Official title

[Introduction to] Monte Carlo Methods

NERS 544

Administrative Stuff

From the bulletin ...

NERS 544. Monte Carlo Methods

Prerequisite: Graduate standing in Engineering, Mathematics or Sciences. (2 credits)

This course is an introduction to Monte Carlo methods, including basic probability and statistics, random number generation, sampling, scoring and tallies, error estimation, variance reduction and importance sampling. Examples are drawn from Monte Carlo particle transport.

Undergraduate standing? (no problem)

"Examples ..."
will be drawn from Math & Medical Physics

NERS 544

Monte Carlo Methods

Announcements:

Please see reading list below, as well as the first assignment

Course-related links:

Tentative Course Schedule (check revision date often)
The Monte Carlo book (Yes! There are missing figures!)
The Dosimetry book (Yes! There are missing figures!)
Course Policy/Grading (check revision date periodically)

Location: G906 White Auditorium
Time: Thursdays 17:30 - 19:30

Instructor: Professor Alex Bielajew
Office: Cooley 2927
Phone call: This is for emergencies only (leave message if no answer)
Phone number: (734) 764-6364 (leave message, I'm usually not there, or ignoring the phone)
e-mail: bielajew@umich.edu This is the best way to get in touch with me
Official Office Hours: TBD

Reference Material:

Matlab refresher material

Lecture 01: Introduction, history, elementary probability theory, random number generation

Read Chapters 1-3 of the Monte Carlo book
Read this chapter on the history of Monte Carlo:
Read this chapter on the basics of Monte Carlo:
Read Chapter 2 revision (in progress)

Assignment 01: Elementary probability theory

All the problems on the last page of this

Alex Bielajew, Cooley 2927, bielajew@umich.edu Last modified: August 29, 2016

NERS544 Schedule Fall 2016

Monte Carlo Methods

Important dates	Reason	
09/08	First lecture	G906
12/01	Schedule variation (working on it!)	TBD
12/08	Last lecture	G906

Date	Topics discussed	Reference material B: Bielajew's "book" H: Handwritten notes online
09/08	Introduction to the course	H: Lecture 01
	What is Monte Carlo?	B:1.1–2, H: Lecture 01
	Probability theory	B:2.1–2, H: Lecture 01
	Random number generation	B:3.1–2, H: Lecture xx
	Sampling theory	B:4.1–4, H: Lecture xx
	Error estimation	B:5.1–5, H: Lecture xx
	Random number and precision anomalies	B:6.1–2, H: Lecture xx
	Ray tracing, rotations and translation	B:7.1–4, H: Lecture xx
	Transport in infinite and mixed media	B:8.1–8, H: Lecture xx
	Lewis theory	B:9.1–2, H: Lecture xx
	Geometry: Planar and quadric surfaces	B:10.1–3,H: Lecture xx
	Building solids from surfaces	B:10.4–6,H: Lecture xx
	Law of reflection	B:10.7, H: Lecture xx
	Monte Carlo evaluation of integrals	B:11.1, H: Lecture xx
	Proof of Monte Carlo superiority for 4+D	B:11.2–4,H: Lecture xx
	Photon Monte Carlo	B:12–13, H: Lecture xx
	Electron Monte Carlo	B:12–13, H: Lecture xx
	Variance reduction techniques	B:17.1–3,H: Lecture xx

NERS544 Class Policy — Fall 2016

Alex Bielajew, Cooley 2927, bielajew@umich.edu Revision: September 1, 2016

Honor Policy

- All students in the College of Engineering are presumed to be decent, honest people, and to abide by reasonable standards of conduct.
- All exam work must be carried out completely on your own, without aid from any of your fellow students. You will be asked to sign the honor code on all exams and quizzes.
- All homework must be completed individually. You are encouraged to form groups and to discuss homework assignments **at the conceptual level** with your fellow students. This includes discussing problem strategies and working out mathematical details. Assignment write-up should be done without help from fellow students. Copying from a current or former student, a former instructor, is an honor code violation.
- You must abide by any special instructions given with any assignment, quiz or exam.

Grading Policy

How grades are determined The grades are determined by assignments only. There will be 10 assignments over the course of the term at an interval of about once per week. They are each worth 10% each, though some longer assignments may count as two assignments. Each will be posted on the class website. The due dates of the assignments are specified in the write up of each assignment.

