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# Multigroup Neutron Dose Calculations for Proton Therapy

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## ABSTRACT

We have developed tools for the preparation of coupled multigroup proton/neutron cross section libraries. Our method is to use NJOY to process evaluated nuclear data files for incident particles below 150 MeV and MCNPX to produce data for higher energies. We modified the XSEX3 program of the MCNPX code system to produce Legendre expansions of scattering matrices generated by sampling the physics models that are comparable to the output of the GROUPR routine of NJOY. Our code combines the low and high energy scattering data with user input stopping powers and energy deposition cross sections that we also calculated using MCNPX. Our code also calculates momentum transfer coefficients for the library and optionally applies an energy straggling model to the scattering cross sections and stopping powers. The motivation was initially for deterministic solution of space radiation shielding calculations using Attila, but noting that proton therapy treatment planning may neglect secondary neutron dose assessments because of difficulty and expense, we have also investigated the feasibility of multigroup methods for this application. We have shown that multigroup MCNPX solutions for secondary neutron dose compare well with continuous energy solutions and are obtainable with less than half computational cost. This efficiency comparison neglects the cost of preparing the library data, but this becomes negligible when distributed over many multigroup calculations. Our deterministic calculations illustrate recognized obstacles that may have to be overcome before discrete ordinates methods can be efficient alternatives for proton therapy neutron dose calculations.

*Key Words*: cross sections, multigroup, coupled proton/neutron, neutron dose, proton therapy

## 1. INTRODUCTION

Neutron dose calculations are not always performed for proton therapy treatment planning due to difficulty and expense [1]. Monte Carlo simulations have shown that these exposures are small but not negligible [2]. Multigroup methods are investigated here as an alternative to the more conventionally used continuous energy Monte Carlo methods of MCNPX [3]. The first obstacle to using multigroup methods is the availability of cross section data. NJOY can be used to prepare multigroup cross sections from the same evaluated nuclear data files used for continuous energy cross section preparation [4]. At energies higher than available in evaluations, physics models can be used to calculate multigroup cross sections thereby eliminating the need for more costly physics model sampling during a transport calculation. With appropriate cross sections multigroup Monte Carlo and deterministic methods become options that can be more efficient. Multigroup cross sections also permit adjoint calculations, which can be more efficient than forward transport for some problems. Importance functions generated by adjoint calculations can also be used to improve efficiency of forward Monte Carlo calculations.

Methods for coupled multigroup proton/neutron cross section preparation spanning the transition from evaluated to model data have been developed. The SADCO-2 code system combines evaluated nuclear data below 20 MeV with cross sections calculated using the Bertini model at higher energies [5]. Our more recent efforts have been the development of tools that allow NJOY to be used to process evaluated data where available up to 150 MeV and then MCNPX to be used to generate higher energy cross section data [6]. Conceptually our methods are similar to those of SADCO-2, but where SADCO-2 is standalone we have built upon the existing capabilities of NJOY and MCNPX.

Coupled multigroup proton/neutron transport capabilities of MCNP were studied before the code was combined with LAHET for MCNPX [7]. Multigroup proton transport with MCNP was also investigated for proton radiography simulation before the advent of MCNPX [8]. The multigroup capabilities of MCNP were carried forward into MCNPX. MCNPX run in the continuous energy forward mode is reputably robust and accurate. By default where evaluated cross section data tables are unavailable it uses the Bertini process. The first step in the process is to decide if a nuclear interaction occurs. This is accomplished as for low energy tabular data transport except that geometric cross sections are used. When an interaction occurs it is then determined whether it is elastic or a reaction using tabulated data generated by an optical phenomenological model. If the interaction is nonelastic, the intranuclear cascade calculation is begun. This calculation is a Monte Carlo random walk for the incident particle, and any secondaries it creates, through the target nucleus itself. Nucleon-nucleon cross sections are used and the primary and secondary particles are tracked until they escape or their energies are below a cutoff. The types, angles and energies of escaping particles define secondary particles initially resulting from the nonelastic nuclear reaction.

A nucleus enters a pre-equilibrium stage following the intranuclear cascade. A pre-equilibrium stage is necessary because the intranuclear cascade model becomes inaccurate at low energies and it can be computationally impractical to track all of the nucleons down to very low energies. The pre-equilibrium calculation begins with the excitation energy and exciton configuration determined at the end of the intranuclear cascade. The pre-equilibrium model is quantum mechanical and in de-excitation of the nucleus emits light ions and more nucleons. The calculation terminates and the equilibrium phase starts when the equilibrium number of excitons is reached. During the equilibrium phase the nucleus may continue to de-excite by evaporating nucleons and light ions or it may fission or fragment. Once the excitation energy is below the particle emission threshold the residual nucleus is decayed by gamma emission using decay data tables.

All stages of the physics model process may produce nucleons that are then tracked outside the nucleus from where they originated. The interaction processing has a computational expense greater than table data sampling. Sampling the physics models before hand to produce multigroup cross sections that can subsequently be used in many transport calculations has potential efficiency benefits and can be thought of as analogous to the condensed history methods used for charged particle slowing down and small angle scattering.

In addition to increasing sampling efficiency for forward Monte Carlo transport, multigroup cross sections allow deterministic methods to be used. Deterministic methods can be advantageous because they provide the entire solution everywhere in a problem. Monte Carlo efficiency is achieved through the application of variance reduction schemes that generally optimize particular solutions. Attila is a discrete ordinates code with charged particle transport capabilities [9]. Interest in coupled proton/neutron transport with Attila for space radiation shielding calculations has been fueled by its ability to import problem geometries directly from the CAD packages being used to design spacecraft, a feature that makes use less difficult. Additionally, large gains in computational efficiency for coupled multigroup proton/neutron transport over Monte Carlo methods have been reported using SADCO-2 cross sections and other discrete ordinates codes [10].

