as SmartScan3D [5].

1.2. Nuclear Background

To determine the active background, the primary source photons and the induced secondary photons and neutrons must be transported. The equation for radiative transport and neutron transport, sometimes referred to as the Boltzmann transport equation, describes how to calculate this result. While exact solutions are difficult to obtain, numerical methods can be used to determine approximate solutions. The Monte Carlo method uses statistical sampling to determine the result by using vast amounts of random numbers to model individual particles. An approximation can also be calculated by the discrete ordinates method which instead discretizes the space, angles, and energy groups to make the calculation feasible by reducing the equation to a linear system.

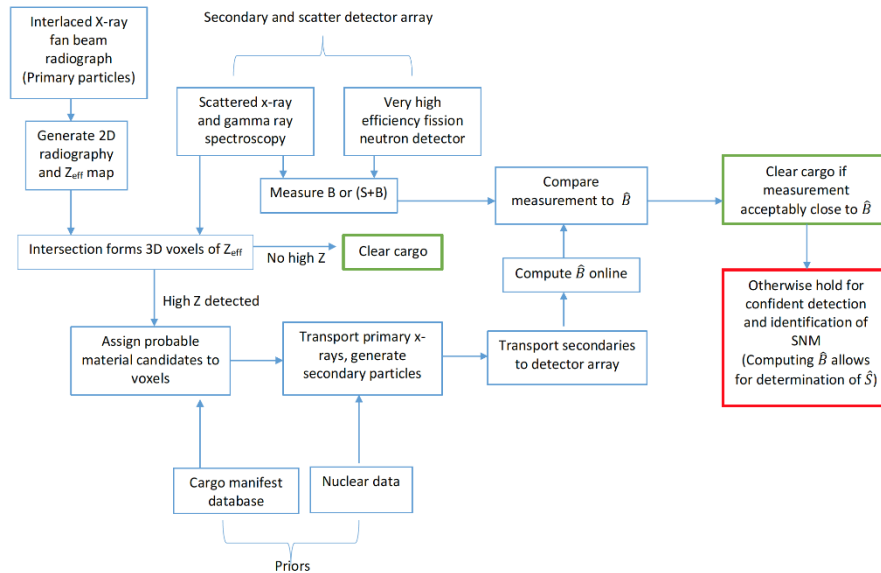


Figure 1.1 Scanning concept of operations [6].

1.3. Nuclear Transport Software

Monte Carlo

The Monte Carlo method uses randomly generated numbers to simulate many particles and tallies the results. The precision increases incrementally as more particles are simulated, with the error decreasing relative to the square root of the number of particles [7]. Monte Carlo N-Particle (MCNP) and Geant4 [8] are two examples of Monte Carlo solvers.

Several physics processes must be implemented when using the Monte Carlo method with some of the key interactions for neutrons including prompt/delayed fission, photofission, and the (n,xn) interactions [9]. For photons key interactions include scattering, pair production, and bremsstrahlung. All of these interactions are modeled in the cross-section tables provided with MCNP and Geant4.

MCNP includes tables from the ENDF/B and ENDL libraries as well as others, which have been preprocessed into a so-called ACE format. The preprocessing changes secondary particle distributions into cumulative density function from a variety of ENDF implementations [10]. Other libraries can be used if processed into the ACE format using NJOY [10].

For photon transport applications, the photoatomic (one table per element) libraries included in MCNP are sufficient. Some photonuclear (one table per isotope) data is also included, but photonuclear physics must be turned on in the user input on

the MPHYS card. MCNP input decks are explained in Chapter 2. For MCNP6, photonuclear tables are only included for 13 nuclides with all other nuclides having to instead use either the physics models provided or external data.

Geant4 provides a selection of reference physics lists for different applications. These physics lists combine different model types to balance performance, accuracy, and precision for different applications. Of interest are the NeutronHP variants which utilize the high precision neutron package for “neutrons below 20 MeV”. Custom physics lists can be made with either custom models or by using the existing models with different energy ranges than the reference lists.

Discrete Ordinates

Discrete ordinates computes an approximate solution to the Boltzmann equation by discretizing the world space, angles, and energy. This allows the solution to be calculated iteratively as it reduces the equation to a system of linear equations [11]. The accuracy of the discrete ordinates method is determined primarily by the number of angles, the energy binning, and how well the discrete geometry matches the desired model. This contrasts Monte Carlo methods, where the accuracy is limited only by the accuracy of the data provided [12]. Attila is one such discrete solver. ADVANTG provides a wrapper around the Denovo solver for accelerating MCNP performance.

Discrete ordinates can also be used to improve Monte Carlo performance. This is achieved by completing a low accuracy, but fast calculation, to obtain biasing parameters for use in the Monte-Carlo simulation [13].

The Consistent Adjoint Driven Importance Sampling (CADIS) and Forward Weighted – CADIS (FW-CADIS) methods are implemented in Attila and ADVANTG for use in MCNP. The CADIS method provides acceleration for an individual tally, while the FW-CADIS method leads to more evenly distributed relative errors across the entire space. The CADIS method uses the adjoint solution as it provides “a measure of the importance of a particle” [14] by measuring the likelihood a particle of a particular energy and location will contribute to the final tally. The adjoint solution is equivalent to transporting from the detector with all processes reversed. By knowing the approximate adjoint solution and therefore the importance, biasing parameters can be selected across the geometry, to weight the MCNP importance of each cell, such that the final variance is reduced. The Forward-Weighted variant uses both the forward and adjoint approximations to further reduce the variance at the desired detector.

ADVANTG provides a wrapper around the Denovo discrete ordinates solver to generate weights either by the CADIS or FW-CADIS method. By accepting MCNP input it is able to add the variance reduction of CADIS or FW-CADIS to most existing MCNP input decks. Denovo discretizes the geometry by defining a grid across the geometry. The spacing for the grid is not required to be uniform which increases flexibility to match the geometry.

Attila discretizes the geometry by defining a mesh over a 3D model that can be imported from various 3D model formats. Then the angular quadrature can be selected, to match the geometry and/or based on the accuracy desired.

Additionally, the energy groups used will determine calculation time and accuracy. Discrete methods use energy groups to discretize the cross sections. Each group covers a range of energies for a single particle. For a run, a range of energy groups must be selected, this determines the physics range with a minimum energy cutoff and maximum energy.

1.4. CAD Modeling Software

Background

To design and model the geometry for simulating in MCNP and Geant4, SoftWare for Optimization of Radiation Detectors (SWORD) was used. SWORD 6.0 [15] allows the geometry to be specified in a CAD-like interface and provides a library of useful predefined object definitions. A Geometry Description Markup Language, GDML, file is output for Geant4 and an input deck is output for MCNP. SWORD6.0 is provided in beta from RSICC without export control restriction.

To verify that optimizations did not negatively impact results, the following target materials were used, lead, tungsten, and uranium. These materials were selected to provide a couple of possible dense neutron interferences and an example fissionable. Material definitions for objects not from the SWORD library are from PNNL's *Compendium of Material Composition Data for Radiation Transport Modeling revision 1* [16]. All SWORD objects used the composition provided by the library.

In a complete system, where 3D Zeff voxels are assigned materials, such objects would be represented instead by voxels, rather than macrobody objects, but using the SWORD library of objects simplifies the process of building the models.

Simple Sphere

To test changes that affected the modeled physics within a material, a simple geometry was used. A simple sphere, with a radius of 3 cm, of target material and a large panel detector in a volume of air provided a simple geometry to verify the physics changes did not affect the desired results. The 3 cm radius was chosen as it approximately corresponds to a 2 kg sphere of SMN, the goal minimum detectable quantity. Figure 1.2 provides a screenshot of this simple sphere model.

Cargo – Pallets

For simulations where the geometry mattered, such as the source direction biasing, a complex model, seen in Figure 1.3, was used. This consisted of a 40 ft container on a truck with 8 wood pallets in a line along the length of the container. Each pallet is loaded with a block of reduced density steel with a density of

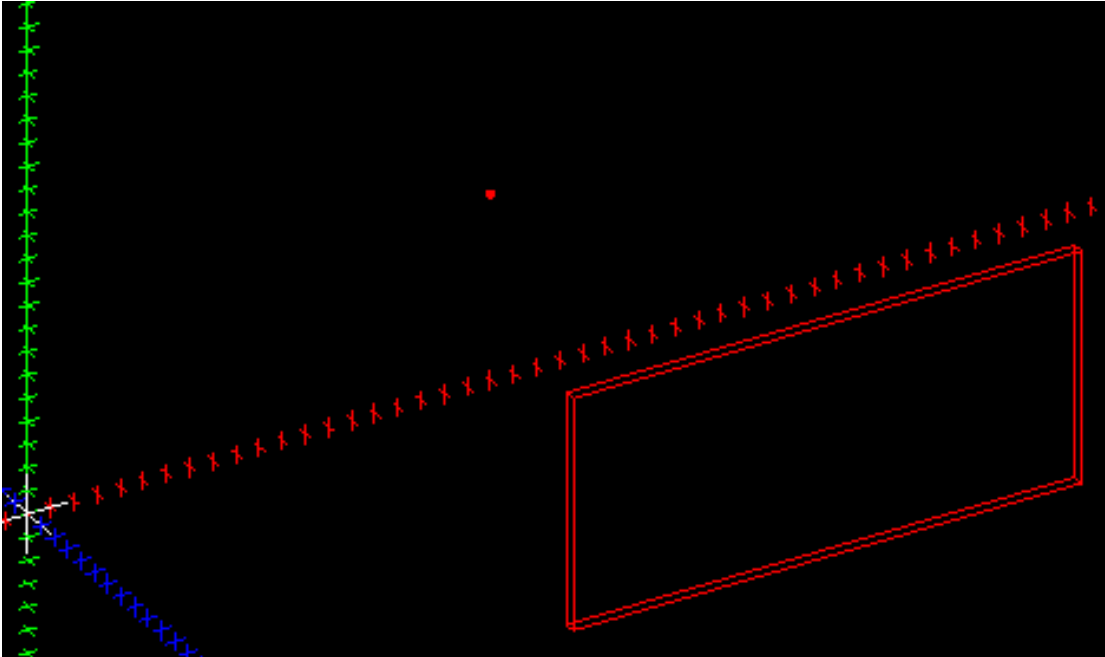


Figure 1.2. Simple sphere model with just a detector panel and a sphere.

