The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
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ELECTRON/PHOTON TRANSPORT AND ITS APPLICATIONS

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ABSTRACT

This paper surveys the wide range of radiation physics topics that involve the transport of energetic electrons and x-rays. Applications in the high-energy range (100 keV to 30 MeV) include: radiation therapy physics (including treatment planning), industrial radiation processing of materials, shielding, experimental and theoretical dosimetry, dose profiles near material interfaces, beta-ray dosimetry, characterization of the photon spectrum from radioisotope sources, bremsstrahlung (x-ray) generation, and radiation charging of insulators. Lower energy applications (from below100eV to 100 keV) include: positron transport, electron probe microanalysis (EPMA), prediction of x-ray tube spectra, x-ray fluorescence analysis (XRF), electron-beam-induced-current (EBIC), auroral phenomena, x-ray lithography, electron beam lithography, Auger electron spectroscopy (AES), x-ray photoelectron spectroscopy (XPS), secondary electron emission, and electron energy loss spectroscopy (EELS). As examples, we briefly discuss (1) radiation therapy physics,(2) dose enhancement at material interfaces, and (3) x-ray target spectrum prediction.

Mathematical methods and models for electron/photon transport are briefly described. These include (1) the Monte Carlo simulation method, (2) numerical solution of the transport equation, (3) analytic or semi-empirical models, (4) several miscellaneous methods, and (5) multidimensional methods. These models must be verified be comparison with benchmark experimental data, such as for electron backscatter and transmission, energy and charge deposition, and x-ray target spectra.

Finally we list some topics where further transport model research would be desirable. We also describe a book in progress, which will provide a broad introduction to the theory of electron/photon transport and its many applications in radiation physics.

Key Words: Electron transport, photon transport, radiation physics, Monte Carlo, radiation therapy physics

1 INTRODUCTION

This intent of this paper is to provide a tutorial overview of coupled electron/photon transport and its applications. In this paper we will (1) show how coupled electron/photon transport unifies many radiation physics topics, (2) summarize the physics and mathematical methods of electron/photon transport, (3) discuss several application areas, such as: radiation therapy physics, dose enhancement at interfaces, and x-ray target spectra, (4) suggest areas for future research, and (5) briefly describe a book which has the goal of providing an "encyclopedic" introduction to electron/photon transport and its applications.

1.1 The Motivation for this Survey Paper

Beside a previous paper [1], this may be the first comprehensive overview of the electron/photon transport field over the broad energy range from 100 eV to 30 MeV. Although low and high-energy Monte Carlo codes utilize different simulation approaches for electron tracks, the physical interactions involved are practically the same. This paper treats high and low energy electron/photon transport as a single field.

This paper gives a brief preview of a book I am writing designed to be both introductory and encyclopedic. It should be a much-needed resource for both beginners and more experienced transport specialists alike. It will be helpful for (1) students interested in the field, (2) instructors, (3) experimentalists needing more understanding of the physical principles behind radiation experiments, and also (4) experienced workers in particular sub-areas of this field. The main purpose of the book will be to demonstrate that the theory of electron/photon transport, though at times complex, provides a clear road to understanding the commonality between widely diverse radiation physics topics.

1.2 What is Radiation Physics?

"Radiation physics" deals with phenomena involving a wide range of particles, e.g., electrons, photons, neutrons, protons, heavy ions, etc. At first glance, radiation physics appears to be a "hodge-podge" of topics involving a wide variety of particles, phenomena, and application topics. Hubbell [2] gives a definition of radiation physics as follows: "*Radiation physics ties together a variety of otherwise separate and compartmentalized scientific, medical and engineering disciplines, all involving aspects of radiation including radiation sources, radiation transport (penetration), radiation detection, and radiation effects.*"

Papers on these topics appear in many journals including: *Radiation Physics and Chemistry, Radiation Measurements, Radiation Protection Dosimetry, Health Physics, Applied Radiation and Isotopes, Medical Physics, Physics in Medicine and Biology, and X-ray Spectrometry*, to name a few. A partial but broad listing of radiation physics topics [2] might include:

