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Development of a GPU-Accelerated Continuous-Energy Monte Carlo Method for BNCT dose calculation

Yuxin Wang[1], Zirui Ye[1], Meitong Wei[1], Xi Pei[2]
Xie George Xu[1*]
1. University of Science and Technology of China, China
2. Anhui Wisdom Technology Co., Ltd., China

ABSTRACT

Purpose: Accurate and efficient dose calculation remains a major challenge in boron neutron capture therapy (BNCT) due to the complexity of neutron transport and the contribution of secondary particles. Conventional Monte Carlo (MC) methods are often too computationally demanding for routine clinical use. This study aims to develop and validate a GPU-accelerated, continuous-energy MC method for BNCT dose calculation with improved computational efficiency while maintaining accuracy.

Methods: A GPU-accelerated continuous-energy MC neutron transport code, ARCHER-Neutron , was developed for BNCT dose calculation. Neutron transport physics and nuclear data were implemented based on Geant4 11.4.0 (physics list: QGSP_BIC_AllHPT), including elastic scattering, inelastic scattering, and capture, while thermal neutron scattering below 4 eV was modeled using the S(α,β) formalism. To improve GPU efficiency, neutron cross-section data were reorganized onto a unified energy grid for fast lookup during particle transport. A phase-space neutron source was used to represent realistic BNCT beam conditions. Secondary photons and electrons were simulated using the GPU-based MC code ARCHER. The method was validated against Geant4 in water phantom and voxelized patient phantom by comparing neutron flux and biologically weighted dose distributions.

Results: The proposed method showed good agreement with Geant4. In the water phantom with B-10 (30ppm), neutron flux distributions exhibited a maximum relative error below 2%. In the patient phantom, a 1 mm/1% gamma passing rate exceeding 99% is achieved. Regarding computational performance, the proposed method achieved up to a 30-78 speedup compared with Geant4 executed on a 128-threads CPU.

Conclusion: This study demonstrates that GPU-accelerated MC approach can simultaneously achieve high accuracy and high computational efficiency for BNCT dose calculations. By enabling fast and reliable dose simulations in patient phantoms, the proposed method shows strong potential for integration into BNCT treatment planning systems and for supporting clinically practical dose evaluation.

CONTACT

Xie George Xu
University of Science and Technology of China
xgxu@ustc.edu.cn

INTRODUCTION

Boron neutron capture therapy (BNCT) is a biologically selective radiation therapy in which thermal neutrons interact with boron-10 to produce high-LET particles with cellular-scale energy deposition. Accurate BNCT dose calculation requires Monte Carlo (MC) simulation due to coupled neutron transport, secondary photon generation, and short-range charged-particle interactions. Although general-purpose MC codes such as PHITS, MCNP, and Geant4 provide accurate neutron transport modeling, patient-specific BNCT simulations remain computationally intensive, limiting clinical applications. While GPU acceleration has improved MC efficiency in photon and charged-particle therapy, GPU-based MC methods for BNCT remain limited. This study develops and verified a GPU-accelerated continuous-energy MC neutron transport code (ARCHER-Neutron) to achieve accurate and efficient BNCT dose calculation within a patient-specific treatment planning framework.

METHODS AND MATERIALS

A GPU-accelerated continuous-energy MC neutron transport code, ARCHER-Neutron, was developed using a CPU+GPU heterogeneous framework. GPU threads performed neutron transport using a history-based parallelization strategy, with neutron physics based on Geant4 11.4.0, including scattering, capture, and S(α,β)-based thermal neutron scattering. Secondary photons were coupled with the GPU-based ARCHER photon transport module. Validation was performed using (1) a 30 ppm B-10 water phantom with a 10 keV monoenergetic neutron source (10^8 histories) and (2) a voxelized glioblastoma patient CT model (2 mm voxel size) irradiated by an accelerator-based BNCT phase-space source (2×10^8 histories). Simulations were benchmarked against Geant4 using an RTX 3090 GPU and an AMD EPYC 7763 64-core CPU (128 threads), with statistical uncertainties below 1%.

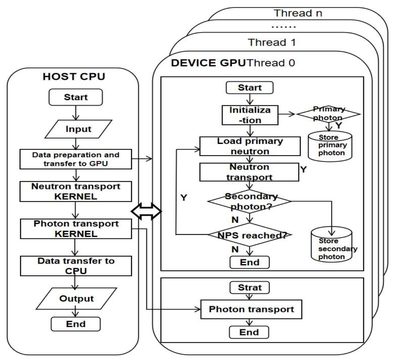

Figure 1. Workflow of the CPU–GPU heterogeneous framework

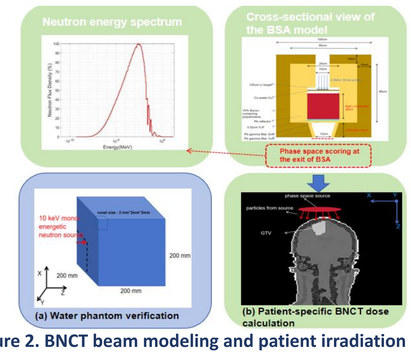

Figure 2. BNCT beam modeling and patient irradiation setup

RESULTS

In the water phantom verification, ARCHER showed good agreement with Geant4 in neutron fluence-depth distributions, with a maximum relative difference below 2%. The neutron transport time was reduced from 66.3 min to 2.21 min, achieving a 30-fold speedup. In the patient-specific model, DVH results for the GTV, skin, and brain demonstrated close agreement between ARCHER and Geant4. For the GTV, ARCHER yielded a mean dose of 39.00 Gy(IsoE), with a relative difference of 1.1% compared with the Geant4 reference value. The differences in D98, D50, and D2 were also within 1.1%, with corresponding deviations of 0.3%, 0.8%, and 0.6%, respectively. For organs at risk, the brain mean dose calculated by ARCHER was 2.86 Gy(IsoE), corresponding to a 1.6% difference from the Geant4 result, while Dmax showed a 3.3% difference (48.39 Gy(IsoE)). The 1 mm/1% gamma passing rate exceeded 99%, confirming the dosimetric consistency between the two methods. The total MC transport time for the patient-specific simulation was reduced from 220.74 min to 2.83 min, achieving a 78-fold speedup.

