Conf-950420--2

UCRL-JC-118754
PREPRINT

ELECTRON TRANSPORT IN RADIOTHERAPY USING LOCAL-TO-GLOBAL MONTE CARLO

M.M. Svatos*, C. T. Ballinger‡, H. Neuenschwander§, T. R. Mackie†,
W. P. Chandler*, C. L. Hartmann Siantar*, and J. A. Rathkopf*

*Lawrence Livermore National Laboratory
7000 East Avenue
Livermore, CA 94550

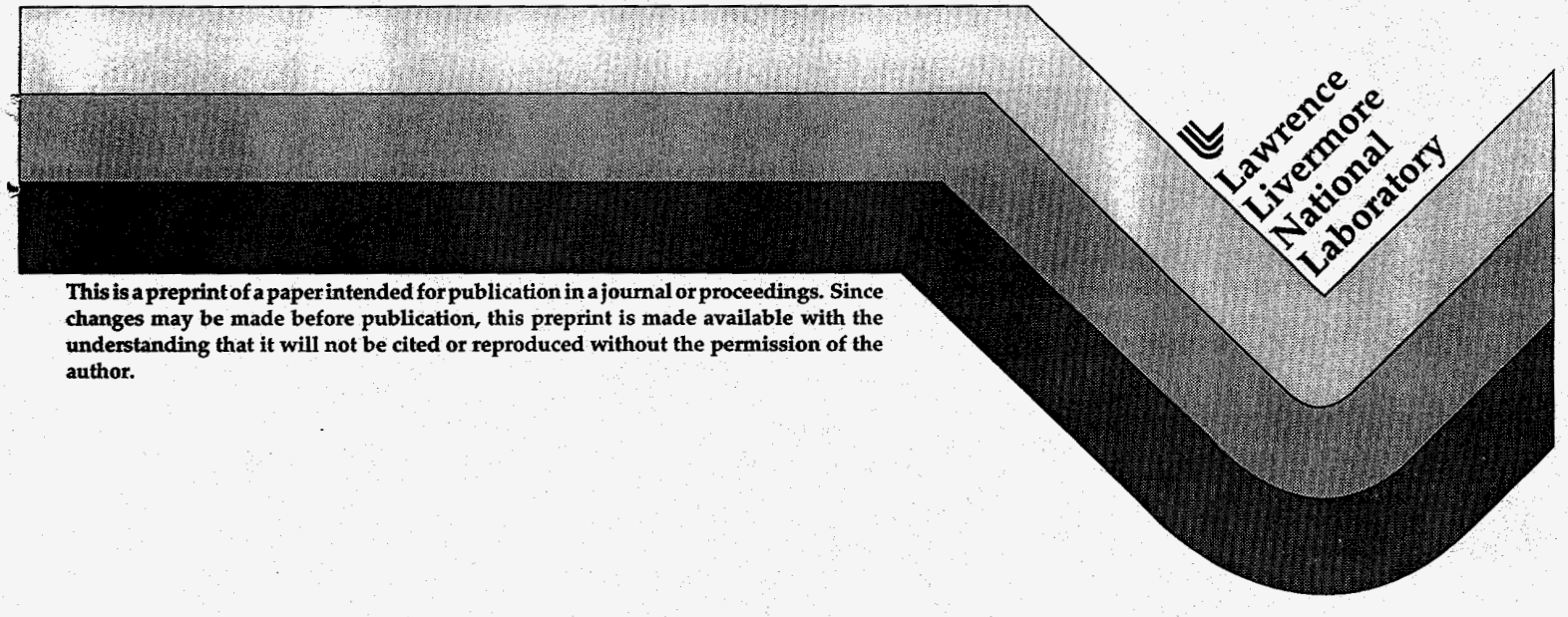
†University of Wisconsin-Madison
1300 University Avenue
Madison, WI 53706

‡Albany Medical Center
Radiation Oncology Department A-137
47 New Scotland Avenue
Albany, NY 12208

§Department of Medical Radiation Physics
University of Bern
Inselspital, CH-3010
Bern, Switzerland

This paper was prepared for submittal to
Proceedings of
International Conference on Mathematics
and Computations, Reactor Physics,
and Environmental Analyses
Portland, Oregon
April 30–May 4, 1995

