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PEREGRINE MONTE CARLO DOSE CALCULATIONS FOR RADIOTHERAPY USING CLINICALLY REALISTIC NEUTRON AND PROTON BEAMS

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Abstract

Lawrence Livermore National Laboratory (LLNL) has developed an all-particle Monte Carlo radiotherapy dose calculation code—PEREGRINE—for use in clinical radiation oncology. For PEREGRINE, we have assembled high-energy evaluated nuclear data bases; created radiation source characterization and sampling algorithms; and simulated and characterized clinical beams for treatment with photons, neutrons and protons. Spectra are available for the Harper Hospital (Detroit, U.S.A.) Be(d,n) neutron therapy beam, the National Accelerator Centre (NAC, Faure, S.A.) Be(p,n) neutron therapy beam and many of the operating modes of the Loma Linda University Medical Center (LLUMC, Loma Linda, USA) proton treatment center. These beam descriptions are being used in PEREGRINE for Monte Carlo dose calculations on clinical configurations for comparisons to measurements. The methods of defining and sampling the beam phase space characterizations are discussed. We show calculations using these clinical beams compared to measurements in homogeneous water phantoms. The state of PEREGRINE's high energy neutron and proton transport database, PCSL, is reviewed and the remaining issues involving nuclear data needs for PEREGRINE are addressed.

1 Introduction

PEREGRINE is an all-particle Monte Carlo radiation transport code developed specifically for the calculation of dose for radiation treatment of cancer. PEREGRINE calculates absorbed dose from clinical photon, neutron and proton therapy beams in complex treatment configurations. The goal of the PEREGRINE Monte Carlo Dose Calculation Project is to deliver the capability for accurate and fast Monte Carlo calculation of radiation therapy dose distributions for routine clinical use and for research into the efficacy of improved dose calculation. Such goals require an efficient method of sampling the radiation source that is a precise representation of the actual source is required. The PEREGRINE teletherapy source package—coupled with state-of-the-art Monte Carlo simulations of treatment heads—makes it possible to describe any teletherapy beam to the precision needed for highly accurate Monte Carlo dose calculations in complex clinical configurations. The accuracy of calculated dose from any radiation type depends on the quality of the atomic and nuclear data, the quality of the transport physics, the statistical accuracy of the requested calculation and, most importantly, the description of the external radiation source. This paper discusses the work-to-date on defining neutron and proton teletherapy sources for use in PEREGRINE.

2 Transport Physics in PEREGRINE

PEREGRINE performs dose calculation with fully-coupled radiation transport. Neutron transport uses a data-driven single-scatter Monte Carlo method with elastic (n,n) and non-elastic reactions (n,Xp) $(n,X\alpha)$ (n,Xd) $(n,X\gamma)$ (n,Xn). Heavy charged particle transport, e.g, p, d, t, ^{3}He, α, uses a class II condensed-history method. This includes continuous energy loss, energy straggling, and multiple scattering. For protons, non-elastic nuclear reactions are also included by use of the PCSL database [1]. Scatter and attenuation from beam modifiers are not yet implemented in PEREGRINE for neutrons or protons. This feature, under development, requires the installation of adequate cross sections for the necessary materials and development of fast methods of tracking radiation through dense materials in which dose information is not needed. Beam modifiers, such as blocks and apertures, are handled with trajectory ray tracing. All event trajectories that pass through solid material are removed from the beam. This technique serves to define the shape of the beam, even through complex apertures.

3 Nuclear Data Files

LLNL has worked together with LANL to assemble a special set of calculational nuclear data files for radiotherapy dose calculation extending to incident energies ≤ 250 MeV. These files gather data from a variety of sources, making considerable use of nuclear model calculations. The resulting transport data tables are referred to as the Production Cross Section Library (PCSL). PCSL contains transport data for photons, neutrons and charged particles: p, d, t, ^{3}He, α. The photon transport data (for $E_\gamma < 250$ MeV) is taken directly from the LLNL Evaluated Photon Data Library (EPDL) [3].

