Research on Hybrid Methods for Variance Reduction in Monte Carlo Dose Calculation of BNCT

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Abstract

Background: Boron Neutron Capture Therapy (BNCT) is a neutron-targeted radiotherapy method for treating cancer. Before radiation therapy, various dose parameters within the patient' s body need to be calculated using a neutron photon dose solver based on parameters such as the patient' s geometric model and neutron source terms, in order to develop an appropriate treatment plan. Purpose: Due to the complexity of neutron-material interactions, most BNCT treatment planning systems utilize dose solvers based on the Monte Carlo method. The Monte Carlo method is a probabilistic statistical method, and thus the statistical variance exists. In BNCT dose calculations, it is necessary to obtain calculation results with as small variance as possible within a limited amount of time in order to develop better treatment plans and ensure the safety and effectiveness of the treatment process. Methods: Therefore, in this study, the Monte Carlo code NECP-MCX was combined with a deterministic code, and the classic hybrid method, the CADIS method was improved to meet the specific requirements of BNCT calculations. Results: To evaluate the effectiveness of the improved BNCT-based Monte Carlo–deterministic coupling variance reduction method, dose-depth curves and Dose and Volume Histogram (DVH) were calculated using a realistic head model. These results were then compared with those obtained from direct calculations. Conclusions: The preliminary findings demonstrate that the proposed method is effective in reducing the relative standard deviation (RSD) and enhancing the computational accuracy in BNCT simulations.

Full Text

Preamble

Research on Hybrid Methods for Variance Reduction in Monte Carlo Dose Calculation of BNCT

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Purpose: Due to the complexity of neutron-material interactions, most BNCT treatment planning systems utilize dose solvers based on the Monte Carlo method. The Monte Carlo method is a probabilistic statistical method, and thus statistical variance exists. In BNCT dose calculations, it is necessary to obtain calculation results with as small variance as possible within a limited amount of time in order to develop better treatment plans and ensure the safety and effectiveness of the treatment process.

Methods: Therefore, in this study, the Monte Carlo code NECP-MCX was combined with a deterministic code, and the classic hybrid method, the CADIS method, was improved to meet the specific requirements of BNCT calculations.

Results: To evaluate the effectiveness of the improved BNCT-based Monte Carlo–deterministic coupling variance reduction method, dose-depth curves and Dose-Volume Histogram (DVH) were calculated using a realistic head model. These results were then compared with those obtained from direct calculations.

Conclusions: The preliminary findings demonstrate that the proposed method is effective in reducing the relative standard deviation (RSD) and enhancing the computational accuracy in BNCT simulations.

Keywords: BNCT; CADIS; dose calculation; Monte Carlo

1. Introduction

Boron Neutron Capture Therapy (BNCT) is characterized by its targeting of tumor cells while having minimal impact on normal tissue cells, and it has been extensively studied both domestically and internationally. In recent years, with the resolution of a series of issues such as accelerator neutron sources and boron

drugs, related research has entered a stage of rapid development [**?**]. Before BNCT treatment, it is necessary to calculate the dose distribution within the patient' s body based on the patient' s geometric model, material distribution, source term, and other relevant information. This calculation enables the formulation of the most appropriate treatment plan, which is the role of the Treatment Planning System (TPS). Currently, the computational cores used in most BNCT treatment planning systems worldwide are Monte Carlo programs. For example, NCTPlan [**?**] and JCDS [**?**] employ MCNP [**?**] to calculate the neutron and photon dose; SERA [**?**] uses SeraMC, which was developed by INEEL specifically for BNCT treatment planning and implements a fast geometry-tracking Monte Carlo method based on Univels. Univel is the uniform volume unit in the SERA model reconstruction technique. This model can operate independently of medical image, with its resolution only limited to the original medical image, exhibiting a high degree of accuracy. Furthermore, the fast geometric ray tracing method enables SERA to avoid calculating the intersection points between ray track and material interfaces. As a result, the computational efficiency of SERA is improved by a factor of 5-10 compared to traditional Monte Carlo method; TsukubaPlan [**?**] utilizes PHITS [**?**] as its solver core, which in addition to neutrons and photons, can simulate the transport of protons and heavy ions with particle energies up to 1 TeV.