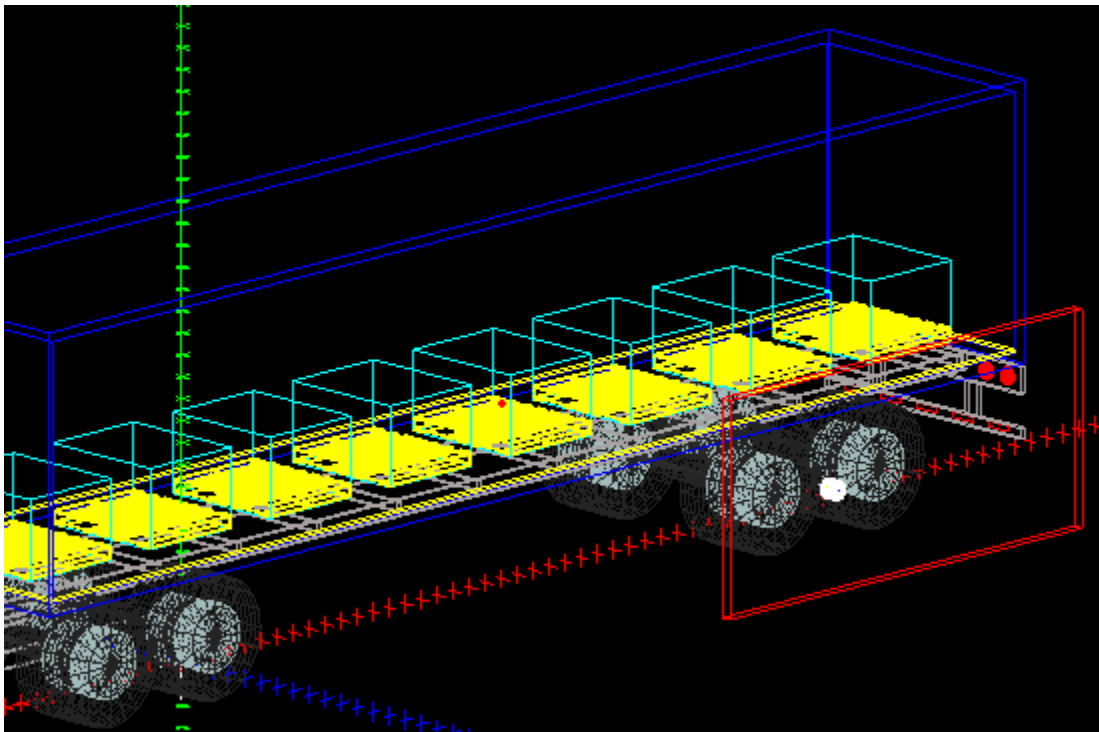


Figure 1.3. Complex pallet model with blocks of reduced density steel.

3 g/cm³, shown in cyan. The block directly in the beam contains a sphere of the target material shown in red. A 5 m x 2 m panel detector, also shown in red, is outside the container, 4 meters away, behind the source. The container and pallets are models included in the SWORD object library. While the container appears mostly empty, the total weight of the cargo amounts to more than 20,000 kg of the maximum allowed 30,480 kg.

Source

The primary source definition for the 9MeV linear accelerator was provided by Varex Imaging as a spreadsheet. This was exported to a comma separated values (CSV) file for use in Geant4 and was input manually for use in MCNP.

As with other electron linear accelerators, the accelerated electrons hit a target material generating a continuous photon bremsstrahlung spectrum. The maximum energy, or endpoint energy, of the resulting photons is the same as the energy of the electrons. For this project an interlaced linear accelerator, the Linatron® Mi-9 [17], provides the source for the active interrogation. Interlaced linear accelerators provide pulses with different energies on each pulse. For the Mi-9 this is a 9MV pulse followed by a 6MV pulse. Figure 1.4 shows the intensity and hardness by angle for the 9MeV pulse. Directly in the center of the cone is significantly more intense and has a harder beam. Figure 1.5 provides another view of the intensity by angle. The increased intensity, or counts, proportionally increase the resulting secondaries. Additionally, the increased hardness results in additional secondaries.

1.5. Thesis Organization

Chapter 2 provides a background for using MCNP; it covers the basics about implementation, fundamentals about the input format, and serves as a guide to interpreting the output. Chapter 3 describes how approximating electrons, minimum energy threshold, source biasing, and parallel computation can be used to accelerate MCNP and examines their impact for modeling active interrogation. Chapter 4 examines alternative methods for computing the active background; Geant4 is an alternative Monte Carlo code, ADVANTG can automatically generate variance reduction parameters for MCNP, and Attila is a discrete ordinates solver. Chapter 5 provides a conclusion and proposals for future work.

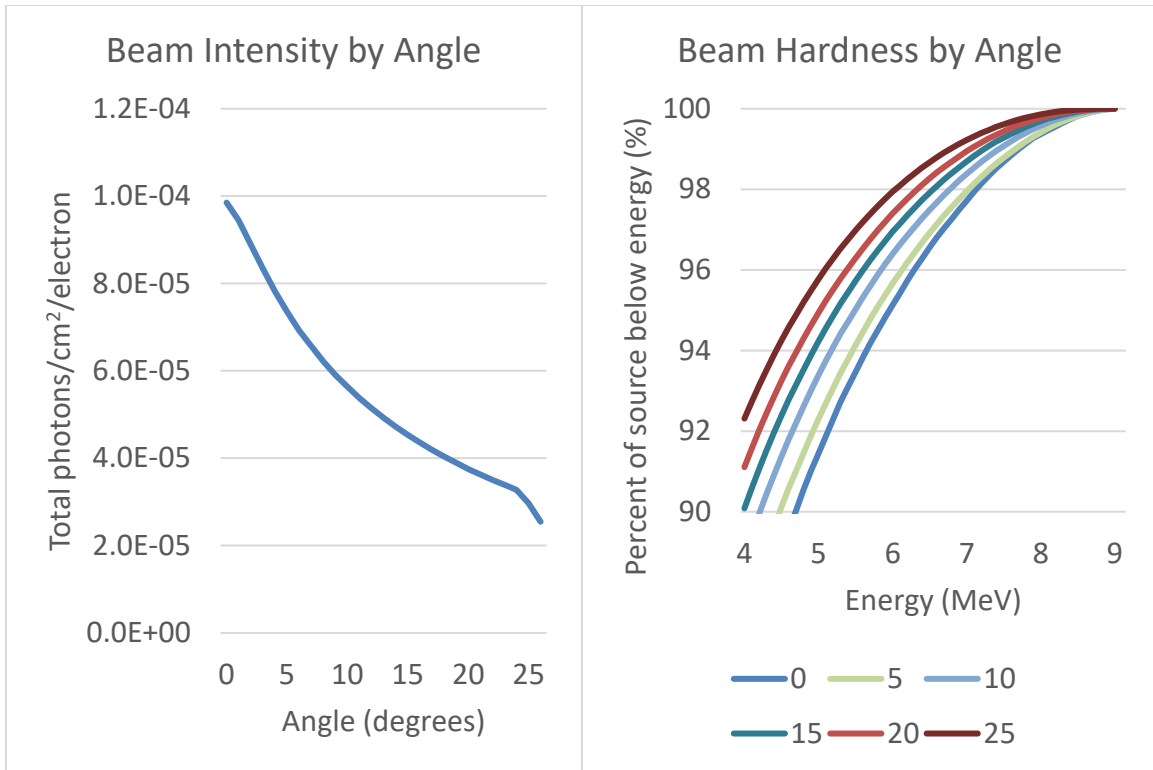


Figure 1.4. Beam intensity and hardness decreases by angle.

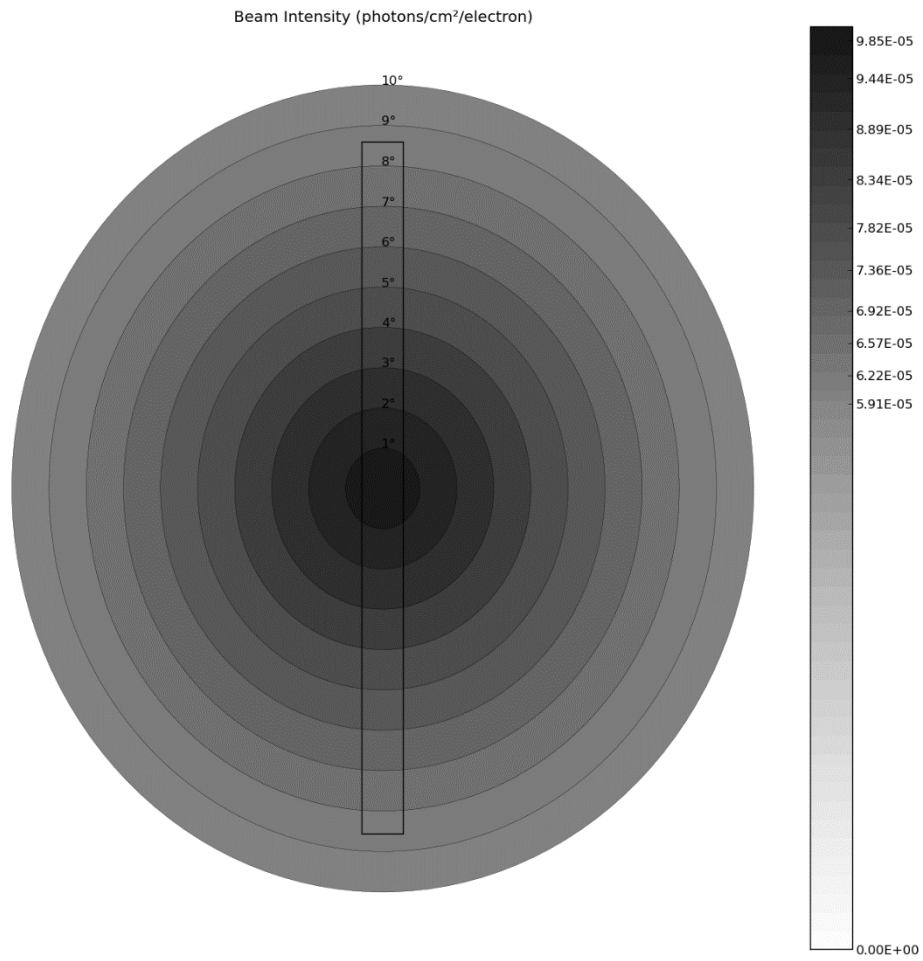


Figure 1.5. Source intensity by angle.