In this paper we investigate the feasibility of, and potential for cost reduction, using multigroup cross sections with MCNPX and Attila for neutron dose calculations resulting from proton therapy treatment. We begin describing the methods used to prepare coupled multigroup proton/neutron cross section data for input to the two codes. We then present a simple calculation testing the validity of the multigroup cross sections followed by one assessing more complex absorbed dose calculation capabilities. We conclude with discussion of observed benefits and limitations of multigroup calculation methods.

## 2. CROSS SECTIONS

Both MCNPX in multigroup mode and Attila in charged particle mode solve the steady state Boltzmann-Fokker-Planck equation.

$$\begin{aligned}\hat{\Omega}\cdot\nabla\varphi(\vec{r},E,\hat{\Omega})+\sigma_t\varphi &= \int_0^\infty\int_{4\pi}\sigma_s(\vec{r},E'\rightarrow E,\hat{\Omega}\cdot\hat{\Omega}')d\hat{\Omega}'dE'+Q(\vec{r},E,\hat{\Omega})\\ &+\frac{\alpha}{2}\left\{\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial\varphi}{\partial\mu}+\frac{1}{1-\mu^2}\frac{\partial^2\varphi}{\partial\phi^2}\right\}+\frac{\partial}{\partial E}S(E)\varphi+\frac{1}{2}\frac{\partial^2}{\partial E^2}T(E)\varphi\end{aligned} \tag{1}$$

The first line of Eq. 1 is the Boltzmann transport equation. The terms on the second line are respectively the momentum transfer, continuous slowing down and energy straggling terms of the Fokker-Planck operator, where as functions of the Coulomb scattering cross section:

$$\alpha = 2\pi\int_{-1}^{+1}\sigma(E,\mu_0)(1-\mu_0)d\mu_0\ , \tag{2}$$

$$S(E)=\int_0^\infty\sigma(E\rightarrow E')(E-E')dE'\ ,\ \text{and} \tag{3}$$

$$T(E)=\int_0^\infty \sigma(E\to E')(E-E')^2\,dE' . \tag{4}$$

These are the momentum transfer coefficient, stopping power, and mean square stopping power. Neither MCNPX nor Attila includes energy straggling directly but it can be modeled in the library data with consistent definitions the scattering cross sections and stopping powers derived from the equations. Minimally, the codes require libraries to include the total and scattering cross sections, and stopping powers for charged particles. The scattering cross sections include all secondary particle production information. These are represented differently for MCNPX and Attila input.

Attila uses the $S_N$ method for which the multigroup discretization of the Boltzmann scattering source is expanded in spherical harmonics requiring Legendre moments of the cross sections to be supplied in the cross section library. The Monte Carlo method employed in MCNPX alternatively requires only the zeroeth moment and then that angular scattering probabilities be supplied using one of two approaches [11]. One is to provide an array of equiprobable cosine bin boundaries and the other is to provide probabilities for an array of discrete angles.

We initially prepared a cross section library in DTF format suitable for Attila input. An upper energy limit of 400 MeV was selected to provide capability for considering Earth orbiting satellite shielding problems. This bounds proton therapy applications as well. The energy group structure includes 5 MeV wide groups over 20 MeV and uses the same 30 group structure below 20 MeV that the coupled multigroup neutron/photon library supplied with MCNPX does. The lower 18 energy groups are omitted for protons establishing a cutoff at 0.823 MeV, approximately the 1 MeV default cutoff for MCNPX continuous energy calculations.

MCNPX is run with the option to turn transport off in order to sample the default physics model process for each nuclide in the library. The outcomes of one million events were written to history files for each proton and neutron group above 150 MeV. The XSEX3 program supplied with MCNPX processes the history files reporting total cross sections and tallying double differential scattering cross sections. The program was modified to calculate $P_{39}$ Legendre expansions of the proton-proton, proton-neutron, neutron-proton, and neutron-neutron scattering matrices. The high order expansion was found necessary and sufficient for faithful representation of the tallies. Evaluated data for each nuclide was then processed using NJOY. The GROUPR routine calculates the required total cross sections and prepares Legendre expansions of the scattering matrices for each reaction in the evaluation. Code was written that reads the GROUPR and modified XSEX3 outputs and prepares the DTF library tables from them.

The code that prepares the DTF library tables includes group stopping powers and heating cross sections read from user supplied input files. For stopping powers we input values interpolated from MCNPX tables. The input heating cross sections were stochastically calculated for all energy groups using MCNPX. For stopping power and energy deposition the goal was to create a multigroup library that was consistent with MCNPX continuous energy data and physics. For momentum transfer however, continuous energy MCNPX uses Rossi theory and as a result multigroup momentum transfer coefficients are not readily obtainable from MCNPX. We calculate values using Eq. 2 and a screened formulization of the differential Rutherford scattering cross section [12]. Finally the code optionally adjusts the stopping powers and cross sections according to a down scatter only straggling model [13]. We have not investigated sensitivity of solutions to the selection of 5 MeV wide group width over 20 MeV. It was selected as a being convenient width, arbitrarily less that the maximum energy transfer computed for the Rutherford cross section. This threshold was shown to be of some significance for accurate multigroup modeling of energy straggling.

