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A modular method to handle multiple time-dependent quantities in Monte Carlo simulations

J Shin¹, J Perl², J Schümann³, H Paganetti³, and BA Faddegon¹

¹University of California San Francisco Comprehensive Cancer Center, 1600 Divisadero Street, San Francisco, CA 94143-1708, USA

²SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA

³Department of Radiation Oncology, Massachusetts General Hospital, Boston, MA 02114, USA

Abstract

A general method for handling time-dependent quantities in Monte Carlo simulations was developed to make such simulations more accessible to the medical community for a wide range of applications in radiotherapy, including fluence and dose calculation. To describe time-dependent changes in the most general way, we developed a grammar of functions that we call “Time Features”. When a simulation quantity, such as the position of a geometrical object, an angle, a magnetic field, a current, etc., takes its value from a Time Feature, that quantity varies over time. The operation of time-dependent simulation was separated into distinct parts: the Sequence samples time values either sequentially at equal increments or randomly from a uniform distribution (allowing quantities to vary continuously in time), then each time-dependent quantity is calculated according to its Time Feature. Due to this modular structure, time-dependent simulations, even in the presence of multiple time-dependent quantities, can be efficiently performed in a single simulation with any given time resolution. This approach has been implemented in TOPAS (TOol for PAricle Simulation), designed to make Monte Carlo simulations with Geant4 more accessible to both clinical and research physicists. To demonstrate the method, three clinical situations were simulated: a variable water column used to verify constancy of the Bragg peak of the Crocker Lab eye treatment facility of the University of California, the double-scattering treatment mode of the passive beam scattering system at Massachusetts General Hospital (MGH), where a spinning range modulator wheel (RMW) accompanied by beam current modulation produces a spread-out Bragg Peak, and the scanning mode at MGH, where time-dependent pulse shape, energy distribution and magnetic fields control Bragg peak positions. Results confirm the clinical applicability of the method.

1. Introduction

Monte Carlo simulation is one of the most accurate methods for fluence and dose calculation in radiation therapy, including proton therapy. Time varying quantities are intrinsic to advanced treatment techniques, including fluence modulations, varying electric and magnetic fields, motions of components in the beam line, motions of the tumor and patient,

and beam gating. Thus, it is necessary to include time as a parameter in Monte Carlo simulations. The diversity of beam delivery systems demands comprehensive handling of multiple time-varying quantities by means of a generic approach.

Several studies have applied 4D Monte Carlo simulation to specific applications. One method is to combine the results of individual static simulations (Verhaegen and Das 1999). However, as pointed out by Paganetti *et al* (2005), this approach is not conducive to a generic solution. Despite its straightforward implementation, the procedure when applied to proton therapy becomes increasingly cumbersome with respect to complexity of geometries and higher time resolution. In addition, the accuracy of simulation is highly reliant on the number of static simulations used to represent the actual treatment. A stochastic approach was proposed by Verhaegen and Liu (2001), used to simulate a dynamic wedge. In this method, the moving jaw position is randomized during simulation based on the known dependence of position on monitor units (MU). This method was applied to simulate dynamic multileaf collimators (Liu *et al* 2001). Belec *et al* (2011) implemented this method to simulate various types of treatment techniques such as 3D conformal, step and shoot intensity modulated radiation therapy (IMRT), helical tomotherapy, and volumetric modulated arc therapy. Another technique for IMRT simulation is to account for MLC motion by simulating particle transmission through the MLC leaves at different positions using a pre-calculated phase space (Keall *et al* 2001).

