

A fast Monte Carlo code for proton transport in radiation therapy based on MCNPX

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ABSTRACT

An important requirement for proton therapy is a software for dose calculation. Monte Carlo is the most accurate method for dose calculation, but it is very slow. In this work, a method is developed to improve the speed of dose calculation. The method is based on pre-generated tracks for particle transport. The MCNPX code has been used for generation of tracks. A set of data including the track of the particle was produced in each particular material (water, air, lung tissue, bone, and soft tissue). This code can transport protons in wide range of energies (up to 200 MeV for proton). The validity of the fast Monte Carlo (MC) code is evaluated with data MCNPX as a reference code. While analytical pencil beam algorithm transport shows great errors (up to 10%) near small high density heterogeneities, there was less than 2% deviation of MCNPX results in our dose calculation and isodose distribution. In terms of speed, the code runs 200 times faster than MCNPX. In the Fast MC code which is developed in this work, it takes the system less than 2 minutes to calculate dose for 10^6 particles in an Intel Core 2 Duo 2.66 GHZ desktop computer.

Key words: Monte Carlo, proton therapy, treatment planning

Introduction

There is currently a growing interest in using proton beam in radiation therapy because of the particular advantages of these heavy particles over photons and electrons.^[1] A major advantage of the proton beam is its relatively low energy deposition in the entrance region, the sharp rise in dose deposition (Bragg peak), and the rapid fall-off of dose at the end. These characteristics incorporate the basic role of radiation therapy which is to concentrate a high dose onto the target volume while minimizing any unnecessary radiation dose to the surrounding normal tissues.^[2-6]

For treatment planning in proton therapy, one needs an accurate dose calculation algorithm. In the early versions of dose calculation for protons, simple and fast methods such as pencil beam algorithm and analytical methods have been used.^[7-13] A general problem for these methods is the large discrepancies near the heterogeneities; however, because of their fast performance, they are currently used in treatment planning systems, especially for intensity modulated proton therapy.^[14-17]

For charged particles, the Monte Carlo (MC) methods generally produce the most accurate results. Most of the general purpose MC codes such as GEANT4,^[18] FLUKA,^[19,20] and MCNPX^[21] have capability of proton transport in clinical conditions and voxel-based phantoms. All these general purpose codes with careful choice of approximations produce accurate results for proton transport compared to experiments.^[22-28]

Review of fast MC codes for proton transport

The general purpose codes are very slow and not suitable for day-to-day clinical treatment planning systems. In recent years, few groups have developed fast MC engine for proton transport in treatment planning such as Fippel and Soukup (VMCpro 2004),^[29] Li *et al.*,^[30] and Tourovsky *et al.*^[31] Most of these codes have been developed from their early versions for electron transport.^[32-35]

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The fast MC code developed by Li *et al.*^[30] is based on track-repeating algorithm for proton beam. This code is an extension of MCSIM code,^[36] which uses pre-generated electron tracks for electron transport. For proton transport, the GEANT4 code is used to create the track of high energy protons in the middle of a large homogeneous water phantom, and tracks of 100000 protons with 250 MeV energy are transported. For each step in the proton track, the location, angle, energy, and deposited energy along the track were recorded for the primary protons and all secondary particles. The cutoff kinetic energy for all particles was 200 keV, and the size of the stored data for 100000 protons was 0.8 Gigabyte (GB).

This work is an extension of the fast MC code Pre-calculated Monte Carlo (PMC) for protons in which one uses pre-generated tracks for particle transport.^[28] The PMC code was initially developed for electron transport with capability of being used for other particles. The main difference between this code and other fast MC codes based on pre-generated tracks is that while the other codes generate the tracks for water and modify them for other materials, in the PMC code, the pre-generated data is collected for each particular material. This technique produces very accurate results near heterogeneities and makes the transport algorithm very simple, since all the physics is handled by a general purpose code. Another difference of the PMC code is that only the track of the primary protons is saved and not the track of the secondary protons as they are treated like a primary proton. This technique decreases the size of the pre-calculated data and makes it possible to generate tracks for various materials. In this work, MCNPX has been used as a reference and for generation of pre-calculated tracks in various materials and energies.

Materials and Methods

Concept of pre-calculated data

This method is based on using pre-generated and stored particle tracks. In this idea, all the possible cases of a particle in clinical range of the energy and materials are transported in MCNPX, and all of data are stored. In Fast Monte Carlo, this information is used and there is no need to calculate the physics of the particle; this saves a lot of time for calculation.