Chapter 2

MONTE CARLO N-PARTICLE TRANSPORT CODE

BACKGROUND

Monte Carlo N-Particle (MCNP) is a radiation transport code produced by the Los Alamos National Laboratory and distributed by the Radiation Safety Information Computational Center (RSICC) [7]. MCNP development at LANL dates back to at least the 1950s [18]; MCNP is written predominantly in Fortran [9] and provides parallel processing with MPI, OpenMP, and PVM. MCNP is only available under export control but can be obtained as either a source or executable release. MCNP 6.1 was used for all simulations reported in this thesis. Since starting the work, MCNP 6.2 became available.

2.1. Implementation

Physics Model

MCNP predominately utilizes tables to model interactions between particles and the geometry. The data in these tables comes from a variety of sources but is used in the A Compact ENDF (ACE) format. The manual notes the name is not always accurate as the files are “often not compact”. The ACE data is processed from other formats using the NJOY or MCPOINT codes.

MCNP offers both photoatomic and photonuclear data. Photoatomic data provides cross-section data per element while photonuclear data has cross-section data per isotope. MCNP, however, only provides limited photonuclear data; if isotopes beyond the 13 provided are needed, then model physics must be used.

Models provide the ability to simulate physics beyond available cross-sections, with additional isotopes, beyond the energy range of the available libraries, or other particles including protons, pions, and muons.

Parallelism

To be able to complete calculations faster, MCNP can be run in parallel. MCNP primarily supports two methods of parallel computation, MPI (Message Passing Interface) and OpenMP. MPI offers process parallelism and can be used across multiple systems while OpenMP provides threading and therefore only works on a single system but can be combined with MPI. In order to use MCNP with MPI it must be compiled from source to link against the local MPI implementation [19]. Use of some MCNP6 features are limited while using OpenMP but not while using MPI, one such feature is model physics, discussed above.

2.2. Input Deck

There are several required components of every MCNP input deck. The first and simplest is the problem title card. The title card is required but can be left blank. Like all cards in an MCNP deck, it is limited to 80 characters prior to MCNP 6.2 which in turn allows 128 characters. Most of the remaining cards follow a standard format with the identifier in the first 5 columns followed by a space. Some other cards are the cell, surface, material, physics, source, tally, and option cards. Figure 2.1 demonstrates an example MCNP deck. The segments of the deck are explained in the following sections, in order of the MCNP deck. Cell, surface, and material cards describe the geometry to be modeled. Physics cards provide the physics configuration for the simulation. The source and tally cards further describe the model. Option cards provide additional run control including termination conditions.

Cell Cards

Cell cards require a number of arguments, a number to identify the cell, a number corresponding to the material for the cell, density, bounds, importance, and others. The cell number is chosen by the user and must uniquely identify the cell. The material number references the material list if the cell is not void; void cells can be specified with a 0. The density of the material can be defined using atom density (10^{24} atoms / cm³) with a positive number or g/cm³ by using a negative number. The bounds of the cell are defined by a list of surface or macrobody identifiers, separated by a space (' ') for intersection, a colon (':') for union, or a number sign ('#') for complement. A negative number represents the opposite side of the surface or macrobody. The importance for each cell must be specified, either all on the cell cards or all on an importance card in the data section. The importance value is used as a geometry-based roulette to kill unimportant particles or split to track more particles in an area of high importance. Numbers greater than 1 split to create extra tracks; numbers less than 1 complete a roulette with that probability to survive. Some additional cell parameters can be set either on the cell card or on the corresponding cards in the data section. Immediately following the cell cards is a mandatory blank line, this is used to distinguish cell cards from surface cards.

Surface Cards

MCNP allows the modeled geometry to be defined with provided macrobodies or surfaces. For simplicity only macrobodies were used. MCNP offers a variety of macrobodies including box, rectangular parallelepiped, sphere, right circular cylinder, right elliptical cylinder, and arbitrary polyhedron. With just a few of these, most geometries can be accurately defined. Commonly used macrobodies include box (an arbitrarily oriented orthogonal box), rpp (a rectangular parallelepiped), and sph (a sphere). Boxes are specified by an x,y,z corner coordinate and three orthogonal vectors. Rectangular parallelepipeds are specified by bounding box x,y,z coordinates. Spheres are specified by center and radius. Macrobody all

Example MCNP Deck

<pre> Problem generated from SWORD XML files C C Cell Data C C void region 10 0 C detector_panel 3 112 -3.67 -3 C target 2 12 -11.34 -2 C WorldVolume 1 6 -0.00129 -1 3 2 IMP:N=0 IMP:P=0 IMP:N=1 IMP:P=1 IMP:N=1 IMP:P=1 </pre>	Cells	<pre> Problem generated from SWORD XML files C C Cell Data C C void region 10 0 C detector_panel 3 112 -3.67 -3 C target 2 12 -11.34 -2 C WorldVolume 1 6 -0.00129 -1 3 2 IMP:N=0 IMP:P=0 IMP:N=1 IMP:P=1 IMP:N=1 IMP:P=1 </pre>	Title Comments Cells Mandatory blank line
<pre> C C Surface Data C C WorldVolume 1 BOX -12500 -12500 -12500 25000 0 0 0 0 25000 C detector_panel 3 BOX -620 108 -505 400 0 0 0 200 0 0 0 10 C target 2 SPH -400 160 0 3 </pre>	Surfaces	<pre> C C Surface Data C C WorldVolume 1 BOX -12500 -12500 -12500 25000 0 0 0 0 25000 C detector_panel 3 BOX -620 108 -505 400 0 0 0 200 0 0 0 10 C target 2 SPH -400 160 0 3 </pre>	Comments
<pre> C C Material Data C C WorldVolume material: Air m6 18040 0.0046615 6012 0.00016529 7014 0.78388 8016 0.21129 C detector_panel material: NaI m112 11023 0.5 53127.42c 0.5 C target material: Pb m12 82206.24c 0.241 82207.24c 0.221 82208.25c 0.524 </pre>	Materials	<pre> C C Material Data C C WorldVolume material: Air m6 18040 0.0046615 6012 0.00016529 7014 0.78388 8016 0.21129 C detector_panel material: NaI m112 11023 0.5 53127.42c 0.5 C target material: Pb m12 82206.24c 0.241 82207.24c 0.221 82208.25c 0.524 </pre>	Comments Materials
<pre> C C Physics Data C MODE n p PHYS:P 100 0 0 -1 0 1 1 cut:p 3 6 0 3 3 </pre>	Physics	<pre> C C Physics Data C MODE n p PHYS:P 100 0 0 -1 0 1 1 cut:p 3 6 0 3 3 </pre>	Comments
<pre> C C Source Data C sdef pos -400 160 -420 PAR=2 VEC=0 0 1 DIR=DZ ERG=D300 C s12 -1 0.999961921 1 sp2 0 0.99998096 0.0001094 sb2 0 0 1 # si300 h sp300 d 5.90E+00 0.00E+00 6.00E+00 2.90E-06 6.10E+00 2.92E-06 6.20E+00 2.87E-06 6.30E+00 2.78E-06 6.40E+00 2.52E-06 6.50E+00 2.52E-06 6.60E+00 2.37E-06 6.70E+00 2.22E-06 6.80E+00 2.10E-06 6.90E+00 2.14E-06 7.00E+00 2.07E-06 7.10E+00 2.10E-06 7.20E+00 1.92E-06 7.30E+00 1.82E-06 7.40E+00 1.73E-06 7.50E+00 1.56E-06 7.60E+00 1.50E-06 7.70E+00 1.43E-06 7.80E+00 1.31E-06 7.90E+00 1.31E-06 8.00E+00 9.18E-07 8.10E+00 9.05E-07 8.20E+00 8.90E-07 8.30E+00 9.00E-07 8.40E+00 8.28E-07 8.50E+00 7.40E-07 8.60E+00 5.10E-07 8.70E+00 4.50E-07 8.80E+00 3.55E-07 8.90E+00 2.65E-07 9.00E+00 1.30E-07 </pre>	Source	<pre> C C Source Data C sdef pos -400 160 -420 PAR=2 VEC=0 0 1 DIR=DZ ERG=D300 C s12 -1 0.999961921 1 sp2 0 0.99998096 0.0001094 sb2 0 0 1 # si300 h sp300 d 5.90E+00 0.00E+00 6.00E+00 2.90E-06 6.10E+00 2.92E-06 6.20E+00 2.87E-06 6.30E+00 2.78E-06 6.40E+00 2.52E-06 6.50E+00 2.52E-06 6.60E+00 2.37E-06 6.70E+00 2.22E-06 6.80E+00 2.10E-06 6.90E+00 2.14E-06 7.00E+00 2.07E-06 7.10E+00 2.10E-06 7.20E+00 1.92E-06 7.30E+00 1.82E-06 7.40E+00 1.73E-06 7.50E+00 1.56E-06 7.60E+00 1.50E-06 7.70E+00 1.43E-06 7.80E+00 1.31E-06 7.90E+00 1.31E-06 8.00E+00 9.18E-07 8.10E+00 9.05E-07 8.20E+00 8.90E-07 8.30E+00 9.00E-07 8.40E+00 8.28E-07 8.50E+00 7.40E-07 8.60E+00 5.10E-07 8.70E+00 4.50E-07 8.80E+00 3.55E-07 8.90E+00 2.65E-07 9.00E+00 1.30E-07 </pre>	Physics Tables
<pre> C C Tally Data C F11:n 3.5 FC11 detector_panel F18:p 3 E18 0.0 0.1 148i 15 </pre>	Tally	<pre> C C Tally Data C F11:n 3.5 FC11 detector_panel F18:p 3 E18 0.0 0.1 148i 15 </pre>	Comments Tallies
<pre> C ngs 1000000000 </pre>	Other		