Geant4 (Agostinelli *et al* 2003) has the ability to handle time-dependent simulation in that a Geant4 job can be composed of more than one “run” (where a “run” is a set of primary histories with identical simulation conditions) and between runs the user can change simulation conditions, such as geometry or beam current. However, exercising this ability is difficult. The user must develop their own code to translate the intended time-dependent changes into a series of discrete values, and must develop their own implementation to control the sequence of runs, to execute the relevant geometrical or other changes and to advise the Geant4 geometry and run-control system that relevant changes have occurred. Paganetti *et al* (2004a, 2005) simulated dynamic proton treatment techniques through such user-written code. Passive scattering and active scanning system were simulated over a series of runs, with geometry or fields adjusted between runs in constant discrete increments to simulate a progression of time. The ad-hoc solutions for time dependence described above become increasingly complex and inter-dependent as the number of time-dependent quantities increases. Each additional time-dependent quantity results in more code that must be written, compiled and debugged. A preferable solution would be a generic approach for 4D Monte Carlo simulation that could:

1. Handle multiple time-dependent quantities in a single simulation.
2. Allow any time resolution, i.e. from a coarse discrete sequence to a randomly sampled continuous sequence.
3. Use a consistent approach to describe all time-dependent quantities.

The purpose of this study was to demonstrate this generic method for the purpose of proton therapy simulation with Geant4. This Monte Carlo toolkit has been rigorously benchmarked for accuracy in proton therapy simulation (Paganetti and Gottschalk 2003, Paganetti *et al*

2004b, Paganetti 2006, and Paganetti *et al* 2008). The focus of the study is the development of the method and demonstration of its use in practical clinical cases. The requirements specified for general 4D simulations could not be met using previous ad-hoc approaches. A new comprehensive approach is presented to simultaneously handle unlimited numbers of various types of time-dependent quantities in any time resolution. This includes translations and rotations, changing volumes, varying electric and magnetic fields, and time varying beam details such as energy, current, and momentum, with time recorded in scored quantities, etc.

The proposed method was implemented on top of the Geant4 toolkit, with no limits on time resolution, using a consistent way to describe time-dependent behaviors. A modular structure of processing was adopted, consisting of time sampling and synchronization. The sampled time is distributed over all time-dependent quantities to be synchronized. This approach was implemented in TOPAS (TOol for PArticle Simulation), a tool for particle simulation using Geant4, currently under development to make Monte Carlo simulation more accessible to both clinical and research physicists (Perl *et al* 2011). This study covers new ground in medical physics computing and in applications of Monte Carlo simulation in proton radiotherapy, including but not limited to dose calculation in radiotherapy. To our knowledge, this is the first published general solution for time-dependent Monte Carlo simulation in radiation therapy.

2. Materials and methods

We first discuss our general approach, which may be applicable to a variety of Monte Carlo codes, then show how this approach has been implemented in TOPAS.

2.1 The Time Feature approach - formulation and operation of time-dependent quantities

To describe time-dependent changes in the most general way, we developed a grammar of functions that we call “Time Features”. When a simulation quantity, such as the position of a geometrical object, an angle, a magnetic field, a current, etc., takes its value from a Time Feature, that quantity varies over time. A Time Feature may consist of a simple time function such as a linear or a sinusoidal change, or it may be composed from a combination of functions, e.g., by summing, multiplying or consecutively joining functions, such that complex time-dependent behavior may be expressed. However simple or complex the Time Feature may be, it has a well-defined time-range and periodicity, such that it yields a well-specified value at any specific time. There are three types of Time Feature to set three types of simulation quantities: numeric, boolean and string.

A numeric Time Feature can be made from a single mathematical equation (a single Time Feature), from the sum or multiplication of more than one other Time Feature or from a series of Time Features arranged consecutively in time. Mathematical functions that have been implemented thus far include step, linear, sinusoidal and square root, as follows, where t is time and a , b , c are coefficients for each function:

$$f(t) = \{C_i, t_i \leq t < t_{i+1}, t=i, \dots, N\}, \quad (1)$$

$$f(t) = a \cdot t + b, \quad (2)$$

$$f(t) = a \cdot \sin(b \cdot t + c), \quad (3)$$

$$f(t) = a \cdot \cos(b \cdot t + c), \quad (4)$$

$$f(t) = a \cdot \sqrt{(b \cdot t + c)}, \quad (5)$$

New library functions such as exponential, logarithmic, or hyperbolic, or complicated equation forms could also be added in C++ code of a numeric Time Feature. A numeric Time Feature can also be made from the sum or multiplication of more than one other Time Feature that act at the same time. The summation Time Feature returns:

$$f(t) = \sum_i f_i(t), \quad (6)$$

where $f_i(t)$ is the i -th Time Feature. The multiplication Time Feature returns:

$$f(t) = \prod_i f_i(t), \quad (7)$$

Finally, a numeric Time Feature can be made from a series of Time Features arranged consecutively in time (a consecutive Time Feature). Only one of its constituent Time Features is active at a given time as follows:

$$f(t) = \{f_i(t), \quad t_i \leq t < t_{i+1}, \quad i=1, N\}, \quad (8)$$

Complex combinations of Time Feature operations are permitted. Summation, multiplication or consecutive Time Features may themselves be made up of other summation, multiplication or consecutive Time Features. For the non-numeric boolean or the string Time Feature, a simple two-column table relates a given time to a given boolean or string value. A boolean Time Feature may be used for features such as gating a treatment beam. A string Time Feature may be used for features such as changing the input file when using Monte Carlo for a set of 4D CT images.

While the Time Features define functions of time, a second element of our grammar, the Sequence, defines what set of time values shall be plugged into these functions over the course of our simulation. The Sequence is defined by the simulation start time, the simulation end time, and a “mode”, which can be either “sequential” or “random”. In Sequential Mode, the time value is sampled in regular, even intervals, from start time to end time, and one or more histories are simulated for each of these evenly-spaced times. In Random Mode, we randomly sample time values between the start and end time, each history is simulated at a different random time, and simulation ends when the desired total number of histories have been handled.

Figure 1 shows how Time Features cooperate with the Sequence. All time-dependent quantities are handled in a single simulation.

When the time value updates, either sequentially or randomly, every Time Feature calculates its new value and this new value is then compared to the previous value of the same Time Feature. If the value has changed, all related time-dependent quantities are updated, and the relevant parts of the simulation (geometries, magnetic fields, beam sources, etc) are then triggered to update themselves. Once all relevant updates are done over all objects, a number of histories is simulated. This number is itself might change in time under control of a Time Feature. (Beam current modulation simulated with Time Features presented in section 3.2 is one application). Even in cases where the random mode will slow down the simulation from having to frequently update many parts of the geometry, random mode can still be a useful way to get a quick, low-statistics, check of the simulation results without having to run the entire sequential simulation.

2.2 Implementation in TOPAS

TOPAS was designed to allow flexible Monte Carlo simulations without requiring users to write C++ code. In TOPAS, details of geometry, particle source characteristics, physics settings, scoring, etc., are not hard-coded into compiled code but are instead read from “Parameter files”. As we described in our introduction, even for Monte Carlo codes that have the ability to handle time-dependence, ad-hoc solutions become increasingly complex as the number of time-dependent quantities increases. Each additional time-dependent quantity results in more user code both outside and inside the simulation job. TOPAS avoids requiring such user code by implementing our Time Feature approach as part of the TOPAS parameter syntax. When any parameter is set to the current value of a Time Feature, rather than to a fixed value, that parameter comes under Time Feature control.

At the beginning of the simulation run, TOPAS automatically notes when any part of the TOPAS code accesses any parameter that depends on a Time Feature. TOPAS maintains a map that correlates the name of each Time Feature with the parts of the TOPAS code that accessed this Time Feature. During the simulation run, TOPAS samples the current time value (using either sequential or random mode) and passes this time value to the *Parameter Manager*. The *Parameter Manager* then instructs each Time Feature to update its current value. If the new Time Feature value is different from its previous value, the *Parameter Manager* signals to any parts of the TOPAS code that have previously accessed this parameter to update their behavior appropriately (change the location or the volume of a geometry, adjust source parameters, gate scoring, etc.).