NeuMANTA [**?**] developed by NEUBORON employs the independently developed Monte Carlo transport code COMPASS [**?**], which is specifically designed for BNCT dose calculation. To improve computational efficiency, COMPASS adopts a simplified voxel geometry, divides continuous neutron energies into multiple groups indexed by a hash table, and uses a well-organized HDF5 cross-section database to model neutron transport with complex cross-section structures. However, to date, none of these dose calculation cores have incorporated variance reduction techniques. This limitation mainly manifests in the following aspects:

The Monte Carlo method requires simulating a large number of particles at the tally locations to achieve convergence of the results. In BNCT treatment, the neutron source spectrum used for patient irradiation is an epithermal neutron spectrum, which has relatively low penetration capability. Consequently, neutrons have difficulty reaching regions far from the source. When the number of simulated particles is insufficient, the statistical results in these regions often fail to converge, resulting in unreliable numerical instability.

In BNCT treatment, it is essential to understand the dose distribution produced by the neutron source throughout all regions of the patient' s body, including both the tumor and the organs at risk (OAR). Therefore, accurate dose calculations are required for the entire body. The simplest method to improve calculation accuracy of the Monte Carlo method is to increase the number of simulated particles. However, this approach inevitably leads to longer computation times. In practical BNCT treatments, the time available for dose calculation within the Treatment Planning System is limited, often constrained to only a few hours.

The TPS is required to compute multiple dose distributions within a limited timeframe in order to select the optimal treatment plan.

Therefore, it is not feasible to simply increase the number of particles simulated in a single calculation. Instead, the goal is to improve calculation accuracy within the same or even shorter computation time.

Currently, various variance reduction techniques for the Monte Carlo method have been developed, including weight windows, source biasing, geometric splitting and roulette wheel selection [**?**], as well as the Consistent Adjoint Driven Importance Sampling (CADIS) [**?**] method based on the adjoint flux. The CADIS method, which hybridizes the Monte Carlo and deterministic approaches, has been implemented in the independently developed NECP-MCX [**?**] code in our laboratory. This study aims to build upon the CADIS methodology by improving and upgrading it for fine voxel models derived from human medical imaging, in order to address the low-count, high-variance problem encountered by conventional Monte Carlo methods in BNCT dose calculations.

2. Methods and Code Development

A commonly used variance reduction technique in the Monte Carlo method is the weight window. The principle of this method is to divide the model region into multiple rectangular grids, with each grid assigned three weight parameters: weight window upper bound, weight window lower bound, and survival weight. When a particle enters a weight window grid, its weight is compared with the weight window parameters to determine whether the particle should be split (if its weight exceeds the upper bound) or subjected to Russian Roulette (if its weight falls below the lower bound). This method effectively guides particle transport toward regions of higher importance, increasing the number of simulated particles in those areas and thereby reducing the overall variance.

For complex problems, it is difficult to empirically define appropriate weight windows. The purpose of coupling the Monte Carlo method with deterministic methods is to automatically generate optimal weight windows. This approach is based on the adjoint flux obtained from the adjoint transport equation.

In Monte Carlo calculations, the target response quantity can be expressed by integrating the product of particle flux and response function over phase space. Based on the relationship between the adjoint transport equation and the forward transport equation, by defining the adjoint source as the response function, the target response quantity can be regarded as the result obtained by weighting the source term with the adjoint flux in the phase space. Therefore, the adjoint flux can be regarded as an importance measure in phase space for Monte Carlo simulation.

Using the adjoint flux to set the weight window parameters, the weight window lower bound is inversely proportional to the magnitude of the adjoint flux. Cor-

respondingly, the survival weight and the weight window upper bound are also determined based on the adjoint flux distribution.

Since the adjoint flux is derived based on the adjoint source, the importance function represents the contribution to the response at the location of the adjoint source. Therefore, the aforementioned method effectively reduces variance for the response at the adjoint source position.

However, for BNCT dose calculation, it is necessary to optimize the tallying across all regions of the model. According to the aforementioned theory, the adjoint source region can be set as the entire model. However, since the variance differs across regions, setting the same adjoint source for all regions does not eliminate the relative differences between them. Therefore, it is necessary to differentiate the source strength of the adjoint sources in different regions with different variance characteristics. The specific approach involves first performing a preliminary forward calculation, which does not require high accuracy but only needs to distinguish the flux levels across different regions. Then, the adjoint source is weighted using this preliminary flux distribution. Under the influence of the weight window, neutrons will transport a greater number of particles to regions with larger importance and larger variances, while reducing the number of particles in regions with relatively lower importance. This balances the number of particles simulated across different regions, thereby improving computational efficiency to a certain extent.

In the aforementioned theory, forward and adjoint calculations are required to generate the importance parameters of the response quantity. Since these importance parameters are primarily used to guide the sampling and transport process for variance reduction, a deterministic method with faster computational speed can be employed. The accurate Monte Carlo method is then used in the final formal calculation. This approach is referred to as the Monte Carlo-Deterministic Coupled Variance Reduction Method, hereinafter abbreviated as the hybrid method.