September 1994



ELECTRON TRANSPORT IN RADIOTHERAPY USING LOCAL-TO-GLOBAL MONTE CARLO

M.M. Svatos*, C.T. Ballinger‡, H. Neuenschwander§, T.R. Mackie†, W.P. Chandler*,
C.L. Hartmann Siantar*, J.A. Rathkopf*, P.J. Reckwerdt†

*Lawrence Livermore National Laboratory
7000 East Avenue
Livermore, CA 94550

†University of Wisconsin-Madison
1300 University Avenue
Madison, WI 53706

‡ Albany Medical Center
Radiation Oncology Department A-137
47 New Scotland Ave
Albany, New York 12208

§Department of Medical Radiation Physics
University of Bern
Inselspital, CH-3010
Bern, Switzerland

ABSTRACT

Local-to-Global (L-G) Monte Carlo methods are a way to make three-dimensional electron transport both fast and accurate relative to other Monte Carlo methods. This is achieved by breaking the simulation into two stages: a local calculation done over small geometries having the size and shape of the "steps" to be taken through the mesh; and a global calculation which relies on a stepping code that samples the stored results of the local calculation. The increase in speed results from taking fewer steps in the global calculation than required by ordinary Monte Carlo codes and by speeding up the calculation per step. The potential for accuracy comes from the ability to use long runs of detailed codes to compile probability distribution functions (PDFs) in the local calculation. Specific examples of successful Local-to-Global algorithms are given.

I. INTRODUCTION

Electron transport is of central importance to calculations in radiotherapy physics. Regardless of whether photon or electron incident beams are used, it is through the electrons that much of the energy is ultimately transferred to the medium. There are at least two distinct physical characteristics of electrons that complicate their simulation: (1) their electric charge, which causes them to interact almost continuously with the medium, and (2) their light mass, which causes them to be deflected through relatively large angles compared to heavier charged particles like protons and alpha particles.

A. Conventional Electron Monte Carlo Algorithms

1. Analog Monte Carlo. Perhaps the most intuitive way to simulate charged particle transport is to assume the point of view of the particle and devise an algorithm which imitates the physics of each interaction while traversing the medium. This "analog" or "single scatter" algorithm is directly analogous to the uncharged particle algorithms that are already widely used for neutron and photon transport. Although the types of interactions are different in the case of charged particles, the code can proceed from interaction to interaction in an exactly analogous manner.

The analog method is potentially the most accurate method of electron simulation if the radiation source and phantom (or patient) are accurately modeled and a large number of histories are run but it is also very time consuming due to the number of interactions that must be modeled: even when excitations are excluded

from the modeled interactions, electrons still collide with the medium $10^4 - 10^5$ times as often as neutrons in the radiotherapeutic energy range. Most of these individual interactions only change the electron energy and trajectory a small amount, but their cumulative effect is significant.

A simulation for radiotherapy using an analog method could take days or weeks to run on a typical workstation. It is thus not appropriate for clinical use; in fact, this method is almost never used for electron transport in any application.

2. Condensed History Monte Carlo. The technique of condensed history [1] is the most prevalent type of electron transport. It circumvents the problem of too many interactions by "condensing" the effect of numerous collisions into a single "step" through the medium. Rather than attempting to model all interactions, a representation of the aggregate effect of multiple collisions after a given step size is made.

In condensed history methods, there are three categories of approximations made concerning the net effect of many interactions on the energy loss and spatial positioning of the electron. A multiscatter angular deflection distribution (usually that of Moliere [2] or Goudsmit-Saunderson [3]) is used to select the scattering angle at the end of a step. A straight-line approximation, modified by a correction to take into account that the electron is not exactly traveling in a straight path during the step, is included. Finally, an expression for energy loss during a step is also required, which should account for the statistical variation in the energy deposited for a given distance traveled.