A key feature of TOPAS is that when geometry has to be updated, TOPAS only updates the specific parts of the geometry that have seen changes. For example, if the change is a rotation of a range modulator wheel or propeller, TOPAS needs to only update one rotation matrix value in one geometry volume. While some component motions in Geant4 require a somewhat time-consuming “geometry reoptimization” (Cosmo, 2004), in which Geant4 recreates its internal map used in making fast decisions about particle navigation, not all motions require re-optimization. A wheel rotation, for example, does not require re-optimization. When re-optimization is required, it needs not to be performed for the entire

geometry, but may be performed only for a specified subset. For a magnetic field change, there is no need to update any geometry component, as the field value is always sampled once per particle step. Each TOPAS geometry component has its own update method, which implements just the minimum change and re-optimization required for that component. The TOPAS geometry system efficiently determines whether to rebuild geometry set-up or to simply update relevant values.

3. Results

To demonstrate the handling of multiple time-dependent quantities in a single simulation, we recorded phase space that includes the sampled time value and then analyzed this phase space to show how fluence, energy, positions, etc., vary over time. All of following simulations were performed on a 2.93 GHz CPU running the operating system OS X server (10.6).

3.1 Water column of the Crocker Lab eye treatment

The University of California San Francisco (UCSF) uses 67.5 MeV protons from the cyclotron at the Crocker Nuclear Laboratory at the University of California, Davis (UCD) for treating ocular tumors (Daftari et al 1996). The treatment beam line, shown in Figure 2, consists of an exit-window, vacuum chambers, propellers, ion chambers, water column, and collimators. The distance from exit-window to isocenter is 236.2 cm. There are four propellers made of plastic layers with a different number of layers to produce different SOBP ranges. A constant beam current is maintained during treatment. A Time Feature simulates the measured rotation speed of 2.41 degree per milliseconds. Since range modulator rotation producing an SOBP is discussed in detail in the next section, only the water column expansion simulation is discussed in this section.

A water column sandwiched between 2 monitor chambers is equipped with a piston to continuously adjust the thickness of the water, used on a regular basis as a fast and reproducible means to confirm constancy of the beam energy (Chu *et al* 1993). The water column increases in thickness at a rate of 5 cm/s. The piston movement was expressed as a Time Feature (Figure 3). Fluence of primary protons was scored by phase spaces located at the upstream (PS1) and downstream (PS2) side of the of the water column, and the result shows that the fluence at PS2 remains relatively constant with the water thickness increasing, up to the range of the 67.5 MeV beam in water, at which point the fluence drops dramatically. This shows that we have simulated energy modulation due to volume changes of the water column.

3.2 Double-scattering simulation

Time-dependent simulations of the double-scattering mode of the Ion Beam Applications S.A. (IBA, Louvain La Neuve, Belgium) universal nozzle at Massachusetts General Hospital (MGH) were performed. This treatment mode generates uniform dose distributions with a spread-out Bragg peak (SOBP) by passing the beam through a varying thickness absorber. The rotating range modulator on this nozzle is synchronized with beam current modulation (BCM) to produce a flat SOBP. The simulation of this system was previously performed

with Geant4 by Paganetti *et al* (2004b) prior to the development of TOPAS. TOPAS provides pre-built generic models of several different rotating range modulator devices in clinical use for this purpose, including propeller (blade) types and wheel types (Koehler 1975, Chu *et al* 1993). The user customizes these generic components by specifying parameters such as number of modulator wheel steps, number of propeller blades, blade angles, materials, etc. The wheel type range modulator has configurable material, number of tracks, and segment angle and height.