1. Atomic and nuclear physics
2. *Medical radiation physics: imaging, therapy
3. Environmental radiation dosimetry
4. Nuclear power engineering,
5. *Radiation shielding (x-rays, neutrons, protons, etc.)
6. *Radiation transport theory, Monte Carlo
7. X-ray crystallography
8. *Industrial radiation processing
9. *Electron microprobe analysis
10. *Fluorescence XRS, XRF materials analysis
11. Proton-induced x-ray analysis (PIXE)
12. Radiation archeometry, dating
13. *Atmospheric electron transport/aurora
14. X-ray, γ-ray astronomy, astrophysics
15. Space vehicle shielding and dosimetry
16. Radiation damage to electronic circuitry

Many of these topics (denoted by *) principally involve high and/or low energy electron/photon transport. In applications where only energetic electrons, photons and positrons are involved, electron/photon transport models that have been developed can now quantify these applications. Thus electron/photon transport physics may be considered as a *unifying theory* for major portions of radiation physics.

2 ELECTRON/PHOTON TRANSPORT PHYSICS

2.1 Coupled Electron/Photon Transport

Why is the term "coupled" useful for describing electron/photon transport? The reason is that, during transport in a medium (solid, liquid, or gas), each particle type produces the other. As we briefly review the physics of electron and photon transport below, we observe that, while electrons often produce photons, photons mainly generate energetic electrons.

2.2 How electrons transport and produce photons

As electrons move through a medium, they experience the following interactions:

(a) They are *elastically scattered* by atomic nuclei, which are to some extent shielded by the electrons in the inner shells of atoms. These collisions produce deflections but essentially no energy loss (except for bremsstrahlung).

(b) They are *inelastically scattered* against other electrons in the medium. In general this involves both an energy loss and a deflection. The deflection is usually ignored. The energy imparted to the other electrons is usually small compared to the initial energy of the electron doing the colliding. These are called "soft collisions".

Electrons with energies above 1 keV are usually regarded as losing their energy continuously to the electrons in the medium. The electron stopping power describes this effect. This is known as the continuous-slowing-down-approximation (CSDA).

(c) Inelastic scattering imparts energy to electrons in the medium and can also produce *secondary electrons*. In so-called "Type II" high-energy Monte Carlo codes [3], these electron-electron collisions are called "hard collisions" which means that a substantial fraction of the initial electron energy is imparted to the secondary electron, also known as a "knock-on" electron.

(d) Electrons produce *bremsstrahlung* radiation. As electrons are deflected by atomic nuclei, energy is radiated and the photons are produced are known as bremsstrahlung radiation. This is observable as background radiation in an x-ray target spectrum at 10 - 50 keV, but only produces a substantial energy loss affecting electron transport at energies above 1 MeV.

(e) During transport, energetic electrons occasionally ionize the inner shells of atoms in a medium. These interactions occur infrequently and can be ignored in calculating electron transport. However, to obtain the results of this ionization, special techniques such as "interaction forcing" have been used [4].

These inner shells return to their normal state by (a) ejection of Auger electrons or (b) emission of fluorescent (characteristic x-ray) photons. The latter process is another way electrons (indirectly) generate photons.

2.3 How photons transport and produce electrons

As photons traverse a medium, they are scattered or absorbed by one of several processes [5]. In most cases, an energetic electron is produced. These interactions include:

(a) The Compton (incoherent) interaction
A major mechanism for photon-produced electron excitation is the Compton interaction (incoherent scattering). In this case, a gamma-ray photon collides with an atom producing an energetic electron and a scattered photon of lower energy. The Compton interactions dominate other photon interactions in the 200 keV to 20 MeV energy range.

(b) Coherent (Rayleigh) scattering
Photons interact with all the electrons in an atom collectively via the Rayleigh interaction. It has a larger cross section than incoherent scattering particularly for low-energy photons and high-Z materials. Because the energy loss to the photon is slight and the scattering angle small, this, Rayleigh scattering is usually neglected in shielding calculations.

