Development of GPU Accelerated Nuclear Fragmentation Model for Dose Calculation in Heavy Ion Therapy

Chang-Min Lee [a], Taewan Kim[a], Yoonho Na[a], Kyuri Kim[a], Sung-Joon Ye[a,b,c,d,*]

[a]*Department of Applied Bioengineering, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, 08826, Republic of Korea*
[b]*Research Institute for Convergence Science, Seoul National University, Seoul, 08826, Republic of Korea*
[c]*Advanced Institute of Convergence Technology, Seoul National University, Suwon, 16229, Republic of Korea*
[d]*Biomedical Research Institute, Seoul National University Hospital, Seoul, 03080, Republic of Korea*
[*]*Corresponding author: sye@snu.ac.kr*

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1. Introduction

The heavy ion therapy is considered as next-generation cancer treatment method due to its high dose locality and relative biological effectiveness. However, heavy ion in therapeutic energy range, up to 400 MeV/u, generates much more secondary ions compared to proton or photon by inelastic nuclear reactions. These secondaries can deliver undesirable dose to surrounded normal tissue. Therefore, Monte Carlo algorithm with considering fragmentation and evaporation model is required to calculate dose precisely in heavy ion therapy.

Unfortunately, conventional Monte Carlo algorithm, such as Geant4 or PHITS cannot be applied in clinical routine due to their computing speed [1]. To resolve this problem, we have developed GPU accelerated relativistic Quantum Molecular Dynamics (QMD) nuclear fragmentation algorithm for the module of GPU accelerated Monte Carlo code under development.

2. Methods and Results

2.1 Quantum Molecular Dynamics (QMD) Model

In QMD, individual nucleon of nucleus is assumed to gaussian wave packet as follow [2]:

$$f_i(\vec{r},\vec{p}) = 8\,exp\left[-\frac{\left(\vec{r}-\vec{R}_i\right)^2}{2\sigma_r^2}-\frac{\left(\vec{p}-\vec{P}_i\right)^2}{2\sigma_p^2}\right] \quad (1)$$

, where $\vec{R}_i$ and $\vec{P}$ represent center of i[th] wave packet in phase-space, σ_r is spatial uncertainty and σ_p is momentum uncertainty. The equation of motion of each packet is

$$\dot{\vec{R}}_i = \frac{\partial H}{\partial \vec{P}_i} \qquad \dot{\vec{P}}_i = -\frac{\partial H}{\partial \vec{R}_i} \quad (2)$$

, where H is Hamiltonian of whole system. With an appropriate timing interval and boundary condition, the phase-space of each nucleon can be calculated for arbitrary time. The Hamiltonian of system are defined as follows:

$$H = \sum_i \sqrt{m_i^2 + \vec{P}_i^2} \quad (3)$$

$$+\frac{1}{2}\frac{A}{\rho_0}\sum_{i,j(\neq i)}\rho_{ij} + \frac{1}{1+\tau}\frac{B}{\rho_0^\tau}\sum_{i,j(\neq i)}\rho_{ij}^\tau$$
$$+\frac{1}{2}\sum_{i,j(\neq i)}\frac{e_i e_j}{\left|\vec{R}_i-\vec{R}_j\right|}\mathrm{erf}\left(\frac{\left|\vec{R}_i-\vec{R}_j\right|}{2\sigma_r}\right)$$
$$+\frac{1}{2}\frac{C_s}{\rho_0}\sum_{i,j(\neq i)}c_i c_j \rho_{ij}$$

Where erf is error function and c_i is isospin, which is 1 for proton and -1 for neutron. ρ_{ij} represents the volume of the overlapped region between two wave packets which is defined as following equation:

$$\rho_{ij} = \frac{1}{(4\pi\sigma_r)^{3/2}}\ exp\left[-\frac{\left(\vec{R}_i-\vec{R}_j\right)}{4\sigma_r}\right] \quad (4)$$

In eq.3, first term represents relativistic energy, second term is Skyrme-type effective N-N interaction, third term is Coulomb repulsion and last is symmetry energy. Since these two-body components except first term can be represented as matrix, which is suitable data structure for GPU architecture, QMD algorithm can show high GPU optimization efficiency.

2.2 Benchmarking Against Geant4

Since the production cross section and dose contribution of pion and delta resonance are neglectable in therapeutic energy range, these particles are not implemented in this work. Maximum collision time cutoff and width of timing interval are set the same as Geant4 QMD (G4QMD) for the fair performance comparison [3].