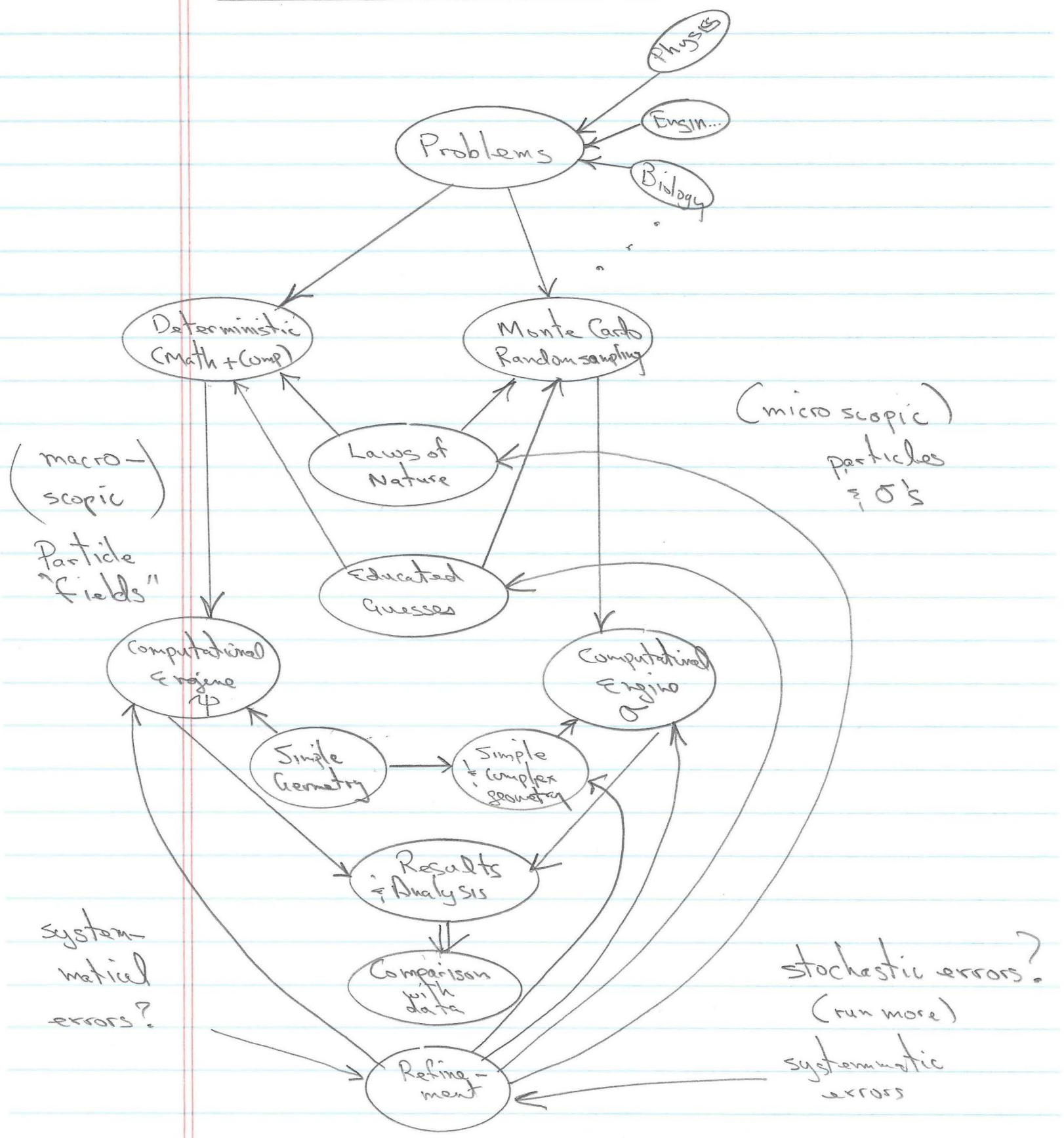
Your final letter grade will be determined according to the following straight scale:

Numerical grade (%)	Letter grade
$97 \leq \% \leq 100$	A+
$90 \leq \% < 97$	A
$85 \leq \% < 90$	A-
$80 \leq \% < 85$	B+
$75 \leq \% < 80$	B
$70 \leq \% < 75$	B-
$65 \leq \% < 70$	C+
$60 \leq \% < 65$	C
$55 \leq \% < 60$	C-
$50 \leq \% < 55$	D+
$45 \leq \% < 50$	D
$40 \leq \% < 45$	D-
$\% < 40$	E

Final project Students have the option of collapsing 4 assignments into one my undertaking a special project of their own design. A proposal is required, and must be approved by the Professor. Presentation of the project will be given on or about the last day of class.

Extra credit Occasionally extra credit points are given. These are typically assigned for going well beyond the requirements of an assignment, or through completion of a special project. Kindly ask if there is something you can do for extra credit.

What is Monte Carlo?



require that the researcher make assumptions about where an audience member would like to sit and attempt to factor in other phenomena such as: a) for some type of performances, people arrive predominantly in pairs, b) audience members prefer an unobstructed view of the stage, c) audience members prefer to sit in the middle, close to the front, *etc.* Each one of these assumptions could then be tested through measurement and then refined. The Monte Carlo method in this case is an adjunct to the basic theory, providing a mechanism to facilitate its development. An example is given in Figure 1.1.

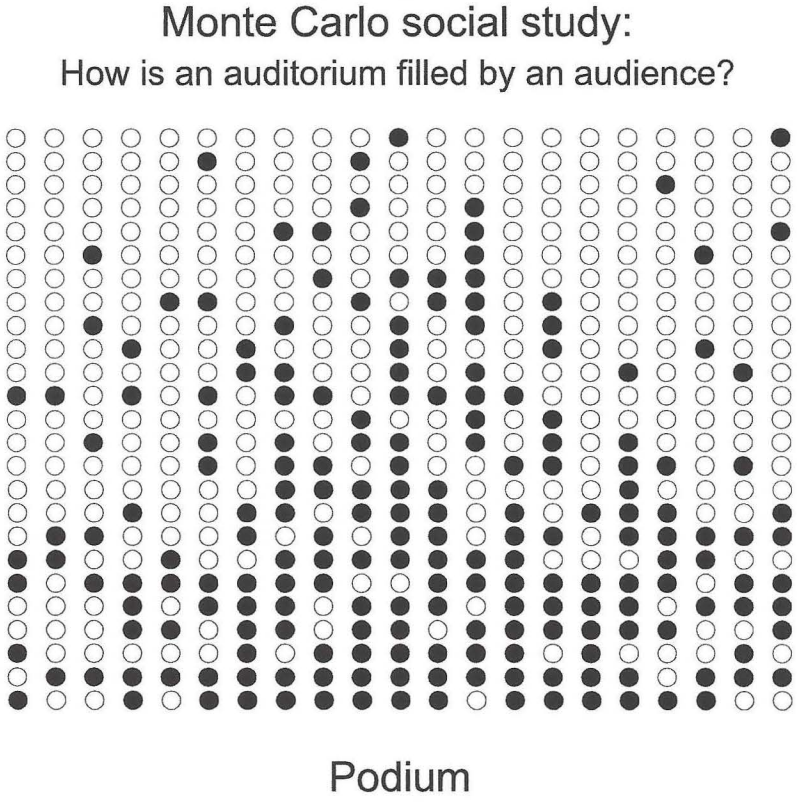


Figure 1.1: Simulation of a seating arrangement in a partially filled small auditorium. An occupied seat is represented by a solid circle and an empty seat by an open circle. The audience members were given a preference to sit in the middle and towards the front with the constraint that only one person could occupy a seat. (This constraint is what makes the mathematical solution difficult but is easy to simulate using Monte Carlo methods.)