The research presented in this paper focuses on the specific application of the aforementioned hybrid method in the context of BNCT dose calculation. Based on the theories discussed previously, this study presents specific customized methods for BNCT dose calculation. The function was developed based on the in-house NECP-MCX code owned by our laboratory. The enhancements encompass the following aspects:

(1) The human models required for dose calculation in BNCT are typically obtained through imaging modalities in hospitals, such as CT, PET, and MRI. These devices generate medical imaging files in DICOM format, which store human model information in a grid-like manner, commonly referred to as a voxel model. For example, in CT, each voxel contains different Hounsfield Unit [**?**] (HU) values, which are closely related to the composition of the materials. Accurate generation of voxel models from DICOM files is critical for BNCT calculations. Therefore, a function for

reading DICOM files and converting them into voxel models has been developed in NECP-MCX. The conversion method is based on Report ICRU46 [**?**], wherein the range of HU is discretized into 24 intervals. For each interval, an interpolation is conducted to determine a specific material density. Ultimately, each voxel' s material is mapped according to the specific HU values present in the DICOM file, resulting in the formation of the voxel model.

(2) Traditional Monte Carlo algorithms for computation employ Constructive Solid Geometry (CSG) models. The process of constructing CSG models involves the following steps: first, various surfaces of different shapes are created, and then a series of Boolean operations are applied to these surfaces to obtain a diverse array of models. CSG models provide high geometric accuracy and can theoretically represent arbitrary shapes. However, particle transport calculations within CSG models require complex surface-crossing computations. In contrast, voxel models consist of relatively simple and regular structured grids, which simplify the surface-crossing calculations during transport simulations. To accelerate BNCT dose calculations, optimizations of the surface-crossing algorithm have been implemented in NECP-MCX [**?**].

(3) In the hybrid method, variance reduction for a specific region requires defining a corresponding adjoint source region. In BNCT dose calculation, the primary focus is on the Gross Tumor Volume (GTV) as well as the dose levels and distributions in various OAR, collectively referred to as regions of interest (ROI). These ROI are stored in DICOM files as contour points. To accommodate the requirements of the hybrid method, a function for automatically constructing ROI models from DICOM files was developed within NECP-MCX. As shown in the left image of Figure 1 [Figure 1: see original paper], the ROI is stored in the DICOM file in the form of contour points. NECP-MCX reconstructs the ROI model by utilizing these points along with a polygon filling function, as shown in the right image of Figure 1. This facilitates the targeted definition of adjoint source regions for the hybrid method and enables convenient output of dose information related to the ROI, including dose levels, distributions, and Dose-Volume Histogram (DVH).

(4) For the global variance reduction hybrid method, it is necessary to employ a deterministic code for the computation of the forward transport equation. The deterministic code utilized in this study is NECP-Hydra with independent intellectual property rights, which employs the Sn method (discrete ordinates method) to solve the three-dimensional neutron transport equation. Since traditional deterministic codes are primarily designed for reactor criticality problems, they can only solve neutron transport equations with isotropic source terms. For BNCT calculations, the sources are primarily unidirectional; therefore, it is necessary to develop the capability to solve the neutron transport equation with unidirectional sources within

the deterministic code. In this study, the unidirectional source calculation capability was implemented in NECP-Hydra by modifying the quadrature sets, thereby enabling NECP-Hydra to accommodate the requirements of unidirectional source calculations and hybrid method in BNCT. Deterministic program calculations require the utilization of a pre-established multigroup cross sections library for computation. Traditional multigroup cross sections are typically employed for reactor-related problems, and their energy group structure is not suitable for the requirements of BNCT calculations. Therefore, this study has reformulated the multigroup cross sections library to meet the specific needs of BNCT calculations.

In summary, the fundamental process of calculating BNCT dose using the NECP-MCX hybrid method is illustrated in Figure 2 [Figure 2: see original paper].