In Geant4, G4QMDReaction::ApplyYourself method is called directly for considering forced interaction situation and for measuring computational time of QMD module. Since evaporation module is not implemented yet in this work, both of two cases, with and without of evaporation module, were simulated in Geant4.

200 MeV/u carbon-12 ion was applied to carbon-12 target. The angular distributions of secondaries were scored in Geant4 and this work respectively. The differential yield of secondary neutron and ^{4}He are illustrated in Fig. 1 and Fig. 2 respectively.

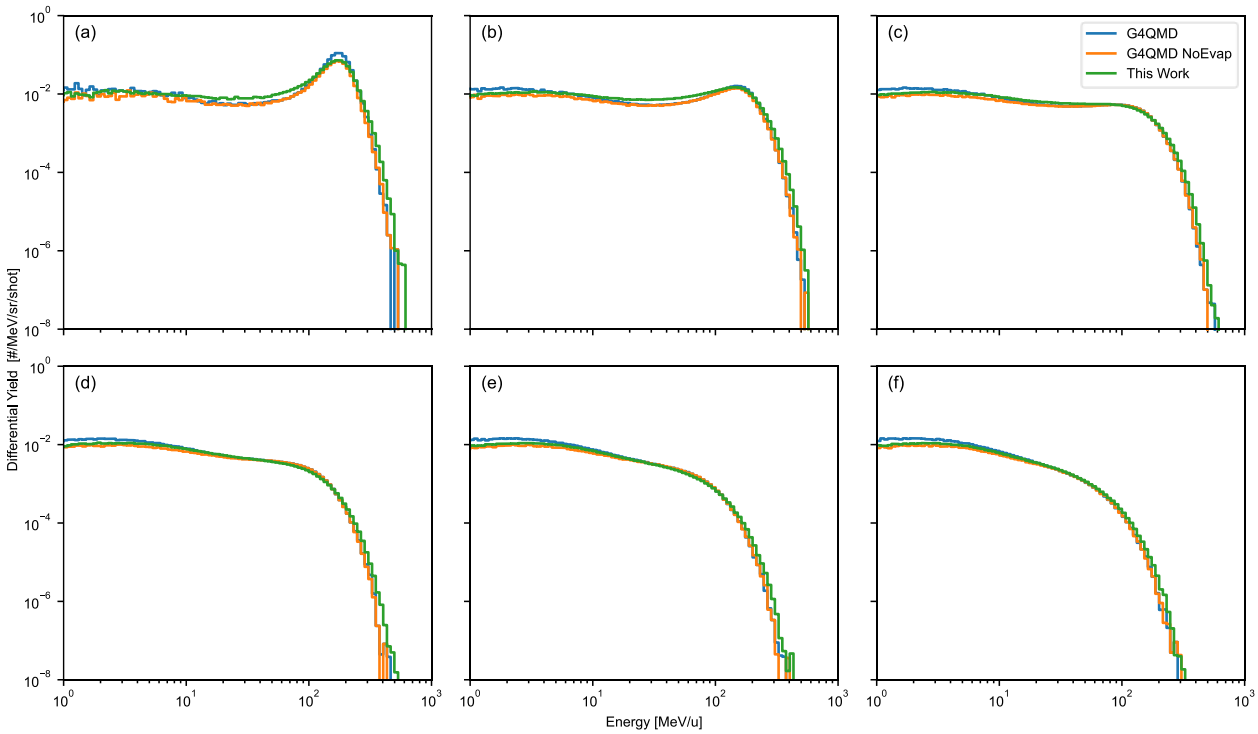

Fig. 2. Differential Yield of secondary neutron in ^{12}C-^{12}C collision with 200 MeV/u. (a) energy distribution in polar angle 0 degree, (b) in 15 degree, (c) in 30 degree, (d) in 45 degree, (e) in 60 degree and (f) in 75 degree.

