Monte Carlo Techniques in Radiotherapy

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Abstract: Monte Carlo techniques for radiation transport in materials are described and several examples of their use in modern radiotherapy dosimetry and treatment planning are presented.

INTRODUCTION

Although the physics of photon and electron interactions in matter is well understood, in general it is impossible to develop an analytic expression to describe particle transport in a medium. This is because the electrons can create both photons (*e.g.*, as bremsstrahlung) and secondary or knock-on electrons (δ -rays) and conversely, photons can produce both electrons and positrons. In addition, both electrons and photons scatter a great deal. Figure 1 shows an example of a single 10 MeV photon incident on a slab of lead and the complexity of the possible interactions is clear.

One widely used technique for solving this problem involves Monte Carlo simulation of radiation transport in which one uses knowledge of the probability distributions governing the individual interactions of electrons and photons in materials to simulate the random trajectories or histories of individual particles. One keeps track of physical quantities of interest for a large number of such histories to provide information about required quantities and their distributions.

Monte Carlo techniques are becoming more and more widely used. In general this is because the cost of computing continues to decrease dramatically. In medical radiotherapy physics this increase is also because of the availability of general purpose and specialised code systems, such as EGSnrc[1, 2] and BEAM[3] described below.

A Simple Example

To understand what is meant by the Monte Carlo technique it is useful to consider a very simple example. Consider the transport of a photon though a large slab of some material. If the energy is high enough (> 1.022 MeV), there are only two significant processes that we need to consider, namely Compton scattering (in which the photon changes direction and loses energy to an electron which is set in motion) and pair production (in which the photon disappears and an electron and positron share its energy). The total probability per cm of a photon interaction is constant and given by Σ_{total} (units are cm⁻¹), which is made up of the probabilities for each of these interactions (*i.e.*, $\Sigma_{\text{total}} = \Sigma_{\text{compton}} + \Sigma_{\text{pair}}$). In our Monte Carlo simulation, we will track many photons as they enter the slab of material. We need to determine how far each photon travels before interacting, and which interaction takes place.

To do this requires the use of random numbers. It is this use of random numbers which first led to the name Monte Carlo for this technique. It is worth noting in passing that a



Figure 1: A 10 MeV photon (dotted line) is incident from the right on a slab of lead. A pair production event occurs and produces an electron (solid line) and a positron (long dashed line). The electron scatters many times and loses energy to low energy particles. The electron gives off a bremsstrahlung photon near the bottom of the figure. The positron also scatters many times and loses energy and then annihilates in flight (if it were at rest, the two 511 keV photons would be given off at 180 degrees to each other). The 511-keV photon coming back towards the surface Compton scatters, creating another electron and scattering, apparently at 90 degrees. The figure is an EGS_Windows output from an EGS4 simulation.

very active field of research is devoted to selecting numbers which really are random, and to determining what it means to be random. Today it is possible to get sequences of random numbers which are 10^{40} numbers long or more (see, for example refs [4, 5] and references therein).

So how do we determine how far a photon goes before it interacts? We know the cross sections and that the pathlengths are exponentially distributed. First we select two random numbers, R1 and R2, which are uniformly distributed between 0 and 1. If we take the distance the photon travels before interacting to be $x = -ln(R1)/\Sigma_{total}$ cm, the set of distances sampled this way is exponentially distributed from 0 to infinity with a mean of $1/\Sigma_{total}$. This is exactly how photons interact in a material and thus we have answered the first question. The second question is, after going x cm, which interaction occurs? We answer this by asserting that if $R2 < \Sigma_{compton}/\Sigma_{total}$, a Compton scattering event occurs. Otherwise a pair production event occurs.

In this simple example we have seen how random numbers are used to make decisions about how the histories of individual particles are simulated. We have had to make use of the known physics. These same principles are applied to all of the other aspects of the simulation, and although the details get more complex, the principles are the same. So, for example, to determine the scattering angle and energy of a secondary electron in a Compton scattering event, we make use of the Klein-Nishina cross section for Compton scattering and use a random number to sample the scattering parameters. As is often the case, very clever techniques need to be developed to do this sampling both accurately and rapidly, since a simulation might have to follow several billion particles to get adequate precision.