Figure 2.1. An example MCNP deck with labels.

define a set of facets with the same orientation as the macrobody (the negative face is the inside the macrobody). Immediately following the surface cards is a mandatory blank line, this is used to distinguish cell cards from surface cards.

Material Cards

Materials are identified by an 'm' followed by a number to uniquely identify the material. To define a material a list of ZAIDs, or nuclide identification numbers, and their corresponding fractions is used. The ZAID includes the atomic number followed by the mass number of the nuclide. Selecting a cross-section table is recommended but is optional; this can be done with a period after the ZAID followed by the table identifier. The last component of the entries for each nuclide is the fraction. The fractions can either be atomic fractions, specified with positive numbers, or weight fractions, specified with negative numbers. Starting in MCNP 6, MX cards can be used to specify the nuclide instead of defining it on the material card. Note the MX cards are not compatible with MCNP 5 and therefore cannot be used with ADVANTG.

Physics Cards

To control the transport, MCNP provides a number of physics options across several cards. The mode card determines what particles will be transported; these are specified by a space separated list of particle designations. The MPHYS card provides a toggle for the use of models by MCNP when cross section tables are unavailable. If the card is omitted and the transported particles specified on the mode card are limited to neutrons, photons, and electrons then by default models are not used. If other particles are specified for transport, then models are used by default. The phys card contains the primary physics options and is specified per particle type. The options per particle also vary. For transport with photons and neutrons an important option to note is the ispn option on the photon phys card to specify photonuclear production. The default option is no photonuclear production but can be specified as analog or biased.

Source Cards

The source is defined by a collection cards but starts with the SDEF card. For simple monoenergetic sources the SDEF card may be the only one required to define the source but more complex sources need to define probabilities. The SDEF card is defined by keyword value pairs rather than a structured argument order. SDEF key arguments are par, pos, erg, vec, and dir. A key feature of the SDEF card is the ability to specify distributions as arguments. To do so, a 'D' and a number are used to define which distribution is to be used. This number should correspond to a pair of following SI (source information) and SP (source probability) cards. The reader is referred to the manual for more details.

Due to the character limit per card and for ease of reading and editing, it is often desirable to represent source probability with a vertical format rather than with

horizontal cards. MCNP allows this by using a '#' in the first 5 columns, this format allows putting any cards into a vertical format. After the '#' the card names should follow. This format allows placing values for multiple cards into a single table. This format is especially useful for defining source probabilities and biasing parameters as the alternative is specifying the source energies, the corresponding probabilities, and the corresponding bias on separate, likely long, cards. Any distribution used for a source is specified with a pair of SI and SP cards and optionally a SB (source bias) card. Each must have the same number of entries and is the card is labeled with the distribution number.

Tally Cards

The primary form of results from MCNP is the tally results. These tallies are defined by a set of tally specification cards. Tallies can be binned by energy, time, or cosine and can represent various . There are several cards used to specify the tally, first the type of tally, particle, and the cell, or surface, must be specified on the Fn card, where n is the tally number. The tally number represents both a unique identifier for the tally and also the type of tally to use. The last digit of the number specifies what type of tally to use. The tally number should match across all tally cards for a particular tally, including the last number. Immediately following the tally number is the particle designator. Depending on the type of tally, a cell or surface will need to be specified, for a surface tally when using macrobodies, the surface number will be appended to the body number and will depend on the macrobody type. Additionally, the energy bins are specified on an En card, where, as before, n represents the tally number. The energy bins are a list of energies on the card. MCNP provides a few shortcut options to avoid long verbose lists. These options, including the ability to repeat a value, insert interpolated values, and multiply the previous entry, are detailed in the "Data Card Horizontal Input Format" section of the MCNP User Manual [20].

Option Cards

MCNP provides additional controls for the calculation itself, including how long to run and what to output. How long the calculation runs can be controlled by a history count, time, or precision with the NPS, CTME, or STOP cards, respectively. There are quite a few output controls provided by MCNP; the PRINT card is notable as it provides access to a number of tables describing many details of the calculation.

2.3. Output

MCNP produces a significant quantity of data in addition to the tallies specified in the input deck. Some of this data is provided to ensure the input was specified correctly, other parts provide details and offer insight into the simulation performed, both for optimization as well as validation. This discussion will focus on the output about the simulation rather than the output describing the input.

Data

One of the most informative tables when tuning physics and biasing parameters is the table describing the creation and loss of the histories simulated. This helps determine whether particle tracks are terminating due to collisions, escaping, a cutoff, or a roulette process and helps explain what produces the tracks. This can help inform decisions about necessary interactions and possible candidates for optimizations, such as, source biasing and energy thresholds.

Another important table for analysis of the geometry is table 126 of the output file. This table provides details about activity per particle per cell. Some important columns to note are the tracks entering, population and collisions for each particle type. Cells with low population or collision count likely don't contribute as much to the final results and as such should be examined as candidates for optimization.

Tallies

For each tally in the input deck MCNP produces a table of results and a brief analysis of the expected precision and some statistical checks to ensure the fluctuation in the tally was as expected. The manual details some secondary verification that can be done if a tally fails any of the statistical checks but warns that the validity of any of those results should be questioned.

Relative error

The relative error for each bin of each tally is as important as the value for that bin. Being an estimate of the precision of the result, the relative error is calculated based on the variance of the tally. That is,

$$R = \sqrt{\frac{1}{N} \left(\frac{x^2}{\bar{x}^2} - 1 \right)}.$$

Note that R decreases relative to the square root of N, the number of particles. Table 2.1 summarizes the MCNP guidance for how to interpret relative error. Performance of biasing parameters was measured by the quantity of results with relative error below 0.1. The manual describes these results as “generally reliable”. Results with a relative error above this value can still be useful but are likely imprecise.

Table 2.1. Guidelines for Interpreting the Relative Error R* [9]

Range of R	Quality of the Tally
0.5 to 1.0	Not meaningful
0.2 to 0.5	Factor of a few
0.1 to 0.2	Questionable
< 0.10	Generally reliable
< 0.05	Generally reliable for point detectors

Chapter 3

EXPERIMENTAL MCNP RESULTS

To improve MCNP performance several MCNP parameters were investigated. First some physics options were tested to establish what physics are relevant for the neutron results. Next, biasing parameters were tested to reduce variance. Finally, MCNP parallelism is investigated.

3.1. Electrons

The first physics option to examine is whether to transport or approximate electrons. By default, in MCNP, when electrons are not designated on the MODE card and photons are, bremsstrahlung photons are generated using a thick-target bremsstrahlung approximation [20]. This model assumes any electrons generated will not leave the material and any secondaries generated by the electron will have the same direction as the electron. This approximation is also used for electrons below the electron minimum energy cutoff if the electron minimum energy cutoff is higher than the cutoff for photons.

Figure 3.1 shows that with the simple model the results with the approximation match that of fully transporting electrons. As the atmosphere surrounding the target sphere is unlikely to interact with any electrons escaping the material this is as expected. With the 0.2 MeV threshold used here for the transported electrons, very few of the electrons (25 million of 3 billion) escaped the sphere so the differences are minimal. As the elements modeled, even in the complex geometry, are relatively large compared to an electron's travel, the approximation is expected to have no notable impact to the final results. In geometries with significant numbers of fine components, on the scale of millimeters, electrons may need to be transported rather than approximated, however, for this model it is not necessary.

Simulation Time

The thick-target approximation is significantly faster than transporting electrons largely due to the large number of electrons and the small step size. Figure 3.2 shows the significant difference in time required between transporting electrons and the thick-target bremsstrahlung approximation when the energy threshold is 0.2 MeV. With 1 billion source photons, there were nearly 4 billion electrons for a total of 714 billion substeps. For comparison, there were 3.8 billion photon collisions. This time reduction is the first step to improving the performance of MCNP.

3.2. Energy Threshold

To further narrow the scope of the modeled physics, the next parameter to examine is energy threshold. The energy threshold setting provides a means to stop transporting particles that do not have sufficient energy to contribute to the

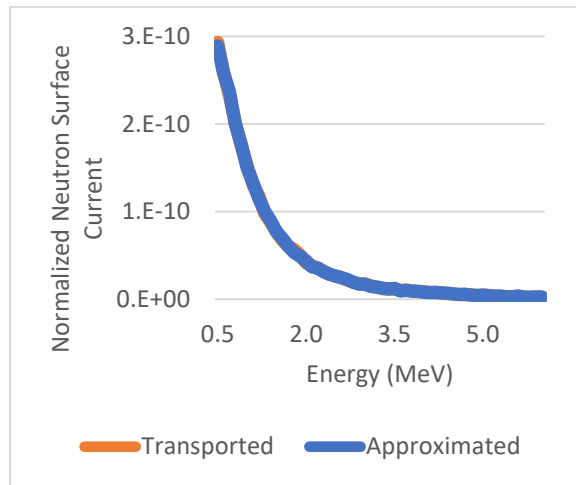


Figure 3.1. MCNP electron transport vs thick-target bremsstrahlung approximation for depleted uranium.