The important role that Monte Carlo methods have to play in this sort of study is illustrated in Figure 1.2. Basic science attempts to understand the basic working mechanisms of a phenomenon. The "theory" is a set of assumptions (with perhaps a mathematical formulation of these assumptions) that can by a measured in an "experiment". Ideally, the connection between theory and experiment is direct so that the interpretation of the experiment in unambiguous. This happens when the mathematical description of the microscopic interactions and the macroscopic measurement involves no further approximation. When this is not

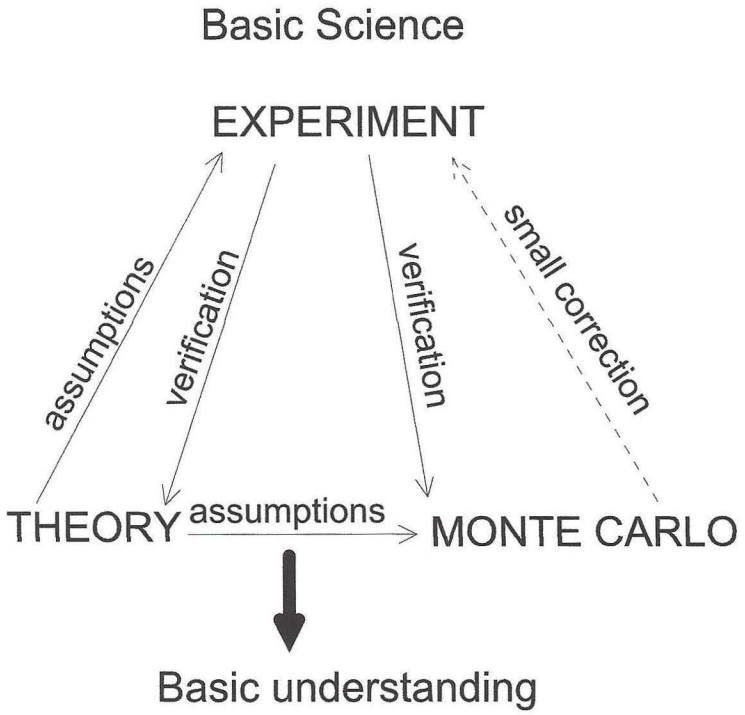


Figure 1.2: The role of Monte Carlo methods in basic science.

possible, as in the example of Figure 1.1 where two people can not occupy the same seat, a Monte Carlo simulation enters the picture in a useful way and can serve a two-fold purpose. It can either provide a small correction to an otherwise useful theory or it can be employed directly to verify or disprove the theory of microscopic interactions.

In some cases, the microscopic interactions are well-known as in the electromagnetic interactions of high-energy electrons and photons and verified by experiment. Monte Carlo techniques in this field are useful for predicting the trajectories of high-energy particles through detectors and other complex assemblies of materials. As an example, consider the experiment by MacPherson, Ross and Rogers [MRR95, MRR96] to measure the stopping power of electrons. The stopping power is the differential amount of energy, $\mathrm{d}E$ deposited in a differential pathlength $\mathrm{d}x$ through some material. Stopping power is a function of the electron energy and the material. The experimental set-up is depicted in Figure 1.3.

Nearly-monoenergetic electrons from a linear accelerator (LINAC) are first scattered in the forward direction by the thin exit window of the LINAC (this produces negligible energy loss). The energy of the electrons are this point is known from a separate experiment. The electron pass through a "thin" foil and are collected in a large NaI detector. The NaI detector completely absorbs the electrons (except the occasional one that is backscattered) although the bremsstrahlung photons produced in slowing down the electrons can escape.

