Chapter 1: History of Monte Carlo

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It is still an unending source of surprise for me to see how a few scribbles on a blackboard or on a sheet of paper could change the course of human affairs.—Stan Ulam, founder of the modern Monte Carlo method, in his 1991 autobiography

Motivating Monte Carlo

Generally speaking, the Monte Carlo method provides a numerical solution to a problem that can be described as a temporal evolution ("translation/reflection/mutation") of objects ("quantum particles" [photons, electrons, neutrons, protons, charged nuclei, atoms and molecules], in the case of Medical Physics) interacting with other objects based upon object-object interaction relationships ("cross sections"). Mimicking nature, the rules of interaction are processed randomly and repeatedly, until numerical results converge usefully to estimated means, moments and their variances. Monte Carlo represents an attempt to model nature through direct simulation of the essential dynamics of the system in question. In this sense, the Monte Carlo method is, in principle, simple in its approach—a solution to a macroscopic system through simulation of its microscopic interactions. Therein is the advantage of this method. All interactions are microscopic in nature. The geometry of the environment, so critical in the development of macroscopic solutions, plays little role except to define the local environment of objects interacting at a given place at a given time.

The scientific method is dependent on observation (measurement) and hypothesis (theory) to explain nature. The conduit between these two is facilitated by a myriad of mathematical, computational, and simulation techniques. The Monte Carlo method exploits all of them. Monte Carlo is often seen as a "competitor" to other methods of macroscopic calculation, which we will call deterministic and/or analytic methods. Although the proponents of either method sometimes approach a level of fanaticism in their debates, a practitioner of science should first ask, "What do I want to accomplish?" followed by "What is the most efficient way to do it?", and then, "What serves science the best?". Sometimes the correct answer will be "Deterministic" and other times it will be "Monte Carlo". The most successful scientist will avail himself or herself of more than one method of approach.

There are, however, two inescapable realities. The first is that macroscopic theory, particularly transport theory, provides deep insight and allows one to develop sophisticated intuition as to how macroscopic particle fields can be expected to behave. Monte Carlo can not compete very well with this. In discovering the properties of macroscopic field behavior, Monte Carlo practitioners operate very much like experimentalists. Without theory to provide guidance, discovery is made via trial and error, guided perhaps, by some brilliant

intuition.

However complexity is measured, when it comes to developing an understanding of a physical problem, Monte Carlo techniques become, at some point, the most advantageous. A proof is given, in the Appendix to this article, that the Monte Carlo method is the more advantageous in the evolution of five and higher dimensional systems. The dimensionality is just one measure of a problem's "complexity". The problems in RTP and Dosimetry are typically of dimension $6.\varepsilon$, or $7.\varepsilon$. That is, particles move in Cartesian space, with position $\vec{x}$, that varies continuously, except at particle inception or expiration. They move with momentum, $\vec{p}$, that varies both discretely and continuously. The dimension of time is usually ignored for static problems, though it can not be for non-linear problems, where a particle's evolution can be affected by the presence of other particles in the simulation. (The "space-charge" effect is a good example of this.). Finally, the ε is a discrete dimension that can encompass different particle species, as well as intrinsic spin.

This trade-off, between complexity and time to solution is expressed in Figure 1.

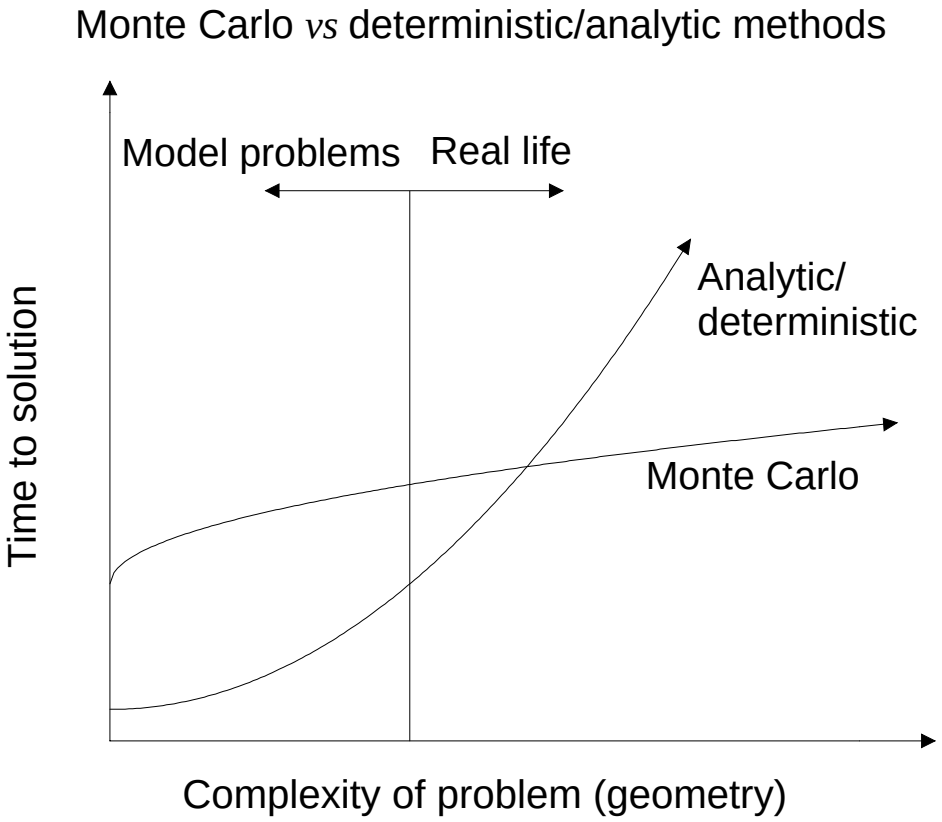


Figure 1: Time to solution using Monte Carlo *vs.* deterministic/analytic approaches.

Although the name "Monte Carlo method" was coined in 1947, at the start of the computer age, stochastic sampling methods were known long before the advent of computers. The first reference known to this author, is that of Comte de Buffon [1] who proposed a Monte Carlo-like method to determine the outcome of an "experiment" consisting of repeatedly tossing a needle onto a ruled sheet of paper, to determine the probability of the needle crossing one of the lines. This reference goes back to 1777, well before the contemplation of automatic calculating machines. Buffon further calculated that a needle of length L tossed randomly on a plane ruled with parallel lines, distance d apart, where $d > L$, would have a probability of crossing one of the rules lines of:

$$p = \frac{2L}{\pi d} \ . \tag{1}$$

Much later, Laplace [2] suggested that this procedure could be employed to determine the value of π, albeit slowly. Several other historical uses of Monte Carlo predating computers are cited by Kalos and Whitlock [3].