For transport of the proton, the pre-generated tracks were repeated, and the energy was deposited along the path in patient geometry built from CT data with voxel size varying between 2-4 mm. In all other materials such as lung tissue, bone, etc., the particle tracks in water are picked up and modified. The scattering angles were repeated for air and soft tissue, although they were adjusted properly for bone, based on the scattering power ratios. The particle step lengths were adjusted based on the density of various materials.

The pre-generated data were obtained by simulating protons with a kinetic energy of 250 MeV. It was necessary to determine where to start track repeating along the proton track if the kinetic energy of an incident proton in a realistic proton beam was lower than 250 MeV.

The fast proton MC code by Li *et al.* runs 13 times faster than the GEANT3 code for energies up to 250 MeV.^[30] The results of the code in homogeneous materials are generally in good agreement with the reference code within 2%. However, there exist relatively large discrepancies near the heterogeneities. The shift of the Bragg peak is handled properly, but the magnitude of the error is up to 10%. Errors of this magnitude are due to various approximation and modification of this code and re-usage of the proton tracks in water for other materials.^[30]

Generation of pre-calculated tracks for proton transport

The general purpose Monte Carlo code MCNPX^[37] is used for generation of the pre-calculated proton tracks. Tracks of 10000 primary protons were generated for various compounds and energies. The proton energy was 20, 40, ... 220, 240, 250 MeV with an energy cut-off of 200 keV. The protons are transported in the middle of a large homogeneous phantom with various materials such as water, lung tissue, bone, and soft tissue.

The ptrac routine of MCNPX writes the various events of each particle in an ASCII file in a particular format. The row format of ptrac file is complicated and very difficult to analyze for beginners; however, it contains the complete information of primary protons and all secondary particles.^[38-42]

An in-house Fortran code was developed to read and extract the needed information from the ptrac file. This code extracts the position, direction, energy, and deposited energy of a particle in each step. The code also extracts the characteristics of all secondary particles generated by primary protons. Post-processing of the data is required to handle the physics of the various secondary particles, as it is discussed in following sections. The track of a few protons and their secondaries are illustrated in Figure 1.

The composition of different materials is taken from ICRU 44 and given in Table 1.^[43] This material is used in MCNPX to fill up the homogeneous phantoms with different materials. Given is the density of materials: Soft tissue $\rho = 1.05 \text{ g/cm}^3$, lung tissue $\rho = 0.3 \text{ g/cm}^3$, and bone $\rho = 1.92 \text{ g/cm}^3$.

Physics of various secondary particles

Unlike electron and photons, protons produce many different secondary particles such as neutrons, deuterons, tritons, alphas, electrons, and secondary protons. From

other studies of MC codes for proton transport^[29,44-49] one can define three categories for handling secondary particles:

1- Secondary protons: They are treated like primary protons and explicitly transported in the PMC code using a track picked up from pre-calculated data. The energy fluence of secondary protons from primary 150 MeV protons in water is illustrated in Figure 2. This is extracted from a ptrac file of 200000 protons in MCNPX. The secondary protons have an energy range from zero to the energy of the primary particle. Therefore, they should be transported explicitly, and their energy cannot be deposited locally or neglected.

2- Neutrons: Since the energy of the neutron is deposited far from the initial point (as illustrated in Figure 1) and their contribution in total dose is less than 0.1%, they can be neglected. This assumption is verified by several groups,^[29,30,44] and it is the case for most of the fast MC codes for proton transport.

3- All other secondaries: Since other secondaries have a very short clinical range of energy and materials, their energy is deposited locally.

An important issue that illustrates the flexibility of the PMC code is that even if all the secondary particles have to be transported explicitly, one just needs to include the track of the particle in the pre-calculated data. This information is already available in ptrac file, and in this case instead of saving just the initial characteristics of secondary particles, the entire track of secondary should be saved in pre-calculated data.