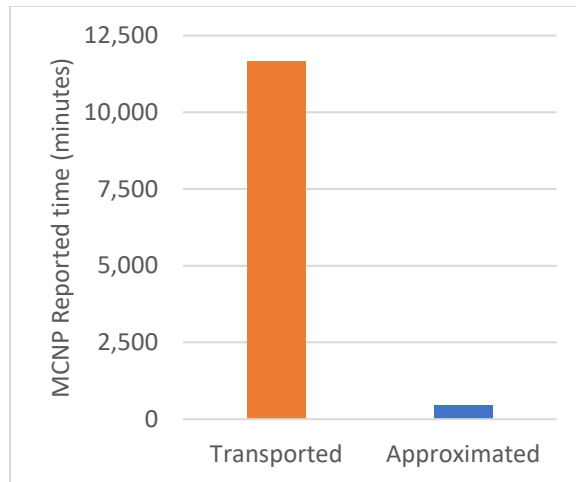


Figure 3.2. Time required to transport and approximate electrons in MCNP.

desired results. When only tallying neutrons, photon tracks that drop below the minimum energy required to generate a neutron track can be terminated, reducing calculation time. Additionally, less memory will be required as lower energy tables don't need to be stored.

Parameters

Energy threshold is specified in MCNP on the CUT card. A single value is selected for each particle type. Higher values may harm the results by eliminating contributions while lower values require more simulation time to obtain reliable results. The ideal value depends on the materials in the geometry as the minimum energy required for interactions varies by nuclide.

6MeV was chosen as the highest value for photon thresholds as it is generally below the minimum reaction threshold for most materials. Some materials, including deuterium, lithium, and beryllium, have reactions below this threshold, however, these materials are low density [1]. Neutron energy threshold was left at default (0.0 MeV [20]) as all neutron results are relevant [6].

Spectrum Comparison

To compare the minimum energy thresholds, a pencil beam was again used with 1 billion source photons on the simple geometry; electrons were not transported as it isn't necessary as shown in the previous section. For the lead results there is a slight difference in the neutron results between 1 and 2 MeV. The source of this discrepancy is not well understood but the difference is minimal. Figure 3.3 shows these results. The higher energy uranium results show additional variation for all thresholds but given sufficient simulation time the results are expected to fully converge.

Simulation Time

As expected, eliminating photons that would not contribute to the neutron tally results in faster computation for all materials tested as seen in Figure 3.4. Further improvement could be gained from further increases to the minimum energy cut but care must be taken to avoid eliminating important photons. If none of the materials being used have photo-nuclear interactions below a higher energy, this value should be raised.

3.3. Energy Roulette

To further improve simulation performance, MCNP's energy splitting and roulette parameter was examined. Many of the simulated particles above the minimum energy threshold may only contribute to a lower energy tally that will have lots of results and therefore have good statistics. By eliminating these, time can be saved without losses to accuracy and only slight increases in the relative error for bins with good statistics. Energy roulette can be used to eliminate these particles and energy splitting can be used to increase the sampling of relevant particles. MCNP

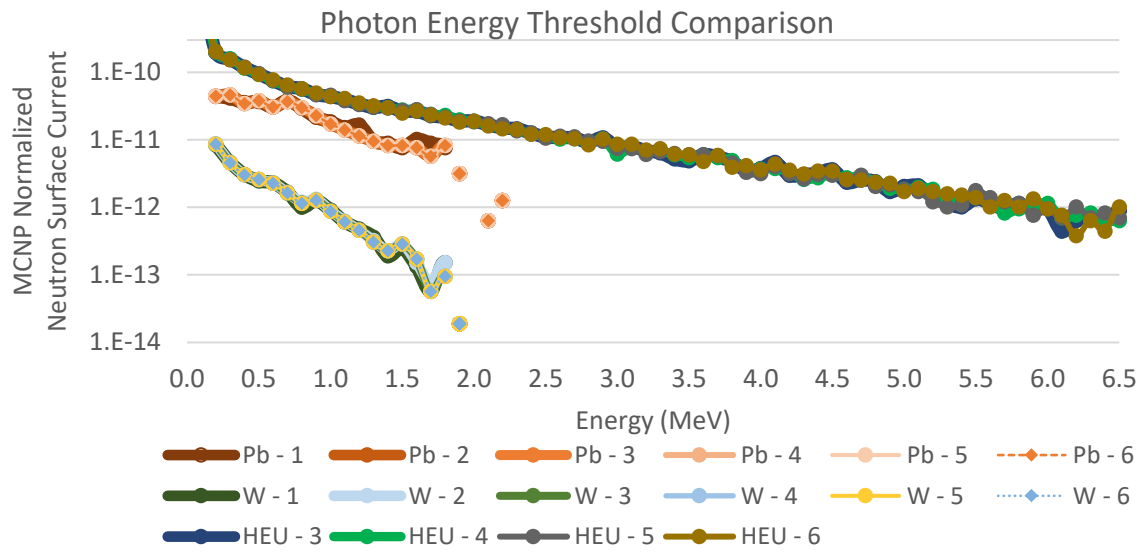


Figure 3.3. Energy threshold comparison for lead, tungsten, and uranium.

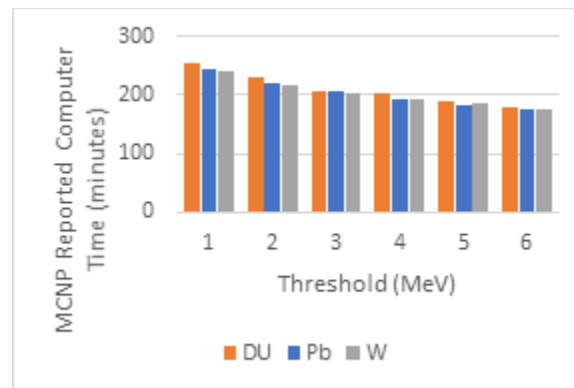


Figure 3.4. MCNP reported computer runtime in minutes by threshold.

energy roulette and splitting are both controlled by the ESPLT card with alternating ratios and energies. Ratios less than 1 are a roulette and greater than 1 result in a split. However, as seen in Table 3.1, most of the photon tracks are from the primary source rather than secondaries. Therefore, source energy biasing is expected to be more effective.

3.4. Source Energy Biasing

Another method to simulate more tracks of the desired energy is to start with more source particles in the optimal ranges. While source particles near the minimum energy threshold set earlier can contribute to the desired tally, they are unlikely to do so yet are much greater in number than the higher energy particles as seen in Figure 1.4. Source energy biasing saves time over an energy roulette as time doesn't need to be spent on tracks that are going to be terminated anyways. Another benefit of source biasing is balancing statistics to achieve better results with lower relative error across the entire desired spectrum.

Parameters

To bias a source in MCNP, a weight must be chosen for each energy bin of the source. Weights chosen are relative to each other as the values are normalized to a total of 1. Each value represents the bias to model for that energy, rather than a bias factor. Like the energy roulette, MCNP also increases weights to compensate for source energy biasing. Care must be still taken to avoid over-biasing the results and, as there is not a direct correlation to a physical process, the correct source energy biasing parameters are non-trivial to determine.

One automated method to determine these parameters is to use the CADIS method as the contributions for each tally from each energy group of the source can be estimated to determine importance. These estimates can be used to bias the source energy as well as regions of the geometry. In this case, only the source energy biasing is used and not the weight windows. ADVANTG, and the process used, is explained further in Chapter 4.

To bias source energy in MCNP a SB card is used, paired with the SI and SP cards used to describe the energy spectra. As such, one parameter must be selected per energy bin.

Comparison

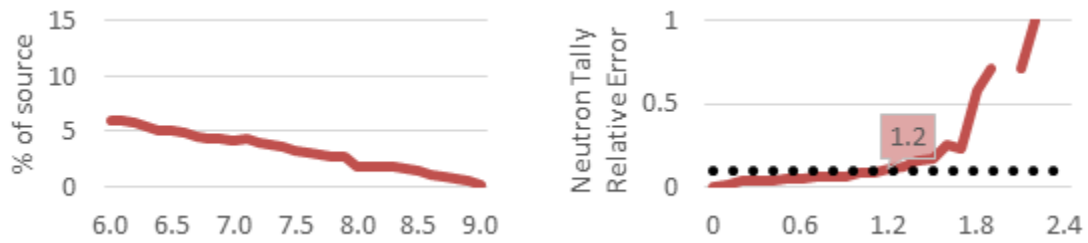
To compare the energy biasing effects, the simple model with the center cone of the Mi-9 source was used. The unbiased source results in a gap in neutron results as seen in Figure 3.5 and only has results below 0.1 relative error to 1.2MeV. With biasing, the result can be made more reliable out to 1.7MeV and the gap can be eliminated. Noticeably better relative error for higher energies was achieved with only minor increases for the lower energies. Unfortunately, such tuning needs to be completed manually to match the materials and, to a lesser extent, the

Table 3.1. MCNP photon track creation by type with lead target.