The charged-particle transport data are combined from four sources: LLNL's Evaluated Charged Particle Library (ECPL) [4] (for $E_{cp} < 20$ MeV); recent evaluations of charged particle production cross sections by Chadwick [5] [6] on ^{12}C, ^{14}N, ^{16}O, ^{31}P and ^{40}Ca; Arndt's SAID program [7] accessed on-line for calculating PP scattering cross sections; and Perkins' and Cullen's formalism for calculating large-angle coulomb PP scattering [8].

The neutron transport data are also taken from a combination of sources: LLNL's Evaluated Neutron Data Library (ENDL) [9] (for $E_n \leq 20$ MeV); recent evaluations of neutron production cross sections by Chadwick for neutrons on ^{12}C, ^{14}N, ^{16}O, ^{31}P and ^{40}Ca (for 20 MeV $< E_n <$ 250 MeV); and the SAID program for NP scattering cross sections > 20 MeV.

The nonelastic neutron and proton data for isotopes heavier than H are stored in the form of production cross sections. All nonelastic production reactions on each isotope are collapsed into a total nonelastic cross section with multiplicities for n, p, d, α, and γ secondaries. The assembled data are maintained in two forms: the Production Cross Section Library (PCSL) [1], stored in the ASCII ENDL format; and a set of binary PMCFyi transport data files, in the LLNL MCF format [10]. The transformation of the ENDL and ECPL data into production cross-section form required the development of a processing code system, PCS [11], to generate production cross-section tables from the reaction cross sections in the existing libraries and combine them with the extended data from Chadwick.

4 Source Characterization

PEREGRINE needs to know the following physical characteristics in the beam coordinate system for each Monte Carlo history to be tracked through the modifiers and dose mesh:

	The radiation type;
(x,y,z)	the starting coordinates;
(u,v,w)	the initial direction cosines with respect to (x,y,z) respectively;
(E)	the particle energy;
(W)	the relative sample weight.

To define a source for PEREGRINE, phase-space history files from Monte Carlo simulations are analyzed and separated into one or more components. In general, we define one direct (unscattered) component and one or more scattered components. Components of contaminant radiation can also be included, i.e., electrons in a photon beam. The direct components are assembled from simulation histories that can be tracked back to within a small distance from a main source—a spallation or bremsstrahlung target, for instance. The scattered component(s) describe the radiation that undergoes further scatter by beamline elements. Separating the scattered and unscattered components simplifies accurately describing and efficiently sampling the different subsources. Further details on the characterization models, sampling methods and treatment of treatment-specific beamline modifiers are given in references [12] and [13].

5 Neutron Beams

The University of Wisconsin-Madison and LLNL are working together to develop detailed phase-space descriptions of beamlines for three neutron therapy facilities: Harper Hospital Cyclotron (d(48.5) Be(48.5)); NAC (p(66) Be(40)); and Fermi National Accelerator Laboratory (FNAL) (p(66) Be(49)). This paper discusses the neutron phase-space analysis for the first two of these locations and represents an extension of work started by Ross [14].

The LAHET Code System [15] and MCNP [16] are being used together to simulate the neutron phase-space at these facilities. LAHET is used to generate neutrons from the charged-particle interaction in the target. *All* neutrons are passed to MCNP for transport through the target, precollimators, flattening filters, etc. A special, limited set of evaluated neutron cross sections for incident energies $\leq$ 100 MeV [17] is used with MCNP to enable tracking of all neutrons produced by the intranuclear cascade models in LAHET. Some materials present in the three beamlines are not available in this data set, but enough are present to approximate all important components. For missing materials, the closest available isotope or composition is used with the actual material density.