Transport of protons

The initial characteristics of the incident proton, such as energy and position, are taken from the input phase-space

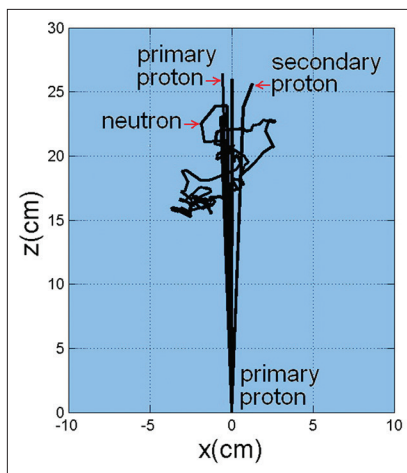


Figure 1: Tracks of few 200 MeV protons in a homogeneous water phantom and their secondary particles. The track information is extracted from the ptrac output file produced by MCNPX

file. One track and the related secondary particle information are picked up from pre-calculated data. After appropriate energy interpolation, the track is rotated and translated to the position of primary proton. In each step of the particle transport, the production of secondary particles is checked. If the secondary particle is a proton and its energy is larger than a user-defined cut-off, it is saved on the stack, otherwise the energy is deposited locally. The energy cut-off for all the simulations of this work is 200 keV. The higher cut-off of up to 500 keV has also given acceptable results in other fast MC code for proton.^[29]

If the particle reaches a new material in its path, according to the energy of the proton, a new track from a related material is picked up. For each voxel, the deposited dose is proportional to the fraction of the step inside the voxel. The pre-calculated track of the particle in the PMC code is saved in Cartesian coordinates (x, y, z) . In the case of new materials with different densities, such as lung tissue which have varying densities in CT-based phantoms, the entire track is scaled proportional to the inverse of density. When the track

Table 1: Composition of different materials (soft tissue, lung tissue, and bone) according to ICRU-44. The numbers are in fraction by weight

	<i>Soft tissue</i>	<i>Lung tissue</i>	<i>Bone</i>
Hydrogen	0.102000	0.103	0.034
Carbon	0.143000	0.105	0.155
Nitrogen	0.034000	0.031	0.042
Oxygen	0.708000	0.749	0.435
Sodium	0.002000	0.002	0.001
Magnesium	-	-	0.002
Phosphorus	0.003000	0.002	0.103
Sulfur	0.003000	0.003	0.003
Chlorine	0.002000	0.003	-
Potassium	0.003000	0.002	-
Calcium	-	-	0.225

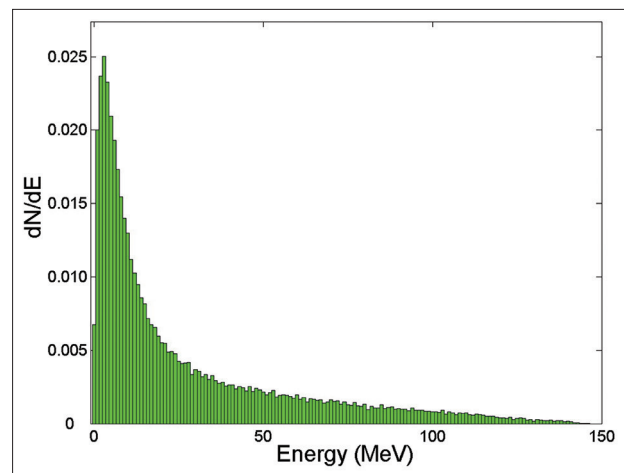


Figure 2: Energy fluence of secondary protons produced by 150 MeV protons in water. The spectrum is extracted from a ptrac file of a MCNPX run for 2×10^5 protons

of the primary particle is terminated, the secondary particles in stack are transported. The neutrons are neglected and the protons are transported one by one like primary proton and other secondary particles are deposited locally.

The energy interpolation could have various approaches. Given a 95 MeV particle a track with closest higher energy neighbor is picked up (i.e. 100 MeV) and within that track, we move down in energy until the step with an energy closest to 95 MeV is met. We then interpolate that step to the 95 MeV point, and the rest of the track is picked up for transport of the particle.

Physics models of MCNPX

In MCNPX, there is an option to choose various physics models through which the particles are transported.^[50-52] The default physics model for proton transport is the Vavilov model for charged-particle straggling,^[53] which is chosen for generation of pre-calculated data in this work. The other option in physics model is based on CSDA (Continuous Slowing Down Approximation) model and as a test the pre-calculated data is generated with this option of MCNPX. The result of 150 MeV protons in water phantom has been compared to MCNPX in Figure 3. In this figure, the PDD of the PMC code with the Vavilov model, the PMC code with CSDA model, and the MCNPX code (Vavilov model) are compared. The results of the PMC code with CSDA models represents generated very sharp peak with respect to the reference, MCNPX.