The idea of using stochastic sampling methods first occurred to Ulam[1], who, while convalescing from an illness, played solitaire repeatedly, and then wondered if he could calculate the probability of success by combinatorial analysis. It occurred to him, that it would be possible to do so by playing a large number of games, tallying the number of successful plays [5, 6], and then estimating the probability of success. Ulam communicated this idea to von Neumann who, along with Ulam and Metropolis, were working on theoretical calculations related to the development of thermonuclear weapons. Precise calculations of neutron transport are essential in the design of thermonuclear weapons. The atomic bomb was designed by experiments, mostly, with modest theoretical support. The trigger for a thermonuclear weapon is an atomic bomb, and the instrumentation is destroyed before useful signals can be extracted[2]. Von Neumann was especially intrigued with the idea. The modern Monte Carlo age was ushered in later, when the first documented suggestion of using stochastic sampling methods applied to radiation transport calculations appeared in correspondence between von Neumann and Richtmyer [5, 6], on March 11, 1947. (Richtmyer was the leader of the Theoretical Division at Los Alamos National Laboratories [LANL].) This letter suggested the use of LANL's ENIAC computer to do the repetitive sampling. Shortly afterward, a more complete proposal was written [8]. Although this report was declassified as late as 1988, inklings of the method, referred to as a "mix of deterministic and random/stochastic processes", started to appear in the literature, as published abstracts [9, 10]. Then in 1949, Metropolis and Ulam published their seminal, founding paper, "The Monte Carlo Method" [11], which was the first unclassified paper on the Monte Carlo methods, and the first to have the name, "Monte Carlo" associated with stochastic sampling.

[1] The direct quote from Ulam's autobiography [4] (p 196, 1991 edition):"The idea for what was later called the Monte Carlo method occurred to me when I was playing solitaire during my illness."

[2] The book "Dark Sun", by Richard Rhodes, is an excellent starting point for the history of that topic [7].

Already by the 1949, symposia on the Monte Carlo methods were being organized, focusing primarily on mathematical techniques, nuclear physics, quantum mechanics and general statistical analysis. A later conference, the "Symposium on Monte Carlo Methods", held at the University of Florida in 1954 [12] was especially important. There were 70 attendees, many of whom would be recognized as "founding fathers" by Monte Carlo practitioners in the radiological sciences. Twenty papers were presented, including two involving gamma rays, spanning 282 pages in the Proceedings. This Proceedings also includes a 95 page bibliography, a grand summary of the work-to-date, with many references having their abstracts and descriptions published in the Proceedings.

The rest, to quote an overused expression, is history. It is interesting to note the wonderful irony: This mathematical method was created for destruction by means of the most terrible weapon in history, the thermonuclear bomb. Fortunately, this weapon has never been used in conflict. Rather, millions have benefited from the development of Monte Carlo methods for medicine. That topic, at least a small subset of it, will occupy the rest of this Chapter.

As of this writing, with the data from 2011 still incomplete, we have found that about 300,000 papers have been published on the Monte Carlo method. If we restrict this search to only those papers related to medicine, the number of publications is almost 30,000. The 10% contibution to the Monte Carlo method seems to be consistent over time, at least since 1970. That represents an enormous investment in human capital to develop this most useful tool. The temporal evolution of this human effort is shown in Figure 2. Before 2005, the growth in both areas appears exponential in nature. The total effort shows three distinct areas of slope, with sudden changes, currently unexplained, though it may be due to the sudden emergence of "vector" and "massively parallel" machines, and the increase in research associated with this fundamentally new computer architecture. The growth in the "Medicine" area has been constant.

Since 2005, both areas are statistically consistent with constant output, with the "Medicine" area leveling out, at greater than 2100 publications/year. It appears that this communication is being written at the pinnacle of this scientific endeavor!

Monte Carlo in Medical Physics

Every historical review has its biases, and the one employed here will restrict the discussion to the applications of radiotherapy and radiation dosimetry. Moreover, the focus will be on the development of electron Monte Carlo, for reasons explained in the following paragraph. There is an abundance of reviews on the use of Monte Carlo in medical physics. A few of the more recent ones that discuss radiotherapy physics and dosimetry are: [13, 14, 15, 16, 17, 18].

The rise of the use of linear electron accelerators (LINACs) for radiotherapy, also ushered in the need to develop Monte Carlo methods for the purpose of dose prediction and dosimetry. LINACs employed in radiotherapy provide an energetic and penetrating source of photons that enter deep into tissue, sparing the surface and attenuating considerably less rapidly than ^{60}Co or ^{137}Cs beams. Relativistic electrons have a range of about 1 cm for each 2

MeV of kinetic energy in water. At its maximum, starting with a pencil beam of electrons, the diameter of the electron energy deposition, pear-shaped "plume" is also about 1 cm per 2 MeV of initial kinetic energy. These dimensions are commensurate with the organs being treated, as well as the organs at risk. The treatment areas are heterogeneous, with

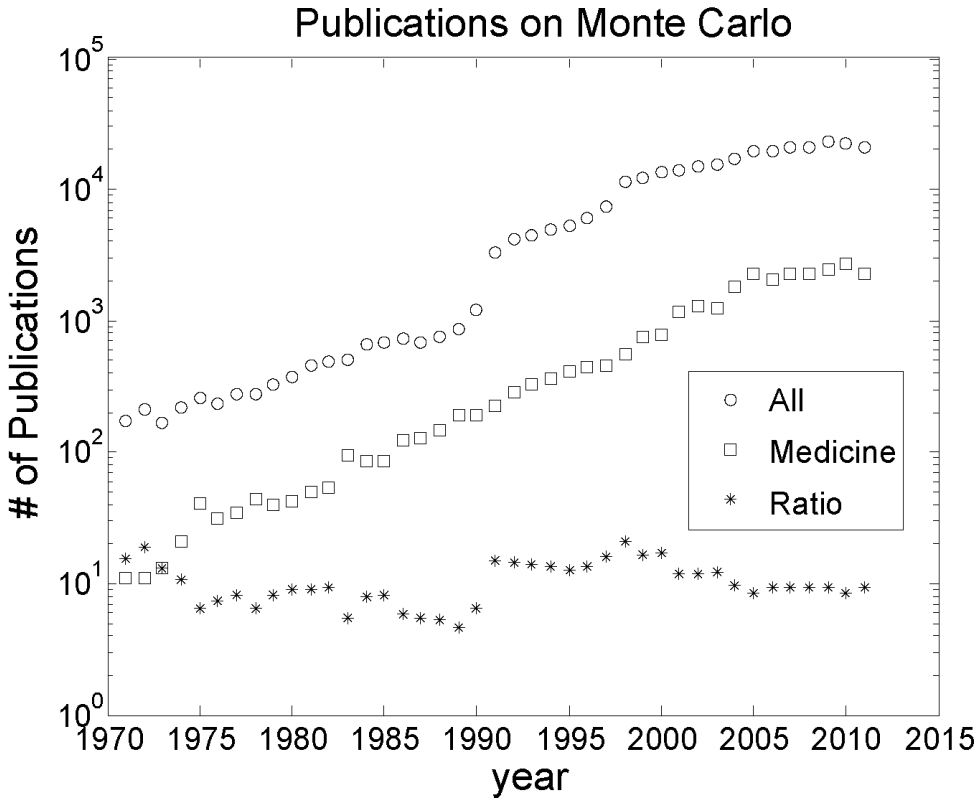


Figure 2: The number of papers published per year garnered from the Web of Knowledge ('All') and MedLine ('Medicine').