For Attila input the DTF library is on a per atom basis and cross sections have units of barns, momentum transfer coefficients have units of steradian barns, and stopping powers and energy deposition cross sections have units of MeV barns. This permits Attila to mix library nuclides. MCNPX in multigroup mode requires total and $P_0$ scattering cross sections in barns per atom but stopping powers and momentum transfer coefficients on a per centimeter basis implying materials must be premixed for library input. We therefore wrote a program to read our DTF library, mix nuclides into materials based on user input and then calculate equiprobable bin boundaries from the resulting weighted $P_{39}$ expansion. Our program outputs MCNPX type 1 cross section files. Multigroup libraries in various formats, including DTF, reportedly can be converted for MCNPX input using the CRSRD program described in Ref. 11, but it was not used for this work.

To investigate the feasibility of multigroup MCNPX and Attila for proton therapy neutron dose calculations we consider only aluminum and water as materials, and make some rather arbitrary cross section processing assumptions that could require additional consideration before proceeding further with library development. For NJOY cross section processing 1/E within group weighting was used, while for MCNPX physics model generated cross sections, constant weighting was assumed. Constant weighting was also used for all group stopping powers, momentum transfer coefficients and energy deposition cross sections. With respect to resonance treatment we assume infinite dilution and process the cross sections at the evaluation temperatures of 296 K.

## 3. CALCULATIONS

Two basic problem geometries were considered. The first is a water cylinder irradiated with a proton beam in which we look at proton slowing down and neutron production comparing continuous energy and multigroup solutions using MCNPX. The second is a water slab irradiated through an aluminum plate where we compare the energy deposition solutions obtained using multigroup MCNPX and Attila with those obtained using continuous energy MCNPX.

### 3.1. Proton Beam on Water

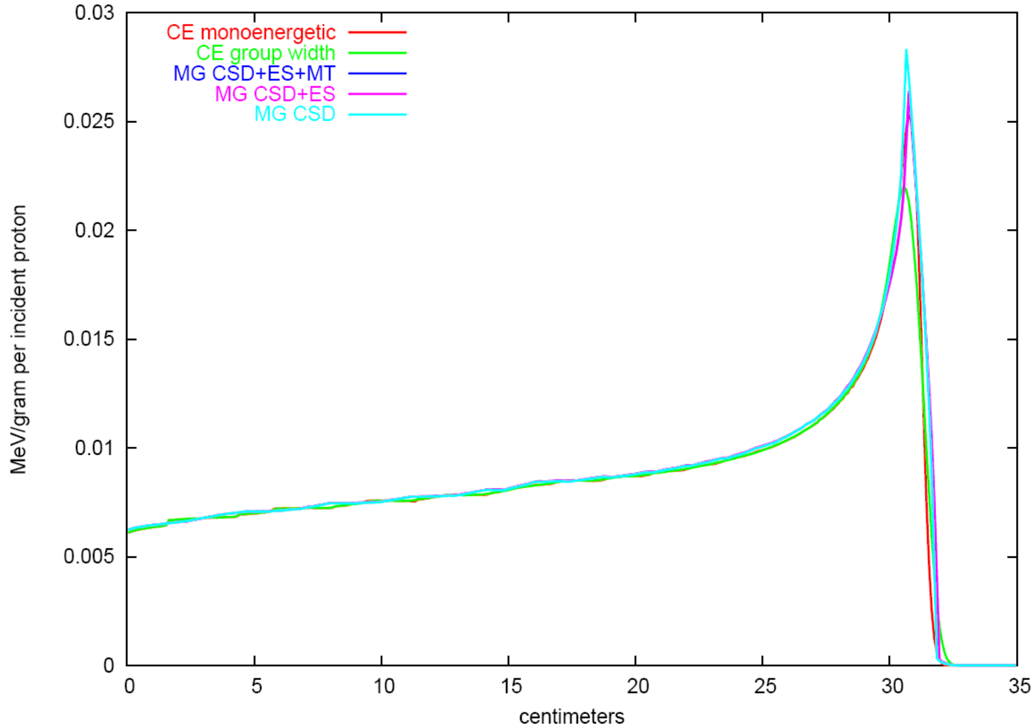
Protons are assumed normally incident at the center point of one end of a cylinder of water, 30 centimeters in diameter and 35 centimeters long. In multigroup calculations the beam energy specification is limited to a group and is therefore not actually monoenergetic. A monoenergetic beam starts off being effectively straggled in energy by the group width. We assume a group at the high end of proton therapy applications, that from 220 MeV to 225 MeV, as a source. The continuous energy transport calculation is run once assuming the beam is monoenergetic at 222.5 MeV and once assuming the beam is uniformly distributed in energy from 220 MeV to

225 MeV. The multigroup calculation is run three times, first with both the energy straggling (ES) model applied to the library data and the calculated momentum transfer coefficients (MT), then with straggling applied but no momentum transfer, and then without either straggling or momentum transfer for a continuous slowing down (CSD) only solution. Results are compared to evaluate the significance of the multigroup monoenergetic beam approximation and second order Fokker-Planck terms to the neutron source solution with respect to what are expected to be greater effects on the proton slowing down solutions. For the multigroup library, 10 equiprobable cosine bins were used to define scattering.