Other groups^[54,55] also have declared such sharp peaks with CSDA model in various homogeneous and heterogeneous mediums. Therefore, although the protons mostly travel through a straight line, the CSDA model is not an appropriate approach for proton transport in clinical range of energies.

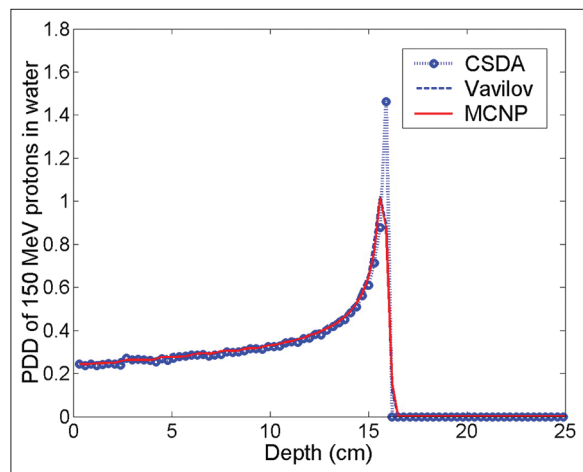


Figure 3: Comparison of the PMC code based on Vavilov model and CSDA model with MCNPX in water phantom. The energy of protons are 150 MeV and the field size is $10 \times 10 \text{ cm}^2$

Results and Discussion

Size of pre-calculated data

The ptrac file generated by MCNPX in ASCII format has a very large size since it contains all the detailed information of each step of the primary proton and all secondary particles. For example, the size of the ptrac file for 10000 protons with 200 MeV is 235 MB (Mega Bytes). Our in-house code to process the ptrac file, reads the file and deletes the header and converts it into a binary unformatted file which is 66 MB in the first step. In the second step, the code extracts the needed information (such as track of primary proton and initial parameters of secondary particle) from the file. Finally all the information is saved in unformatted file as an input for the PMC code and the size of file at this stage is 23 MB.

For a primary particle, in each step, the code saves five parameters: Position (x, y, z), energy of the particle in the beginning of the step, and deposited energy during the step. The initial characteristics of secondary particles such as particle type, position, direction, and energy are saved in a separate file. The total size of the pre-calculated library for each material is on the order of 100-200 MB. This compact size of the data is reached, since in pre-calculated data of the PMC code, the track of secondary particles is not saved.

Result of the code for homogeneous phantoms

For verification of the PMC code results, the MCNPX code version 2.5 is used as a reference. An important reminder for MCNPX run is that, in the default setting, the maximum energy of the code for all particles is 100 MeV. This number has to be changed manually in the input file of the code to highest possible energy of the problem (250 MeV in our case) otherwise the physics is wrong. The size of each voxel is 0.3 mm in each direction, and the size of the phantom is $21 \times 21 \times 30 \text{ cm}^3$.

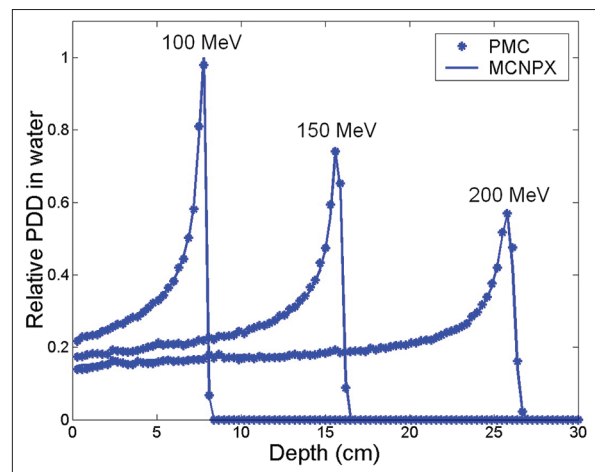


Figure 4: The relative PDD of monoenergetic protons in water phantom. The field size is $10 \times 10 \text{ cm}^2$ and the size of the voxel is $(3 \text{ mm})^3$

The comparison of the PMC code results with MCNPX for various energies in water is illustrated in Figure 4. A monoenergetic incident proton beam with an energy of 100, 150, and 200 MeV and a field size of $10 \times 10 \text{ cm}^2$ are used. All the field sizes are defined in the surface of the phantom and the incident particles are distributed uniformly in the surface. The graph represents the relative percentage depth dose (PDD) along the central axis. There is generally a very good agreement between the PMC code results, and the difference is in the order of 2%.