But the example is not yet complete since we have not collected any information. The second component of any Monte Carlo simulation of radiation transport is to keep track of, or "score" the quantities of interest. In our simple example we might score the average distance travelled before an interaction, or the fraction of interactions which are pair production events. In this case the scoring is close to trivial, but in more realistic simulations, efficiently scoring quantities of interest can become an art as well as a science.

Geometry Considerations and Electron Transport

In this simple example we have not introduced the other major complication in real simulations, namely handling the geometry of the problem. In principle this is a straightforward issue for Monte Carlo techniques, since the particle track can be broken up into individual segments, each of which can be considered to occur in a single material and region. As one crosses the geometric boundary one needs to change cross-sections if the material changes, and one has the choice of reselecting a new distance x to travel in the new medium, or of keeping track of how many mean free paths were traversed in the previous medium and converting the remaining mean free paths into the physical distance in the new medium using the new cross-sections. This choice comes about because once a particle has reached a given point, the probability of interacting in the new medium is independent of how far it travelled in the previous medium. Although a great strength of Monte Carlo is that the geometry and transport problems can be separated, handling the geometry can, in general, be very complex, but it is essentially book-keeping.

However, the geometry can introduce one severe complication for electron transport simulations. This is a result of how electron paths are simulated. As an electron slows down in a material, it can undergo hundreds of thousands of scattering events in which it is deflected slightly but loses virtually no energy. Berger[6] first introduced the condensed history technique in which electron histories were "condensed" into a series of steps in which the effects of many scattering events were considered at once and a multiple scattering theory used to account for the elastic and inelastic scattering during this step. Although the individual steps of an electron are simulated as if they go in a straight line, this straight line only represents the net effect of an ensemble of curved paths. Away from boundaries this model can be very accurate, but near boundaries between media that differ substantially, the model breaks down because it doesn't account for the part of the ensemble of paths which actually occurs in the second medium. Solving this problem has been very complex in the general case and has required the development of new multiple scattering theories and very complex algorithms for transporting electrons, including reverting to modelling single scattering events near boundaries. The problem has been solved, primarily by Kawrakow and Bielajew working at NRC and a paper by Kawrakow describes his implementation of these advances into EGSnrc, a new version of the EGS4 code system[1]. The same paper gives a complete set of references to the various prior papers.

THE EGS CODE SYSTEM

The EGS (Electron-Gamma-Shower) code system for Monte Carlo simulation of electron and photon transport[2, 7, 8, 9] is one of three main general purpose code systems (the others are PENELOPE[10] and various codes based on Berger and Seltzer's ETRAN code[11], *e.g.*, the ITS[12] and MCNP4[13] systems). The EGS system started as a high-energy physics tool which was developed at the Stanford Linear Accelerator Center (SLAC) by Richard Ford and Ralph Nelson in the mid-seventies. During the eighties NRC and SLAC collaborated to make EGS also work in the energy regime of interest in medical physics, *viz* 10 keV to 50 MeV rather than just that of high-energy physics (100 MeV to 100 GeV).

The beauty of the EGS system is that a structured set of subroutines handles all of the physics in the simulation in a manner which allows users to write their own geometry and scoring routines without actually touching the EGS system itself. Figure 2 presents this structure. The user is responsible for writing the routines which define the geometry using a very simple but general interface (HOWFAR and HOWNEAR) and a scoring routine (AUSGAB) which is called under well-specified conditions which allow the user to score virtually any parameter of interest. For example, the user can arrange to have the scoring routine called before and/or after any class of interaction, to score where they occur, how often they occur,



Figure 2: Structure of the EGSnrc code system. The components of the user-code above the dashed line are written by the user and those below the dashed line are part of the EGSnrc code system. From ref [2].

what happened during the interaction, etc.

The figure provides a summary of all the physical processes modelled by the EGS system: annihilation of positrons at rest or in flight; inelastic Moller and Bhabha scattering of electrons and positrons (respectively) from atomic electrons; bremsstrahlung production by positrons and

electrons from interactions with the nucleus and atomic electrons; elastic multiple and single scattering of electrons and positrons from nuclei and atomic electrons; pair production by photons; Compton scattering of photons from bound atomic electrons; photoelectric interactions of photons with atomic electrons; Rayleigh coherent scattering of photons from atoms; and relaxation of the atom by production of fluorescent x-rays and Auger electrons. For a general introduction to these processes, see any radiation physics textbook such as Attix[14] and for detailed information on how they are modelled in EGSnrc, see the manual[2]. The figure also highlights an important component of any simulation system, *viz* the generation of cross section data for all the physical processes involved. The EGSnrc system uses a variety of data sources, some prepared ahead of time by the PEGS4 data preparation package, the rest picked up from individual data bases. All of these data are picked up by the routine HATCH.