The Harper Hospital Cyclotron neutron source is modeled with all beamline components starting at the target down to the entrance of the field-shaping W multirod collimator. To date, 255,000 neutron histories have been generated representing ~1500 hours of CPU time. The image of the precollimation system is a 19cm×19cm rectangle at the entrance to the multirod collimator. This neutron phase space is described to PEREGRINE as a two component source. Figure 1 shows the energy spectrum and fluence distributions of direct neutrons at $z = 112.8$ cm downstream from the Be target. These distributions include only neutrons arriving at the collimator directly from the target without subsequent scatters. The analysis of the direct component assumes cylindrical symmetry and accounts for the area cropped by the square by assigning higher weight—based on the fraction of arc inside the square—to particles at radii greater than 9.5 cm but still within the precollimator image. In the simulation-history file, 91.5% of the total neutron energy within the limits of the pri-

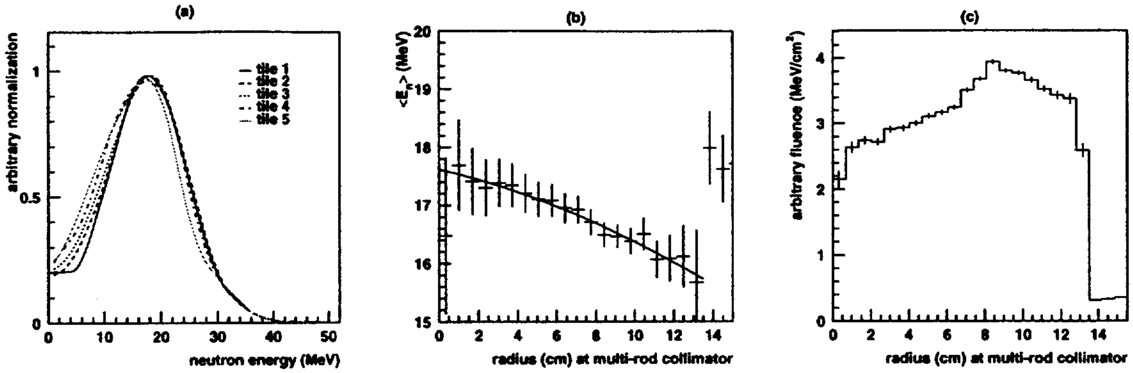

Figure 1: Harper Cyclotron direct neutron distribution at the entrance to the multirod collimator ($z = 112.8$ cm from the target). (a) Energy spectra for six radial annuli defined by the set $r = \{0.0, 2.7, 5.4, 8.1, 10.8, 13.5\text{ cm}\}$; (b) Average neutron energy vs. radius; (c) Total energy fluence vs. radius.

mary collimator system is in the form of direct neutrons. Neutrons scattered by the precollimators and/or flattening filter (8.5% of total energy) are described as a second component. This scattered neutron component has a lower average energy of ~13 MeV/neutron and an almost flat energy fluence. Currently ignored are all neutrons that arrive at the entrance to the multirod collimator outside the diagonal limit of the precollimation system ($r > 13.5$ cm). Neutrons, both direct and scattered, outside this limit will be blocked by the multirod collimator. In the absence of transmission or transport through the collimator, there is no need to include this portion of the fluence and it is ignored in the characterization.

The structure seen at small radii in the simulation-derived energy fluence—the hole in the very center and the notch at the fourth bin (Figure 1c)—is not seen in shallow dose-profile measurements. However, if these features are left in the PEREGRINE source description, they clearly show in calculated profiles, which points to a need for much higher statistics in the simulation-history file. Figure 1 shows a comparison between PEREGRINE calculations and measurements of neutron depth-dose and profiles. A smoothed fluence function was used in the calculation. Excellent agreement in depth-dose is seen to a depth of 15 cm, with a small, noticeable deviation at larger depth.