As a result of relying on empirical approximations, condensed history methods have a limited range of validity. For example, Ballinger has shown [4] that at low energies (below a few keV) the results of Class I condensed history codes such as ETRAN [5], ITS [6], and MCNP [7] are inaccurate. This is primarily because they rely on a Landau distribution [8] for energy loss, which allows the possibility of large energy losses, but deposits the energy locally instead of transferring it to secondary electrons. It is thus not valid for situations involving secondary disequilibrium. Class II electron transport codes, such as EGS4, explicitly transport secondary electrons above a threshold energy, but they also break down at low energies. This is due in part to the small sub-step sizes that are used at low energies; very small sub-steps do not contain enough interactions to make the (Moliere) multi-scatter distributions valid. [1] Short sub-steps not only cause the simulation to slow down, they often cause inaccurate electron energy loss. In both class I and class II algorithms, large sub-steps increase the efficiency, but the results can be inaccurate due to poor representation of the electron location, since the straight flight path approximation becomes worse as the step size increases.

B. Principles of Local-to-Global Transport

Recently several charged particle transport algorithms have emerged which can generally be classified as Local-to-Global Monte Carlo transport. The purpose of Local-to-Global Monte Carlo codes is to provide much of the accuracy of other Monte Carlo codes without carrying out the same time–consuming calculations. It will be shown that this can lead to speed up factors sufficiently large to make analog codes practical for use in part of the L-G transport.

Local-to-Global Monte Carlo methods use a "local" calculation, carried out only once, to generate data that can be read by the patient-specific "global" calculation. The technique consists of completing high-statistic runs of a traditional Monte Carlo code having initial conditions (such as material type and energy) that are likely to be needed in future calculations. The net result of running a series of local calculations is a permanent library of probability distribution functions (PDFs), each of which represents the change in a phase space variable that the electron experiences upon exiting a selected volume. A separate PDF is computed for each incident energy of interest and for each relevant material type. The volume through which the local calculation is carried out is termed the "local geometry". The shape of the local geometry must be chosen judiciously because it will determine the shape of the steps in the global calculation.

[1] An exception is Bielajew's recent single-scatter extension of the Moliere theory for EGS4 [9].

The global calculation is done every time a user wants to simulate electrons traveling through a mesh such as a CT scan. The code selects a step size based on the distance to a boundary in the global geometry and the sizes available in the PDF library. The output state after a step is then determined by interpolating between the PDFs appropriate for the energy and material of the electron.

For each step, the incident phase space on the local geometry is the exit phase space of the previous step. Transport is thus reduced to sampling PDFs, updating the electron's phase space and depositing the energy difference between steps. This continues until the electron is either below the cut-off energy or has escaped the global geometry.

II. OVERVIEW OF TWO SUCCESSFUL L-G ALGORITHMS

At least two examples of Local-to-Global Monte Carlo transport codes have achieved excellent results. On the fast end of the spectrum is the Macro Monte Carlo (MMC) method, which was conceived to improve the speed of condensed history codes without a significant loss of accuracy. It has obtained results in very good agreement with EGS4 [10] for radiotherapy dose distributions in times that are a factor of 10-20 faster [11]. On the highly accurate end of the spectrum, the Response History method has yielded results that are in very good agreement with single electron scattering (analog) results, which has been instrumental in exploring the situations under which the assumptions in other algorithms break down [4]. Together, these two codes illustrate that the Local-to-Global Monte Carlo method is capable of achieving both speed and accuracy.

A. Macro Monte Carlo

1. Algorithm. The concept of Local-to-Global Monte Carlo was first proposed in the literature by Mackie and Battista [12] in 1984. They proposed an algorithm called Macro Monte Carlo (MMC) which would use cubical voxels as the local geometry. The proposal was never implemented due to (what seemed in 1984 to be) unfeasibly large memory requirements to store the PDFs.

The Macro Monte Carlo method was implemented more recently (1992) by Neuenschwander and Born [13], who reduced the storage required. This was possible by using a more symmetric spherical local geometry and assuming perpendicular incidence. The spherical volume elements were dubbed "kugels". (*Kugel* means "sphere" in German.) Several other clever enhancements have made this method extremely fast and a viable option for clinical electron simulation [11].

The improved MMC algorithm of Neuenschwander *et al* features a range of possible kugel sizes from 0.05 to 0.3 cm in radius. This allows the user to take smaller step sizes as a significant boundary is approached, providing accuracy where it is important. At the same time it is possible to take large, efficient steps through the homogeneous portions of the patient or phantom. In order for this adaptive step-size algorithm to work efficiently, the volume is pre-processed and a maximum kugel size index assigned to each zone. Although the pre-processing requires an initial computational investment, the investment is more than returned in seconds or minutes into the transport calculation.