The EGSnrc and EGS4 systems are on-line at http://www.irs.inms.nrc.ca/inms/irs/irs.html.

APPLICATIONS OF MONTE CARLO IN MEDICAL PHYSICS

The Monte Carlo technique has been used very extensively in medical physics applications. These have been described in a variety of review articles[15, 16, 17, 18, 19] and only a few highlights will be mentioned here.

Brachytherapy Calculations

Brachytherapy is the use of encapsulated radioactive sources to treat cancer (see the paper by Beaulieu in this same issue or Williamson[20]). Many problems occur when trying to measure the dose around such sources and Monte Carlo has been used extensively to sort these problems out. For example, Williamson and colleagues have developed a very sophisticated photon Monte Carlo code which is optimised for dose calculations around a brachytherapy source (see [20] and references therein). They have used this code to calculate extensive tables of dose distributions around brachytherapy sources. The dose drops off rapidly with distance from the source and the variation of dose with angle must be accounted for since routine measurements are made in one orientation and this does not represent the entire 4π geometry of the source. These calculations, and others like them have become the basis of a detailed dosimetry protocol for brachytherapy (TG-43[21]). Not only are Monte Carlo calculations used to provide detailed dose distributions, they are used to calculate such things as the relationship between the air kerma (or exposure) measured in-air on the transverse axis (which is what can be routinely measured in a clinic) and the absorbed dose in a water or tissue phantom surrounding the source (the clinically relevant quantity). Monte Carlo has also been used to identify and explain the effect of ignoring the existence of fluorescent x-rays created in the material used to encapsulate the $^{125}\mbox{I}$ sources.

Ion Chamber Dosimetry

lon chambers are the most commonly used devices to measure the amount of radiation present in both radiotherapy physics and radiation protection situations. The charge measured from the ion chamber is used to determine either the absorbed dose in a medium (such as tissue or water) or the air kerma when the beam is in air (the kerma is a measure of how much energy is transfered to the electrons in the air). Monte Carlo calculations have become an essential component of the conversion from measured charge to the dose or the air kerma. In the next two sections we describe 2 specific examples of how Monte Carlo has become an essential part of dosimetry.

STOPPING-POWER RATIOS

One of the earliest and most critical applications of Monte Carlo techniques in medical physics has been in the calculation of stopping-power ratios, denoted $(\overline{L}/\rho)_{air}^{med}$, where the stopping power of a medium quantifies how much energy an electron loses per unit pathlength. Stopping-power ratios relate the dose measured in the air in an ion chamber, D_{air} (proportional to the measured charge), to D_{med} , the dose in the medium, via $D_{med} = (\overline{L}/\rho)_{air}^{med} D_{air}$. They must be known for dosimetry in electron beams because the dose per unit signal varies by about 15% as a function of incident beam energy and depth. The first step in the calculation of stopping-power ratios is to use Monte Carlo techniques to obtain the fluence of electrons in the undisturbed medium at the point of the ion chamber and from this the stopping power is averaged over the fluence spectrum (see ICRU Report 35 for a detailed discussion[22]). Berger[22, 23] provided extensive sets of calculated stopping-power ratios for use in radio-therapy electron beams. He made the approximation that the incident electron beams were mono-energetic. Nonetheless, these values were used for many years by major protocols for clinical reference dosimetry since this was the best there was[23, 24].