(c) The photoelectric interaction (also called “photo-ionization”)
Here photons interact with the inner shells of atoms in the solid and eject a “photoelectron”. Depending on the inner shell involved, the electrons are called K-, L- and M-photoelectrons. Their energy is equal to the energy of the incoming photon less the binding energy of the inner shell. The K-shell photoelectric interaction varies with atomic number Z and photon energy E as Z^4/E^3 and is dominant in medium-to-high Z materials below 200 keV.

(d) Electron–positron pair production.
Photons with energy of at least twice the electron rest mass are able to create electron–positron pairs. This process becomes increasingly important above 2 MeV and is the dominant interaction above 30 MeV. This is another mechanism by which photons produce electrons.

2.4 Electron and Photon Sources

Another way we see the coupling between electrons and photons is through examining different types of electron and photon radiation sources.

(a) Electron sources can be regarded as either *externa*l or *internal*. An external source is an incident electron beam impinging on a medium. Some examples of internal sources are (1) beta-emitting sources inside a medium and (2) the electrons excited by incident x-ray or gamma-ray photons via the Compton, photoelectric and pair-production interactions.

(b) An example of an external photon beam sources would be: (1) gamma-rays from radioactive isotopes sources (e.g. a Co^{60} irradiator). Electron-produced photon sources include (2) high-energy bremsstrahlung generators (as used, e.g., in radiation therapy) and (3) x-ray tubes, where characteristic and continuum x-rays (bremsstrahlung) are important. Internal photon sources might include (4) gamma rays from imbedded radioactive isotopes, (5) positron annihilation radiation and (6) fluorescent x-rays.

3 ELECTRON/PHOTON TRANSPORT CATEGORIES

The various features of electron/photon transport and its applications have been organized into four main categories. These are (a) Input Data (cross sections for the physical interactions which we discussed in **2**), (b) Mathematical Methods and Models, (c) Benchmark Experimental Data, and (d) Applications. We further subdivide the applications into four types ranked by energy plus a fifth consisting of "other" (miscellaneous) application areas. I have named these application types as: (a) High-Energy Applications (1 - 30 MeV), (b) Medium-to-High Energy applications (100 keV - 10 MeV), (c) Medium-Energy Applications (1 - 100 keV), (d) Low-Energy Applications (~100 eV - 50 keV), and (e) Other Application Areas. An extensive listing of topics in these areas is given below:

3.1 High-Energy Applications

- Radiation therapy physics
- Fermi-Eyges theory (for electron pencil beams)
- Radiation treatment planning
- Industrial radiation processing

3.2 Medium-to-High Energy Applications

- Radiation shielding, deep penetration and gamma ray buildup
- Polarized photon transport
- Beta-ray dosimetry
- Determination of the photon spectrum of Co^{60} and bremsstrahlung radiation sources
- Theoretical dosimetry and cavity chamber theory
- Dose perturbations and dose enhancement at material interfaces
- X-ray photoemission yields and spectra
- Experimental dosimetry and dosimeters
- Detectors and their response to radiation
- Radiation charging of insulators

3.3 Medium-Energy Applications

- Positron transport in solids
- X-ray target spectrum prediction
- Electron probe microanalysis (EPMA)
- X-ray fluorescence (XRF)
- Electron-Beam-Induced-Current (EBIC)
- Atmospheric electron transport and the aurora
- Electron beam and x-ray lithography

3.4 Low Energy Applications

- X-ray photoelectron spectroscopy (XPS)
- Auger electron spectroscopy (AES)
- Positron-Annihilation-Induced Auger electron spectroscopy (PAES)
- Secondary electron emission
- Low energy electron transport in conducting media
- Low energy transport in dielectrics (including charging effects)

3.5 Other Application Areas

- Electron-hole pair creation
- Electron slowing down
- W-values in gases (energy to create an ion pair)
- Microdosimetry

- Track structure of electrons (including near ion tracks)
- Proton and ion beam transport (where there are analogues to electron transport)
- Electron energy loss spectroscopy (EELS)
- Reflection electron energy loss spectroscopy (REELS)
- Elastic peak electron spectroscopy (EPES)

4 MATHEMATICAL METHODS AND MODELS

In this section we briefly summarize several types of mathematical models for calculating electron/photon transport. These include: (1) the Monte Carlo method, (2) numerical solution of the transport equation, (3) analytic or semi-empirical models, (4) miscellaneous mathematical methods and (5) multidimensional transport models.