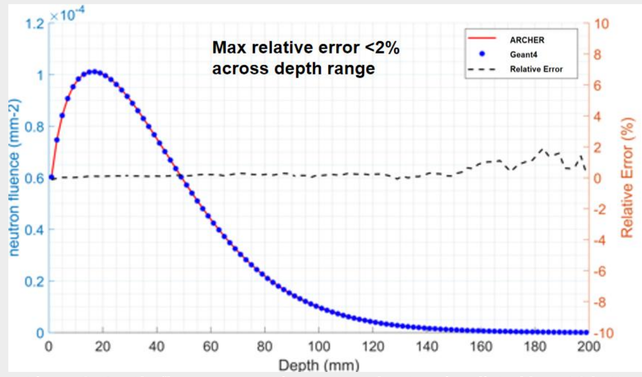

Figure 3. Depth–fluence curves in a water phantom irradiated by a 10 keV monoenergetic neutron source

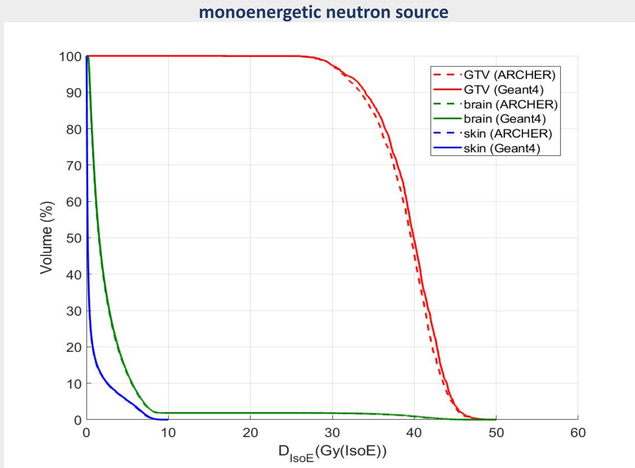

Figure 4. Dose-volume histogram (DVH) comparison in a patient-specific model

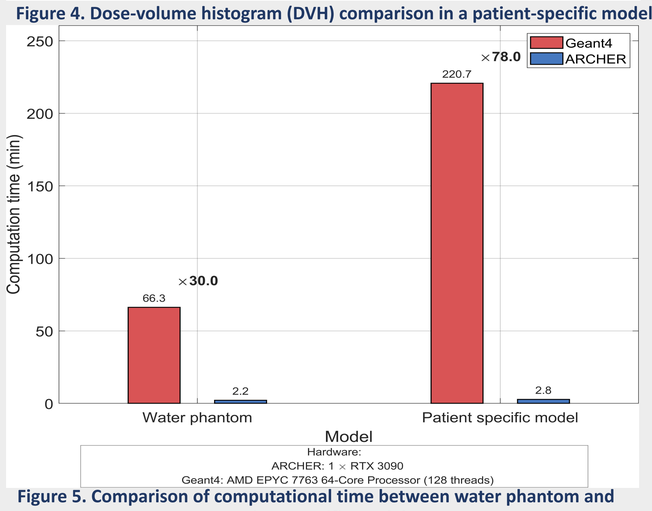

Figure 5. Comparison of computational time between water phantom and patient-specific model

DISCUSSION

This study demonstrates that GPU-accelerated MC simulation can achieve high accuracy and computational efficiency for BNCT dose calculation. The water phantom validation confirmed that ARCHER reproduces reference MC neutron transport behavior with good agreement in fluence-depth distributions, while the patient-specific model showed consistent DVH characteristics and dosimetric metrics compared with Geant4. The close agreement in target dose coverage and organ-at-risk doses supports the reliability of the GPU-based approach for patient-specific BNCT dose evaluation. ARCHER achieved substantial computational acceleration, reducing simulation time by approximately 30-fold for the water phantom and 78-fold for the patient-specific model, enabling more practical dose calculation and plan evaluation workflows. Several limitations remain: the patient evaluation was based on a single glioblastoma case and does not represent inter-patient variability. Boron distribution was assigned using region-based values rather than individualized PET-derived heterogeneous distributions, and the current workflow does not include inverse plan optimization or patient-specific boron pharmacokinetics. Future studies will extend validation to larger patient cohorts and incorporate more realistic boron distribution modeling.

CONCLUSIONS

A GPU-accelerated continuous-energy Monte Carlo neutron transport code (ARCHER-Neutron) was developed and validated for BNCT dose calculation. The code was benchmarked against Geant4 in both a boron-containing water phantom and a voxelized glioblastoma patient CT model, showing good agreement in neutron fluence distributions and biologically weighted dose metrics, with maximum relative errors below 2% in the phantom and approximately 1-2% for key dosimetric parameters in the patient case. The proposed method achieved an overall speedup of approximately 78-fold compared with Geant4 executed on a multi-thread CPU, reducing the total MC transport time from 7.8 hours to 3.8 minutes. These results demonstrate that GPU-accelerated MC simulation can simultaneously achieve high accuracy and high computational efficiency for BNCT dose calculations, showing strong potential for integration into BNCT treatment planning systems and for supporting clinically practical dose evaluation workflows.

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