FRED: a fast Monte Carlo code on GPU for quality control in Particle Therapy

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Abstract. Charged Particle Therapy is a non-invasive technique for radio-resistant tumor treatment performed with protons or light ions, aiming to deliver a high precision treatment. Compared to conventional radiotherapy, ions allow for a higher dose deposition in the tumor region while sparing the surrounding healthy tissue. To really exploit the potential benefits of this technique, the highest possible accuracy in the calculation of dose and its spatial distribution is required in treatment planning. Commonly used Treatment Planning Software solutions adopt a simplified beam–body interaction model. An alternative is the use of Monte Carlo simulations which explicitly take into account the interaction of charged particles with actual human tissues hence providing highly accurate results. However, Monte Carlo simulations are used in a restricted number of cases due to substantial computational resources required. The code FRED has been developed to allow a fast optimization of the treatment plans in Charged Particle Therapy while profiting from the dose release accuracy of a Monte Carlo tool. Currently, the most refined module is the transport of proton beams in water. A comparison with measurements shows that the lateral dose tails are reproduced within 2\% in the field size factor test up to 20 cm. Models for the interaction of ion with the matter are currently under development in the FRED code. The status of new developments and the performance of FRED will be presented.

1. Introduction

Particle Therapy (PT) uses charged particle (usually proton or Carbon ion) beams to release energy into the tumour volume causing the diseased cells apoptosis [1]. According to recent statistic (PTCOG [2]) by the end of 2018 more than 220 000 patients have been treated worldwide with PT. About 190 000 have been treated with protons, about 28000 with C-ions and about 3 500 with He, pions and other ions. The number of clinical centers dedicated to this treatments is rapidly increased. The main difference with a conventional radiotherapy is in the high spatial selectivity and in the biological damage, related to the released energy, the ionization density and the type of projectile used. Usually one talks about dose which is the measure of the energy deposited in matter by ionizing radiation per unit mass. While the dose deposition obtained with a conventional radiotherapy (photon beams), as a function of depth in the transverse matter, is...
continuous during all the path in a target, the dose deposited by beams of protons and Carbon ions is concentrated in few millimeters at the end of the particle range, in the so call Bragg Peak (BP, Fig.1). Therefore PT allows for a higher dose deposition in the tumor region while sparing the surrounding healthy tissue, achieving a lower complication probability. To cover the entire tumor volume, which usually is larger than few millimeters and has an arbitrary shape, an overlap of beams at different energies is used, obtaining a wider irradiation profile called Spread Out Bragg Peak (SOBP, Fig.2).

![Figure 1. Dose deposited by a photon beam (in black), a proton beam (in blue) and a Carbon ion beam (in red) as a function of depth in the transverse matter.](image1)

![Figure 2. Spread Out Bragg Peak using a combination of proton beams with different energies.](image2)

To really exploit the potential benefits of PT, the highest possible accuracy in the calculation of dose and its spatial distribution is required. Sophisticated software tools, called Treatment Planning System (TPS) have been developed in order to produce a patient-specific set of particle beams. Routinely the analytic TPSs are used, tuning the algorithm on measurements taken at each treatment center. Usually the system is based on a pencil beam algorithm, where an accurate dose depth profile is remapped in the transverse direction using analytic functions. The short time required to realize this treatment planning is a huge advantage in a clinical context but, for a restrict number of difficult cases, where there is a large density gradients and non-uniform materials, Monte Carlo Treatment Planning System are preferred. In fact a Monte Carlo, which explicitly take into account the interaction of charged particles with actual human tissues, is considered the most reliable tool to address the complexity of mixed field irradiation in a heterogeneous environment [3][4][5]. However, presently, it is impossible to use full Monte Carlo calculations routinely because they typically demand substantial computational resources. Monte Carlo usually used for this purpose are FLUKA [7][6] or TOPAS [8]. The latter is a software platform, based on GEANT4, produced by the interfacing of MC tools with accelerator machine and patient data in order to have a code which could be more easily introduced in clinical environments. The advent of general programming Graphics Processing Units (GPU) has prompted the development of MC codes that can dramatically reduce the plan recalculation time with respect to standard MC codes in CPU hardware [9][10].