differences in composition and density. Moreover, the instruments used to meter dose are even more diverse. It is true now, as it was then, that the Monte Carlo method provides the only prediction of radiometric quantities that satisfies the accuracy demand of radiotherapy.

Thus, the history of the utility of the Monte Carlo method in medical physics is inextricably tied to the development of Monte Carlo methods of electron transport in complex geometries and in the description of electromagnetic cascades[3].

The first papers employing the Monte Carlo method using electron transport, were authored by Robert R. Wilson [19, 20, 21], who performed his calculations using a "spinning wheel of chance".[4] Although apparently quite tedious, Wilson's method was still an improvement

[3]Certainly there are important applications in brachytherapy and imaging that ignore electron transport. However, we shall leave that description to other authors.

[4]R. R. Wilson is also acknowledged as the founder of proton radiotherapy [22].

over the analytic methods of the time—particularly in studying the average behavior and fluctuations about the average [23]. Hebbard and P. R. Wilson [24] used computers to investigate electron straggling and energy loss in thick foils. The first use of an electronic digital computer in simulating high-energy cascades by Monte Carlo methods was reported by Butcher and Messel [25, 26], and independently by Varfolomeev and Svetlolobov [27]. These two groups collaborated in a much publicized work [28] that eventually led to an extensive set of tables describing the shower distribution functions [29]—the so-called "shower book".

For various reasons, two completely different codes were written in the early-to-mid 1960's to simulate electromagnetic cascades. The first was written by Zerby and Moran [30, 31, 32] of the Oak Ridge National Laboratory, motivated by the construction of the Stanford Linear Accelerator Center. Many physics and engineering problems were anticipated as a result of high-energy electron beams showering in various devices and structures at that facility. This code had been used by Alsmiller and others [33, 34, 35, 36, 37, 38, 39] for a number of studies since its development.[5]

The second code was developed by Nagel [41, 42, 43] and several adaptations have been reported [44, 45, 46]. The original Nagel version, which Ford and Nelson called SHOWER1, was a FORTRAN code written for high-energy electrons ($\leq$ 1000 MeV) incident upon lead in cylindrical geometry. Six significant electron and photon interactions (bremsstrahlung, electron-electron scattering, ionization-loss, pair-production, Compton scattering, and the photoelectric effect) plus multiple Coulomb scattering were accounted for. Except for annihilation, positrons and electrons were treated alike and were followed until they reached a cutoff energy of 1.5 MeV (total energy). Photons were followed down to 0.25 MeV. The cutoff energies were as low as or lower than those used by either Messel and Crawford or by Zerby and Moran.The availability of Nagel's dissertation [42] and a copy of his original shower program provided the incentive for Nicoli [45] to extend the dynamic energy range and flexibility of the code in order for it to be made available as a practical tool for the experimental physicist. It was this version of the code that eventually became the progenitor of the EGS Code Systems [47, 48, 49, 50, 51].

On a completely independent track, and apparently independent from the electromagnetic cascade community, was Berger's e-γ code. It was eventually released to the public as ETRAN in 1968 [52], though it is clear that internal versions were being worked on at NBS (now NIST) [53] since the early 60s, on the foundations laid by Berger's landmark paper [54]. The ETRAN code then found its way, being modified somewhat, into the Sandia codes, EZTRAN [55], EZTRAN2 [56], SANDYL [57], TIGER [58], CYLTRAN [59], CYLTRANNM [60], CYLTRANP (unpublished), SPHERE [61], TIGERP [62], ACCEPT [63], ACCEPTTM [64], SPHEM [65] and finally the all-encompassing ITS [66, 67] codes. The ITS electron transport code was incorporated into the MCNP code at Version 4, in 1990 [68]. The MCNP code lays claim to being a direct descendant of the codes written by the origi-

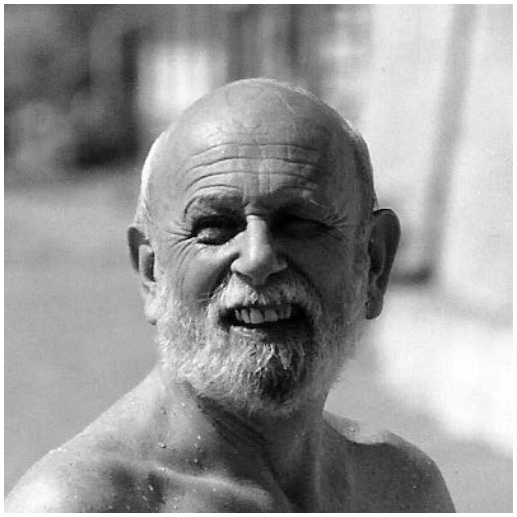
[5] According to Alsmiller[40], the Zerby and Moran source code vanished from ORNL and they were forced to work with an octal version.

nators of the Monte Carlo method, Fermi, von Neumann, Ulam, as well as Metropolis and Richtmyer [69]. Quoting directly[6],

> *"Much of the early work is summarized in the first book to appear on Monte Carlo by Cashwell and Everett in 1957.*[a] *Shortly thereafter the first Monte Carlo neutron transport code MCS was written, followed in 1967 by MCN. The photon codes MCC and MCP were then added and in 1973 MCN and MCC were merged to form MCNG. The above work culminated in Version 1 of MCNP in 1977. The first two large user manuals were published by W. L. Thompson in 1979 and 1981. This manual draws heavily from its predecessors."*

[a] 1959, to be exact [70].

The first appearance of electron transport in MCNP occurred with Version 4, in 1990 [68]. After that time, MCNP became an important player in medical-related research, to be discussed later.



