POST-PROCESSING OF MONTE CARLO SIMULATIONS FOR RAPID BNCT SOURCE OPTIMIZATION STUDIES

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ABSTRACT: A great advantage of some neutron sources, such as accelerator-produced sources, is that they can be tuned to produce different spectra. Unfortunately, optimization studies are often time-consuming and difficult, as they require a lengthy Monte Carlo simulation for each source. When multiple characteristics, such as energy, angle, and spatial distribution of a neutron beam are allowed to vary, an overwhelming number of simulations may be required. Many optimization studies, therefore, suffer from a small number of datapoints, restrictive treatment conditions, or poor statistics.

By scoring pertinent information from every particle tally in a Monte Carlo simulation, then applying appropriate source variable weight factors in a post-processing algorithm, a single simulation can be used to model any number of multiple sources. Through this method, the response to a new source can be modeled in minutes or seconds, rather than hours or days, allowing for the analysis of truely variable source conditions of much greater resolution than is normally possible when a new simulation must be run for each datapoint in a study. This method has been benchmarked and used to recreate optimization studies in a small fraction of the time spent in the original studies.

INTRODUCTION: Neutronics studies in BNCT have strived to improve the tumor dose to tissue dose ratio of a given treatment by careful tailoring of the neutron spectrum. Many different beam shaping designs have been used or proposed, resulting in a great variety of different neutron spectra to be compared. Two such spectra are shown in Fig. 1, a typical reactor-produced beam(1) and an accelerator-produced beam(2), demonstrating the large differences in spectra that different sources can provide. While most analyses have shown(3, 4) that neutrons in the range of about 2 keV to 20 keV are most desirable, detailed optimization studies that analyze the effects of energy, angle, spatial distribution, RBEs, and phantom geometries are usually tedious, involving hundreds or even thousands of Monte Carlo simulations. Each of these simulations can take hours or days to complete.

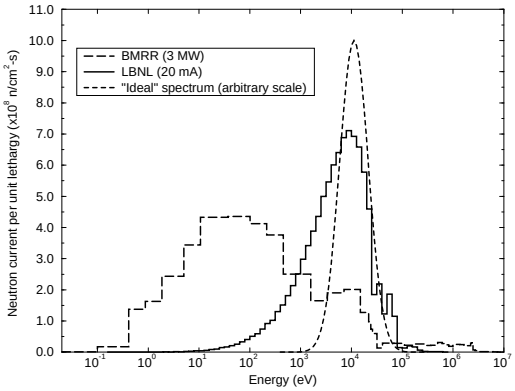

FIGURE 1. Neutron energy spectra for the BMRR beam, an LBNL acclerator-based design, and an "ideal" spectrum which produces the greatest tumor dose at the brain midpoint as determined from extensive Monte Carlo optimization

To facilitate more rapid optimization studies, the "ubertally" method was developed. This method involves post-processing of individual particle tallies in a Monte Carlo simulation to reweight the fluxes to reflect a new neutron or photon source. The calculations that are performed are identical to those that would be performed in a normal MCNP run, except in a different order.

MATERIALS AND METHODS: The first step is the "master" MCNP simulation, which produces the "ubertally" files. In most respects, the master MCNP input file is like a normal input file with a few exceptions. First, a FILES card is used to create two unformatted, sequential files, UBERTALE and UBERTALF. It is into these files that particle information is stored. Second, the source is modeled probabilistically as isotropic, isoergic, and evenly spatially distributed. However, this source is then biased so that an adequate number of particles across the entire spectrum from 0.001 eV to 15.84893 MeV will be modeled. The biasing is performed over the whole spectrum with ten equiprobable, equal lethargy bins per energy decade. Finally, the tallies of interest are affected by the "FU" card, which calls a custom TALLYX subroutine.

To record pertinent information on each particle that encounters a tally volume, a custom TALLYX subroutine is written. Source information is written into the UBERTALE file: particle history number, source position (Y and Z), source energy, and source angle. This data is written only once per source particle. Tally information is written to the UBERTALF file for every particle track in any tally cell: particle history number, cell number, particle type, energy, and flux (track length divided by cell volume). These files can obviously get quite large, so before recording, floating point variables are converted into four byte real numbers, and particle type and cell number are converted into single byte integers.

The individual particle tallies recorded by the TALLYX subroutine can then be post-processed, applying kerma factors and new source weights corresponding to any neutron and/or photon energy spectrum, angular distribution, and/or spatial distribution within the limits of the original master MCNP run.(5)

RESULTS AND DISCUSSION: The "ubertally" method was benchmarked against a normal MCNP simulation of equivalent source and geometry. Because the exact same calculations are made in each case, only in a different order, any differences are be due to the equilethargy biasing of the "ubertally" method.

A specific LBNL accelerator-based source was also simulated using both a normal, unbiased MCNP simulation and the "ubertally" method, to determine the effect

the biasing would have on the results. Dosage in small tally volumes along the centerline of the beam are shown in Fig. 2, along with the percent discrepancy between each value for each dose in Fig. 3. Doses were calculated using BMRR's treatment planning protocol.(1) As the relative error represents a single standard deviation in the expected solution, it is expected that approximately 63% of the error bars should overlap the origin. This appears to be the case, with the lowest agreement occuring in the hydrogen doses, especially at deep depths, where the dose approaches zero.