The treatment head was modeled and simulated in the current study with TOPAS, employing Time Features for time-dependent behaviors of the spinning range modulator wheel (RMW) and the BCM (Figure 5). The time dependence of RMW rotation was described using a simple Time Feature. The Time Feature for the BCM was made by multiplication of two Time Features: a beam weight factor array (with integers ranging from 0 to 256), to specify the change in beam current within a single pulse, and a beam on and off, to specify the start time and width of the pulse. Composing the BCM Time Feature from these individual Time Features allowed adjustment of the width of a SOBP just by adjusting the beam pulse time.

Two phase spaces, upstream and downstream of the RMW, were used to record particles with sampled time values to prove that all those time-dependent quantities are done in a single simulation. The beam energy to the treatment head was $214.86 \text{ MeV} \pm 0.52 \%$ FWHM. The average kinetic energy of the primary particles decreases as the absorber height increases due to rotation of the RMW (Figure 6, left).

One advantage of including time in the simulation is the ability to analyze results as a function of time, as shown in the plots of the dependence of the full depth dose curve on time (Figure 7). Such information facilitates understanding the physics behind the SOBP depth dose curve and can be used for such applications as component design or beam current modulation optimization (Lu *et al* 2007). The simulation results are for 9 million histories, with dose scored in a segmented cylinder (10 cm diameter and 0.5 mm thickness) and statistical uncertainty less than 1 %. The simulation time was 98.5 hours.

3.3 Scanned beam simulation

In addition to passive scattering mode, the MGH universal nozzle is capable of delivering scanned beams controlled by two orthogonally oriented magnetic fields. The dynamic behavior of the magnetic fields (MAG in Figure 4) was simulated with TOPAS.

TOPAS provides an interface to simulate three kinds of magnetic fields from Geant4: a dipole magnet, a quadrupole magnet, and a three-dimensional parameterized field map. Through the TOPAS interface, users can select and configure a differential equation of motion of a particle to compute a curved trajectory in the presence of the magnetic field. By default, the 4th order of a Runge-Kutta method with 0.1 mm as “chord distance” is applied. A shorter chord distance approximates the curved path with higher precision. In order to simulate scanned proton beam in two directions, two TOPAS dipole magnetic fields were used and their field strength values in tesla were handled via a TOPAS Time Feature.

Various target patterns at iso-center were generated to demonstrate the flexibility of the presented method. For each pattern, one Time Feature was implemented for each dipole magnetic field and a continuous beam was used. We demonstrated the raster and sawtooth (Figure 8), Lissajous (Figure 9), and an arbitrary pattern (Figure 10). To show that the protons are driven by the two magnetic fields in a single simulation, the phase space at isocenter was recorded with sampled time values. The mean position of primary protons in every millisecond is displayed on top of normalized energy fluence maps (1 mm × 1 mm voxel).

In addition, a spot scanning simulation was performed with pulsed beam current, magnetic fields, energy, energy spread and spot size all varying with time (Figure 11). All of this information was obtained from the treatment control software and manually converted to Time Features in TOPAS parameter files.

4. Summary and Conclusions

A general method was developed to facilitate accurate dose calculations in Monte Carlo simulation of proton therapy that involves time-varying quantities. We have applied this approach to simulate volume changes, rotational motion, current variation, magnetic fields, energy spot size, etc.

Through this novel method's clean separation of the time-sampler, the Sequence, and the time-handlers, the Time Features, any number and type of time-dependent quantities can be controlled in a single simulation. The user can set a specific time increment (sequential mode) or perform continuous simulation (random mode).

We have shown that TOPAS can be used to simulate source and geometries varying simultaneously in time for real clinical situations, applying TOPAS to various proton beam lines. In each case we demonstrated that multiple time-dependent quantities were handled in a single simulation. The results are qualitatively reasonable. To our knowledge benchmark data is not yet available to quantitatively validate the time varying result for complex clinical situations. We expect this method is suitable for other clinical applications such as calculation of tissue phantom ratios (Karzmark *et al* 1965), 4D treatment planning (i.e., with patient motion from 4D CT), tracking a moving target with a moving beam, advanced x-ray therapy techniques such as Tomotherapy, etc.