The MMC algorithm also uses energy partitioning across each boundary to account for differences in collision stopping powers on both sides of that boundary. This provides a reasonably accurate and very fast way to deposit energy on either side of the boundary.

For each material, kugel size and electron energy, the distributions of primary electrons emerging from the kugel are stored in 100 equi-probable bins for efficient sampling. Thus the determination of particle parameters after an MMC transport step is reduced to determination of a table index, which is much faster than random interpolation of cumulative PDFs.

Secondary energy for both photons and electrons is released into the local kugel and scored "on the fly". Later it is "transported" (smeared forward in the incident direction and exponentially attenuated) and deposited in a post-process ray-tracing step after the actual simulation. Like the pre-processing step, the post-processing step gives a large gain in efficiency. Although this type of secondary transport is extremely quick, it is also probably the most significant limitation on the accuracy of the MMC method. By not explicitly modeling secondary electrons, the MMC code tends to flatten out discontinuities in dose across interfaces. It ignores the secondary electrons that are sensitive to changes in the scattering properties of different materials. New algorithms for secondary transport are being explored.

2. Results of Macro Monte Carlo. The MMC algorithm has been proven to be both accurate and fast. In phantom studies, MMC results agreed to within 5% of EGS4 calculations [11]. While differences of up to 10% were observed in small air cavities, the dose to air is not usually relevant for radiotherapy planning. It is possible that a 5% discrepancy with EGS4 near tissue inhomogeneities may be of clinical significance in a few cases, since EGS4, like other condensed history codes, is known to underestimate the dose at boundaries due to its inability to model backscatter properly [14]. However, for most cases this difference is not clinically relevant.

The most impressive aspect of MMC is its efficiency. It has shown speed-up factors of 10-20 over EGS4, depending on the complexity of the geometry in the global calculation [15]. As an example, a CT-based calculation of a 10 MeV electron beam incident on a 5 cm x 3 cm sinus field took about 11 minutes on a DEC AXP 400, with an average statistical accuracy of 2% in voxels near the maximum dose. The dose grid resolution in this example was 0.25 cm; the same simulation was done over a dose grid resolution of 0.5 cm took only 1.8 minutes. The MMC code takes approximately 10 MBytes of memory for an 80x80x80 density grid and a 64x64x64 dose grid.