4.1 Monte Carlo Methods

The principal computational method used for calculating electron/photon transport is the Monte Carlo method. This method consists of computer simulation of electron and photon tracks (also called "histories") by randomly choosing the outcome of each scattering event and following the paths of the primary particle and all its secondary particles down to some cutoff energy. Two main types of Monte Carlo models are used: (1) "Single scattering" Monte Carlo, also known as "analog" Monte Carlo and used only for low energy transport, which follows each collision event sustained by each particle, and (2) "Condensed history" Monte Carlo which lumps many individual deflections of electrons against the nuclei of the medium into a single "multiple scattering" event. We note that the Monte Carlo method is a statistical method and often requires millions of particle histories to obtain the desired accuracy for, e.g., radiation therapy applications. A more recent Monte Carlo model (3), exemplified by the PENELOPE [6] code, utilizes a "random-hinge" which allows a smooth transition to be made from the analog to condensed history approach.

The Monte Carlo method has undergone extremely rapid development in the past ten years. One reason for this is the interest in modeling the radiation dose in three dimensions for radiation therapy planning and to reduce the computation time as much as possible consistent with the high accuracy required. Because it simulates complex physical interactions and is applicable for general geometry, Monte Carlo is the principal method used for electron/photon transport calculations and is under continual development as witnessed by this conference (also see [7]). I have observed that, of the many journal references I have surveyed, roughly 80 to 90% involve the Monte Carlo method one way or another.

Beside well-established Monte Carlo codes like ETRAN, EGS4, MCNP, ITS, and GEANT, other programs described in recent literature include: (1) new general-purpose codes such as EGSnrc [8] and PENELOPE [6], (2) algorithms specifically tailored for radiation therapy treatment planning [9-11], and (3) specialized models involving (a) x-ray fluorescence (XRF) [12], (b) electron transport below 1 kev [13, 14], and (c) specific materials, such as water (used for track structure studies [15]).

4.1.1 Some advantages of the Monte Carlo method

- All known physical interactions can be modeled fairly well.
- It is practical for most applications.

- It can be utilized for general geometries in 1-D, 2-D, and 3-D

4.1.2 Some disadvantages of the Monte Carlo method

- Depending on the desired accuracy or resolution required (particularly for fine grids in the space, energy, and/or angle variables), running times can be excessively long.
- No finite amount of running time will eliminate statistical uncertainties from the results.
- Because of these statistical uncertainties, determining the effect of small parametric variations may be difficult. Occasionally "correlated histories" have been used to deal with this situation.
- At high energies, the "condensed history" approach is necessary, but this an approximation that can introduce "artifacts" particularly near material boundaries and interfaces..
- For deep penetration problems or for regions where too few particles contribute to the solution, the statistical error may be unacceptable. Accuracy can sometimes be improved using variance reduction techniques.
- A Monte Carlo code cannot be treated as a "black box" and correct answers are not always easy to obtain. Parameters for describing energy steps and path step sizes should be chosen carefully. The algorithm may need to be modified and adapted for a particular problem. The beginning user will need time to develop the experience needed to make reliable Monte Carlo calculations.

4.2 Transport equation solutions

A method almost as physically rigorous as Monte Carlo is to solve the transport equation for coupled electrons and photons. The starting point is the time-independent Boltzmann transport equation with four terms: (1) a source term, (2) a "collision-in" term (an integral over all particle fluxes that contribute particles into the energy of interest), (3) a "collision out" term which describes the rate that particles are scattered out of the energy of interest, and (4) a "drift" term that describes the rate that particles leave a region of phase space. This integro-differential equation is directly applicable for treating photon transport.

For electron transport, the full Boltzmann equation is only used at very low energies [e.g., secondary electron emission]. At higher energies, approximations to the Boltzmann equation are used such as the Spencer-Lewis equation (which uses the CSDA), the Fokker-Planck equation, and the Boltzmann-Fokker-Planck equation.