Martin Berger, on a beach near Erice, 1987[7]

Berger's contribution [54] is considered to be the *de facto* founding paper (and Berger the founding father) of the field of Monte Carlo electron and photon transport. That article, 81 pages long, established a framework for the next generation of Monte Carlo computational physicists. It also summarized all the essential theoretical physics for Monte Carlo algorithm development. Moreover, Berger introduced a specialized method for electron transport. Electron transport and scattering, for medical physics, dosimetry, and many other applications, is subject to special treatment. Rather than modeling every discrete electron interaction (of the order of 10^6 for relativistic electrons), cumulative scattering theories, where by $10^3 - 10^5$ individual elastic and inelastic events are "condensed" into single "virtual" single-scattering events, thereby enabling a speedup by factors of hundreds, typically. Nelson, the originator of the EGS code system, is quoted as saying [71], "Had I known about Berger's work, I may not have undertaken the work on EGS!".

As for general-purpose uses in medical-related fields, with multi-material, combinatorial geometries, the two historically dominant players in RTP/Dosimetry[8], are the EGS and MCNP codes, introduced above. In the last decade, GEANT [78, 79] has also made significant contributions as well, presently equal in use to MCNP. A plot of the number of papers published,

[6] The codes and manuals referred to in this quote appear to have vanished.

[7] Photograph courtesy of Ralph Nelson.

[8] There are some very relevant, alternative approaches, that the reader should be aware of, namely FLUKA [72, 73, 74] (that traces its roots to 1964 [75]), and the Penelope code [76, 77]. As of this writing, the number of papers produced using these codes in medical-areas is about 240, about half that of MCNP.

using these methods is charted in Figure 3. Once MCNP introduced electron transport, we see, from Figure 3, that usage of MCNP experienced exponential growth in its use in medical-related areas. That exponential growth ended in about 2000. Since then, both the EGS and MCNP code systems seem to be experiencing steady use, with GEANT still, arguably, on the increase. If one considers all of the non-medical literature related to Monte Carlo, MCNP is undeniably the most cited Monte Carlo code, by about a factor of 7 over EGS.

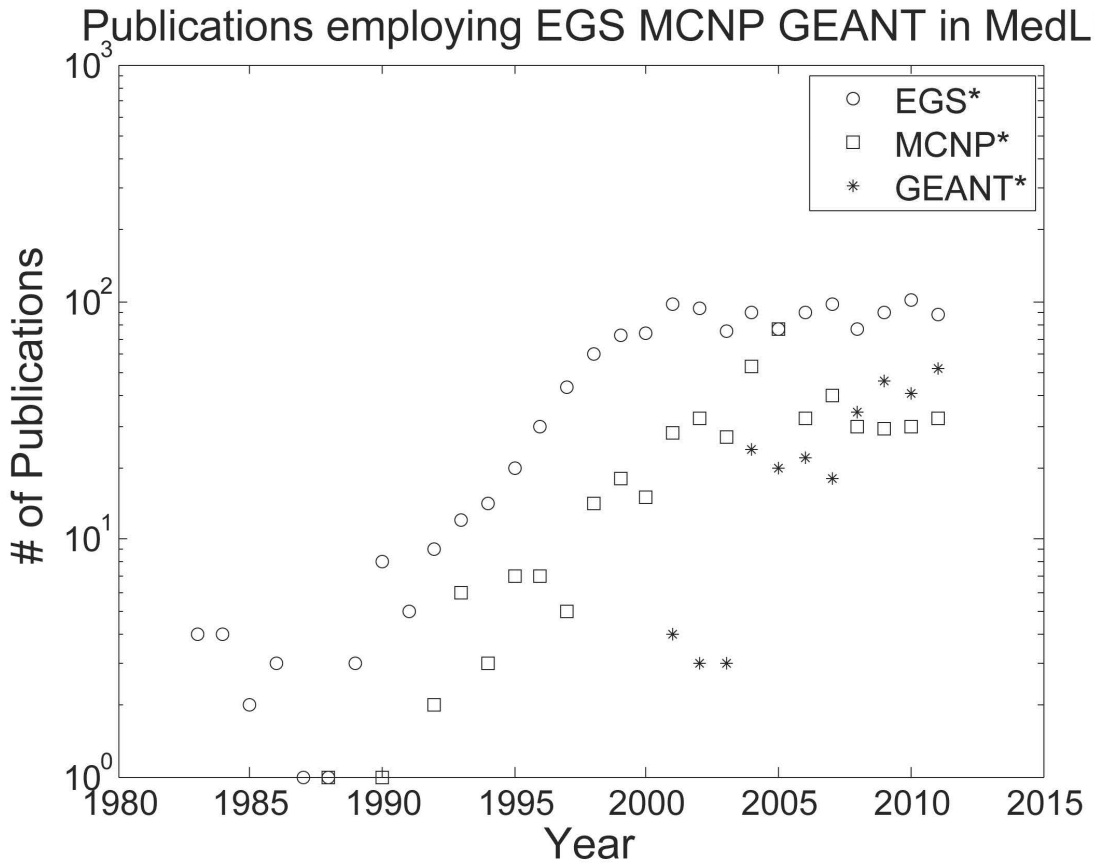


Figure 3: Papers using EGSx, MCNPx, and GEANTx, as captured on MedLine.

It should be emphasized that these two code systems are very different in nature. EGS has specifically targeted the medical area, since 1984, though it has enjoyed some use in other areas of physics as well. Some features are genuinely unique, such as the tracking of separate electron spins, a feature introduced [80] in EGS5 [51], as well as Doppler broadening [81], both inclusions of great interest to those doing research in synchrotron radiation light sources. Overall, however, considering Monte Carlo uses over all areas, MNCP's state-of-the-art neutron transport, makes it the world leader in the Nuclear and Radiological Sciences conglomerate. The EGS code systems are supported by practitioners representing a panoply of scientific disciplines: Medical Physics, Radiological Scientists, Pure and Applied Physicists. MCNP serves these communities as well, but also enjoys the support of

a vibrant Nuclear Engineering profession, where transport theory of neutrons is a rich and active research area.

The EGSx Code systems

The history of how EGS, a code developed primarily for high-energy physics shielding and detector simulations, came to be used in medical physics, has never appeared in text, in its entirety. Rogers' [82] humility probably interfered with its exposition in his article. However, I was an observer at those early events, and think I may offer some insights. In 1978, SLAC published EGS3 [47], and Rogers employed it in several important publications [83, 84, 85, 86, 87]. Of particular importance was the publication that offered a patch to the EGS3 algorithms to mimic a technique employed in ETRAN, making electron-dependent calculations reliable, by shortening the steps to virtual interactions. At the time, electron transport step-size artefacts were completely unexplained. Shortening the steps is understood to solve the problem, as explained most eloquently by Larsen [88], but at the cost of added computational time. These "step-size artefacts", attracted the attention of Nelson, who invited Rogers to participate in authoring the next version of EGS, EGS4 [48], along with Hirayama, a research scientist at the KEK, the High Energy Accelerator Research Organization, Tsukuba, Japan.