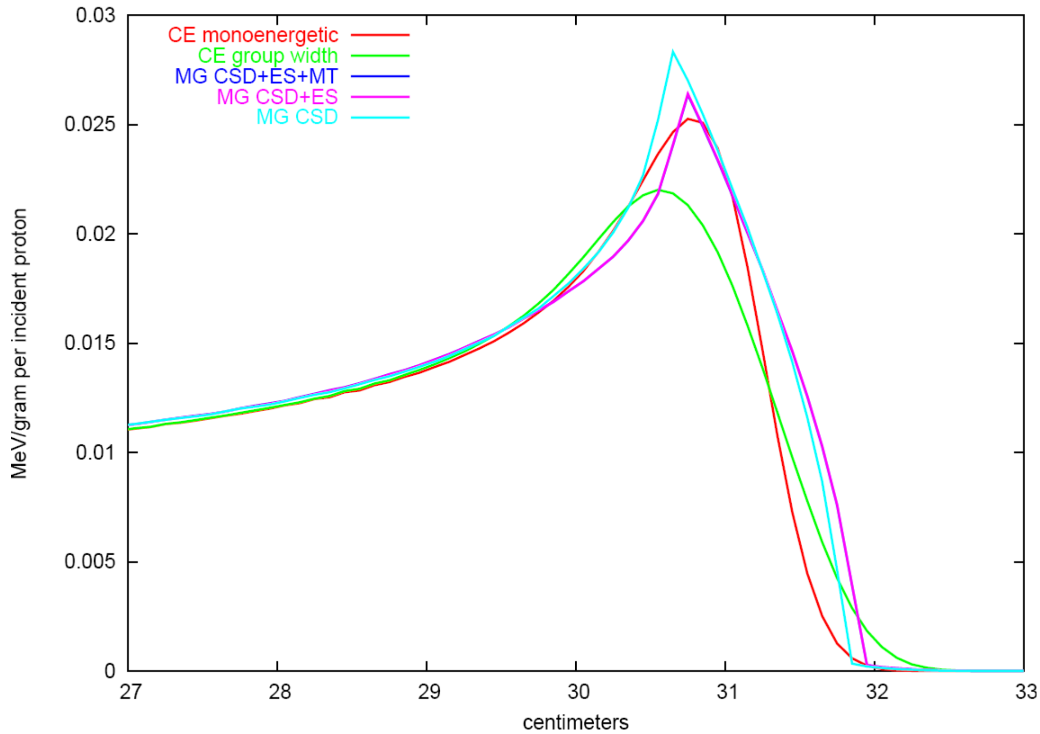
In each calculation three tallies were made for one million incident proton histories. Proton energy deposition was tallied through the cylinder in 1-millimeter thick segments. Energy dependent proton flux was tallied at a depth of 27.25 centimeters, about 90 percent of the proton range. Finally the neutron flux spectrum averaged over the entire water volume was tallied. The results are plotted in Figures 1, 2 and 3. The transport was analog for all cases. The run times required were 5 times longer for the continuous energy calculations than for the multigroup calculations.

As shown in Figure 1 the dose depth curves are comparable through most of the range, but significant differences are observable in the Bragg peak. Calculation errors were generally 0.1 percent or less and to 30 centimeters the calculations were within 3 percent of each other. Neither the continuous energy slowing down solutions nor the multigroup are particularly smooth over the first 25 centimeters. This appears to be a numerical affect of the stepwise algorithm employed in MCNPX [14]. Presumably the differences in the Bragg peak shapes result from differences between continuous energy and multigroup slowing down algorithms. Comparing the Figure 2 energy distributions at 27.25 centimeters where the multigroup peak appears to be slightly higher energy, suggests something other than constant weighting may be more appropriate for the multigroup stopping powers. Errors for the data plotted in Figure 2 were less than 1 percent in the 60 MeV to 75 MeV range. Momentum transfer did not observably affect the multigroup solutions. The plotted CSD+ES solutions lie on top of the CSD+ES+MT solutions. This is not surprising since the tally was not radially segmented. The energy straggling model does broaden the multigroup proton energy spectrum, but clearly this is of little consequence to the secondary neutron spectrum.

Figure 3 plots the tallied neutron spectra. The tally errors are less than 1 percent below 30 MeV and remain less than 5 percent up to 200 MeV. Group by group the agreement between the multigroup and continuous energy calculations is to within 10 percent, except for the three groups below 0.4 eV. In the lowest energy groups the multigroup solutions were one third to one quarter the continuous energy solutions. This is also not surprising, considering that 1/E weighting was assumed through thermal energies for the multigroup data and no thermal scattering treatment was applied, where for the continuous energy calculations a light water scattering kernel was used for hydrogen and free-gas treatment was used for oxygen. More thoughtful cross section weighting and thermal scattering treatment would certainly improve the very low energy spectra agreement but will not significantly affect integral neutron energy deposition calculations.