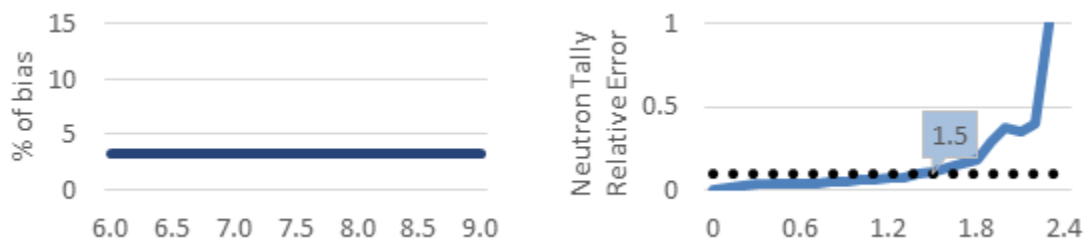
Photon Creation	tracks
source	10,000,000,000
nucl. interaction	52,034
particle decay	0
weight window	0
cell importance	0
weight cutoff	0
e or t importance	0
dxtran	0
forced collisions	0
exp. transform	0
from neutrons	27,236
bremsstrahlung	4,168,228
p-annihilation	0
photonuclear	1,963
electron x-rays	0
compton fluores	0
muon capt fluores	0
1st fluorescence	0
2nd fluorescence	0
(gamma,xgamma)	0
tabular sampling	0
prompt photofis	0
total	10,004,249,461

Source Energy Biasing - Lead

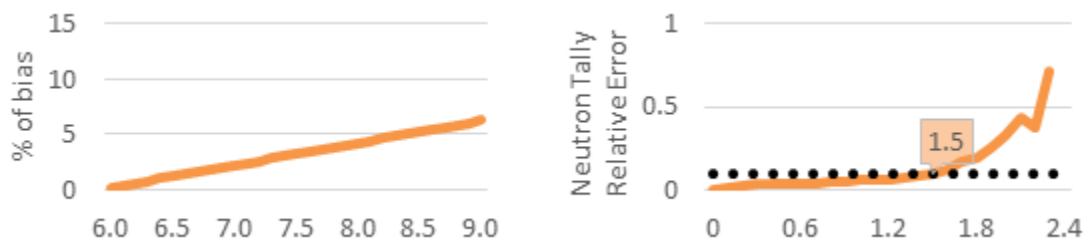
True Source



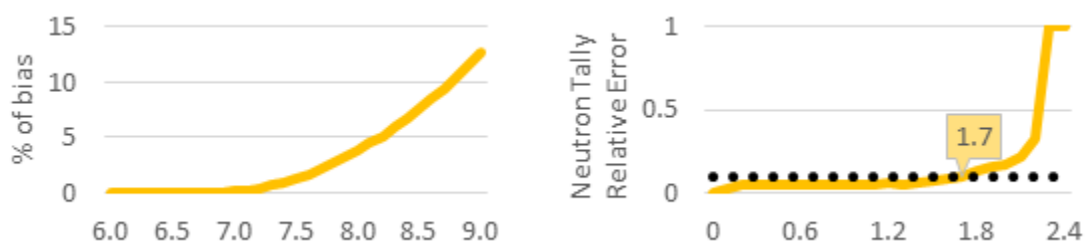
Uniform



Linear



χ^2



ADVANTG

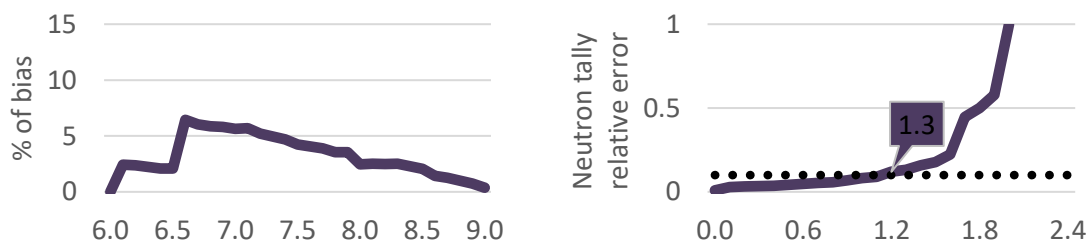


Figure 3.5. Source energy biasing parameters and neutron relative error.

shielding. ADVANTG offers an automated process for generating a source bias but for this application it selects a conservative bias that doesn't perform as well as the manually selected bias. Additionally, there is significant risk of over-biasing, as seen in the exponential results in Figure 3.6. The exponential bias did result in better precision at higher energies but introduced significant error to the lower energy bins resulting in a very unreliable result.

Simulation Time

The time required increases as simulating more higher energy source particles results in more secondary particles. For this comparison a fixed time was selected to offer a better comparison of biasing options. This comparison was also run on a single core to eliminate parallelization timing inconsistencies. Even with the increase in secondaries, transporting the primary photons dominates the runtime. The x^2 bias runs 7% less particles in the fixed time than the true source but still has much better statistics for the neutron tally as it generates 4 times as many neutrons.

3.5. Source Direction Biasing

To be able to model a complete cargo container, the fan source must also be modeled. While previous tests were completed with a pencil beam, which leads to many of the photons hitting the target material, a fan beam covers the entire container, resulting in many of the source particles not hitting a material of interest. By biasing the direction of the source, computation can be focused to the desired materials.

Parameters

Like the biasing parameters used for source energy biasing, source direction biasing provides a mechanism to focus the simulation towards source particles that are more likely to contribute to the tally. Source direction biasing, however, biases, as the name implies, the direction of the source. This is used for cone beams to focus on particular angles of the source. To bias the direction of the source a SB card is used, as with source energy biasing, each entry must correspond to a value on the SI and SP cards used to specify the direction of the source.

Spectrum comparison

With the complete cargo model, fan beam, and an ideal detector, material discrimination is possible even without source direction biasing. As seen in Figure 3.7, source direction biasing eliminated the fluctuation in the uranium results while maintaining the trends of the results. The same result would be achievable by significantly increasing the number of particles modeled as the fluctuation in the unbiased results are from poor sampling. The convergence rate improves significantly by biasing the source direction.

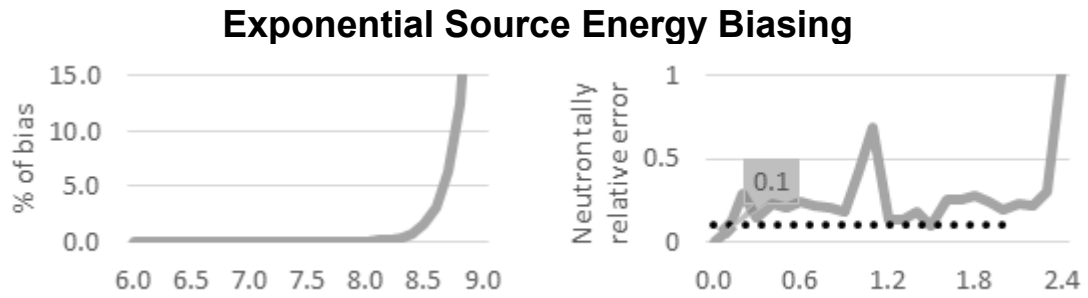


Figure 3.6. Exponential source energy biasing.

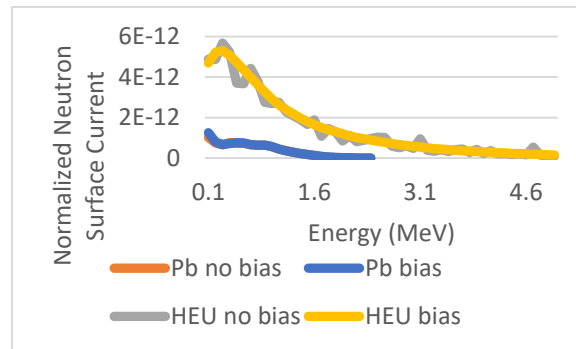


Figure 3.7. Increased reliability from source direction biasing.

Total Simulation Time

Again, the time required increases as more secondaries are generated by focusing the beam to the target material. Unlike the source energy biasing, this was not run on a single core as these runs are much longer due to the geometry being more complex. To achieve reliable results for the uranium target, many CPU days are required while the previous comparisons required only days.

3.6. Parallel Computation

OpenMP multi-threading requires disabling of the physics models (MPHYS card). This limits which isotopes can be used as not all isotopes are supported for photonuclear without models. In order to use MPI, which supports distributed computing, MCNP must be built from source as support is not included in the executable version.

MCNP MPI

Monte Carlo simulations are embarrassingly parallel [21] as histories are independent. There are however some limiting factors to scaling to many cores. Initialization, checkpointing, and gathering the final solution may require a less scalable implementation that may become a limiting factor.

For sufficiently long runs MCNP scales well to many cores but other factors limit the scaling for short runs. Figure 3.8 shows the improved scaling for longer runs. While short runs do not suffer from the additional cores, the cores do not contribute and in a cluster environment may be better utilized elsewhere.

To control synchronization, MCNP provides the PRDMP card. The card controls a few different options that together decide how often synchronization is necessary, including checkpointing with the RUNTPE, printing tallies, and the MCTAL file.

By setting the history cutoff to 1, nearly all the compute portion of the run can be eliminated. For 72 processes, when run on a quad Xeon Gold 6140 system, the single history run required an average of 5 seconds; as the 1 billion history run was about 2 minutes this is a notable portion and contributes to the loss in efficiency when scaling to many cores.

In a production system, some of the initialization time may be eliminated by storing the geometry in a format that doesn't need to be translated, as a voxel-based cargo would always have the same geometry. Further profiling would be required to determine the potential speed-up.

3.7. Discussion

By approximating electron interactions rather than transporting electrons, setting a minimum energy threshold for photons, and biasing the source energy and direction, the MCNP calculation can be completed much more quickly. These

improvements enable distinguishing materials in a complete cargo model but don't facilitate real-time simulation. Further tuning may be achievable with further adjustment of the parameters investigated. Additionally, scaling to more cores can further decrease runtime, but the scalability of adding more cores is limited.