Following its release in December 1985, Rogers' institution (a Radiation Standards' Laboratory, and a sister laboratory to Berger's NIST) became a nucleus of medical physics and dosimetry Monte Carlo dissemination. It took over support and distribution of the EGS4 code, and began offering training courses all over the world. Hirayama was engaged in similar efforts in the Asian regions.

Yet, the step-size artefacts in EGS4 remained unexplained. Nahum, who was interested in modeling ionization chamber response, visited Rogers' laboratory in the spring of 1984, to collaborate on this topic. Nahum already had a scholarly past in electron Monte Carlo [89], producing what would eventually be realized, through a Lewis [90] moments analysis [91], to be a far superior electron transport algorithm. While using EGS4 to predict ionization chamber response, EGS4 would predict responses that could be 60% too low. Quoting Nahum, "How could a calculation that one could sketch on the back of an envelope, and get correct to within 5%, be 60% wrong using Monte Carlo?". Step-size reduction solved the problem [92, 93], but the search for a resolution to step-size anomalies was commenced, resulting in the PRESTA algorithm [49, 94]. The release of PRESTA was followed by the demonstration of various small, but important, shortcomings [95, 96]. There were improvements over the years [97, 98, 99, 100], eventually resulting in a revision of the EGS code, known as EGSnrc [50] and EGS5 [51]. A PRESTA-like improvement of ETRAN [101, 102] was even developed.

Application: Ion Chamber Dosimetry

The founding paper for applying Monte Carlo methods to ionization chamber response is attributed to Bond, Nath and Schulz [103], who, using an in-house Monte Carlo code, cal-

culated ionization chamber response as a function of wall thickness, to ^{60}Co γ irradiation. While validating the EGS code for this application, it was found that the EGS code had fundamental algorithmic difficulties with this low energy regime, as well as this application. The resolution of these difficulties, not patent in other general-purpose Monte Carlo codes, became of great interest to this author. While general improvements to electron transport ensued, the fundamental problem was quite subtle, and was eventually described elegantly by Foote and Smythe [96]. In a nutshell, the underlying algorithmic reason that was identified arose from electron tracks being stopped at material boundaries, where cross sections change. EGS used the partial electron path to model a deflection of the electron, from the accumulated scattering power. The result was a rare, but important effect, the spurious generation of fluence singularities.

The literature on ionization chamber dosimetry is extensive. A partial compilation of very early contributions is: [92, 93, 104, 105, 106, 107]

Presently, the calculation of ionization chamber corrections is a very refined enterprise, with results being calculated to better than 0.1%. The literature on this topic is summarized by Bouchard and Suentjens in their chapter in this book, "Applications of Monte Carlo to radiation dosimetry". That chapter also summarizes the contribution of Monte Carlo to dosimetry protocol and basic dosimetry data, some of the earliest applications of Monte Carlo to medicine.

Early Radiotherapy Applications

For brevity, only the earliest papers are cited in this section, and the reader is encouraged to employ the comprehensive reviews already cited earlier in this article. Some of the very early history of radiotherapy applications is rarely mentioned, and I have attempted to gather them here.

The Monte Carlo modeling of Cobalt-60 therapy units was first mentioned in the ICRU Report # 18.[108]. However, a more complete descriptive work followed somewhat later [109, 110].

The modeling of LINAC therapy units was first accomplished by Petti *et al.* [111, 112] and then, soon after by Mohan *et al.* [113].

Photoneutron contamination from a therapy unit was first described by Ing *at al.* [114], although the simulation geometry was simplified.

Mackie *et al.* pioneered the convolution method [115] and then with other collaborators, generated the first database of "kernels" or "dose-spread arrays" for use in radiotherapy. [116] Independently, these efforts were being developed by Ahnesjö *et al. et al* [117]. These are still in use today.

Modeling of electron beams from medical LINACs was first accomplished by Teng *et al.* [118], Ho *et al.* [119], and then Manfredotti *et al.* [120]

An original plan to use Monte Carlo calculation for "target button to patient dose" was proposed by Mackie *et al.* [121]. That effort became known as "the OMEGA (an acronym for Ottawa Madison Electron Gamma Algorithm) Project". However, early on in that project, a "divide-and-conquer" approach was adopted, whereby the fixed machine outputs ("phase-space files") were used as inputs to a patient specific target (applicators and patient), to generate a full treatment plan. This bifurcation spawned two industries, treatment head modeling, of which the BEAM/EGSx code is the most refined [122] and is the most cited paper in the "Web of knowledge" with "Monte Carlo" in the title, and "radiotherapy" as a topic. The second industry spawned by the OMEGA project was the development of fast patient-specific Monte Carlo-based dose calculation algorithms. [123, 124, 125, 126]. For more discussion on the current fast Monte Carlo methods in use, the reader is encouraged to see the excellent review by Spezi and Lewis [127].

The Future of Monte Carlo

The first step in predicting the future is to look where one has been, extrapolate the process, thereby predicting the future. The second step in predicting the future is to realize that the first step involves some very specious, and problematic reasoning!

The progress of time, with the events that it contains, is intrinsically "catastrophic" in nature. A scientific discovery can be so earth-shattering, that new directions of research are spawned, while others dissolve into irrelevance. Yet, we persist in the practice of prediction. Therefore, allow me to be very modest in this effort.

Amdahl's Law [128]: Amdahl may be saturating due to multiprocessor intercommunication bottlenecks. Gains in single chip speeds are also slowing. We are nearing the limits of what we can do, and what new challenges we can address.

Harder to predict is algorithm development, specific to Monte Carlo applications in RTP. There is historical precedent for this in the citation data. In 1991, there was a 2.8 factor increase in productivity in only one year, followed by another in 1998, by a factor of 1.6. These increases are large, and unexplained. Yet, they illustrate the chaotic nature of the field.

There is a strong suggestion that research in Monte Carlo is saturating. Both the medical and "all" data have been flat since about 2005. The EGS and MCNP output has been flat since 2000. Perhaps we are at the pinnacle?

We can safely predict, while the approach to the pinnacle may have been somewhat chaotic, the decline will be gradual. Monte Carlo codes have gotten easier to use, packaged with more user-friendly interfaces, and developing into "shrink-wrapped", "turn-key" software systems. This is how it should be. The fact that a Monte Carlo method is the "engine" beneath a computational algorithm, should be transparent, but not invisible, to the researcher using the tool.