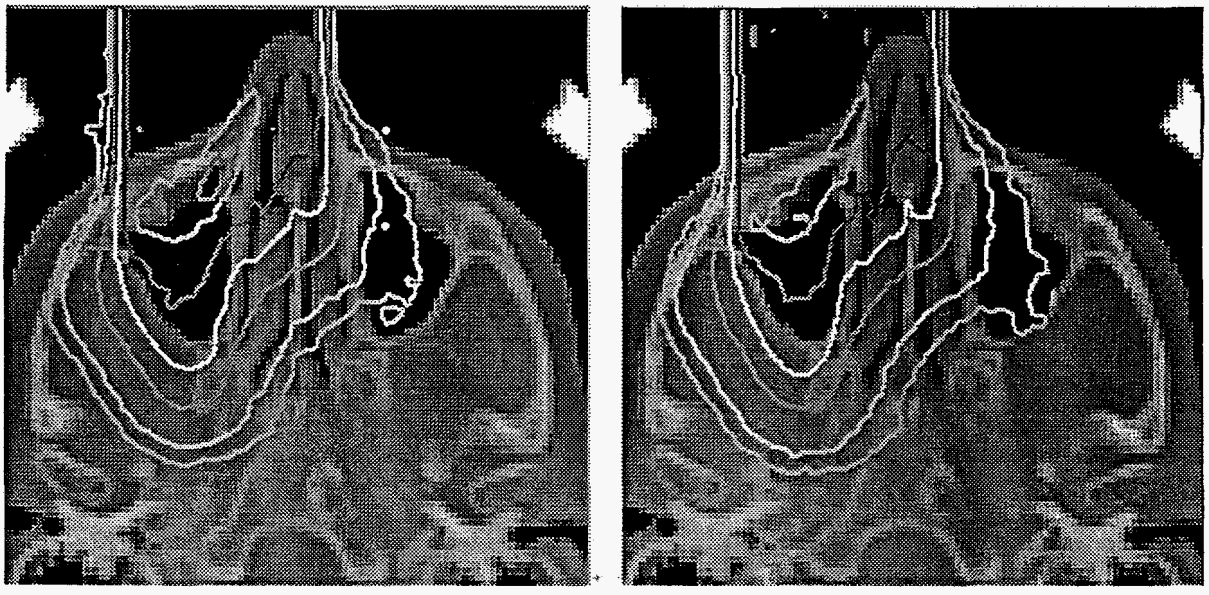


Figure 1: A comparison of dose distributions in a patient head. On the left is the result from an EGS4 calculation. The highest isodose line is a small 90% contour in the anterior region of the left sinus, followed outward by the 80%, 70%, 60%, 50%, 40% and 30% contours. On the right is the same calculation done with the MMC method; the central isodose line is 80%, the rest are analagous to the MMC case.

B. Response History

The Response History Monte Carlo (RHMC) method, although pursued completely independently of the Macro Monte Carlo method, shares its underlying philosophy and a few of its design features. It was developed at Lawrence Livermore National Laboratory (LLNL) in 1991 by Ballinger[14] *et al.* It began as a marriage of an obscure "response matrix" Monte Carlo algorithm [16] and a Class I condensed history algorithm.

1. Algorithm. The local geometry in RHMC is a hemisphere, which was chosen because it was believed to be more suitable than a sphere for two reasons: (1) to match boundary conditions for normally incident electron beams in the global calculation; and (2) to avoid tracking low–energy backscattered electrons in the local calculation that add to the computation time without contributing much information to the overall probability distribution being generated; it is more efficient to tally them immediately as they cross the planar boundary. In addition to these reasons, the hemisphere still allows a modest degree of symmetry for decoupling the energy and angle distributions. [2]

The local calculation in RHMC is done using a custom analog code, rather than using a condensed history code as in the Macro Monte Carlo method. The analog code is based entirely on LLNL databases for cross sections [17],[18],[19], rather than on empirical approximations as is condensed history. Thus the RHMC method has the potential to replicate the accuracy of high-quality data.

Unlike typical Class I transport algorithms, RHMC permits knock-on electrons to be tracked as regular (primary) histories. The knock-on electrons are recorded in separate PDFs during the local calculation, and these distributions are sampled in the global calculation to determine the "birth state" of the knock-on. There is no capability to model bremsstrahlung in the RHMC algorithm, because it was designed for use in low-energy regimes where bremsstrahlung interactions do not account for an appreciable fraction of the total cross section.

The most significant strength of RHMC is its analog-type accuracy at a fraction of the time required to do an analog calculation. Since the hemispheres are quite small in size ($1.67\text{x}10^{-7}$cm – $1.69\text{x}10^{-3}$cm in radius), the RHMC method is able to attain excellent spatial resolution. It is one of the few codes in existence that has been shown to model backscatter realistically, which has great appeal for radiotherapy applications that involve severe inhomogeneities.

A limitation of using the RHMC code currently for radiotherapy applications is that it does not explicitly model bremsstrahlung events. Instead it handles this energy loss in a Class I - type manner; *i.e.*, the energy is locally deposited, which is not a good approximation for photons. Photon transport could be accommodated by storing the birth states of photons and passing them to a photon Monte Carlo code.

2. Results of Response History. The RHMC code has been shown to be in excellent agreement with experiment even under very severe conditions, such as high atomic number interfaces and low incident energy. This is shown in Figure 2. The time required for these calculations was slightly faster than the condensed history code MCNP4 [7] for the same calculations. For example, to simulate 10,000 electrons normally incident on thick gold took 63.5 cpu seconds on a Cray YMP computer. The corresponding calculation with MCNP took 110.9 seconds, and the analog code took 18,629 cpu seconds. Thus the RHMC resulted in a speed up factor of 293 over the analog code, while still inheriting most of its accuracy.