3. Numerical Results

This study employs the NECP-MCX hybrid method to calculate two different voxel models and analyze the absorbed doses of four different dose types, relative standard deviation (RSD), and the Figure of Merit (FOM). The medical imaging data were obtained from The First Affiliated Hospital of Xi' an Jiao Tong University, with patient names and other identifying information anonymized. The absorbed dose is calculated based on energy deposition. The RSD quantifies the numerical convergence of the Monte Carlo simulation results; a smaller RSD indicates lower statistical uncertainty in results. The FOM evaluates [**?**] the computational efficiency of the Monte Carlo simulations. As defined in Equation (10), the FOM represents the ability to achieve a smaller RSD in less computational time; therefore, a relatively higher FOM corresponds to greater computational efficiency. Dose-depth curves and DVH for ROI were generated based on the results. These outcomes were then compared with those obtained from direct Monte Carlo calculations without the hybrid method to validate the variance reduction and optimization effects of the hybrid method in BNCT dose calculation. To ensure comparability, both methods employed Intel(R) Xeon(R) CPU E5-2670 v3, utilizing 2 nodes and a total of 128 cores for parallel computation. Additionally, to visually demonstrate the effectiveness of the hybrid method in reducing RSD, the computation times for both methods were kept approximately equal.

3.1.1 Computational Parameters

The voxel model 1 consists of a grid of 512 × 512 × 69 voxels, with overall dimensions of 30 cm × 30 cm × 20.4 cm. The locations of the GTV and OAR are illustrated in Figure 3 [Figure 3: see original paper]. The red region represents the GTV, while other regions represent OARs. In order to simulate the actual computational scenario for BNCT, the boron concentration in the GTV region is set as 70 ppm, while the concentration in the surrounding tissue regions is 20 ppm. The source term is a neutron surface source with a radius

of 5 cm, positioned directly on the upper surface of the head, with the GTV located beneath it. The emission direction is oriented along the negative z-axis, and the energy spectrum utilizes the actual exit source distribution following collimation through a Beam Shaping Assembly (BSA) [**?**]. The position of the source term is indicated by the circular plane in Figure 3.

3.1.2 Computational Results

The distribution of the forward flux and adjoint flux calculated by the deterministic program NECP-Hydra is illustrated in Figure 4 [Figure 4: see original paper], where a distinct unidirectionality of the forward flux is evident.

Based on the calculation results, the overall improvement in the FOM was first evaluated for all voxel grids. Since BNCT primarily focuses on the dose generated within the human body, to avoid the influence of doses outside the body on the statistical results and conclusions, only the voxel grids within the human body were included in the analysis. The statistical results are summarized in Table 1 . The hybrid method improves the computational efficiency of over 96% of the voxel grids for all four dose types. Except for the photon dose, the FOM for the other dose types shows a maximum increase of 5176.74-fold and an average improvement of 147.41-fold, indicating a significant enhancement. In contrast, the photon dose exhibits a maximum FOM increase of 5.01-fold and an average improvement of 1.29-fold, reflecting a less pronounced enhancement. This is attributed to the fact that the photon dose is indirectly generated through the (n, γ) reaction, which does not fully conform to the theoretical framework of the hybrid method. Moreover, due to the high penetration ability of photons, they can reach nearly all regions within the human body. The RSD of the photon dose is already sufficiently low compared to that of neutron doses.

Then, the overall spatial distribution of the variance reduction effect of the hybrid method was analyzed by calculating the average dose and average RSD within a series of grids below the source term, producing dose-depth curves as illustrated in Figures 5, 6, 7, and 8. The blue curve in the figures represents the results obtained from direct Monte Carlo calculations without the hybrid method, while the red curve corresponds to the results computed using the hybrid method. Aside from the photon dose, the remaining doses utilize the hybrid method to achieve a uniform reduction in global RSD, thereby enhancing computational efficiency. The extent of this enhancement is proportional to depth, as the directly computed RSD in shallower regions is already sufficiently small. For photon dose, the hybrid method can achieve a proportional reduction of RSD at different locations.

Finally, the impact of the hybrid method on dose calculation within local ROI was specifically analyzed. The average dose, average RSD, and average FOM for the ROI were calculated, along with the dose deviation and the fold increase in FOM, as presented in Tables 2, 3, 4, and 5. The tables show that, except for the photon dose, the FOM of the other dose types exhibits varying degrees

of improvement across different ROI, consistent with the results of the dose-depth curves. The maximum enhancement in computational efficiency reaches up to 276.91-fold. The FOM improvement for photon dose calculations is relatively uniform across different ROI. These results demonstrate that the hybrid method effectively improves the computational efficiency within ROI. Finally, DVH for different ROI and dose types were generated. In Figures 9, 10, 11, and 12, the curves represent the DVH obtained by the hybrid method, while the scatter points correspond to those from direct calculations. The close agreement between curves and scatter points confirms the accuracy of the calculation results.