Paraphrasing the comment made by Martin Berger, the founder of our field, during his

speech at his retirement *Festschrift* symposium [129],

> *"I am not used to so much public attention. Tonight is quite unusual for me. I hope that, after tonight, I can disappear into the anonymity that I so assuredly crave."*

And so it may be, for Monte Carlo research—at least, until the next great thing comes along.

A very astute student once said to me, "We no longer have Departments of Railroad Engineering.", in an effort to explain the (then) decline of Nuclear Engineering Departments, before the "nuclear renaissance". It may be that the *development* of the Monte Carlo method is bound to decline as it matures, but it will remain an essential component of our scientific infrastructure, forever.

Appendix: Monte Carlo and Numerical Quadrature

In this Appendix, we present a mathematical proof that the Monte Carlo method is the most efficient way of estimating tallies in 3 spatial dimensions when compared to first-order deterministic (analytic, phase-space evolution) methods. Notwithstanding the opinion that the Monte Carlo method is thought of as providing the most accurate calculation, the argument may be made in such a way, that it is independent of the physics content of the underlying algorithm or the quality of the incident radiation field.

A.1 The dimensionality of deterministic methods

For the purposes of estimating tallies from initiating electrons, photons, or neutrons, the transport process that describes the trajectories of particles is adequately described by the linear Boltzmann transport equation [130]:

$$\left[\frac{\partial}{\partial s} + \frac{p}{|p|}\cdot\frac{\partial}{\partial x} + \mu(x,p)\right]\psi(x,p,s) = \int \mathrm{d}p'\,\mu(x,p,p')\psi(x',p',s)\ , \tag{2}$$

where x is the position, p is the momentum of the particle, $(p/|p|)\cdot\partial/\partial x$ is a directional derivative (in three dimensions $\vec{\Omega}\cdot\vec{\nabla}$, for example) and s is a measure of the particle pathlength. We use the notation that x and p are multi-dimensional variables of dimensionality N_x and N_p. Conventional applications span the range $1 \le N_{p,x} \le 3$. The macroscopic differential scattering cross section (probability per unit length) $\mu(x,p,p')$ describes scattering from momentum p' to p at location x, and the total macroscopic cross section is defined by:

$$\mu(x,p) = \int \mathrm{d}p'\,\mu(x,p,p')\ . \tag{3}$$

$\psi(x,p,s)\,\mathrm{d}x\,\mathrm{d}p$ is the probability of there being a particle in $\mathrm{d}x$ about x, in $\mathrm{d}p$ about p and at pathlength s. The boundary condition to be applied is:

$$\psi(x,p,0) = \delta(x)\delta(p_0 - p)\delta(s)\ , \tag{4}$$

where p_0 represents the starting momentum of a particle at $s = 0$. The essential feature of Equation 2, insofar as this proof is concerned, is that the solution involves the computation of a $(N_x + N_p)$-dimensional integral.

A general solution may be stated formally:

$$\psi(x,p,s) = \int \mathrm{d}x' \int \mathrm{d}p'\, G(x,p,x',p',s) Q(x',p') \ , \tag{5}$$

where $G(x,p,x',p',s)$ is the Green's function and $Q(x',p')$ is a source. The Green's function encompasses the operations of transport (drift between points of scatter, $x' \rightarrow x$), scattering (*i.e.* change in momentum) and energy loss, $p' \rightarrow p$. The interpretation of $G(x,p,x',p',s)$ is that it is an operator that moves particles from one point in $(N_x + N_p)$-dimensional phase space, (x',p'), to another, (x,p) and can be computed from the kinematical and scattering laws of physics.

Two forms of Equation 5 have been employed extensively for general calculation purposes. Convolution methods integrate Equation 5 with respect to pathlength s and further assume (at least for the calculation of the Green's function) that the medium is effectively infinite. Thus,

$$\psi(x,p) = \int \mathrm{d}x' \int \mathrm{d}p'\, G\left(|x-x'|, \left[\frac{p}{|p|}\cdot\frac{p'}{|p'|}\right], |p'|\right) Q(x',p') \ , \tag{6}$$

where the Green's function is a function of the distance between the source point x' and x, the angle between the vector defined by the source p' and p and the magnitude of the momentum of the course, $|p'|$, or equivalently, the energy.

To estimate a tally using Equation 6 we integrate $\psi(x,p)$ over p, with a response function, $\mathcal{R}(x,p)$ [131]:

$$T(x) = \int \mathrm{d}x' \int \mathrm{d}p'\, F(|x-x'|,p') Q(x',p') \ , \tag{7}$$

where the "kernel", $F(|x-x'|,p')$, is defined by:

$$F(|x-x'|,p') = \int \mathrm{d}p\, \mathcal{R}(x,p) G\left(|x-x'|, \left[\frac{p}{|p|}\cdot\frac{p'}{|p'|}\right], |p'|\right) \ . \tag{8}$$

$F(|x-x'|,p')$ has the interpretation of a functional relationship that connects particle fluence at phase-space location x',p' to a tally calculated at x. This method has a known difficulty—its treatment of heterogeneities and interfaces. Heterogeneities and interfaces can be treated approximately by scaling $|x-x'|$ by the collision density. This is an exact for the part of the kernel that describes the first scatter contribution but approximate for higher-order scatter contributions. It can also be approximate, to varying degrees, if the scatter produces other particles with different scaling laws, such as the electron set in motion by a first Compton collision of a photon.

For calculation methods that are concerned with primary charged particles, the heterogeneity problem is more severe. The true solution in this case is reached when the pathlength steps, s in Equation 5 are made small [88] and so, an iterative scheme is set up:

$$\psi_1(x,p) \ = \ \int \mathrm{d}x' \int \mathrm{d}p'\, G(x,p,x',p',\Delta s) Q(x',p')$$

$$
\begin{aligned}
\psi_2(x,p) &= \int \mathrm{d}x' \int \mathrm{d}p'\, G(x,p,x',p',\Delta s)\psi_1(x',p') \\
\psi_3(x,p) &= \int \mathrm{d}x' \int \mathrm{d}p'\, G(x,p,x',p',\Delta s)\psi_2(x',p') \\
&\vdots \\
\psi_N(x,p) &= \int \mathrm{d}x' \int \mathrm{d}p'\, G(\psi_{N-1}(x',p') \qquad (9)
\end{aligned}
$$

which terminates when the largest energy in $\psi_N(x,p)$ has fallen below an energy threshold or there is no x remaining within the target. The picture is of the phase space represented by $\psi(x,p)$ "evolving" as s accumulates. This technique has come to be known as the "phase-space evolution" model. Heterogeneities are accounted for by forcing Δs to be "small" or of the order of the dimensions of the heterogeneities and using a $G()$ that pertains to the atomic composition of the local environment. The calculation is performed in a manner similar to the one described for convolution. That is,

$$
T(x) = \sum_{i=1}^{N} \int \mathrm{d}x' \int \mathrm{d}p'\, F(x,x',p,p',\Delta s)\psi_i(x',p') \ , \qquad (10)
$$

where the "kernel", $F(x,x',p,p',\Delta s)$, is defined by:

$$
F(x,x',p,p',\Delta s) = \int \mathrm{d}p\, \mathcal{R}(x,p) G(x,p,x',p',\Delta s)) \ . \qquad (11)
$$