**a: entire range.**




**b: expansion about Bragg peak.**

**Figure 1: Proton energy deposition versus depth.**

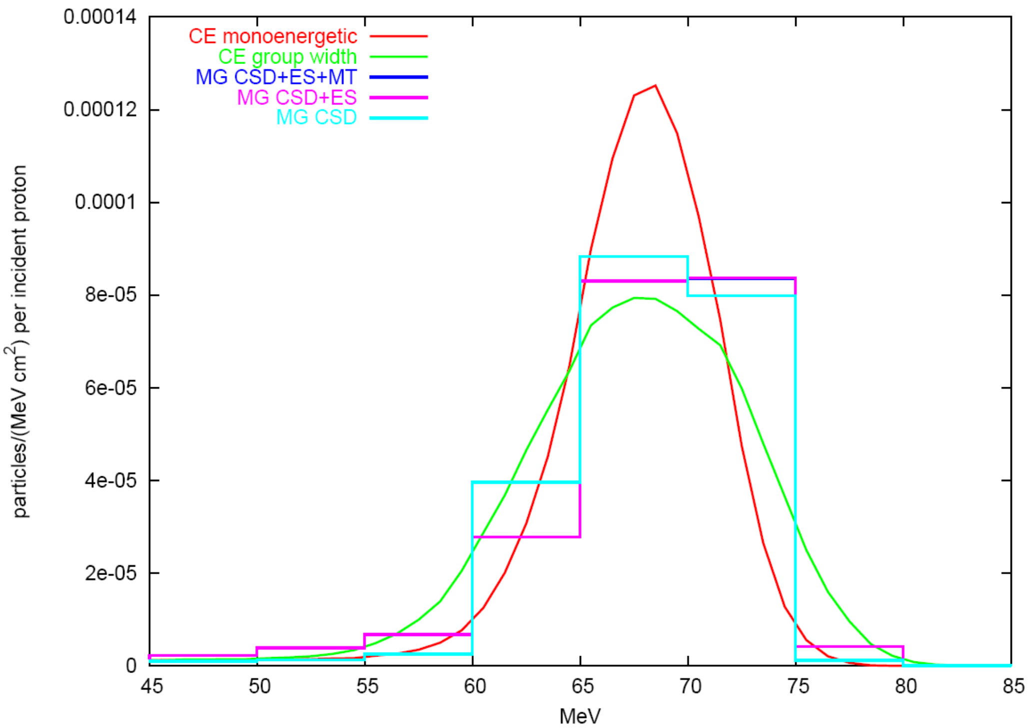



**Figure 2: Proton energy spectrum at 27.25 centimeters.**

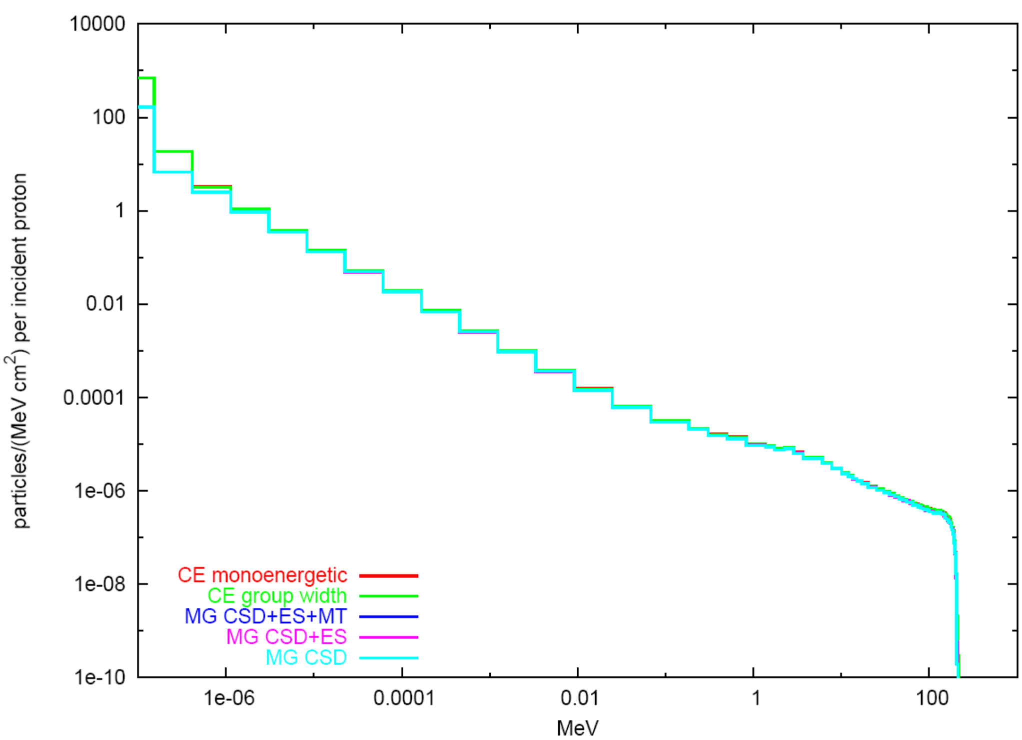



**Figure 3: Secondary neutron spectrum.**

### 3.2. Energy Deposition in Water Slab Through Aluminum

For the second problem we look at the spatial neutron and proton energy deposition solutions in a large water slab grossly approximating a proton therapy patient. The beam is assumed incident on a 1-centimeter thick aluminum plate accounting for neutron production that might occur in a therapy nozzle. The problem geometry is illustrated in Figure 4. For the continuous energy MCNPX solution the source is assumed a monoenergetic 222.5 MeV proton beam. For the multigroup solutions with MCNPX and Attila the 220 MeV to 225 MeV group is assumed. In all of the calculations the beam was assumed uniformly incident on the same 25 square centimeter area near the center of the aluminum plate. The area was matched to two boundary sides of tetrahedral mesh elements in the Attila problem geometry.