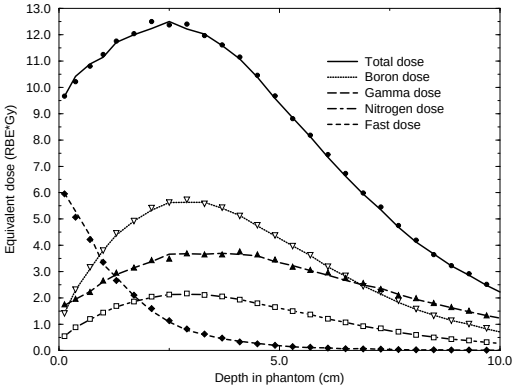

FIGURE 2. Comparison of depth-dose components for healthy tissue in an accelerator-produced neutron beam. Data points represent values generated by the "ubertally" method while the lines represent values of a normal MCNP run.

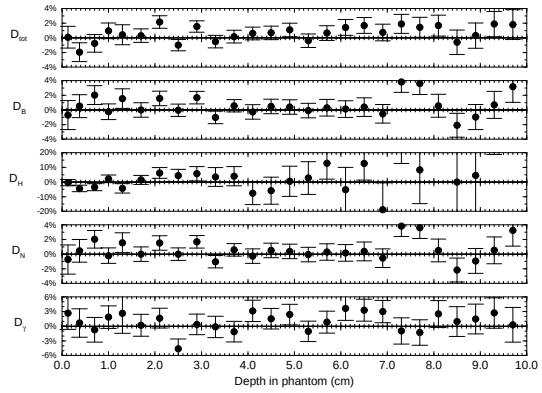

FIGURE 3. Percentage variations of depth-dose values from Fig. 2, with error bars representing one standard deviation statistical error, added in quadrature from each simulation.

The same study was conducted with the BMRR beam from Fig. 1, with simliar results. The agreement of the hydrogen dose, which is primarily dominated by fast (>10keV) neutrons undergoing proton-recoil collisions, was also not as good (about 50% error bar overlap). Because the BMRR beam has a larger fast dose component at deeper depths, this affected the total tissue dose more prominantly. Future use of the "ubertally" method should therefore benefit from additional biasing of higher energy neutrons to provide greater statistics for the hydrogen reaction.

These benchmark comparisons were conducted assuming no external photon beam. An external photon beam can be added, however, by an additional photon "ubertally" simulation, in which the results of both components of the beam are combined after post-processing. This was done for an optimization study to determine the best thickness of Fluental^{TM}(6) for neutrons created in the $^{7}Li(p,n)^{7}Be$ reaction with 2.4 MeV protons, and compared to the same optimization study using the INEEL treatment planning code, RTT.(7) Fig. 4 shows that the "ubertally" method produces the same results, though in minutes rather than hours or days and with much greater accuracy due to much larger particle sampling (fifty million neutrons and three hundred million photons versus two million of each particle in the RTT simulation).

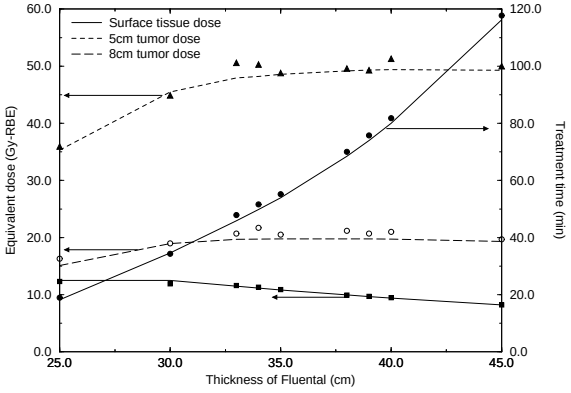

FIGURE 4. Optimization study using "ubertally" (lines) and RTT (data points).

While the "ubertally" method is a powerful tool in optimization studies for BNCT and other fields with variable sources, great care must be taken to ensure the results are reliable and errors are low. Results may be misleading as a single MCNP simulation is used for multiple sources and errors may become systematic. Sources with narrow energy, angle, and/or spatial distributions may be particularly suspect, since a great number of simulated particles may be discarded or given low weight.

The "ubertally" method will used in future studies to produce response functions to the changing of multiple variables in BNCT treatments, such as the energy spectra, angular distribution, spatial distribution, RBE, patient geometry, etc. Greater error analysis will be conducted to ensure the results of this method are reliable.

REFERENCES:

1. Coderre, J. A., et. al. *J. Neuro. Oncol.* **33**, pp. 93-104 (1997).
2. Bleuel, D. L., et. al. *Applications of Accelerators in Research and Industry*, Nov. 4-7, 1998, Denton, Texas, AIP Conference Proceedings **475** Vol. 2, pp. 1050-1055 (1999)
3. Bleuel, D. L., Donahue, R. J., Ludewigt, B. A., and Vujic, J., Proceedings of the 8th International Symposium on NCT for Cancer in La Jolla, CA, Sep. 13-18, 1998.
4. Yanch, J. C., Harling, O. K., *Radiation Research* **135**, pp. 131-145 (1993).
5. Bleuel, D. L., Donahue, R. J., Ludewigt, B. A., and Vujic, J., Proceedings of Monte Carlo 2000 Conference in Lisbon, Portugal, Oct. 23-26, 2000.
6. Auterinen, I., and Hiismaki, P., *Proceedings of the CLINCT BNCT Workshop*, TKK-F-A718, Helsinki, 14-24, 1993.
7. Nigg, D. W., Wheeler, F. J., Wessol, D. E., Capala, J., Chada, M., *J. Neuro-Oncol.*, **33**, pp. 93-104 (1997).