[2] This means that the electrons that reach the surface of the hemisphere have traveled approximately the same distance, so that the electrons leaving the curved surface have then suffered approximately the same number of collisions so energy and trajectory are only loosely related and can be treated independently. The backscattered electrons are considered a completely separate case in this method.

III. THE MACRO RESPONSE METHOD

The Macro Response Monte Carlo method is a new algorithm being developed particularly for radiotherapy simulation. It will be implemented as the electron package in a new all-particle Monte Carlo Monte Carlo code being developed at LLNL called PEREGRINE [20]. Although still in its developmental stages, it is likely that the results of this code will prove it to be a compromise between RHMC and MMC with regard to accuracy and speed.

A. Local Calculation

The MRMC local calculation code is an analog scatter code, similar in philosophy to the RHMC analog code since it relies directly on the LLNL databases [19],[17],[18]. The local geometry chosen for the MRMC method is spherical. A range of spheres, or *kugels* in the MMC vernacular, having diameters from approximately 10 μm to 1 cm may tabulated in a "bootstrapped" configuration – the smallest kugel is generated from the single scatter code, and these small kugels are then used to generate the next larger kugel size, and so forth, until the largest kugels are generated. This allows MRMC to be efficient in both transport stages, since it speeds up the calculation of large kugels in the local calculation, which in turn speed up the global calculation. The primary electron is assumed to be incident in the center of the kugels, unlike MMC which assumes normal incidence on the surface. This geometry reflects perfect symmetry, which allows added decoupling of phase space so that the global calculation will not need an extra transformation and can be faster still. The kugel will be divided into several surface zones, and separate PDFs will be generated for each zone.

B. Global Calculation

1. Boundary Crossing Algorithm. There are at least two options for handling the simulation across a boundary between significantly different media. It should be emphasized that the kugel size will be reduced as the the electron approaches the boundary, which will greatly minimize the error associated with either boundary crossing algorithm.

- Statistical Interpolation
  Statistical interpolation simply dictates that the kugel is considered to be either entirely of the first material or entirely of the second material (or third, and so forth). The material is chosen by assigning a probability of each possible material type based on the percentage of the kugel's volume that is overlapping with that material type. Then a random number is generated to make the decision. For example, suppose a kugel has 80% of its volume in bone and 20% of its volume in soft tissue. If the random number is less than 0.8, the kugel is taken to be of material type bone, otherwise it is considered soft tissue. This is a relatively efficient but less accurate scheme.

- Partial Volume Ray Tracing
  A more accurate method for modeling the boundaries, at least as far as energy deposition is concerned, is a method similar to that described by Neuenschwander *et al* [11] and Ballinger [21]. Here the electron is assumed to travel in a straight ray from the center of the kugel to the sampled edge position, with part of the ray being in one material and part of the ray being in another material. The pathlengths are then scaled according to their linear stopping power, $l' = \frac{S}{\rho} \cdot \rho \cdot l$, where l is the true length and l' is the scaled length. The energy deposited in each voxel is simply the energy available to be deposited times the fractional scaled pathlength.

Energy determined to be absorbed by the medium in a particular kugel will be deposited be a straight path from the center of the kugel to the outside edge of the kugel. The path will be "blurred" by a Gaussian that has a width corresponding to the pathlength of the cut-off energy for the electrons if the cut-off range is large.

2. Treatment of Secondaries. As secondary electrons are created, they will be tracked if they have enough energy to escape the present kugel. Their phase space will then be tabulated in PDFs in a manner directly analogous to the primary case. If the secondary electrons do not have enough energy to escape the

current kugel, their history will be terminated immediately and their energy deposited inside the kugel. A PDF will also be formed for the number of secondaries escaping the kugel, so that the stepping code will know how many times to sample the secondary phase space PDFs.

For secondary photons (from bremsstrahlung) a separate series of PDFs will be constructed which will include their creation position in the kugel, initial energy, and initial trajectory. Again, the number created in each kugel will also be tallied. The photons will not be transported in the electron code, only tabulated so that their transport can be assumed by an external Monte Carlo routine with photon capabilities, such as PEREGRINE.