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Figure 1.

Diagram showing the interaction between the Sequence and the Time Features. When a time value is sampled by the Sequence, Time Features are then told to update their values as a function of the sampled time. Time-dependent components such as moving geometries, magnetic fields, beam source, etc., are then told to update their time-dependent quantities to the latest values of the relevant Time Features. Note that one Time Feature may affect more than one time-dependent quantity, e.g., quantity 3 of time-dependent simulation component 2 is synchronized with quantity 1 of time-dependent simulation component K.

Figure 2.

Proton beam line used by UCSF for eye treatment as modeled in TOPAS, showing the exit-window (X), wire chamber (WIC), ion chambers (IC1 and IC2), rotating propeller (PR), collimators (CO) and the position of the water column (H2O). Protons are entering from the left.

Figure 3.

Monte Carlo calculations of the proton fluence in phase space planes placed on each side of the water column in figure 2 (lines) as the water column expands from 0 to 3.2 cm (filled circles); PS1 is located upstream (dashed line) and PS2 is placed downstream. A screen capture of the water column as it is expanding is embedded. A total of 16 million histories were simulated and the statistical uncertainty was less than 0.5%.

Figure 4.

MGH Universal nozzle used for both passive scattering and active scanning treatment; Ionization chamber 1 (IC1), First scatterer (FS), range modulator wheels (RMW), scanning magnets (MAG), second scatterer (SS), variable collimator (VC), ionization chamber 2 and 3 (IC 2 &3), snout (SN), and water column (H2O). Protons travel from left to right.

Figure 5. Time Features for a range modulator wheel (RMW) rotation at 28.6 degree per a second (straight line) and normalized beam current modulation (BCM) (stepped curve). One of the modeled RMW's is embedded.

Figure 6.

(Left) The mean kinetic energy of primary protons at nozzle entrance (PS1) and downstream of RMW (PS2). Thickness and material types of the RMW on the beam axis as the RMW rotates, starting with the brass block and followed by increasing thicknesses of carbon. The decreasing energy at the PS2 position is a consequence of the RMW rotation. (Right) Energy spectra from PS2: A total of eight intervals are shown.

Figure 7.

Calculated Bragg peaks over the same time-intervals shown in Figure 6 and the accumulation of all Bragg curves over all intervals produces a SOBP. Dose was normalized to result in a maximum of 100% in the SOBP.

Figure 8.

Raster and Saw-tooth pattern; (Top) The Time Feature for magnetic field X was made out of a consecutive combination of two single linear Time Features with opposite slopes. The Time Feature for the magnetic field Y was made of a single Time Feature moving spots to the right either discretely for a raster pattern or continuously for a saw-tooth pattern. (Bottom) The resulting energy fluence map (color wash) and the mean particle position at each 1 ms time interval (points with dashed lines).

Figure 9. Lissajous pattern; (Left) Time Features for two magnetic field X and Y made out of trigonometric functions with different phases. (Right) Energy fluence map and mean position of primary particles at each 0.5 ms, as in Figure 8.

Figure 10.

Arbitrary pattern; (Left) User defined Time Features for the magnetic field X and Y, composed of several Time Features. (Right) Energy fluence map shows that protons are delivered at a certain point, then moved in a circle about this point, with the motion repeated in a grid pattern.

Figure 11.

Spot scanning simulation; (Top left) Time Features for magnetic field X and Y. (Middle left) Number of simulated histories. (Middle right) Time Feature energy and peak width with mean kinetic energy from phase space at isocenter. (Bottom left) Energy fluence map at isocenter with averaged positions per every 10 milliseconds. (Bottom right) Energy spectra at isocenter for each of the time intervals $T1$, $T2$, $T3$, etc.