The PMC code results for various materials such as bone, lung tissue, and soft tissue are illustrated in Figure 5. There is generally a good agreement between the results with discrepancies up to 2.5%.

Result of the code for in-homogeneous material

Figure 6 illustrates an example of proton transport in heterogeneous phantom. This phantom contains water with a 4-cm slab of bone embedded at a depth of 3 cm. The

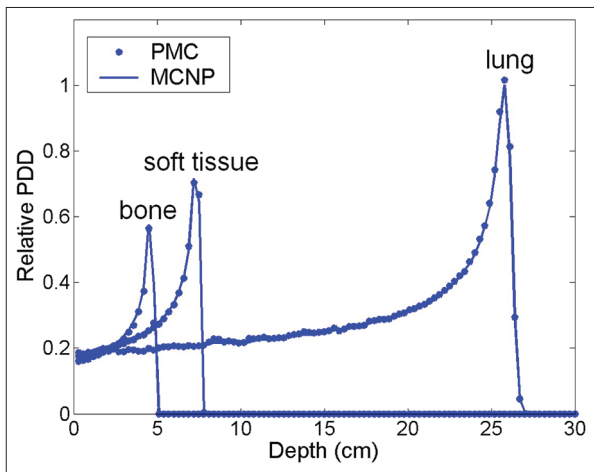


Figure 5: PDD of 100 MeV protons in various materials. The density of materials are 1.92, 1.06 and 0.3 g/cm³ for bone, soft tissue and lung tissue, respectively

field size in this case is $4 \times 4 \text{ cm}^2$ and the proton energy is 150 MeV. In this phantom, there are both higher to lower and lower to higher density interfaces. The comparison of PDD with MCNPX for the same geometry but with a lung slab is illustrated in Figure 7. An example of lateral dose profile for a bone and lung slab in water phantom is illustrated in Figures 8 and 9. The difference is between 2%-3%, and the shift of Bragg peak due to the slab of bone and lung is handled very accurately.

Time of calculations

Transport of 1 million protons with the PMC code takes approximately 60-100 s for various homogeneous and inhomogeneous materials. All the runs, including MCNPx runs, were done in a desktop computer with Intel Core 2 Duo 2.66 GHZ CPU.

In terms of speed, the PMC code for protons runs 200 times faster than MCNPX on the same computer. This

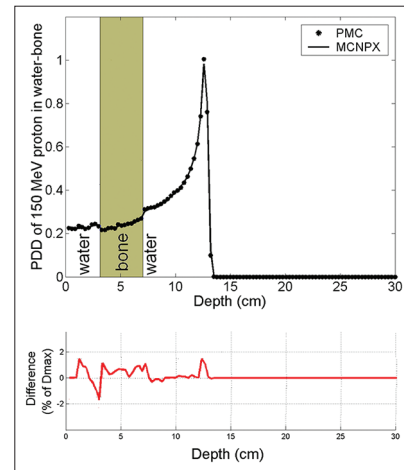


Figure 6: PDD of 150 MeV protons in the water phantom in which a 4 cm slab of bone is embedded. Figure (b) illustrates the lateral dose calculation for this phantom

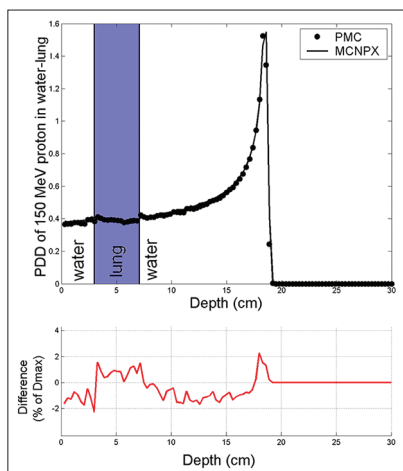


Figure 7: PDD of 150 MeV protons in water-lung phantom, and $4 \times 4 \text{ cm}^2$ field size

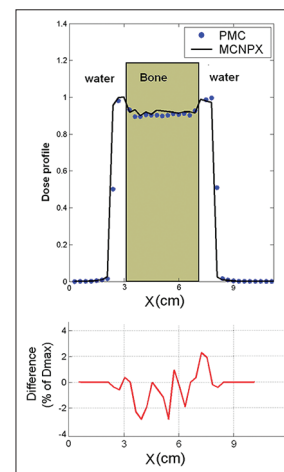


Figure 8: The comparison of dose lateral profile at the middle of the bone slab for $6 \times 6 \text{ cm}^2$ field size. The energy of the proton beam is 150 MeV and the profile is compared at depth of 2 cm