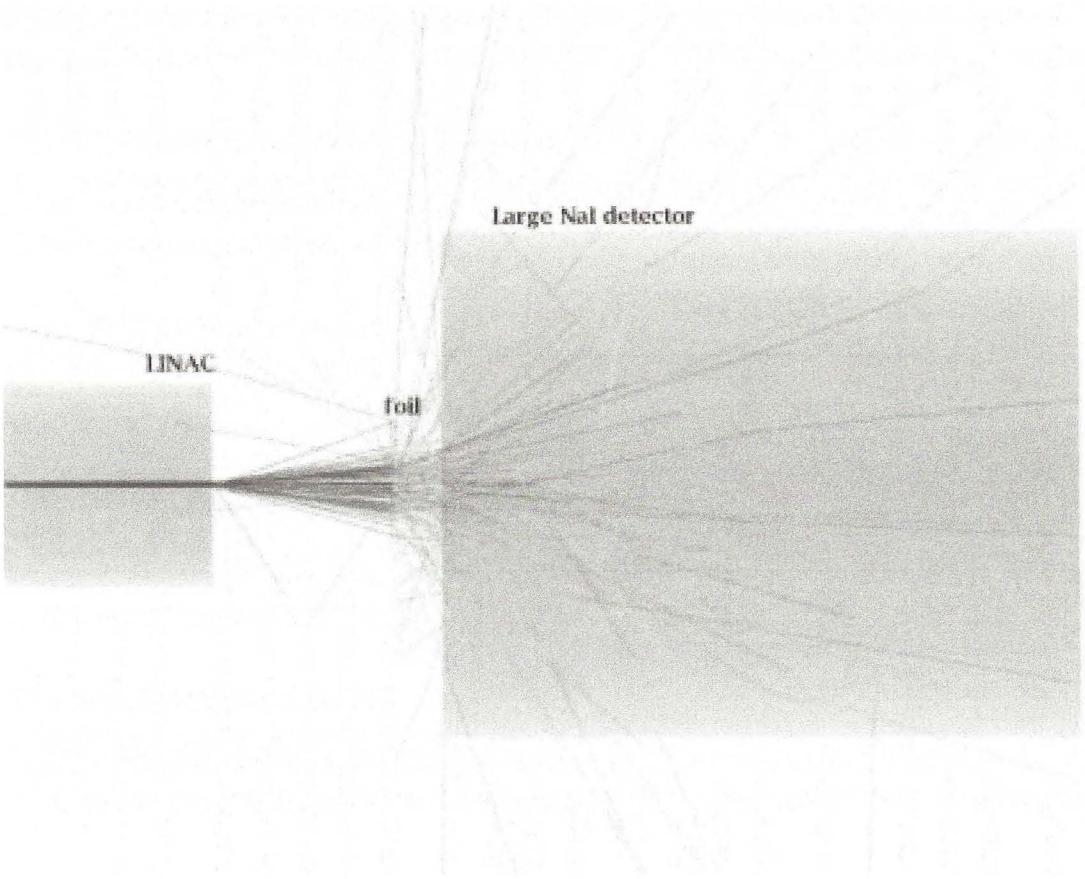
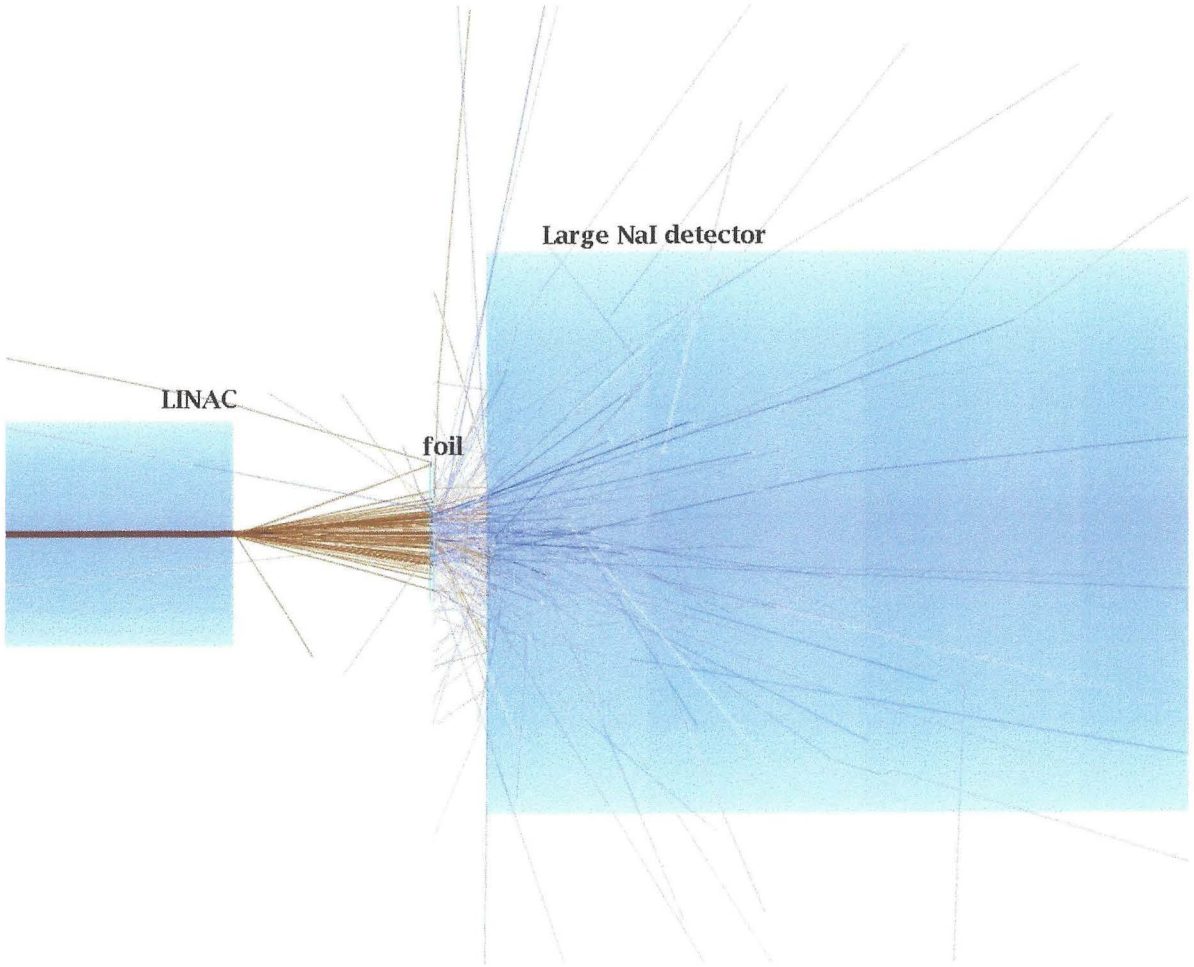


Figure 1.3: Experimental set-up of the MacPherson *et al.* stopping-power measurement.

The photon trajectories are represented by straight-line segments in the figure[2]. A close-up of the electron and photon trajectories in the foil is represented in Figure 1.4. In this case, 20 MeV electrons passed through a thin plastic foil.

We can note several features: 1) the electron trajectories through the foil are nearly straight (there is little elastic scattering) although the angular distribution following the accelerator's exit window is evident, 2) some electrons backscatter from the foil and the NaI detector, 3) some bremsstrahlung, which is produced in either the foil or the NaI detector, escapes detection, 4) some electrons scatter into large angles in the foil and escape detection. Since the amount of energy lost in the foil is determined by how much energy is captured by the NaI detector *less* the known input energy, items 2)–4) are corrections to the experiment that can be determined by Monte Carlo methods and the skewness of the electron trajectories in

[2]The trajectories depicted in Figure 1.3 and some subsequent ones were produced by the EGS4 code [NHR85, BHNR94] and the system for viewing the trajectories is called EGS_Windows [BW91]. Color renditions of this and subsequent figures make it easier to distinguish the particle species and color versions may be viewed on the web at `http://www-ners.engin.umich.edu/info/bielajew/EWarchive.html`.