In the following analysis, we will not consider further any systematic errors associated with the treatment of heterogeneities in the case of the convolution method, nor with the "stepping errors" associated with incrementing s using Δs in the phase space evolution model. Furthermore, we assume that the Green's functions or response kernels can be computed "exactly"—that there is no systematic error associated with them. The important result of this discussion is to demonstrate that the dimensionality of the analytic approach is $N_x + N_p$.

A.2 Convergence of Deterministic Solutions

The discussion of the previous section indicates that deterministic solutions are tantamount to solving a $\mathcal{D}$-dimensional integral of the form:

$$
I = \int_{\mathcal{D}} \mathrm{d}u\, H(u) \ . \qquad (12)
$$

In $\mathcal{D}$ dimensions, the calculation is no more difficult than in two dimensions, only the notation is more cumbersome. One notes that the integral takes the form:

$$
I = \int_{u_{1,\min}}^{u_{1,\max}} \mathrm{d}u_1 \int_{u_{2,\min}}^{u_{2,\max}} \mathrm{d}u_2 \cdots \int_{u_{\mathcal{D},\min}}^{u_{\mathcal{D},\max}} \mathrm{d}u_{\mathcal{D}}\, H(u_1, u_2 \cdots u_{\mathcal{D}})
$$

$$= \sum_{i_1=1}^{N_{\rm cell}^{1/\mathcal{D}}} \int_{u_{i_1}-\Delta u_1/2}^{u_{i_1}+\Delta u_1/2} \mathrm{d}u_1 \sum_{i_2=1}^{N_{\rm cell}^{1/\mathcal{D}}} \int_{u_{i_2}-\Delta u_2/2}^{u_{i_2}+\Delta u_2/2} \mathrm{d}u_2 \cdots \int_{u_{i_\mathcal{D}}-\Delta u_\mathcal{D}/2}^{u_{i_\mathcal{D}}+\Delta u_\mathcal{D}/2} \mathrm{d}u_\mathcal{D} \sum_{i_\mathcal{D}=1}^{N_{\rm cell}^{1/\mathcal{D}}} H(u_1, u_2 \cdots u_\mathcal{D}) \tag{13}$$

The Taylor expansion takes the form

$$\begin{aligned} H(u_1, u_2 \cdots u_\mathcal{D}) &= H(u_{i_1}, u_{i_2} \cdots u_{i_\mathcal{D}}) + \sum_{j=1}^{\mathcal{D}} (u_i - u_{i_j}) \partial H(u_{i_1}, u_{i_2} \cdots u_{i_\mathcal{D}})/\partial u_j + \\ & \sum_{j=1}^{\mathcal{D}} \frac{(u_i - u_{i_j})^2}{2} \partial^2 H(u_{i_1}, u_{i_2} \cdots u_{i_\mathcal{D}})/\partial u_j^2 + \\ & \sum_{j=1}^{\mathcal{D}} \sum_{k \neq j=1}^{\mathcal{D}} (u_i - u_{i_j})(u_i - u_{i_k}) \partial^2 H(u_{i_1}, u_{i_2} \cdots u_{i_\mathcal{D}})/\partial u_i \partial u_j \cdots \end{aligned} \tag{14}$$

The linear terms of the form $(u_i - u_{i_j})$ and the bilinear terms of the form $(u_i - u_{i_j})(u_i - u_{i_k})$ for $k \neq j$ all vanish by symmetry and a relative $N^{-2/\mathcal{D}}$ is extracted from the quadratic terms after integration. The result is that:

$$\frac{\Delta I}{I} = \frac{1}{24 N_{\rm cell}^{2/\mathcal{D}}} \frac{\sum_{i_1=1}^{N_{\rm cell}^{1/\mathcal{D}}} \sum_{i_2=1}^{N_{\rm cell}^{1/\mathcal{D}}} \cdots \sum_{i_\mathcal{D}=1}^{N_{\rm cell}^{1/\mathcal{D}}} \sum_{d=1}^{\mathcal{D}} (u_{d,\max} - u_{d,\min})^2 \partial^2 H(u_{i_1}, u_{i_2} \cdots u_{i_\mathcal{D}})/\partial u_d^2}{\sum_{i_1=1}^{N_{\rm cell}^{1/\mathcal{D}}} \sum_{i_2=1}^{N_{\rm cell}^{1/\mathcal{D}}} \cdots \sum_{i_\mathcal{D}=1}^{N_{\rm cell}^{1/\mathcal{D}}} H(u_{i_1}, u_{i_2} \cdots u_{i_\mathcal{D}})} \,. \tag{15}$$

Note that the one and two-dimensional results can be obtained from the above equation. The critical feature to note is the overall $N_{\rm cell}^{-2/\mathcal{D}}$ convergence rate. The more dimensions in the problem, the slower the convergence for numerical quadrature.

A.3 Convergence of Monte Carlo solutions

An alternative approach to solving Equation 2 is the Monte Carlo method whereby $N_{\rm hist}$ particle histories are simulated. In this case, the Monte Carlo method converges to the true answer according to the central limit theorem [132] which is expressed as:

$$\frac{\Delta T_{\rm MC}(x)}{T_{\rm MC}(x)} = \frac{1}{\sqrt{N_{\rm hist}}} \frac{\sigma_{\rm MC}(x)}{T_{\rm MC}(x)} \,, \tag{16}$$

where $T_{\rm MC}(x)$ is the tally calculated in a voxel located at x as calculated by the Monte Carlo method and $\sigma_{\rm MC}^2(x)$ is the variance associated with the *distribution* of $T_{\rm MC}(x)$. Note that this variance $\sigma_{\rm MC}^2(x)$ is an intrinsic feature of how the particle trajectories deposit energy in the spatial voxel. It is a "constant" for a given set of initial conditions and is conventionally estimated from the sample variance. It is also assumed, for the purpose of this discussion, that the sample variance exists and is finite.