As will be discussed below, the BEAM code has allowed for detailed simulations of realistic beams from clinical radiotherapy accelerators. This has allowed for more accurate calculations of stopping-power ratios in these realistic beams and the new stopping-power ratios have been shown to be different from the values for mono-energetic beams used previously. Figure 3 shows what happens when a realistic model of the accelerator beam is used. The differences could lead to nearly 2% errors in the clinic and thus these new, more accurate stopping-power ratios have been used in the most recent dosimetry protocols[25, 26]



Figure 3: Variation of stopping-power ratios and hence dose per unit charge measured by an ion chamber in a 20 MeV electron beam used for radiotherapy. The 15% change with depth is why calculated stopping-power ratios are critical for clinical dosimetry. The differences of up to 1.6% between using a mono-energetic beam of electrons in the calculations and using a full simulation of the electron beam, is an example of how the BEAM code is being used to improve clinical dosimetry. From [27].

WALL ATTENUATION CORRECTIONS FOR PRIMARY STANDARDS OF AIR KERMA

It is important that the measurement of dose delivered in cancer radiotherapy in Canada give the same results as that in the US, France, the UK and the rest of the world. To accomplish this, each major country has primary standards of air kerma which have been the basis of calibrations for ion chambers used in the clinic. Air kerma is the kinetic energy released in the air in the absence of the ion chamber. Until recently, all clinical dosimetry was based on these calibrations. The primary standards in each country (maintained at NRC in the case of Canada) are independent of other standards, but there is an extensive history of comparisons of the standards around the world to ensure that each country is coming as close as possible to measuring the air kerma accurately.

To establish the primary standards for air kerma, each lab uses a graphite walled ion chamber and requires a variety of correction factors, the most important of which is the correction for the attenuation and scatter of photons in the walls of the ion chamber, K_{wall} . Traditionally this correction was determined by adding a series of extra walls around the ion chamber. As this is done, the response of the ion chamber decreasess linearly with the extra wall thickness. The instinctive reaction of any good physicist is to linearly extrapolate the readings back to a zero wall thickness and assert that this corrects for the attenuation and scatter by the walls. This was the technique used by most labs, including NRC, for many years.

However, by the mid-eighties it was possible to calculate wall attenuation corrections using Monte Carlo techniques. One of the advantages of the Monte Carlo technique is that you don't need to model the physics in accordance with nature. To evaluate the wall attenuation and scatter correction one does two separate calculations, one with the correct physics and one which ignores the attenuation and scatter in the wall (i.e., after each photon interaction, the original photon continues in its original direction and no scattered photon is created). The ratio of the dose to the air in the cavity in these two situations is, by definition, the correction for attenuation and scatter in the walls of the chamber. These calculations agreed very well with the experimental data as the extra wall thickness was added, but they failed to agree with the extrapolation to zero wall thickness by up to 1%, which is considered a huge error in this type of work[28].

The resolution of the mystery was provided by Alex Bielajew who used a simple model for spherical chambers to demonstrate that the extrapolation was non-linear and agreed with the Monte Carlo results for spherical chambers[29]. Despite this, people in standards labs were reticent to accept the Monte Carlo approach for over 10 years. The astute reader will be asking, "Why didn't they just do the measurements with much thinner walls and verify the extrapolation directly?" The problem is that ion chamber walls must be a minimum thickness to allow for electron buildup, or else there is virtually no response from the ion chamber. Thus, making the walls thinner is not an option.

At their biennial meeting in 2001, the various standards labs (finally) agreed to change to using the Monte Carlo corrections because of convincing new experimental evidence. On the one hand, an NRC group led by John McCaffrey and Ken Shortt did a series of measurements with a flat, so-called pancake ion chamber. They showed that irradiating the chamber from the front or the side caused a 9% change in the chamber reading. The EGSnrc Monte Carlo calculations predicted this change within 0.2% and showed that the change was almost entirely

due to the change in the attenuation and scatter correction. A group from the German and Hungarian standards labs (PTB and OMH) led by Ludwig Büermann and Michael Krammer presented data demonstrating that using the linear extrapolation technique to determine the wall correction factors led to 5% inconsistencies in the reading corrected for wall attenuation and scatter if the beam was incident from the side or end of cylindrical or pancake chambers. In contrast, their data showed that the Monte Carlo technique led to a consistent result.

The change to using the wall attenuation and scatter corrections is also accompanied by a change to using Monte Carlo corrections, K_{an} to account for the fact that real photon beams are diverging from a point source rather than being parallel beams as assumed in the underlying theory. The combination of these two changes implies an increase in the air-kerma standards of the world which averages 0.9% (see figure 4), a remarkable change given that previously most standards were thought to agree within 0.2% with the global average. Fortunately, such a change, although large by standards labs criteria, has little clinical impact.