In this framework FRED (Fast paRticle thErapy Dose evaluator) has been developed [11]. It is a code on GPU to recalculate and optimize ion beam treatment plans. Rapidly recalculating a complete treatment plan within minutes, instead of hours, it paves the way for many clinical
applications where the time-factor is important. Developing the algorithm, the goal is to balance accuracy, calculation time and GPU execution guidelines. To do it, the most effective physical models from the literature have been chosen. For many processes, FRED relies on a library precomputed look-up tables instead of performing an explicit calculation. This approach performs extremely well on GPU cards where hardware interpolation can be exploited using the so called texture units.

2. Comparison with other MC softwares and with data
The implemented models and FRED performance were tested against the full-MC codes FLUKA and GEANT4 for protons in liquid water.

In Fig.3 the Bragg curves for monoenergetic proton beams in a water phantom had been simulated with different initial energies in order to observe all them together. They are the result of the simulation of FRED, FLUKA and GEANT4 considering different models. In fact, to check each interaction model separately, the elastic and inelastic nuclear interactions were switched on and off. Profiles closely overlap for most of the particle range. Only near the peak there are slight differences but however the agreement with FLUKA is within 1.5% of the Bragg peak value for all models in the energy range of PT (50-250 MeV).

Since the dose in a single voxel depends on the contribution from many thousands of pencil beams closely bundled on the transverse direction, it is important to take care of the accuracy of the lateral dose distribution. In Fig.4 the dose distribution for a single pencil beam of proton at 150 MeV in water is shown. The first panel (a) is in logarithmic scale in order to clearly see the tracks of secondary particles emitted (protons and deuterons). In the second panel (b) the dose line profile along the beam axis for FRED (in red) and for FLUKA (black) is represented. The figure shows the lateral beam spreading due to multiple scattering. The transverse lineouts at the Bragg peak position (z=15.6 cm), respectively in linear (c) and logarithmic (d) scale, are also represented. The tails of the distributions are mainly due to nuclear interactions. Comparison with FLUKA simulations, in the same condition (same scoring grid and same statistics), shows good agreement up to four orders of magnitude in lateral dose distribution at a distance of 3 cm from the beam axis.

To be sure to have under control the contribution of long-range lateral tails in the dose distribution, the Field Size Factor (FSF) test has been performe (Fig.5). The test is realized in homogeneous conditions, placing a dose detector inside a liquid water phantom. A set of pencil beams with the same energy and fluence are delivered to the phantom, distributing the
Figure 4. Dose in water for a 150 MeV proton beam with 0 FWHM. It is possible to observe: the dose map a), the central voxel lineout along beam axis b), the lateral lineout at 15.6 cm depth in linear c) and logarithmic d) scale. In particular with the logarithmic scale is it possible to observe the tails of the distributions, mainly due to nuclear interactions.[11]

Figure 5. The Field Size Factor test. The detector (a Markus chamber) is positioned inside a box of water and its depth can be changed. The beam is shot on a grid configuration with a spot interspacing of 2 mm and a spot intensity of $5 \times 10^7$. The measurement has been repeated for different energies, fields size and depths.

Figure 6. FSF test for a 226.62 MeV/n proton beam with the dose detector at a depth of 20 cm in the CNAO water phantom. FSF is normalized to 10 cm size value and computed with FRED and measured data (left), and relative error (right). [11]
Computed and collected data points were normalized to their respective value at 10 cm field size. FRED reproduces the experimental data within 2% for the field size up to 20 cm. In the Tab.1 temporal performances of FRED for different hardware architectures are represented in comparison with a simulation with a code full MC (FLUKA). Using the same CPU hardware, FRED is 20 times faster than FLUKA. This is possible due the fact that FRED is a "fast" Monte Carlo. It means that the physics models implemented in the code are simplified, simulating only what is needed for a treatment planning in Particle Therapy. Moreover, running on GPU, there is a gain in time of 50 times compared with an execution in a single CPU. Moreover, using a combination of 4 GPU cards it is possible to simulate a primary particle in 0.05 $\mu$s.