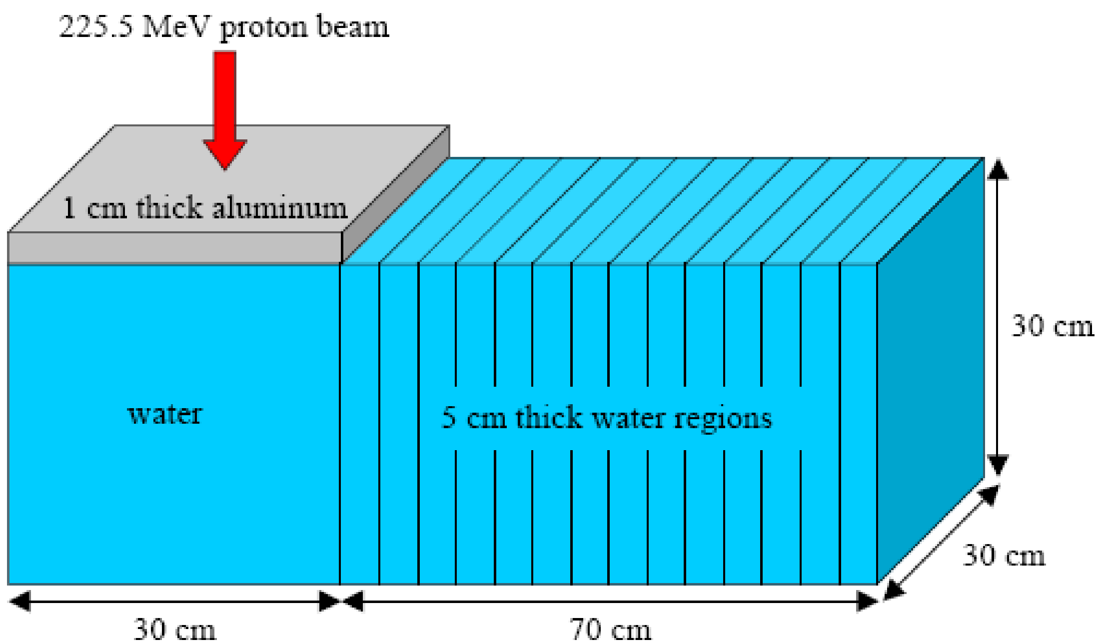



**Figure 4: Geometry for secondary neutron energy deposition calculations.**

The MCNPX calculations were run assuming the proton source is normally incident on the aluminum slab. Angular approximation is however necessary for deterministic solution with Attila. Attila features a plane wave boundary source applicable to surface element sets. A set was defined consisting of the sides of tetrahedra upon which the source was defined. The plane wave direction was defined normal to the aluminum slab. For solution this results in equal weighting of the forward directions of the assumed angular quadrature set. This does not result in a monodirectional beam definition but is an approximation that might be sufficient for reasonable secondary neutron solutions away from the proton source.

Average neutron energy depositions in the 5-centimeter thick regions illustrated in Figure 4 were calculated. The results are plotted in Figure 5. The calculation errors are less than 1 percent. The results are modified track length flux tallies. In the continuous energy case this is calculated from heating cross sections below 150 MeV and physics models above with the addition of heating by proton slowing down using track length heating tallies. In the multigroup cases the track length flux tallies are modified by the calculated multigroup heating cross sections included in the libraries at all energies. The multigroup MCNPX calculations were run with aluminum and water cross sections prepared assuming 10, 20 and 40 equiprobable cosine bins for the scattering distributions. The results indicate that many equiprobable bins are necessary for good agreement with the continuous energy solutions far from the beam. This is because the scattering cross sections are highly anisotropic, and with increasing secondary particle energy, forward production probabilities become increasingly larger than higher angle particle production probabilities. So in order to adequately define large angle production with respect to distant solutions using the equiprobable bin approach, many bins are needed. Alternatively, fewer angles might be necessary using the discrete angle approach but it is less robust because it can lead to ray effects [11].