Simulation of the NAC neutron therapy beam and generation of a source description for PEREGRINE is in progress. Figure 3 shows the current understanding of the radial variation in neutron fluence and average energy at a plane located 35.25 cm downstream from

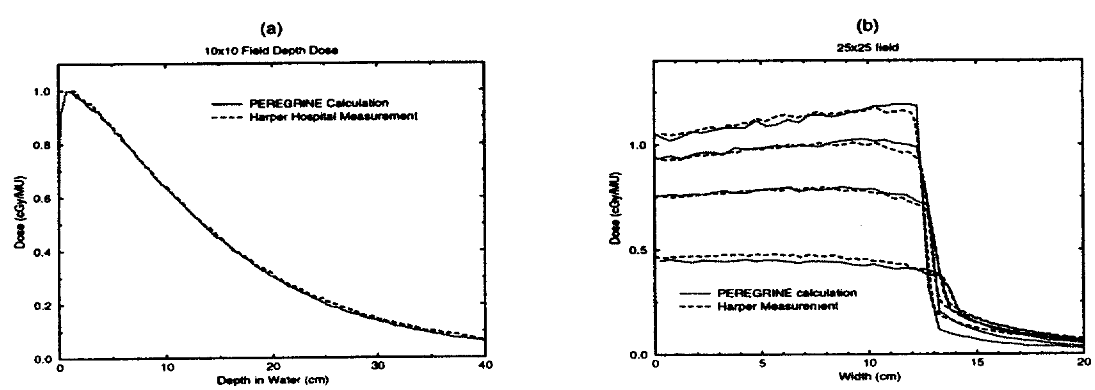

Figure 2: Harper Cyclotron neutron dose comparison between PEREGRINE calculations and measurements. (a) Depth-dose for 10×10 field; (b) 25×25 field profiles at depths of 1.2, 5.0, 10.0 and 20.0 cm (top to bottom).

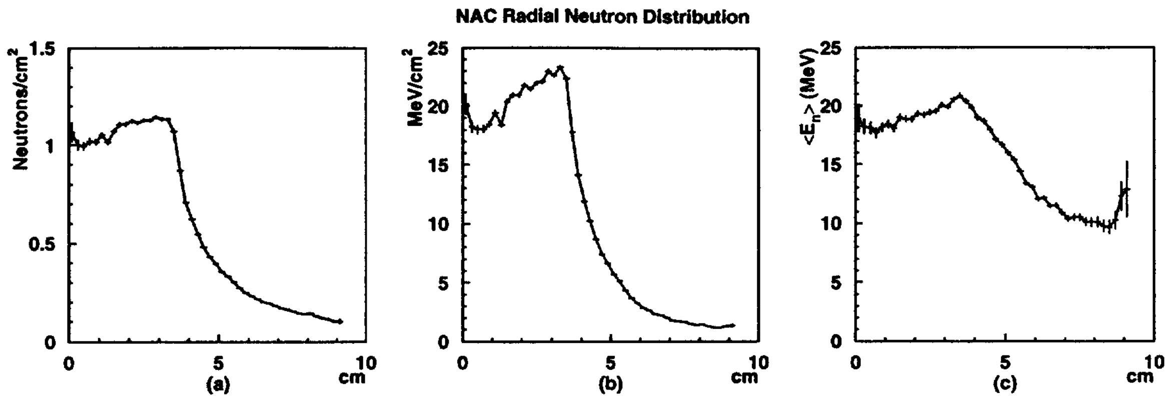

Figure 3: NAC radial neutron distributions at $z = 35.25$ cm. (a) neutrons/cm^2; (b) total energy/cm^2; (c) average neutron energy. Azimuthal symmetry is assumed in the analysis.

the Be target. This plane is just in front of the secondary, treatment-dependent collimation system, and after the precollimators and flattening filter assembly. Analysis of the beam for direct and scattered components is not yet complete, but the NAC beam appears to have a larger scattered component, as evidenced by the long tail outside the projected image of the precollimator image—3.5 cm radius at this z location. These results are preliminary pending clarification of some missing structural details on the precollimation system and comparison of calculations to measurements.