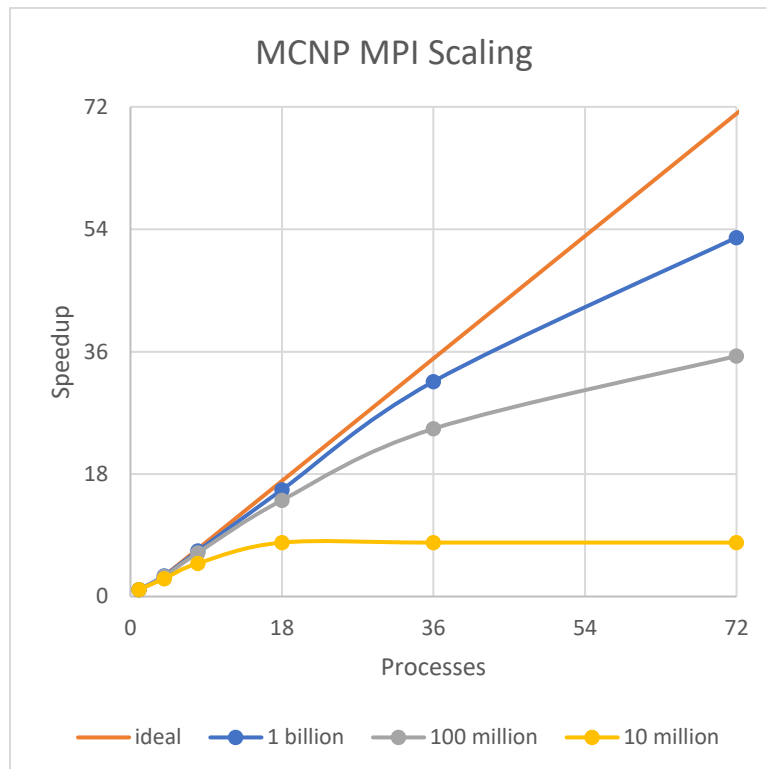


Figure 3.8. MCNP MPI scaling vs particle count on quad Intel Xeon Gold 6140 system (72 total cores).

Chapter 4

ALTERNATIVE TRANSPORT METHODS

This chapter examines three potentially faster alternatives to MCNP, namely, Geant4 which is an open-source Monte Carlo code that allows broader modifications and optimizations, ADVANTG which generates variance reduction parameters for MCNP, and Attila which is a discrete ordinates solver.

4.1. Geant4

Geant4 is an open-source Monte Carlo toolkit developed by CERN with an object-oriented design [8]. Geant4 was investigated with the goal of determining the feasibility of utilizing this design to further optimize Geant4 specifically to this application. This section discusses Geant4's implementation, the input used, the tally methods, validation efforts, and the physics lists.

Implementation

Geant4 geometry is defined using C++ objects [22], either by coding the geometry directly or using a reader to translate a format to those C++ objects. Geant4 provides one such reader to read Geometry Description Markup Language, GDML, files.

Geant4 uses a Run object to manage a collection of Track objects which manage the state for a particle through a series of Step objects. The Track object is “a snapshot of a particle” [23] containing the location and any applicable quantities of the particle, such as the weight, energy, time, or velocity. At each step, each process is applied in order to determine the step length and energy loss and also to create secondary particles. To cross boundaries between volumes, the end point of the step is placed on the volume boundary. The start and end point both link to the material of their respective volume so that processes such as refraction can be modeled.

Input

The GDML format provides an alternative to using C++ objects for defining the Geant4 geometry. The GDML format is an XML schema for defining the materials, solids, and structure [24]. By using an XML format, changes to the geometry can easily be implemented programmatically. Similar to the MCNP input described in Chapter 2, the solids are defined separately from the structure. The format provides a number of preset solids for defining boxes, cones, spheres, and other basic shapes but also allows for much more complex definitions by either combining shapes or defining more complex polyhedra. The structure provides geometry nesting and links the materials to the shapes, also similar to MCNP. Detector volumes can be defined within the GDML by providing “auxiliary” volume information.

As Geant4 is only a toolkit, how it is run will vary by implementation. Some common implementations include pure command-line or one of the graphical interfaces provided for visualization and some input.

Tally methods

The SensitiveDetector class enables defining a method that will be called for every Step within the flagged logical volumes. The results are stored as hits which store the information about the detected particle to be processed at the end of the run. Additionally, scorers can be used to track occurrences of events rather than particles within a volume. For all runs, Sensitive Detectors were used.

Random Number Generators

For longer simulations, the default random number generator for Geant4 caused the output to include duplicate results. With reference to Figure 4.1, this trend was first noticed because the neutron counts didn't trail down to 1 for higher energies as expected. Further examination showed that each entry is duplicated an average of 5.712 times for 100 Million starting photons as shown in Figure 4.2. These duplicated entries were never repeated immediately but were thousands of entries apart and were often repeated in clusters.

Geant4 provides other random number generators [22]. The MixMaxRng and RanecuEngine random number generators were both found to not produce any duplicate results for 100 Million starting photons.

Physics Lists

Even using an appropriate random number generator, the Geant4 results never seemed to match the MCNP results. Further examination of literature discovered this was a known issue in Geant4 as the provided physics lists do not provide sufficiently accurate photofission cross-sections [25]. Updated cross-sections were not available via RSICC at the time of writing.

Discussion

Geant4 allows greater flexibility than MCNP but also requires more validation as the parts must be put together with C++ by the end-user, and this process can introduce errors. Additionally, the provided physics lists are not suitable for use for the SNM application. When improved physics list become available, perhaps Geant4 should be re-evaluated, but care will need to be taken to ensure appropriate selections are made at every step and the result will need to be validated.

4.2. ADVANTG

AutomateD VArIaNce reducTion Generator (ADVANTG) is, as it sounds, an automated tool for generating variance reduction parameters for MCNP [13] developed by Oak Ridge National Laboratory (ORNL). ADVANTG accelerates

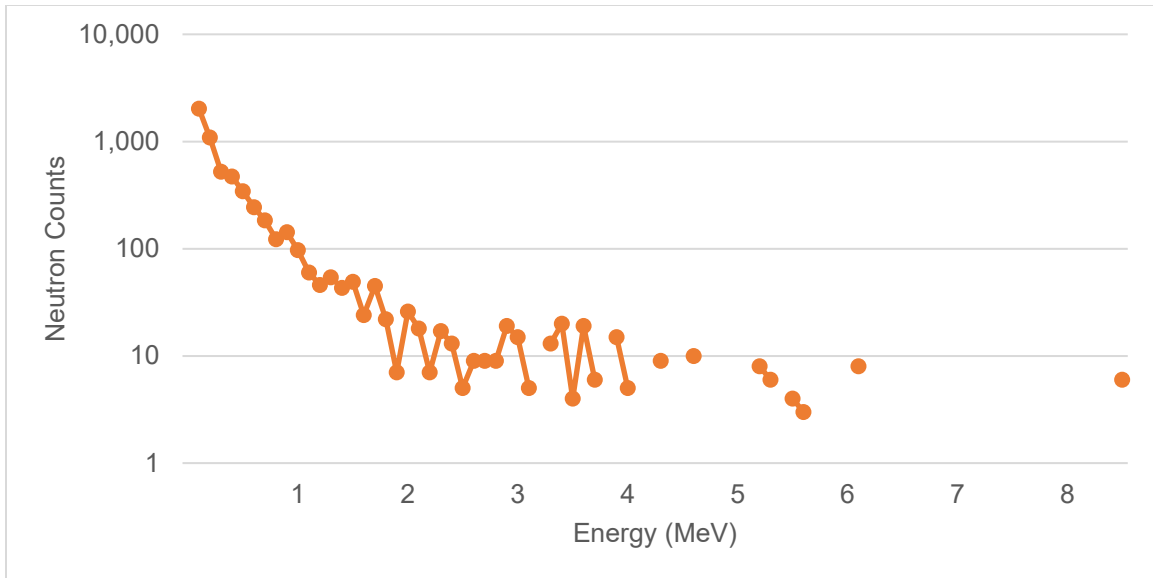


Figure 4.1. Geant4 default random number generator.

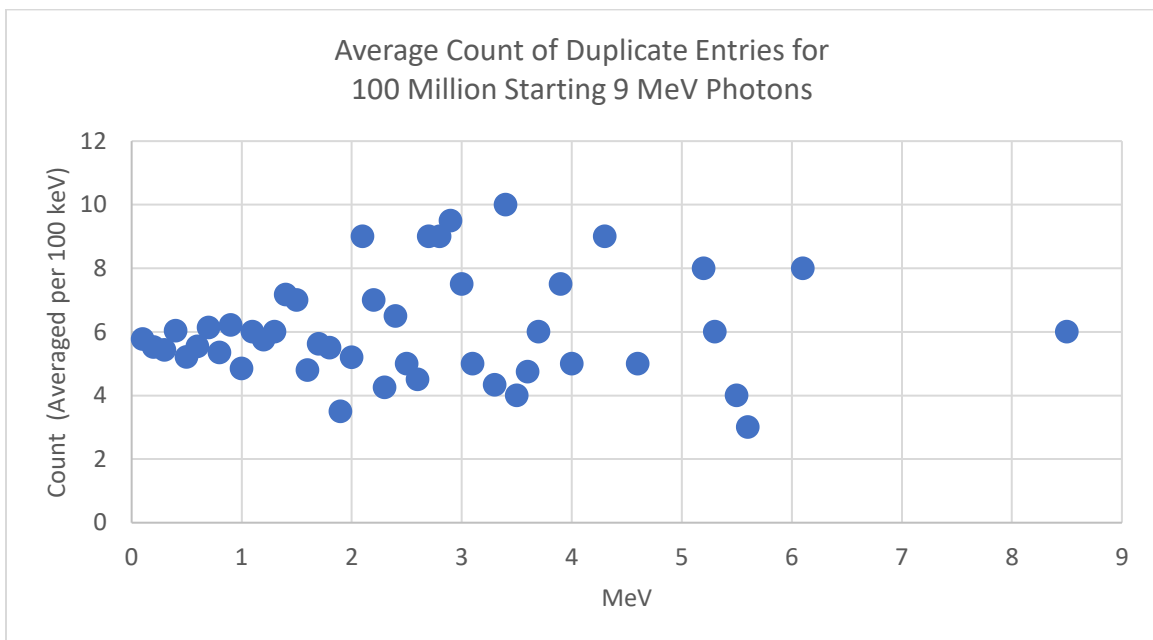


Figure 4.2. Duplicate Counts by Energy.