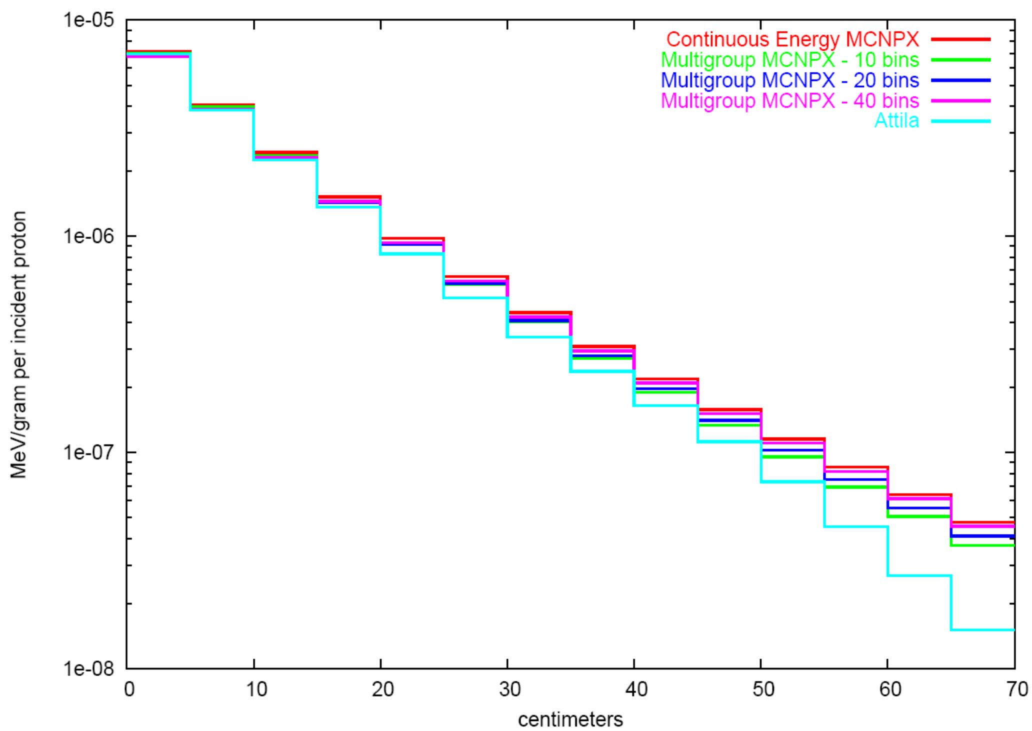


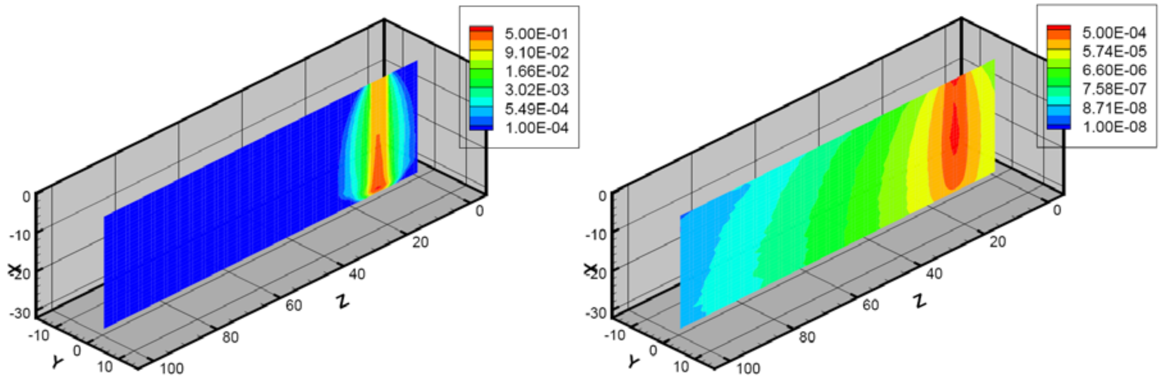

**Figure 5: Average neutron energy depositions in slab.**

The continuous energy and multigroup MCNPX solutions for neutron heating are comparable but the multigroup solution falls off faster with distance from the beam when an inadequate number of angular bins are used to define the scattering cross sections. With only 10 bins the multigroup MCNPX solutions are about 20 percent lower than the continuous energy solutions at the far end of the slab. With 40 bins the multigroup MCNPX solutions are within 5 percent of the continuous energy solutions through the entire slab. Also plotted is the Attila solution obtained for a reflected mesh of 2,520 cells using the $S_{12}$ Chebyshev-Legendre quadrature set with $P_3$ Galekin scattering treatment and the extended transport correction. The solution also diverges from the continuous energy MCNPX solution suggesting much higher angular quadrature order is needed for accurate solution far from the beam.

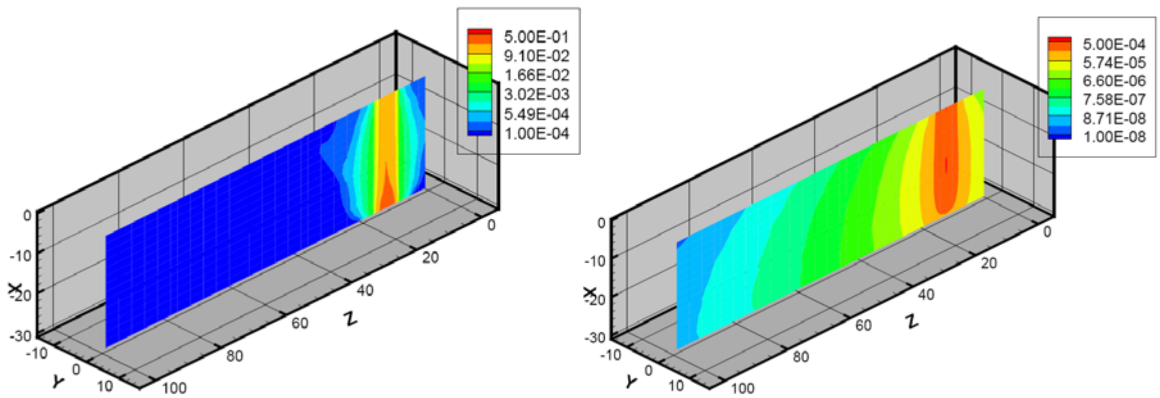
Continuous energy and multigroup MCNPX mesh tally solutions are plotted in Figure 6 for both proton and neutron energy depositions. The results are again modified track length flux tallies. The continuous energy and multigroup MCNPX solutions for neutron heating are virtually indistinguishable. The plotted solutions are for the 40-anglar bin cross section definitions. The differences in the features in the proton heating solutions are consistent with the observations made from Figure 1 for the first calculation. Also plotted in the figure is the heating node field generated from the Attila solution. The much broader proton heating illustrated for the Attila solution is primarily the result of the crude beam approximation. The Attila neutron heating solution is similar to the Monte Carlo solution but the increasing underestimate with distance is apparent.

For the multigroup and continuous energy MCNPX calculations the same energy independent spatial importance function was used for variance reduction. The multigroup histories required on average half the run time that the continuous energy histories required. As a measure of efficiency, the figure-of-merit for the multigroup neutron solutions were about twice that of the continuous energy solution. To achieve a continuous energy solution error in the last region of one percent required 24 hours of run time on a 3.6 GHz processor using the precompiled Linux version of MCNPX. Less than half the time was required for the multigroup solutions. The Attila deterministic solution was produced in less than 1 hour on a Windows machine with a 3.2 GHz processor and 4 GB of memory.