IV. CONCLUSIONS

Local-to-Global Monte Carlo is a transport method that has been proven to have the ability to make electron transport simultaneously fast and accurate. This is achieved by breaking the simulation into a "local" stage and a "global" stage. The results of the local stage are stored in a library, which is sampled by the global calculation. Like condensed history, this method allows the transport to proceed by taking macroscopic steps representing the result of many collisions. Unlike condensed history, however, this method does not require analytic approximations which limit the validity of the code. In fact, it is possible to base L-G transport entirely on data, as is seen in the Response History and Macro Response Monte Carlo methods.

Examples of the promise of this technique can be seen in the results of Macro Monte Carlo method and the Response History method. Macro Monte Carlo has the ability to improve the speed of traditional condensed history methods without much loss in accuracy. Response History has the ability to make the accuracy of analog scatter codes practical. The Macro Response method combines many features of these algorithms to create a compromise between the two and specifically address electron transport in the new All-Particle radiotherapy simulation code, PEREGRINE.

In summary, Local-to-Global methods have three potential advantages over traditional Monte Carlo Methods: they are fast, accurate and simple to understand. The same simple code is used for any step size, and accuracy is not sacrificed by using larger step sizes, unlike condensed history methods. A potential disadvantage is the amount of memory required to store the results of the local calculation, but for a radiotherapy-specific code this problem can be reduced to a manageable level (under 15 MBytes – as little as 1.5 MBytes for MMC at runtime) for mid-size workstations.

ACKNOWLEDGMENTS

The LLNL authors would like to thank R.M. White, M.B. Chadwick, D.E. Cullen, L.J. Cox and D.A. Resler for their contributions to the databases and for many helpful discussions. The Macro Response Monte Carlo method, the Response History method, and PEREGRINE are performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

The Macro Monte Carlo method was partially funded by NIH grant CA52692.

REFERENCES

[1] M.J. Berger. Monte Carlo calculation of the penetration and diffusion of fast charged particles. *Methods in Computational Physics*, 1:135–215, 1963.

[2] G. Moliere. Theorie der streuung schneller geladener. *Naturforsch*, 2a:133, 1947.

[3] S. Goudsmit and J. L. Saunderson. Multiple scattering of electrons. *Physical Review*, 57:24–29, jan 1940.

[4] C.T. Ballinger, D.E. Cullen, S.T. Perkins, J.A. Rathkopf, W.R. Martin, and S.J. Wilderman. Single-scatter Monte Carlo compared to condensed history results for low energy electrons. *Nuclear Instruments and Methods in Physics Research B*, pages 19–27, 1992.

[5] M.J. Berger and S.M. Seltzer. Bremsstrahlung and photoneutrons from thick tungsten and tantalum targets. *Physical Review*, C(2):621–631, 1970.

[6] J. Halbleib. Structure and operations of the ITS code system. In Theodore M. Jenkins, Walter Nelson, and Alessandro Rindi, editors, *Monte Carlo Transport of Electrons and Photons*, New York and London, 1988. Plenum Press.

[7] J.F. Briemeister. MCNP4 - a general Monte Carlo code for neutron, photon, and electron transport. In *LA-7936-M Rev. 4*, Los Alamos National Laboratory, 1991.

[8] L. Landau. On the energy loss of fast particles by ionization. *Journal of Physics USSR*, 8(4):201–5, 1944.

[9] A. Bielajew, R. Wang, and S. Duane. Incorporation of single elastic scattering in the EGS4 Monte Carlo code system: tests of the Moliere theory. *Nuclear Instruments and Methods*, 1994.

[10] W.R. Nelson, H. Hirayama, and D.W.O. Rogers. The EGS4 code system. *Stanford Linear Accelerator Center Report 265*, 1985.

[11] H. Neuenschwander, T.R. Mackie, and P.J. Reckwerdt. MMC - a high performance Monte Carlo code for electron beam dose calculations. *Medical Physics – submitted*, 1994.

[12] T.R. Mackie and J.J. Battista. A Macroscopic Monte Carlo method for electron beam dose calculations: A proposal. In *Eighth International Conference on the Use of Computers in Radiation Therapy*, Toronto, 1984. IEEE.

[13] H. Neuenschwander and E.J. Born. A Macro Monte Carlo method for electron beam dose calculations. *Physics of Medicine and Biology*, 37(1):107–125, 1992.