MCNP calculations using the CADIS (Consistent Adjoint Driven Importance Sampling) and FW-CADIS (Forward Weighted - CADIS) methods discussed in Chapter 1 to generate weight-window and source biasing parameters. ADVANTG uses the Denovo discrete ordinates solver to generate these parameters.

Input

As ADVANTG is intended to automate variance reduction for MCNP, it directly accepts an MCNP deck to describe the geometry and source. It also requires a separate input to describe the desired grid and options to be used for Denovo. Unfortunately, ADVANTG only supports MCNP 5 decks rather than MCNP 6 decks. This means that the MPHYS card (enable model physics) and MX cards (material nuclide control) cannot be used. While MPHYS card is critical when using materials beyond the limited available photonuclear tables, the MX card can be substituted by specifying the nuclides with the material on the materials' cards.

ADVANTG is run from the command-line with the ADVANTG input file as an argument.

Output

ADVANTG outputs an MCNP deck with weight windows and source biasing added to the deck. This enables direct use of the output in MCNP5. For use with newer features added in MCNP6, the output will need to be changed to reflect those features.

Discussion

The lack of support for photonuclear reactions and fission products in Denovo [13] limits the usefulness of ADVANTG for accelerating MCNP for the SNM application. To avoid the lack of support for either issue, the calculation can be broken into components, the first transporting the source photons to the material, the second transporting the neutron products. This adds significant complexity to the process as the intermediate must be calculated and formed into an MCNP input deck.

4.3. Attila

Developed by Silver Fir Software, Attila is a discrete ordinates solver for use in medical and industrial imaging applications [26]. Attila is intended for use as a graphical interface as opposed to the previously discussed packages but does support command-line operation. One of the significant advantages of Attila over other discrete ordinates solvers is the visualization built directly into it and the ability to compare with MCNP results for the same model.

Input

Attila uses CAD models for geometry input and cannot read models generated by SWORD. As it is primarily intended for graphical use, many of the parameters are selected in the interface, rather than a config file, as seen in the other packages.

Some of the notable geometry options in the interface are the “Max allowable edge length” and the curvature refinement options. Both refine how the mesh is generated over the model. Figure 4.3 shows a CAD model and the resulting mesh.

Attila4MC

Attila is also able to provide an interface for MCNP. This allows the use of the meshes generated by Attila from the base models to be used with MCNP and the results to be visualized using the Attila tools. This can either be used just for running MCNP or for validating Attila results as it enables simulating the same 3D mesh within both MCNP and Attila and provides the same output format for both. Figure 4.4 shows an example MCNP visualization.

Physics

Like ADVANTG, Attila is currently unable to model photo-nuclear reactions. This limits the applicability of Attila directly for this application as to correctly model these reactions the processing again needs to be split into two steps, transporting primaries and transporting secondaries, as with ADVANTG.

Discussion

The rapid photon solution that can be calculated by Attila’s use of discrete methods and ability to use Attila4MC to compare the discrete ordinates results directly to MCNP generated results, using the exact same model, shows promise for future use. Attila and other discrete solvers, however, do not currently handle the necessary processes to determine if cargo contains just benign materials or special nuclear material. Implementing photo-nuclear reactions into a discrete solver could offer a method to rapidly clear cargo.

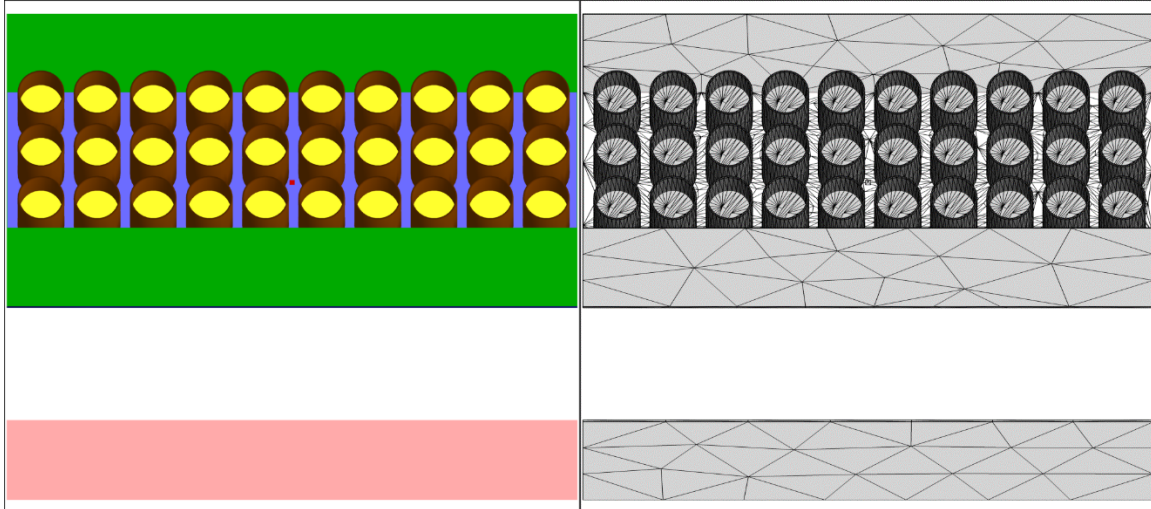


Figure 4.3. CAD model and mesh generated by Attila. This model is a 20 ft container (ceiling removed for visualization) with barrels, partially filled with water and a 20 ft detector.

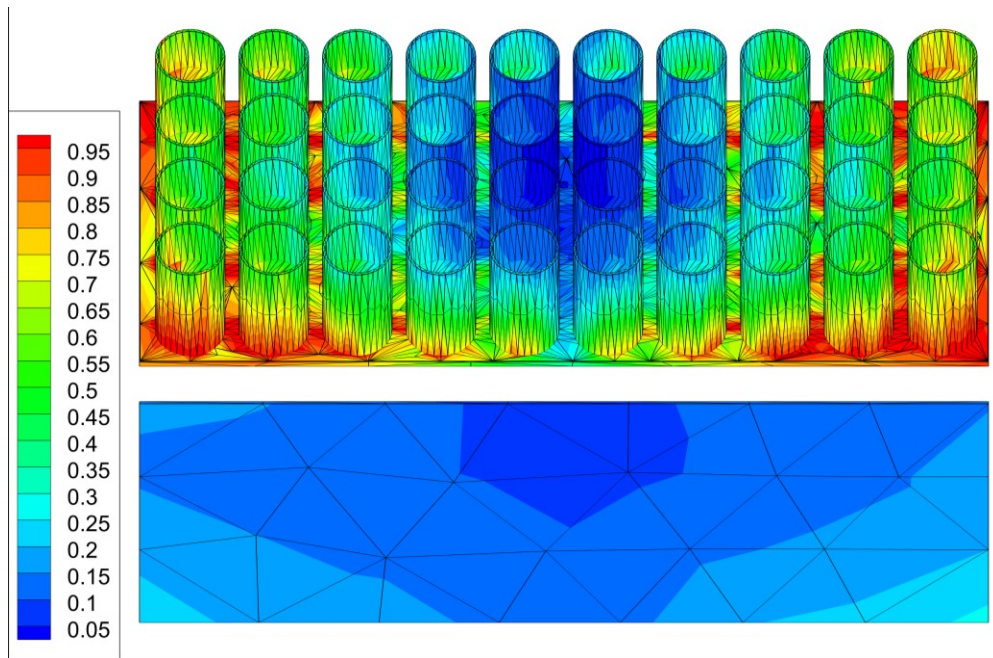


Figure 4.4. MCNP relative error, visualized using Attila4MC (ceiling and walls removed for visualization).

Chapter 5

CONCLUSIONS AND RECOMMENDATIONS

Conclusion

MCNP can be used to estimate the active background given a cargo model. With careful selection of parameters and biasing, the simulation can finish in a reasonable amount of time, albeit not fast enough for real-time determinations. This parameter study can be useful for rapid validation of other methods.

Geant4 offers increased flexibility over MCNP but also comes with the additional challenges of associated with building up from a framework rather than a complete working system. Additionally, instead of configuring defined parameters for tuning performance, those features must be developed from code and functionality must be validated rather than just the effects of the selected value or values. Various complete packages built upon Geant4 exist, each offering a different selection of features, but, for this application, largely limited by the available physics libraries.

ADVANTG can be used to generate biasing parameters for MCNP and improve MCNP performance, however, the multi-stage process required for this application prevents use in real-time. Attila and other discrete solvers show promise for this application if photo-nuclear reactions are implemented.

Future Work

Discrete solvers can offer great performance, but accuracy doesn't improve with greater iteration counts. Instead, discretization errors are introduced from the first step. This challenge is largely overcome when considering a voxelized cargo as generated from a 3D Zeff map. As there is little potential for geometry loss from discretization, minimal error is introduced. Unfortunately, before a discrete solver can be applied to active background estimation, the appropriate photonuclear cross-sections must be added.

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VITA

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