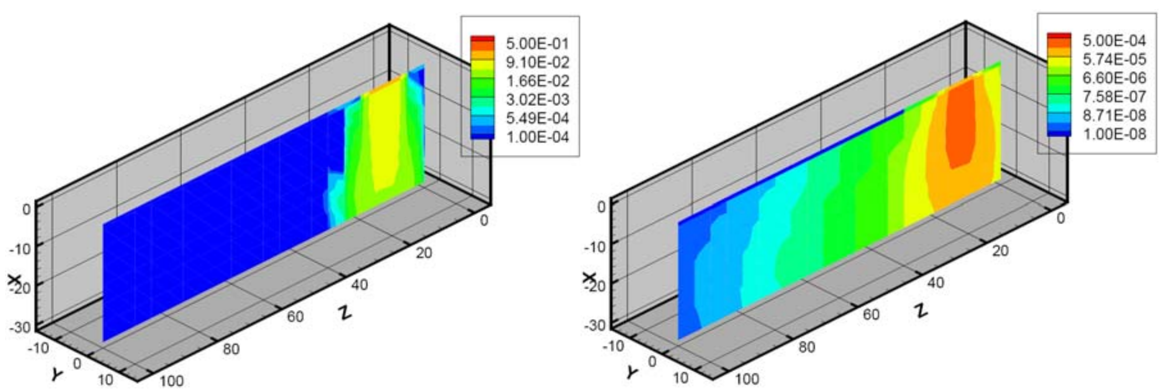
The deterministic solution we present is not considered adequate for proton therapy neutron dose calculations. Increasing the scattering degree and quadrature order, and selecting one with points more uniformly distributed, could be expected produce better results for this problem. Memory requirements and run times increase with increasing scattering degree and quadrature order. With the spatial and angular discretizations and scattering degree we used the problem fit in the memory of our machine. Refining the mesh and angular quadrature would have required more memory or execution in low memory mode resulting in longer run time. Extrapolating, it is unlikely an accurate solution is achievable any more efficiently than it is with Monte Carlo methods. Adaptive discrete ordinates algorithms being developed address this by only adding to the quadrature points needed for accurate solution [15]. That our deterministic solution is as close to the Monte Carlo solutions as it is may be attributed to the fact that more neutrons are produced in the aluminum and at shallow depths of the problem before the proton solution completely degrades. The deterministic proton solution is poor foremost because of the gross angular approximation that was made for the beam that could be better with more quadrature points, but also because of apparent numerical straggling effects resulting from linear discontinuous differencing of the continuous slowing down term of the Fokker-Plank operator. Improved differencing methods have been developed but they are also computationally more costly [16].




a: continuous energy Monte Carlo




b: multigroup Monte Carlo




c: deterministic

**Figure 6: Energy deposition solutions, protons on left and neutrons on right (MeV/gram per incident proton).**

To ascertain whether Monte Carlo multigroup efficiency gains are simply a result of not having to sample the physics models at energies over 150 MeV or are more generally a function of the continuous energy verses multigroup algorithms, the same problem was run assuming a 147.5 MeV proton beam. The multigroup and continuous energy solutions again compared favorably and the figure of merit for the multigroup solution was three times that of the continuous energy solution. For the higher energy beam the difference was only a factor of two. The observed increase was unexpected and warrants further investigation, which we have not yet undertaken, but it appears that the multigroup gains are not limited to higher energy problems.

## 3. CONCLUSIONS

We have developed tools and methods for the preparation of coupled multigroup proton/neutron cross section libraries suitable for use with the MCNPX and Attila codes. The physics models of the MCNPX code run in its continuous energy mode are used to generate cross sections above evaluated table data energy limits. NJOY is used to prepare multigroup data directly from evaluations. We combine data from MCNPX and NJOY in a DTF cross section library and apply an energy straggling model and include calculated momentum transfer coefficients. The DTF library is directly usable with Attila. We have written a program to mix library nuclides into material cross section library data formatted for MCNPX input. These tools have permitted us to investigate the feasibility and potential benefits of using multigroup methods for calculating secondary neutron doses from proton therapy.

Secondary neutron doses from proton therapy have been described as small but not negligible, however due to difficulty and expense are not always calculated during treatment planning. We considered multigroup methods for their potential of being more computationally efficient than the more conventional continuous energy Monte Carlo approach. Comparing our forward multigroup and continuous energy Monte Carlo calculations we observed efficiency gains of factors of two to five for secondary neutron solutions with agreement to within five percent for total energy deposited by secondary neutrons. This does not consider the expense required to prepare the multigroup data, but once a library is built it can be used over and over for multigroup calculations and this expense becomes negligible. A factor of two or better increase in computational efficiency could lead to more frequent inclusion of secondary neutron dose calculations in the treatment planning process.

Though discrete ordinates methods can be very efficient, further development may be necessary for them to be viable alternatives for proton therapy neutron dose calculations. Attila is a state-of-the-art radiation transport tool that we found easy to use. It can import geometric models directly from CAD systems. Its features alleviate some of the difficulty associated with performing calculations, but the computational expense may be higher than that of Monte Carlo methods when used for proton therapy secondary neutron dose problems. This is due to the very high quadrature order that appears necessary for accurate coupled multigroup solutions. Ease of use could be more important than computational expense, in which case discrete ordinates codes may presently be an alternative.

## ACKNOWLEDGMENTS

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