

Development of GPU-Accelerated Monte Carlo for Simulating Dose and Distribution of Beta Emitter in Hadron Therapy

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1. Introduction

Carbon ion radiotherapy is characterized by the presence of a sharp Bragg peak, accompanied by a high linear energy transfer (LET) value at the vicinity of the peak, where the biological effectiveness is maximized. By exploiting this property, carbon ions can achieve superior therapeutic efficacy compared to conventional radiotherapy modalities such as X-ray irradiation, and extensive research and development efforts are currently underway in this field [1].

In carbon ion radiotherapy, positron-emitting isotopes such as ^{11}C , ^{10}C , and ^{15}O are produced through nuclear reactions along the beam path. Although their production occurs upstream, these isotopes tend to slow down and accumulate near the Bragg peak, where they ultimately come to rest. Leveraging this effect, the concept of Particle Therapy Positron Emission Tomography (PT-PET) has been proposed as a method to perform real-time quality assurance during treatment [2].

In the present work, heavy-ion transport capabilities were implemented into the GPU-accelerated Monte Carlo code RT², and the feasibility of providing computational indices applicable to PT-PET was investigated [3].

2. Methods and Results

This section provides a concise overview of the nuclear reaction models implemented in RT². Subsequently, the results obtained from the implemented code are compared with those from Geant4, PHITS, and experimental data in terms of dose profiles, β -emitter distributions, and computational performance.

2.1 Quantum Molecular Dynamics

In the Quantum Molecular Dynamics (QMD) model, protons and neutrons constituting both the target and projectile nuclei involved in a nuclear reaction are represented as Gaussian wave packets. Each packet is assumed to form a two-body problem with all other packets, and the interaction potentials are defined by the strong nuclear force and the electromagnetic force. The

equations of motion are then solved within this potential matrix to update the positions and momenta of the packets at successive time steps. This procedure is iteratively performed up to 100 fm/c with a time interval of 1 fm/c. Owing to its repeated matrix operations, the QMD algorithm is well suited for efficient implementation on GPU architectures.

2.2 De-Excitation Model

Through the QMD process, stable nuclei may undergo proton or neutron separation or addition, leading to the formation of unstable nuclei. These unstable nuclei subsequently de-excite by emitting light particles such as protons, neutrons, or alpha particles, or by releasing gamma rays. The Weisskopf–Ewing model is one of the theoretical frameworks describing this de-excitation process and is commonly employed as a default option in Monte Carlo algorithms such as Geant4.

In the Weisskopf–Ewing model, the calculation of decay widths requires the inverse-reaction cross section. In RT2, both the Dostrovsky and Chatterjee cross-section models have been implemented, and their performance has been compared.

2.3 Depth-Dose Profile

A 290 MeV/u ^{12}C beam was irradiated onto a PMMA phantom. The same scenario was simulated using Geant4, FLUKA, and RT². Geant4 and FLUKA calculations were performed on a single Intel Xeon Gold 6342 node utilizing all 48 threads, while RT2 was executed on a single NVIDIA RTX 4090 GPU. The results are presented in Fig. 1.

The dose contribution of primary ^{12}C , secondaries, total dose, and computational time of each codes and models are listed in Table I.

Table I: Dose contribution and tracking rate of Geant4, FLUKA, and RT²

	Total Dose [MeV/u]	Prim Dose [MeV/u]	Sec Dose [MeV/u]	Tracking Rate [ms ⁻¹]
G4 BIC	254.80	179.36	75.45	0.70
G4 QMD	253.29	186.15	67.13	0.97
FLUKA	255.55	180.37	75.18	2.51

RT ² Dostr	253.34	179.97	73.37	69.52
RT ² Chatt	250.62	179.29	71.33	65.20

In Geant4, simulations were performed using both the Binary Cascade (BIC) and QMD models, while FLUKA operates on a QMD-based framework. RT² is also based on the QMD model, with calculations performed separately for the two implemented de-excitation models. The tracking rate, defined as the number of histories processed per millisecond, was used as a measure of computational performance. Using the Dostrovsky model, RT² demonstrated markedly higher efficiency, achieving approximately 27 times the performance of FLUKA and about 70 times that of Geant4 QMD.

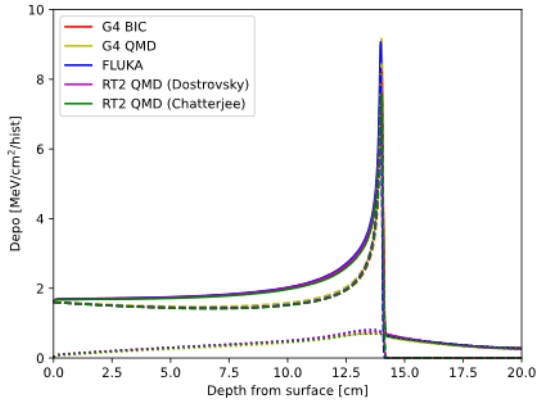


Fig. 1. Depth-dose profile of the 290 MeV/u ¹²C ion in PMMA, calculated by Geant4, FLUKA, and RT².