Figure 4: The "as reported" ratios of air-kerma rates of various primary standards laboratories to the rate at the international standards laboratory (BIPM) and the same results after applying both the K_{wall} and K_{an} corrections as obtained from Monte Carlo calculations. Note that not only has the average value gone up with the revised values, but there is a change in the baseline of the BIPM of 0.4%. The solid horizontal lines are averages of the results. From [30].

Modelling Radiotherapy Beams

Radiotherapy beams from linear accelerators are very complex. Some are high energy electron beams, made uniform by one or two thin scattering foils and shaped by thick metal devices called applicators. More commonly they are high energy x-ray or photon beams cre-

ated as bremsstrahlung as the electrons are stopped in thick high-Z targets and then made uniform across the field by a flattening filter designed to attenuate the centre of the beam much more than the edges and shaped by thick jaws or multi-leaf collimators. Researchers had successfully modelled various clinical accelerators but in the past these models required significant simplifications of the accelerator, or were applicable to only one type of accelerator. In 1995 the BEAM code[3] was released for general use and has become very widely used for many research purposes. BEAM was designed to model all types of radiotherapy accelerators (as well as 60 Co units and x-ray units). Figure 5 shows a model of an electron beam from a Therac 20 accelerator which was manufactured in Canada. The model of the accelerator is built from a series of component modules (CMs), each of which can be re-used several times in the accelerator and each of which has two surfaces perpendicular to the axis of the accelerator (eg the JAWS CM is used to model the jaws which limit the beam when used in photon beam mode and in this case the electron applicator made of parallel bars, or the CHAMBER CM is used to model the details of the monitor ion chamber that controls the total dose delivered in a treatment). The primary output of the simulation is a large file containing the phase space information about all the particles leaving the accelerator as well as information about where each particle has interacted in the accelerator. This file can be used directly in further BEAM calculations (eg to determine the effect of beam modifiers such as lead blocks or cutouts to shape an electron beam) or as input to a simulation to determine the dose distribution in a model built from the CT scan of the patient.



Figure 5: Model of an AECL Therac 20 accelerator as produced by BEAM and the EGS_Windows graphics package, a general purpose tool for tracking EGS simulations in 3D. Sitting at a terminal one had full 3D control of the display: rotation, zoom, various particles on/off etc. For a colour version, see the cover of the Sept 1995 edition of Physics in Canada (Vol 54 (#4)).

Since the BEAM code was designed from the beginning to model radiotherapy sources, its geometry routines are optimised for these simulations and the code has a variety of built-in variance reduction techniques which can improve the efficiency of a given calculation by a factor of more than 25. For example, electrons below a specified energy which cannot reach the patient plane are discarded rather than needlessly tracked, and bremsstrahlung splitting is used to increase the number of photons created each time an electron gives off a brem photon since tracking electrons takes much more time than tracking photons.

The code is also designed to run in parallel on an arbitrary number of linux machines. This is essentially a trivial procedure (except for bookkeeping) for Monte Carlo calculations since each simulated history is independent of the others and hence in the limit, one could do each history on a different machine and just add up the results at the end. This capability is dependent on the fact that modern random number generators are capable of initiating a very large number of sequences which are known to be independent[5].

The BEAM code has been used for a wide variety of research projects, from developing models of radiotherapy beams (which are then used as part of the PEREGRINE commercial treatment planning system[31]), to doing dosimetry studies such as that mentioned above regarding stopping-power ratios, to helping to develop improved accelerator characteristics.