These equations can be solved by several numerical methods. The principal method used is the S_n or discrete ordinates method. (The P_n method and the method of moments have also been applied.) This method suffers from discretization errors due to the small but *finite* spatial, angular and energy intervals used. The discrete ordinates solution will always differ somewhat from the correct solution. A more accurate solution may require a larger mesh than can be handled on small computers. Examples of 1-D discrete ordinates codes for coupled electron/photon transport (from Sandia National Laboratory) are the CEPXS-ONELD code [16] and its successors.

4.2.1 Some transport solution advantages

- Solutions are exactly reproducible from one run to another (unlike Monte Carlo).
- The method lends itself well for making parameter changes for a given application.
- When it applies, it can be more rapid than Monte Carlo.
- It generates a solution for all points in phase space (although the solution

may not be accurate for "deep penetration" problems, such as in shielding).

4.2.2 Transport solution disadvantages

- This approach is pretty much limited to 1-D (including spherical).
- Little progress has been made on 2-D, 3-D transport.
- Solution errors are generally not easy to estimate.
- Some physics can be hard to model (e.g. straggling, when the CSDA approximation is used).
- Very large grids may be needed for solutions of sufficient accuracy.
- Higher-order schemes are subject to oscillations, instabilities.

4.3 Semi-empirical Models

Many different analytical models that calculate specific quantities, such as the energy deposition profile or backscattering coefficient, have been developed. They are called "semi-empirical" because they involve general physical parameters such as Z, E, incident beam angle, material thickness, etc. An example for energy deposition in multilayered materials is the EDMULT code [17]. Models for such quantities as backscatter, transmission, positron "implantation", x-ray target spectra, etc. have also been developed. They usually are only applicable for simple 1-D geometries, allow rapid calculations, and often provide insight into the behavior of a quantity as a function of incident particle energy and angle and material parameters.

4.4 Other mathematical methods

Other techniques exist for formulating transport problems. Examples of these methods include (a) the method of invariant imbedding (used, e.g., for studying electron backscattering [18] and x-ray microanalysis [19], (b) solution of the one-speed transport equation utilized in XPS/AES [20], and (c) the phase-space-evolution method [21].

4.5 Multidimensional transport (2-D,3-D)

Both Monte Carlo and transport equation methods have been used to obtain solutions for the 3-D spatial-energy-angle flux distribution of electrons and photons in a medium. In the case of the coupled electron/photon transport equations, Drumm [22] has developed production discrete ordinates codes for solving 3-D problems. Here the computer memory requirements are far exceed those for 1-D problems. The 2- and 3-D transport equations for *photons* have also been applied to several medical dosimetry applications [23, 24].

5 BENCHMARK EXPERIMENTAL DATA

Due to space limitations, we must omit a description of benchmark experimental data available for verifying the physics in electron/photon transport codes. Types of benchmarks data include (a) backscatter, (b) transmission, (c) energy deposition, (d) charge deposition, and (e) the x-ray target spectra. Some recent papers where Monte Carlo codes are compared with experimental benchmarks are given in references [25, 26, 27].

6 APPLICATIONS

As illustrations, we briefly describe three specific applications: (1) radiation therapy physics, (2) dose enhancement at material interfaces, and (3) x-ray target spectrum prediction.

6.1 A High-Energy Application (1 – 30 MeV): Radiation Therapy Physics

A high-energy application example is the (enormous) field of radiation therapy physics. Radiation therapy treatment requires both careful measurement and calculation of absorbed dose (2% or less accuracy) to a patient. It is important to maximize the dose to a cancerous tumor while minimizing the dose to the surrounding tissues. Often the only way to do this is to use a number of different photon beams with different angles with respect to the patient. Finding the optimal beam configuration and radiation parameters is an example of "radiation treatment planning".

Human bodies are highly individual and each tumor is different. It is critical to determine the radiation dose delivered to a patient as accurately as possible. Because of steep dose-response curves, 5%-10% errors in the dose can be fatal [28]. Up until the present time, commercial treatment planning systems have handled 3-D geometry well but more or less empirical "pencil-beam" models can underestimate the dose by as much as 20% because of inhomogeneities in lungs, bone, tissue, air cavities, etc. Monte Carlo algorithms, now under intensive development, may be expected to eliminate or reduce these errors.