Large NaI detector
LINAC
foil

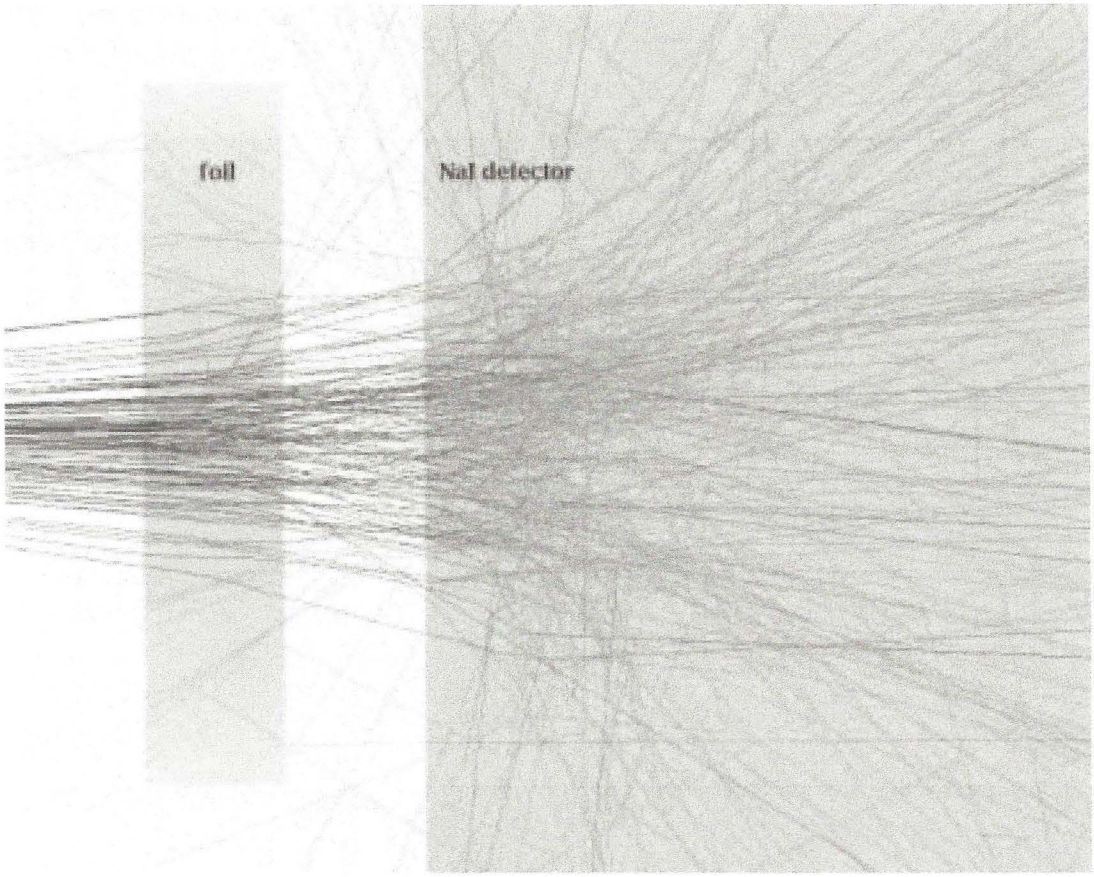
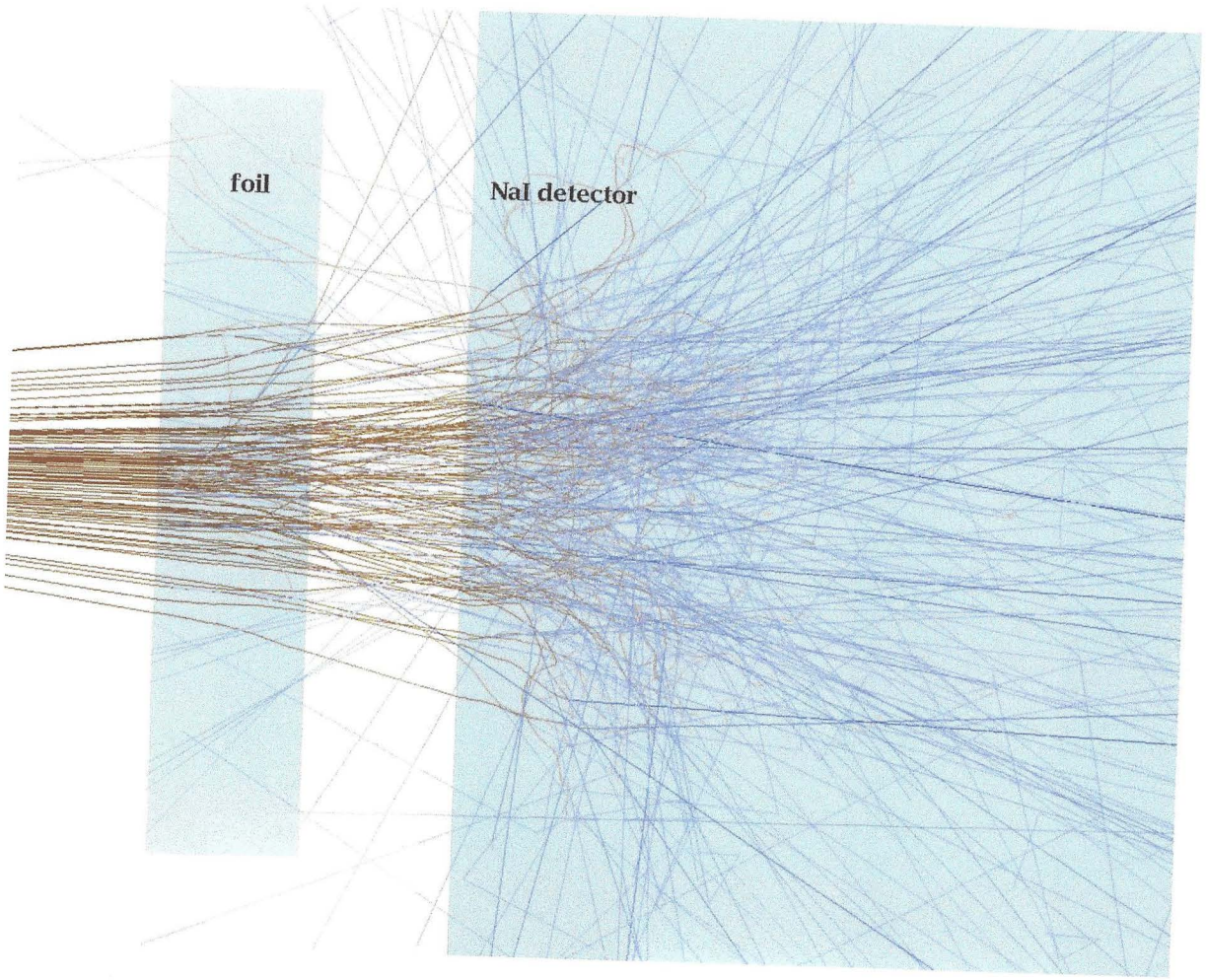