Monte Carlo Treatment Planning

THE OMEGA PROJECT

When the BEAM code was developed in the early nineties, it was within the larger OMEGA project (a collaboration between NRC, the University of Wisconsin and the Ottawa Cancer Clinic) which was to develop a 3-D dose calculation engine for use in clinical treatment planning systems for electron beam therapy. The goal of clinical treatment planning is to find the best way to maximise the dose to the tumour and minimise the dose to the healthy tissue and, in particular, to minimise the dose to radiation sensitive organs such as the spine or eyes. An important step in this process is to calculate the dose distribution in the patient accurately. Most current commercial systems for electron beams use an analytic calculation to determine these dose distributions. These can have significant errors near inhomogeneities in the patient (10 to 20% errors in bad cases). In addition, Monte Carlo calculations for electron beam dose distributions are about an order of magnitude faster than for photon beams (where the analytic models are also much more accurate). Hence the OMEGA project's goal was to develop electron beam dose calculation capabilities, although the resulting codes work equally well for electron and photon beam therapy. The project developed a code, called DOSXYZ, which calculates the dose distribution in a patient defined by a CT data set. The program handles the complexities of the accelerator beam coming in at an arbitrary angle and the problem of defining the materials and densities to be used in the Monte Carlo simulation based on the CT data, but otherwise is a relatively simple Monte Carlo code which only needs to simulate rectangular parallelepipeds with different materials. While BEAM and DOSXYZ are still used to define the "gold standard" for many Monte Carlo calculations, there have been some truly remarkable developments in the last few years which have taken the concept of using Monte Carlo for clinical treatment planning out of the research lab and into commercial implementations.

VMC and VMC++

Starting in the mid-nineties, Kawrakow and Fippel, originally working in Germany, started work on what they called the voxel Monte Carlo method to allow for much faster Monte Carlo calculations of dose in a patient phantom. Their code for electron beam calculations, VMC, was a factor of about 30 to 40 faster than the standard EGS4 calculations and maintained comparable accuracy in patient phantoms[32]. Shortly thereafter, Kawrakow moved to NRC and worked on improving highly accurate Monte Carlo techniques for what became EGSnrc. In the meantime Fippel created a code he called XVMC to allow fast Monte Carlo calculations using the principles developed for the VMC code. In the summer of 1999 Fippel came to NRC for 4 months to work with Kawrakow. By the end of the summer they had sped up the photon beam code system by an order of magnitude so that a Monte Carlo calculation for photon beams could be done in a matter of minutes on a 500 MHz PC[33]. The code made use of some highly innovative variance reduction techniques including photon splitting, electron history repetition, Russian Roulette and quasi-random numbers. Over the next year Kawrakow reworked the code into C++ and called it VMC++ which has a variety of further improvements, in particular a technique called STOPS (Simultaneous Transport Of Particle Sets)[34]. With all of the improvements made to the code, it runs 50 to 80 times faster than EGS on a similar calculation and has almost the complete accuracy of EGSnrc. For some standard benchmark calculations, the VMC++ code does an electron beam calculation in about 35 s on a 500 MHz machine (and 3.5 times faster machines are available today for about \$1000) and photon beam calculations take about 360 s. This code represents such a significant advance that it was almost immediately commercialised by Ottawa based MDS Nordion which is one of the major players in the world market for treatment planning systems, Figure 6 shows a simulation of a treatment. The system is currently under test in some clinics (Dec 2001) and will be available soon.

With these developments reaching clinics in the next few years, the issue of accuracy in dose calculations for external beam radiotherapy, long an area of intense research interest, will be behind us and the search will be on for more accurate and effective delivery of the treatments (as discussed elsewhere in this issue).

CONCLUSION

Monte Carlo techniques have become widely used in Medical Physics because of the availability of powerful codes such as BEAM, EGSnrc, PENELOPE and ETRAN/ITS/MCNP and because of the massive increase in computing power in the last decades. Both trends can be expected to continue so that Monte Carlo techniques for radiation transport will only continue to increase in importance in the next decade or two. In the short term, the commercial application of codes such as VMC++ should start to make Monte Carlo the standard technique for clinical treatment planning calculations. As computing power continues to increase it is likely that the research emphasis will change from studying dose deposition and other physical processes using Monte Carlo simulation of the passage of radiation through matter to studying biological processes induced by this same radiation.



Figure 6: Cutaway rendering of an electron beam dose calculation for the chest wall. The goal is to adjust beam parameters to avoid dose to the lung. The patient's anatomy is represented by a CT scan which is used to map the beam interaction properties for the individual patient. Lines to represent calculated isodose levels are superimposed on the CT scan for visualization and evaluation. The Monte Carlo dose engine was developed by Iwan Kawrakow of NRC and is driven by a new electron beam model developed by MDS-Nordion. The complete system is commercialized within the treatment planning system of MDS-Nordion. Rendering produced by Tomas Lundberg of MDS-Nordion.

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