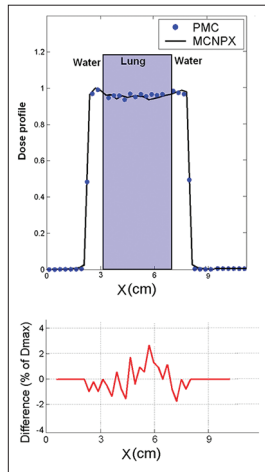


Figure 9: The comparison of dose lateral profile at the middle of the lung slab. The energy of the proton beam is 150 MeV and the profile is compared at depth of 2 cm

factor is reasonable considering the fact that MCNP is a relatively slow code.^[48] For electron transport, the code runs 40-60 times faster than EGSnrc.^[28]

Result of dose calculation in a CT-based phantom

The PMC code has been employed for proton transport in a CT-based head. The head contains various materials such as soft tissues, bones, and air cavity. The density of each voxel is determined after appropriate calibration using Hounsfield numbers.^[48] Hounsfield numbers are closely related to attenuation coefficients that range from -1000 (air) to $+1000$ (dense bone or tooth enamel). CT uses water as its standard value, and it is assigned a Hounsfield number of 0.^[48]

The input for the PMC code is a 3D matrix of real numbers related to the density of each voxel. In a typical phantom, we may have different materials with various densities. For example, bone density may vary from 1.6 g/cm^3 to 3 g/cm^3 . For proton transport in one material with various densities as mentioned in Section 3.5, the pre-calculated track is scaled using the density of each voxel on the fly. The image of the head and related isodoses are illustrated in Figure 10. The resolution of the phantom is 2 mm^3 . The isodose curves represent the dose distribution of 100 MeV protons incident on $5 \times 5 \text{ cm}^2$ field size. The effect of the air cavities and bony structures on the isodose curves is handled properly and can be observed.

Advantages and limitations

The most important advantage of using pre-calculated data from a general purpose MC code is the accuracy of the results. It is mentioned before other fast MC codes for proton have up to 10% errors in heterogeneous materials.^[36] The accuracy of this method is due to the fact that when, for example, during the transport of a particle in a tissue if we come to a boundary of a new material, bone, we do not modify the track of the particle in tissue for bone transport;

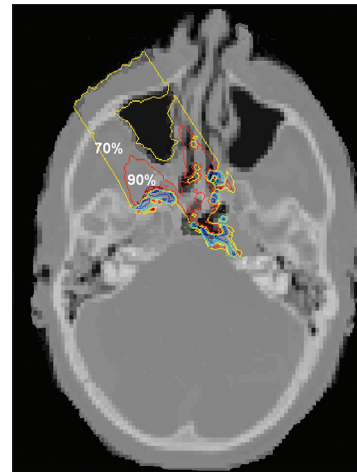


Figure 10: Dose distribution in the patient's head irradiated with 100 MeV protons. The field size is $5 \times 5 \text{ cm}^2$ and the resolution of the voxels is 2 mm in each dimension

a new track is picked up from the pre-calculated tracks of bone.

On the other hand the large size of the pre-calculated data, in the range of the 1 GB, makes some limitations in application. For parallel processing, the code needs huge amount of RAM for each core. The load of the data on the RAM for itself for the first run takes some time; however, this task is done once for all runs as long as the computer is not turned off. Because of the large amount of data, it is not possible to run the codes in a graphics processing unit (GPU) that has very fast calculation times as well.

Conclusions

The fast MC code, PMC has been developed for proton particle. The pre-calculated data is generated by the general purpose MC code, MCNPX. The major difference between the PMC code and other fast MC codes based on pre-generated data is that the pre-generated data is calculated for each particular material; therefore, all the physics is calculated by the general purpose code. This fact makes the physical calculation of the code very simple especially for proton particles since there are many different types of secondary particles that are produced. The pre-calculated data contains tracks of 10000 protons for various energies and materials and the size of the pre-calculated data is in the order of 100 MB for each material with the size of the entire data being as high as 1 GB. The PMC code generally produced accurate results, and the transport of protons near the heterogeneities was performed accurately.

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