Figure 1.4: A close up of the electron and photon trajectories in a thin foil in the MacPherson *et al.* stopping-power experiment.

the foil would have to be accounted for. However, these corrections are small in this case and the Monte Carlo methods assist in the determination of the stopping power, a basic physics parameter, and the scientific method outlined in Figure 1.2 still applies[3].

If one makes the foil thicker and/or reduces the energy, the electron trajectories become considerably more complicated. A close up of a tungsten foil irradiated by 10 MeV electrons in the same experiment is depicted in Figure 1.5. The electrons develop very curved trajectories owing to multiple Coulomb elastic scattering. Indeed, some of them even stop *in the foil!* Since the corrections in this case would be large (The dx in the stopping power is a measure of the electron pathlength, **not** the thickness of the foil.) and to some extent circular, this measurement is not useful as a determination of the stopping power. However, this does not mean that the energy deposition in the thick foil is not accurate! Assuming

[3]There is some circular logic in using Monte Carlo calculations to assist in the determination of stopping power since the Monte Carlo calculations itself relies upon knowledge of the stopping power. However, if the foil is thin enough, the sensitivity to the assumed stopping power in the Monte Carlo calculations is minimal.


foil
NaI detector

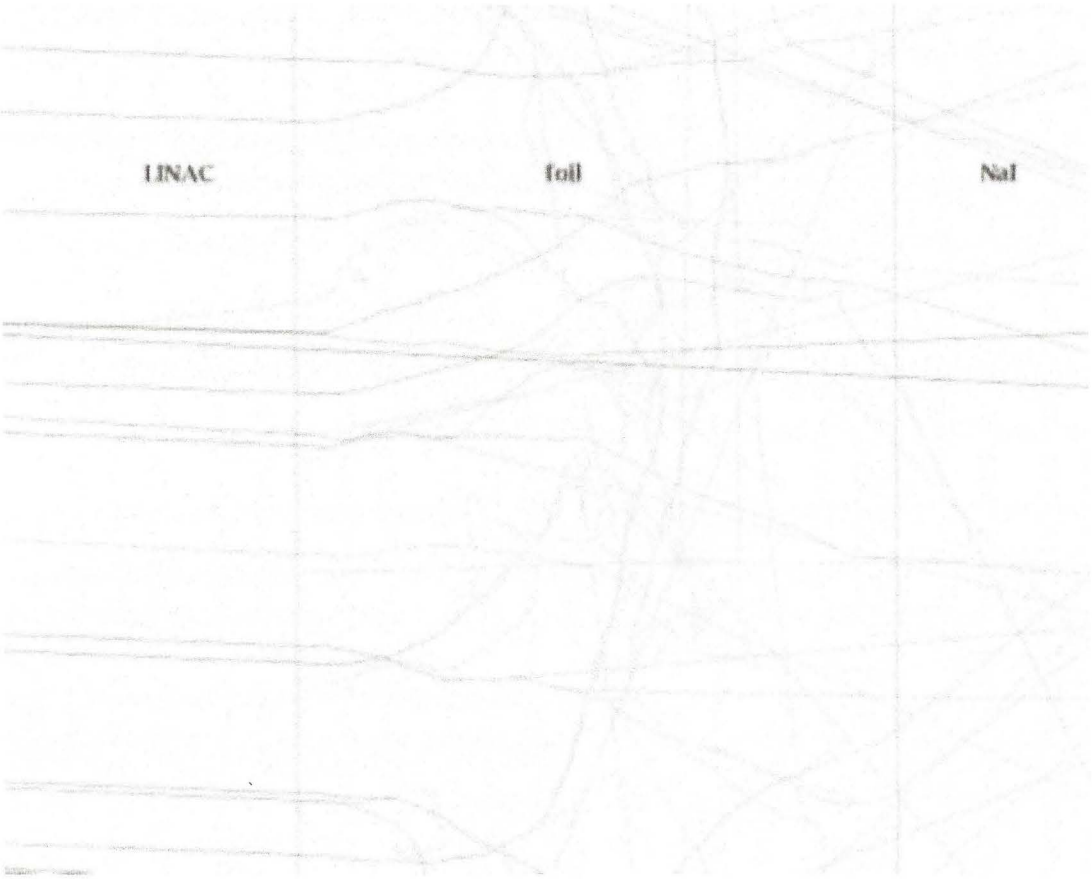
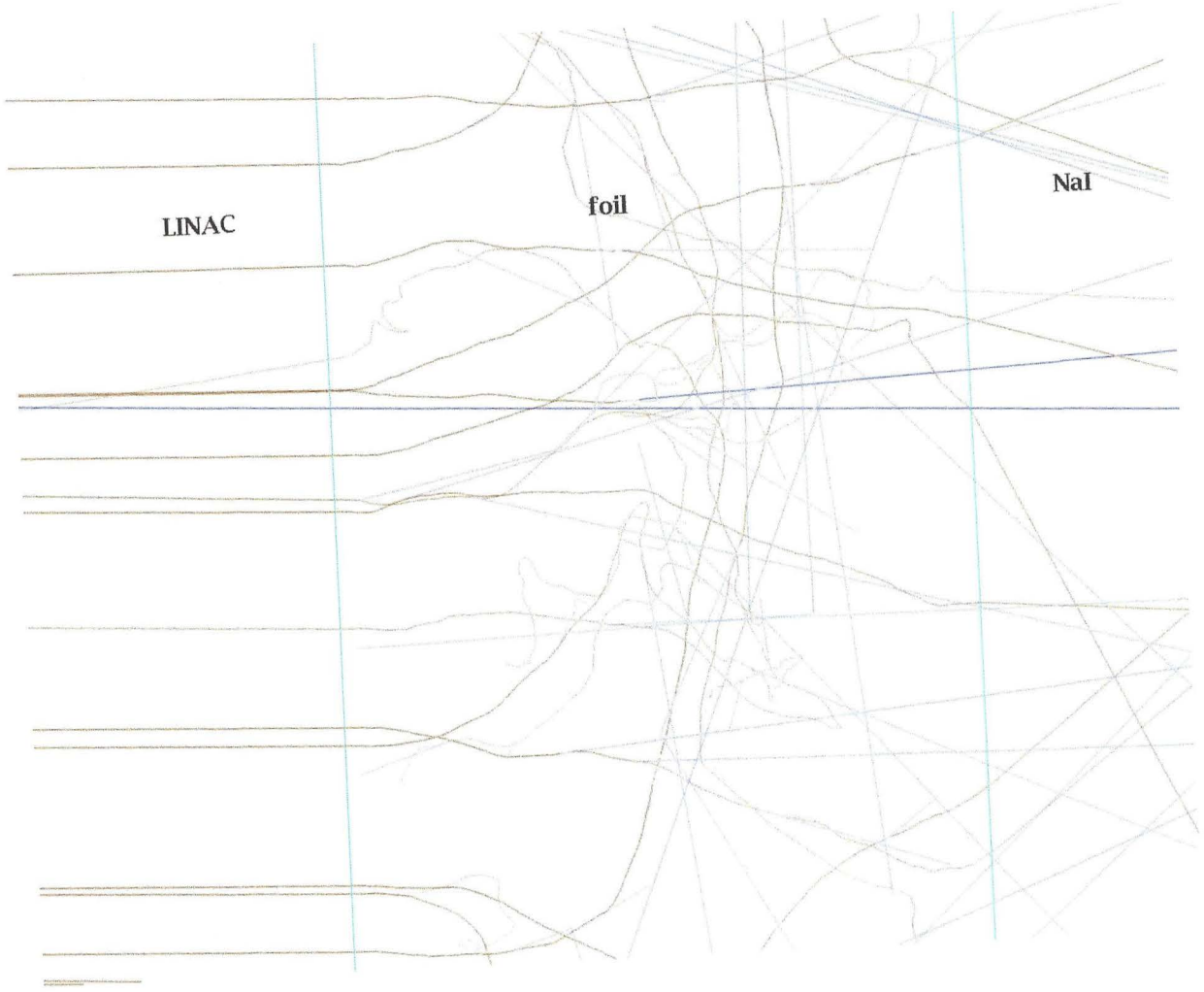


Figure 1.5: A close up of the electron and photon trajectories in a thick foil in the MacPherson *et al.* stopping-power experiment.

we believe the accepted value of the stopping power, the energy deposited in the foil may be predicted with accuracy. However, the calculated result depends in a complicated and coupled way on all the physics of electron and photon transport.

This use of the Monte Carlo method is depicted in Figure 1.6. In this case, theory can not provide a sufficiently precise and entire mathematical description of the microscopic and macroscopic physics. Theory can, however, provide intuition for the design of the measurement. Monte Carlo methods are an adjunct to this process as well, serving in the analysis of the experiment and verifying or invalidating the design.


LINAC
foil
NaI

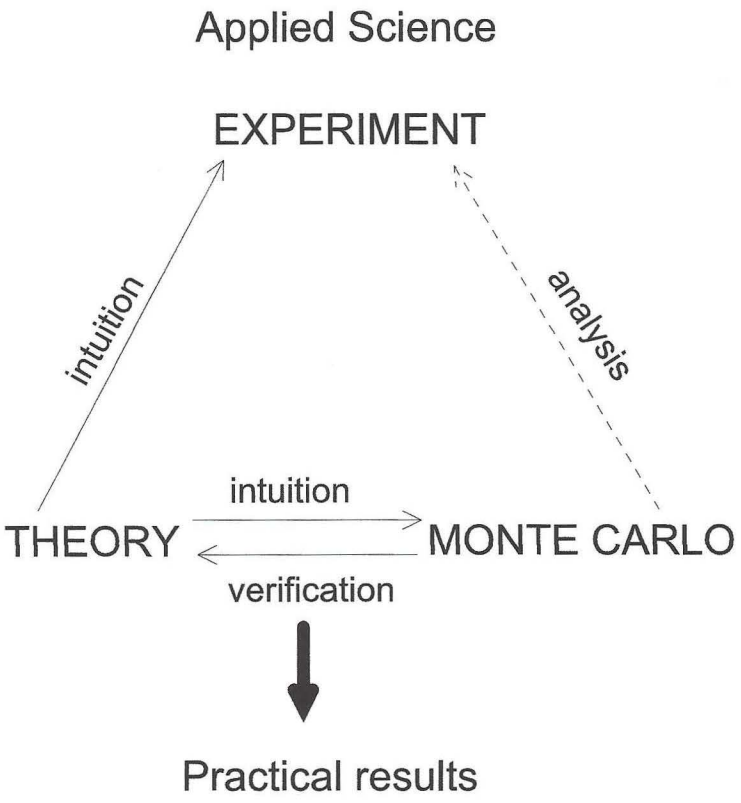


Figure 1.6: The role of Monte Carlo methods in applied science.