6.2 A Medium-to-High-Energy Application (100 keV – 10 MeV): Dose Enhancement at Material Interfaces

When x-rays or gamma-rays irradiate a region involving an interface between two media, the dose profile near the interface is seen to undergo rapid spatial variations with respect to the "equilibrium dose" value away from the interface. This effect is called "dose perturbation" or "dose enhancement". If this effect is overlooked, depending on the photon energy, the dose on the low-Z side of an interface can be underestimated by a factor of two or even much more. However, dose perturbations close to the interface are not entirely easy to evaluate. A recent reference [29] discusses some of the difficulties involved in calculating or measuring this effect.

This effect is especially important for x-ray energies in the 50 - 500 keV range where the photon absorption in a high atomic number medium will usually be many times the photon absorption in the lower atomic number medium. Medical examples where dose enhancement can play a role include x-ray irradiation of tissue near a lead pin or of a tooth with a gold inlay.

Dose enhancement also occurs in electronic devices [30], when there is a high Z material close to a silicon/silicon dioxide interface. Typical Co^{60} irradiators with a primary energy of 1.25 MeV nearly always contain a large component of lower energy (Compton-scattered) photons. To decrease dose enhancement effects, a lead-aluminum filter container has been used to reduce the fraction of low energy photons reaching a dosimeter or device being tested.

6.3 A Medium-Energy Application (1 keV – 100 keV): X-ray target spectrum prediction

Knowing the spectrum of x-rays produced in an electron-irradiated target (usually one element) is of great interest. X-ray tubes produce x-rays for many purposes, such as diagnostic x-rays and x-ray fluorescence analysis. The target spectrum consists of characteristic x-ray lines and a "background" x-ray continuum. Both Monte Carlo [27] and semi-empirical models [31] have been used for calculating x-ray spectra. The spectrum is dependent on the energy and angle of incidence of the electron beam and the exit angle of the x-rays.

A field closely allied to x-ray generation is the popular analytical technique of electron probe microanalysis (EPMA). Here the measured energies and intensities of various characteristic x-ray lines from an electron-beam irradiated sample are used to determine the elemental composition of a small portion of the sample material [32]. More or less simplified, transport-based “correction" models are required to perform this quantitative analysis.

7 SUGGESTIONS FOR FUTURE RESEARCH

Here we list several areas where more research is recommended:

(1) There are almost no reports where the sensitivity of transport calculations has been studied as a function of changes in the electron scattering cross sections. For example, how much will a 10% variation in the magnitude of the elastic scattering cross section change the electron backscattering coefficient? We need to understand how much uncertainties in cross sections affect the accuracy of transport calculations in different scenarios.

(2) Better knowledge of K, L, and M ionization cross sections are needed for more accurate x-ray spectrum prediction and quantitative electron probe microanalysis.

(3) Electron transport in high atomic number materials is not well understood [33]. More experimental and theoretical studies are needed at all electron energies.

(4) Numerical solution of the coupled electron/photon transport equation in 2-D and 3-D geometry continues to be a major challenge. Will more progress be made on this?

(5) The “ultimate” solution for transport is the full energy-angle-spatial Boltzmann flux distribution function. To date, little or no information about this function has been obtained, possibly because it isn’t needed for obtaining observable transport quantities. It would nevertheless be valuable to have, at least, approximate solutions for this general function, both for a better understanding of the transport process and as a reference solution for comparing different transport models.

8 BOOK PROJECT SUMMARY

The author is currently writing an introductory book on the physics of the transport of electrons, photons and positrons. About fifty distinct topics will be discussed. The basic physical interactions, mathematical models and methods, benchmark experimental data and applications from below 100 eV to 30 MeV will be described. We have accumulated a bibliographic database of over 3100 references to be included with the book. If feasible, we hope to include one or more working Monte Carlo codes and other transport algorithms on a CD-ROM.

9 CONCLUSIONS

We have surveyed the physics, mathematics and applications of coupled electron/photon transport. To our knowledge, an overview treating the full energy range from about 100 eV to 30 MeV has not been given previously. We have shown that electron/photon transport provides a flexible theoretical model and a unity for a wide variety of radiation physics topics.

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