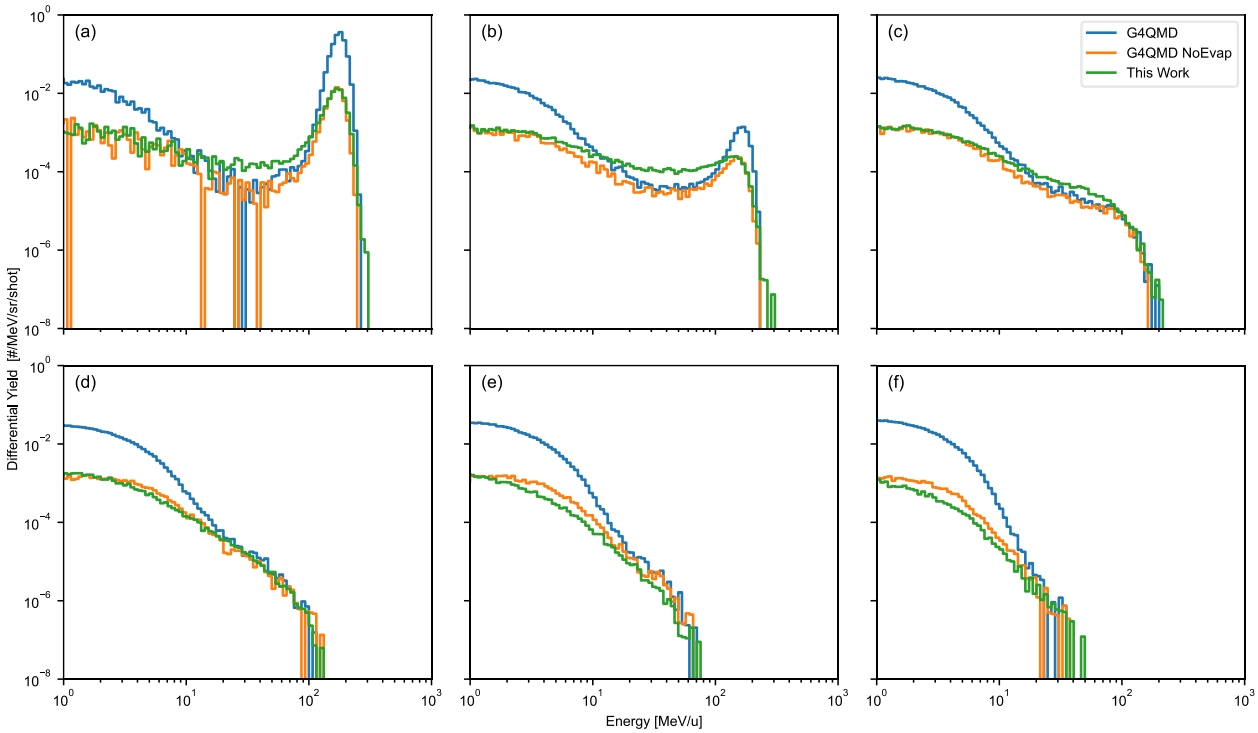

Fig. 1. Differential Yield of secondary ^{4}He in ^{12}C-^{12}C collision with 200 MeV/u. (a) energy distribution in polar angle 0 degree, (b) in 15 degree, (c) in 30 degree, (d) in 45 degree, (e) in 60 degree and (f) in 75 degree.

In evaporation stage, excited or neutron-proton unbalanced nucleus are commonly decay with α emission. Therefore, the emission probability of single nucleon is much smaller than ^{4}He in evaporation phase, G4QMD and G4QMD without evaporation was shown no significant difference in neutron yield.

In Fig. 2-(a), peaks in right and left side represents remnant nucleus of projectile carbon and target carbon respectively. Differences between G4QMD and G4QMD NoEvap are contribution of evaporation. In ^{4}He yield, this work shows slight difference compared to G4QMD NoEvap in intermediate energy from 10 MeV to 100 MeV. The reason of these differences is under investigation.

In Geant4 calculation, all 20 threads of single Intel i9-10900k node were used. Single Nvidia RTX 4090 card was used for this work. 432 seconds were taken for computing 10^6 collisions in G4QMD simulation and 55 seconds for computing 8.2×10^6 collisions in this work. Therefore, time per shot were 432 μs and 6.71 μs respectively. Therefore, relative performance of GPU-accelerated QMD algorithm was 64.4 times higher than G4QMD in these computing platforms.

3. Conclusions

The GPU-accelerated relativistic Quantum Molecular Dynamics (QMD) code was developed for heavy ion therapy dose calculation. Developed code was benchmarked against to Geant4 QMD module (G4QMD) and energy-angle difference at 10-100 MeV region was found in ^{4}He secondaries. Relative performance of GPU-accelerated QMD algorithm was 64.4 times higher than G4QMD.

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