3.2.1 Computational Parameters

The voxel model 2 consists of a grid of 512 × 512 × 73 voxels, with overall dimensions of 30 cm × 30 cm × 21.6 cm. The locations of the GTV and OAR are illustrated in Figure 13 [Figure 13: see original paper]. The red region represents the GTV, while other regions represent OARs. The boron concentration in the GTV region is set at 70 ppm, while the concentration in the surrounding tissue regions is 20 ppm. The source term is a neutron surface source with a radius of 5 cm, positioned directly on the upper surface of the head, with the GTV located beneath it. The emission direction is oriented along the negative z-axis, and the energy spectrum utilizes the actual exit source distribution following collimation through a BSA. The position of the source term is indicated by the circular plane in Figure 13.

3.2.2 Computational Results

The distribution of the forward flux and adjoint flux calculated by the deterministic program NECP-Hydra is illustrated in Figure 14 [Figure 14: see original paper], where a distinct unidirectionality of the forward flux is evident.

Similar to voxel model 1, based on the calculation results, the overall FOM improvement for the four dose types across the entire voxel grid was first evaluated. As shown in Table 6 , the hybrid method improves the computational efficiency of over 97% of the voxel grids for all four dose types. Except for the photon dose, the FOM for the other dose types exhibits a maximum increase of 4338.60-fold and an average improvement of 168.42-fold. The photon dose shows a maximum FOM increase of 12.76-fold and an average improvement of 1.89-fold.

Subsequently, the overall spatial distribution of the variance reduction effect achieved by the hybrid method was analyzed by generating dose-depth curves, as shown in Figures 15, 16, 17, and 18. The blue curve in the figures represents the results obtained from direct calculations, while the red curve corresponds to the results computed using the hybrid method. The observed phenomena are consistent with those in voxel model 1.

Finally, the impact of the hybrid method on dose calculation within local ROI

was specifically analyzed. The statistical results are presented in Tables 7, 8, 9, and 10. The tables indicate that, except for the photon dose, the computational efficiency within ROI can be improved by up to 243.86-fold. The FOM improvement for photon dose calculations is relatively uniform across different ROI. DVH for different ROI are shown in Figures 19, 20, 21, and 22.

4. Conclusion

In this study, we applied the Monte Carlo-deterministic hybrid method to BNCT dose calculation and constructed test cases to validate its effectiveness. The results demonstrate that the hybrid method significantly improves the efficiency of calculating boron neutron dose, achieving maximum speedups of 5165.74-fold and 4189.45-fold, and average speedups of 139.31-fold and 155.30-fold for the two voxel models, respectively. Similar efficiency improvements were observed for thermal neutron dose and total neutron dose calculations. For photon dose calculations, the method achieved maximum speedups of 5.01-fold and 12.76-fold, with average improvements of 1.29-fold and 1.89-fold, respectively. Additionally, dose calculations within different ROI were analyzed, showing that the hybrid method markedly enhances computational efficiency across ROI, with maximum speedups of 275.85-fold and 227.35-fold for boron neutron dose in the two voxel models. In summary, these results confirm the effectiveness of the Monte Carlo-Deterministic hybrid Variance Reduction Method for BNCT dose calculation.

Author Contribution Statement
Bojin Zhao: Conceptualization, Investigation, Methodology, Software, Validation, Formal Analysis, Writing-Original Draft; Qi Zheng: Conceptualization, Funding Acquisition, Project Administration, Supervision, Writing-Review & Editing; Qingming He: Supervision, Writing -Review & Editing; Liangzhi Cao: Supervision, Writing -Review & Editing; Tiejun Zu: Funding acquisition; Yongping Wang: Funding acquisition.

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Conflict of Interest Statement
The authors have no relevant conflicts of interest to disclose.

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Figure Captions:

Figure 1. Schematic illustration of ROI model construction by NECP-MCX (left: contour points of the ROI; right: ROI model).

Figure 2. The process of calculating BNCT dose using the NECP-MCX hybrid method.

Figure 3. Schematic diagram of voxel model 1. (The left image illustrates a schematic diagram of the head, while the right image depicts the schematic representations of the GTV and OAR.)

Figure 4. Schematic diagram of the forward flux and adjoint flux calculated by NECP-Hydra (left: forward flux; right: adjoint flux).

Figure 5. Comparison of Boron Neutron Dose Depth Curves (Left: Dose Mean Comparison; Right: RSD Comparison).

Figure 6. Comparison of Thermal Neutron Dose Depth Curves (Left: Dose Mean Comparison; Right: RSD Comparison).

Figure 7. Comparison of Total Neutron Dose Depth Curves (Left: Dose Mean Comparison; Right: RSD Comparison).

Figure 8. Comparison of Photon Dose Depth Curves (Left: Dose Mean Comparison; Right: RSD Comparison).

Note: Figure translations are in progress. See original paper for figures.