### Table 1. FRED performances in comparison with FLUKA and different hardware.

| MC     | Hardware       | Primary/s | $\mu$s/primary |
|--------|----------------|-----------|----------------|
| FLUKA  | single CPU core| 0.75k     | 1340           |
| FRED   | single CPU core| 15k       | 68             |
| FRED   | single GPU cards| 800k   | 1.35           |
| FRED   | 4 GPU cards    | 20000k    | 0.05           |

### 3. FRED for Carbon beams

The excellent results achieved with protons determined the interest of the CNAO (Centro Nazionale di Adroterapia Oncologica) center (Pavia, Italy) to develop FRED also for Carbon therapy applications. Models for the interaction of $^{12}$C ions with matter are currently under development to be implemented in the FRED code.

In particular, the main difference is in the fragmentation of the projectile since protons do not fragment while ions do. The result of the projectile fragmentation is a small tail of dose after the Bragg Peak (Fig.1). While fragments emitted by the target have a kinetic energy almost zero, and so they release dose close to the point of emission, fragments emitted by the projectile have a kinetic energy of the same order of the energy per nucleon of the beam. The consequence is that they travel in the body releasing energy far from the emission point. For this reason, the beam fragmentation process is related to the dose release outside the tumor region and its description is of paramount importance and has to be accurately modeled.

Currently, the development of the model is based on the use of data taken during experiments at Ganil (laboratory of CAEN, France) where the fragmentation of Carbon ions on thin targets (H, C, O, Al and Ti) has been studied [12][13]. The experiment provided data about the angular and energy cross section of a Carbon beam of 95 and 50 MeV/n and with a detection angles in the rage $\left[-43^o, 43^o\right]$. To tune the algorithm in the energy range used in PT treatments, and not only at beam energies of the Ganil experiment, an appropriated scaling has been used, obtaining energy and angular cross-sections specific for every energies:

\[
K_f = K_f^{Ganil} R, \quad \theta_f \propto \sqrt{\frac{p_f}{p_b}} \approx \sqrt{\frac{K_f}{K_b}}; \tag{1}
\]

where: $R = K_b^{Ganil}/K_b$. $K_f$ and $\theta_f$ are respectively the kinetic energy and the emission angle of a fragment emitted with a beam of a chosen energy, $K_f^{Ganil}$ is the kinetic energy of a fragment emitted by the Ganil’s beam (95 or 50 MeV/n), $K_b$ is the kinetic energy of the beam at the chosen energy,
$p_f$ and $p_b$ are the transverse momentum of the fragment and of the beam.
In the next future the model will be improved using more data from new experiments (i.e. FOOT experiment) in order to have more information of the fragmentation of the projectile for different energies, targets and angles.

References

[1] Durante M and Loeffer J S 2010 Nat. Rev. Clin. Oncol. 7 37
[2] https://ptcog.ch/index.php/patient-statistics
[3] Paganetti H 2009 Phys. Med. Biol. 54 4399–421
[4] Parodi K et al. 2012 Phys. Med. Biol. 57 3759–84
[5] Grassberger C et al. 2015 Phys. Med. Biol. 60 633–45
[6] Agostinelli S et al. 2003 Nucl. Instrum. Methods A 506 250-303
[7] Ferrarin A et al. 2005 CERN-2005-10 INFN/TC-5/11, SLAC-R-773
[8] Perl J et al. 2012 Med. Phys. 39 6818–37
[9] Jia X et al. 2014 Phys. Med. Biol. 59 R151–82
[10] Giantsoudi D et al. 2015 Phys. Med. Biol. 60 2257–69
[11] Schiavi A et al. 2017 Physd. Med. Biol. 62 7482
[12] Dudouet J et al. 2013 Phys. Med. Biol. 88 1-15
[13] Divay C 2017 Physical Review C 95 044602