2.4 Beta Emitter Distributions

Experimental data and PHITS simulation results were referenced from H. Rohling et al. [4]. The distribution of radioactive isotopes produced by a 266 MeV/u ¹²C beam irradiated onto a water phantom was calculated using RT². In the PHITS calculations, nuclear reactions were modeled with the same QMD framework as in RT², while de-excitation was treated using the Generalized Evaporation Model (GEM) and the Statistical Decay Model (SDM). The dominant β -emitters were identified as ¹¹C, ¹⁵O, and ¹⁰C, and their respective distributions are shown in Fig. 2, Fig. 3, and Fig. 4.

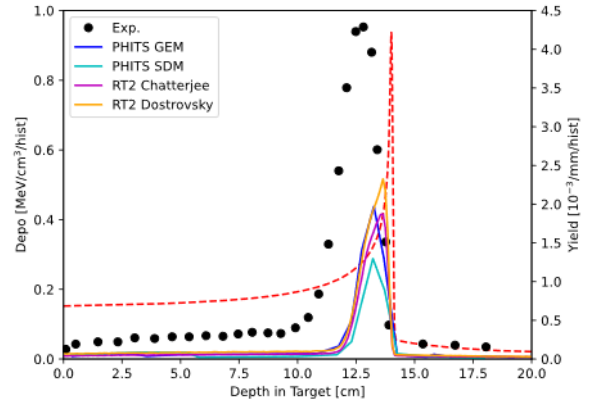


Fig. 2. Calculation and experimental data of ¹¹C yield. The red dashed line represents the depth-dose profile.

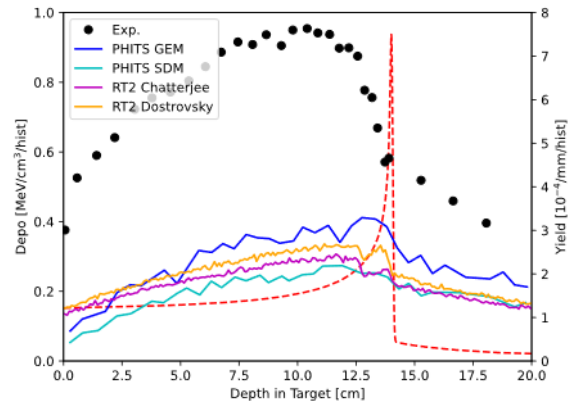


Fig. 3. Calculation and experimental data of ¹⁵O yield. The red dashed line represents the depth-dose profile.

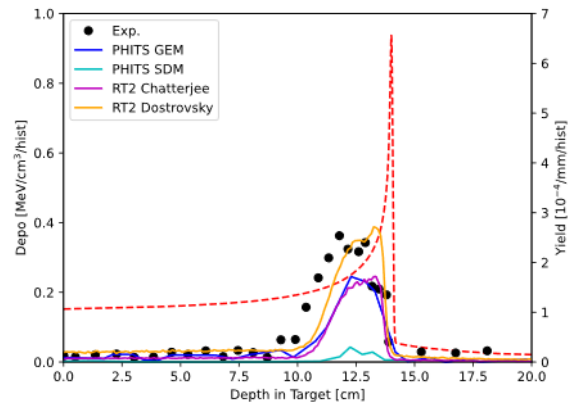


Fig. 4. Calculation and experimental data of ¹⁰C yield. The red dashed line represents the depth-dose profile.

3. Conclusions

Heavy-ion transport and β -emitter calculation capabilities were newly implemented in the GPU-accelerated Monte Carlo code RT². The primary and secondary dose profiles of ¹²C beams were validated against Geant4 and FLUKA, yielding consistent results

while demonstrating performance improvements of approximately 27-fold over FLUKA and 70-fold over Geant4. By leveraging this computational efficiency, RT2 is expected to be applicable to Monte Carlo-based dose calculations in hadron therapy.

The spatial distributions of ^{11}C , ^{15}O , and ^{10}C induced by ^{12}C irradiation were also calculated, showing good agreement with PHITS results. Compared to experimental data, both ^{11}C and ^{15}O yields were underestimated, consistent with the PHITS predictions. Since both PHITS and the present work employ the QMD model for nucleus–nucleus reaction calculations, this discrepancy is attributed to intrinsic characteristics of the QMD approach.

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