6 Proton Beams

Using LAHET [15] to simulate the proton accelerator and stationary components of the beam delivery head, LLUMC and LLNL are working to improving the understanding of the proton phase-space for all of the operating modes of the LLUMC proton treatment facility [18]. The goal of these investigations is to determine what improvements are needed in PEREGRINE to adequately handle beam modifiers such as blocks and compensators.

The version of LAHET in use is one modified by Siebers to use Landau-Vavilov energy straggling [19] in place of the default LAHET range straggling. The results of these simulations have been used to make source description files for use in PEREGRINE. Figure 4 shows a comparison of measurements and calculations of central axis depth-dose in water

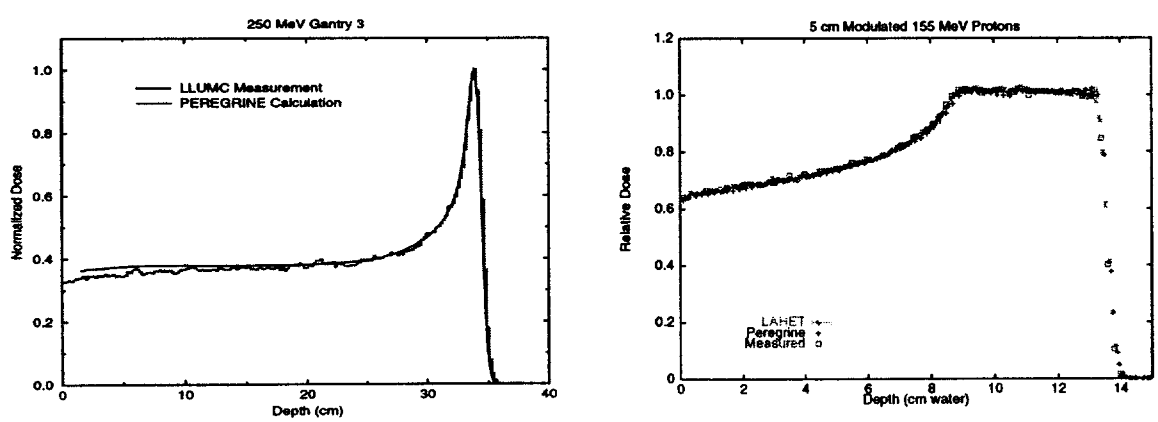

Figure 4: Relative proton depth-dose comparison of ion chamber measurement and PEREGRINE calculation are shown (a) for the 250 MeV LLUMC Gantry 3 beamline and (b) for a 5-cm range-modulated 155 MeV proton beam (includes LAHET calculation.)