A.4 Comparison between Monte Carlo and Numerical Quadrature

The deterministic models considered in this discussion pre-calculate $F(|x-x'|,p')$ of Equation 8 or $F(x,x',p,p',\Delta s)$ of Equation 11 storing them in arrays for iterative use. Then, during the iterative calculation phase, a granulated matrix operation is performed. The associated matrix product is mathematically similar to the "mid-point" N_x+N_p-multidimensional integration discussed previously:

$$T(x) = \int_{\mathcal{D}} \mathrm{d}u\, H(u,x) \ , \tag{17}$$

where $\mathcal{D} = N_x + N_p$ and $u = (x_1, x_2 \cdots x_{N_x}, p_1, p_2 \cdots p_{N_p})$. That is, u is a multidimensional variable that encompasses both space and momentum. In the case of photon convolution, $H(u,x)$ can be inferred from Equation 7 and takes the explicit form:

$$H(u,x) = \int \mathrm{d}p\, F(|x-x'|,p')Q(x',p') \ . \tag{18}$$

There is a similar expression for the phase space evolution model.

The "mid-point" integration represents a "first-order" deterministic technique and is applied more generally than the convolution or phase space evolution applications. As shown previously, the convergence of this technique obeys the relationship:

$$\frac{\Delta T_{\mathrm{NMC}}(x)}{T_{\mathrm{NMC}}(x)} = \frac{1}{N_{\mathrm{cell}}^{2/\mathcal{D}}} \frac{\sigma_{\mathrm{NMC}}(x)}{T_{\mathrm{NMC}}(x)} \ , \tag{19}$$

where $T_{\mathrm{NMC}}(x)$ is the tally in a spatial voxel in an arbitrary N_x-dimensional geometry calculated by a non-Monte Carlo method where N_p momentum components are considered. The D-dimensional phase space has been divided into N_{cell} "cells" equally divided among all the dimensions so that the "mesh-size" of each phase space dimension is $N_{\mathrm{cell}}^{1/\mathcal{D}}$. The constant of proportionality as derived previously is:

$$\sigma_{\mathrm{NMC}}(x) = \frac{1}{24} \sum_{i_1=1}^{N_{\mathrm{cell}}^{1/\mathcal{D}}} \sum_{i_2=1}^{N_{\mathrm{cell}}^{1/\mathcal{D}}} \cdots \sum_{i_{\mathcal{D}}=1}^{N_{\mathrm{cell}}^{1/\mathcal{D}}} \sum_{d=1}^{\mathcal{D}} (u_{d,\max} - u_{d,\min})^2 \partial^2 H(u_{i_1}, u_{i_2} \cdots u_{i_{\mathcal{D}}}) / \partial u_d^2 \ , \tag{20}$$

where the u-space of $H(u)$ has been partitioned in the same manner as the phase space described above. $u_{d,\min}$ is the minimum value of u_d while $u_{d,\max}$ is its maximum value. u_{i_j} is the midpoint of the cell in the j^{th} dimension at the i_j^{th} mesh index.

The equation for the proportionality factor is quite complicated. However, the important point to note is, that it depends only on the second derivatives of $H(u)$ with respect to the phase-space variables, u. Moreover, the non-Monte Carlo proportionality factor is quite different from the Monte Carlo proportionality factor. It would be difficult to predict which would be smaller, and almost certainly, would be application dependent.

We now assume that the computation time in either case is proportional to N_{hist} or cell. That is, $T_{\mathrm{MC}} = \alpha_{\mathrm{MC}} N_{\mathrm{hist}}$ and $T_{\mathrm{NMC}} = \alpha_{\mathrm{NMC}} N_{\mathrm{cell}}$. In the Monte Carlo case, the computation

time is simply N_{hist} times the average computation time/history. In the non-Monte Carlo case, the matrix operation can potentially attempt to connect every cell in the $\mathcal{D}$-dimensional phase space to the tally at point x. Thus, a certain number of floating-point and integer operations are required for each cell in the problem.

Consider the convergence of the Monte Carlo and non-Monte Carlo method. Using the above relationships, one can show that:

$$\frac{\Delta T_{\text{MC}}(x)/T_{\text{MC}}(x)}{\Delta T_{\text{NMC}}(x)/T_{\text{NMC}}(x)} = \left(\frac{\sigma_{\text{NMC}}(x)}{\sigma_{\text{MC}}(x)}\right)\left(\frac{\alpha_{\text{NMC}}^{\mathcal{D}}}{\alpha_{\text{MC}}}\right)^{1/2} t^{(4-\mathcal{D})/2\mathcal{D}} \ , \tag{21}$$

where t is the time measuring computational effort for either method. We have assumed that the two calculational techniques are the same. Therefore, given enough time, $D_{\text{MC}}(x) \approx D_{\text{NMC}}(x)$. One sees that, given long enough, the Monte Carlo method is always more advantageous for $\mathcal{D} > 4$. We also note, that inefficient programming in the non-Monte Carlo method is severely penalized in this comparison of the two methods.

Assume that one desires to do a calculation to a prescribed $\varepsilon = \Delta T(x)/T(x)$. Using the relations derived so far, we calculate the relative amount time to execute the task to be:

$$\frac{t_{\text{NMC}}}{t_{\text{MC}}} = \left(\frac{\alpha_{\text{MC}}}{\alpha_{\text{NMC}}}\right)\left(\frac{[\sigma_{\text{NMC}}(x)/T_{\text{NMC}}(x)]^{\mathcal{D}/2}}{\sigma_{\text{MC}}(x)/T_{\text{MC}}(x)}\right)\varepsilon^{(4-\mathcal{D})/2} \ , \tag{22}$$

which again shows an advantage for the Monte Carlo method for $\mathcal{D} > 4$. Of course, this conclusion depends somewhat upon assumptions of the efficiency ratio $\alpha_{\text{MC}}/\alpha_{\text{NMC}}$ which would be dependent on the details of the calculational technique. Our conclusion is also dependent on the ratio $[\{\sigma_{\text{NMC}}(x)/T_{\text{NMC}}(x)\}^{\mathcal{D}/2}]/[\sigma_{\text{MC}}(x)/T_{\text{MC}}(x)]$ which relates to the detailed shape of the response functions. For distributions that can vary rapidly, the Monte Carlo method is bound to be favored. When the distributions are flat, non-Monte Carlo techniques may be favored.

Nonetheless, at some level of complexity (large number of N_{cell}'s required) Monte Carlo becomes more advantageous. Whether or not one's application crosses this complexity "threshold", has to be determined on a case-by-case-basis.

Smaller dimensional problems will favor the use of non-Monte Carlo techniques. The degree of the advantage will depend on the details of the application.

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