[14] C.T. Ballinger, J.A. Rathkopf, and W.R. Martin. The Response History Monte Carlo method for electron transport. *Nuclear Science and Engineering*, pages 283–95, 1992.

[15] H. Neuenschwander, T.R. Mackie, P.J. Reckwerdt, and J. Yang. MMC – a high performance Monte Carlo code for electron beam dose calculations. *Physics of Medicine and Biology: Abstracts of the World Congress on Medical Physics and Biomedical Engineering*, 39a:674, 1994.

[16] W.C. Wan. *Response Matrix Monte Carlo.* PhD thesis, University of Michigan, Ann Arbor, Michigan, 1988.

[17] S.T. Perkins and D.E. Cullen. The Livermore electron impact ionization database. UCID-21628, 1989. Lawrence Livermore National Laboratory.

[18] S.T. Perkins and D.E. Cullen. The Livermore electron elastic scattering database. UCRL-ID-103170, 1990. Lawrence Livermore National Laboratory.

[19] D.E. Cullen and S.T. Perkins. The Livermore bremsstrahlung database. UCID-21627, 1989. Lawrence Livermore National Laboratory.

[20] C.L. Hartmann Siantar, W.P. Chandler, J.A. Rathkopf, M.M. Svatos, and R.M. White. PEREGRINE: An All Particle Monte Carlo code for radiation treatment planning. *this conference*, 1995.

[21] C.T. Ballinger. *The Response History Method for Electron Transport.* PhD thesis, University of Michigan, Lawrence Livermore National Laboratory, 1991.

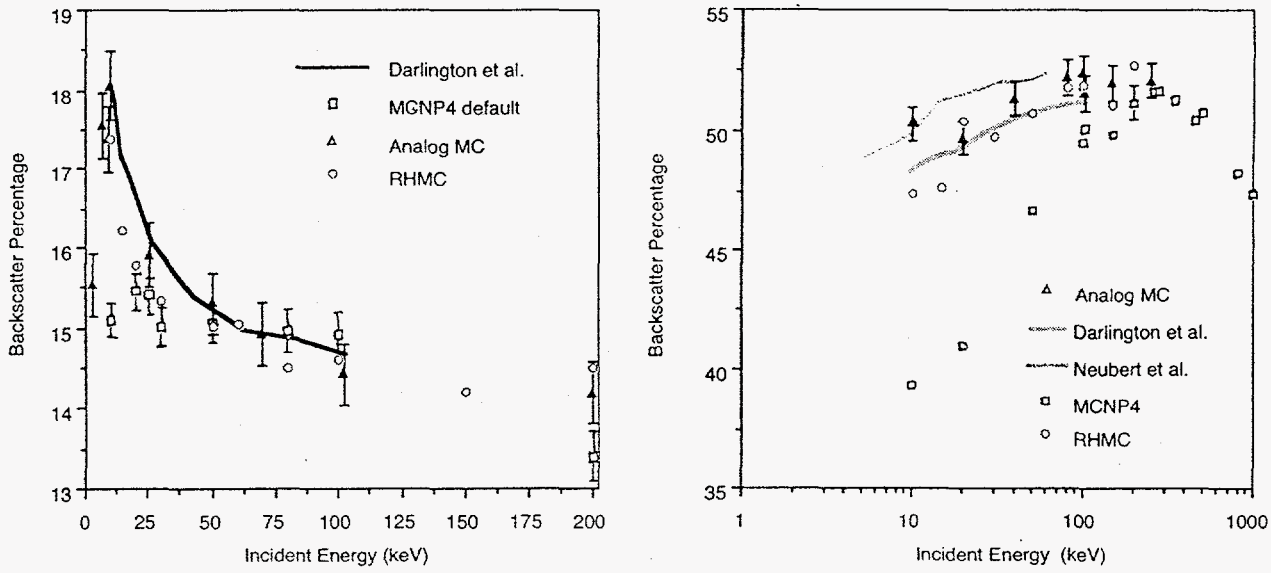


Figure 2: The agreement of the Response History method with experiment compared to other Monte Carlo codes under very stringent test conditions in aluminum (left) and gold (right).