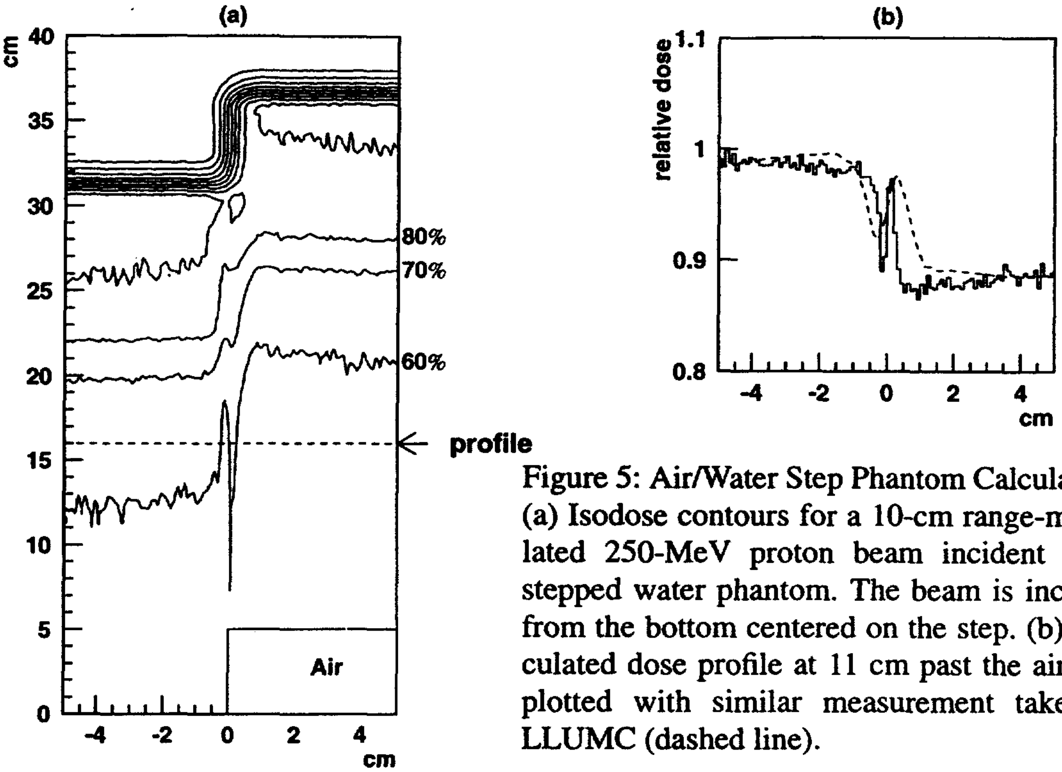

Figure 5: Air/Water Step Phantom Calculation. (a) Isodose contours for a 10-cm range-modulated 250-MeV proton beam incident on a stepped water phantom. The beam is incident from the bottom centered on the step. (b) Calculated dose profile at 11 cm past the air step plotted with similar measurement taken at LLUMC (dashed line).

for 250-MeV double-scattered protons and 5-cm range-modulated 155-MeV protons. A source file of approximately 1.6 million proton events was created for each configuration using the modified LAHET. The resulting sources were then used in LAHET and PEREGRINE to calculate depth-dose in configurations similar to those used for the measurements. The differences between LAHET and PEREGRINE are attributed to the absence of scatter off of apertures in PEREGRINE. As with neutrons, a lack of evaluated cross-section data for necessary materials has delayed the development of a full-physics modifier transport package in PEREGRINE for protons. For the LLUMC proton facility, charged particle interaction cross sections for energies up to 250 MeV are required. Neutron cross sections to the same energy are also needed for tracking of neutron secondaries.

Comparisons of dose profiles for various apertures and phantom configurations have been done. In general, calculations and measurements are in reasonable agreement. The current lack of aperture scatter affects the accuracy of the penumbra region of profile calculations, but field width and absolute profile height is accurately reproduced.

In addition to homogeneous comparisons, we are studying the effects of inhomogeneities in density or materials. These variations can cause distant effects in dose distributions, which are easily illustrated by introducing an air inhomogeneity in a water phantom. Figure 5 shows a PEREGRINE calculation of such a phantom compared to a similar, but not identical, ion-chamber measurement taken at LLUMC. The proton beam was incident parallel to and centered on the air step. The effect of the step is clearly visible in the measurement and the calculation.

7 Summary

The combination of data, modeling and measurements has enabled us to develop source descriptions that accurately and compactly describe all types of teletherapy sources. While this paper has concentrated on neutron and proton therapy beams, similar work has been done on bremsstrahlung photon therapy sources. The same descriptive models and analysis techniques do an excellent job of preserving important aspects of the different source types. In generating source descriptions for clinical use, it will be necessary to combine the simulations with measurements to "tune" the source description to match a set of site-specific measurements. Our experience with photon therapy sources leads us to expect excellent agreement for all field shapes and sizes with a single description that is properly adjusted to match such measurements.

Future directions will include the acquisition of reaction data for more materials, the development of accurate, fast models for handling treatment-specific modifier configurations and extensive comparison to clinical treatment planning dose calculation techniques.

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