1.1 Why is Monte Carlo?

If Monte Carlo did not exist there would be strong motivation to invent it! As argued previously, the products of both basic and applied science are dependent upon the trinity of measurement, theory and Monte Carlo. 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?" 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 avenue attack on a problem.

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 behaviour, Monte

Carloists operate very much like experimentalists. Without theory to provide guidance the process of discovery is trial and error, guided perhaps, by some brilliant intuition.

However, when it comes to complexity of a problem, however that is measured, Monte Carlo techniques become advantageous as the complexity of a problem increases. Later in this book, in section 11, a mathematical proof is given. This "idea" is expressed in Figure 1.7.

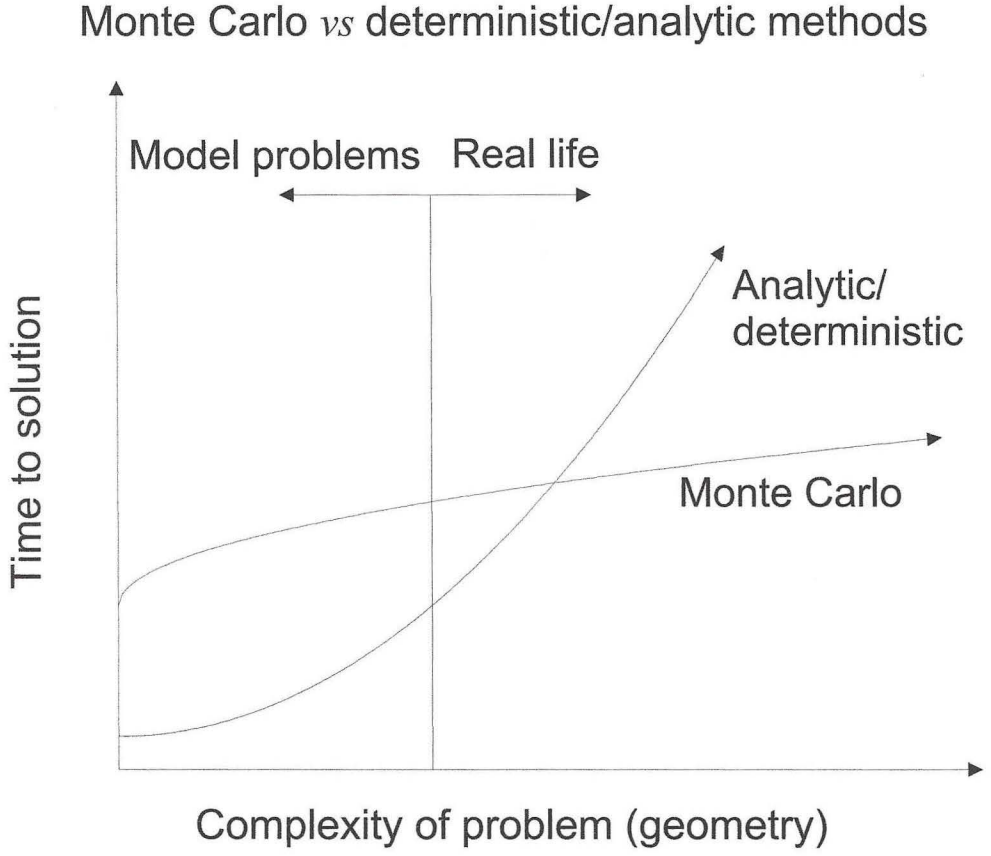


Figure 1.7: Time to solution of Monte Carlo *vs.* deterministic/analytic approaches.

The other inescapable reality is that computers are getting faster and cheaper at an geometric rate. This is known as Moore's Law[4].

A demonstration of Moore's Law for the radiotherapy application has been maintained for about 10 years now, through a timing benchmark of the `XYZDOS` code [BR92, Bie95], a "user

[4]Gordon E Moore (one of the co-founders of Intel) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 12. This was based upon observation of silicon manufacturing during the previous few years. Moore's Law is not actually a law—it is a prediction based on the observation. Computers doubled in speed/unit cost every 12 months from 1962–1970 and every 18 months thereafter.

"It can be shown" [ICBS] [Proof given in the book in Ch. 11]

Monte Carlo is more efficient than deterministic methods in 4+ dimensional problems.

Real life applications are

6, 8 dimensions

3 for space $\vec{x}$
3 for momentum $\vec{p}$
8 for # of particles involved
$e^-, \gamma, p, n, \alpha \ldots$

or 7, 8 (1 for time)

[time is necessary when the beam can modify the target]

History of Monte Carlo

See book 1.2
Online chapter "History"
← Wiki it!

Comte de Buffon [1707–1789] proposed (in 1777!) a random process – toss a needle of length L onto a ruled sheet of paper with

↕ d interline spacing

Probability of intersecting any line is (proof due to Pierre-Simon Laplace [1749–1927])

$$P = \frac{2L}{\pi d}, \text{ where } L < d$$

1.2 Some history

The usual first reference to the Monte Carlo method is usually that of Comte de Buffon [dB77] who proposed a Monte Carlo-like method to evaluate the probability of tossing a needle onto a ruled sheet. This reference goes back to 1777, well before the contemplation of automatic calculating machines. Buffon calculated that a needle of length L tossed randomly on a plane ruled with parallel lines of distance d apart where $d > L$ would have a probability

$$p = \frac{2L}{\pi d} . \qquad (1.1)$$

A computer simulation of 50 needles (where $L/d = \frac{3}{4}$) on a finite grid of 5 lines is shown in Figure 1.9.

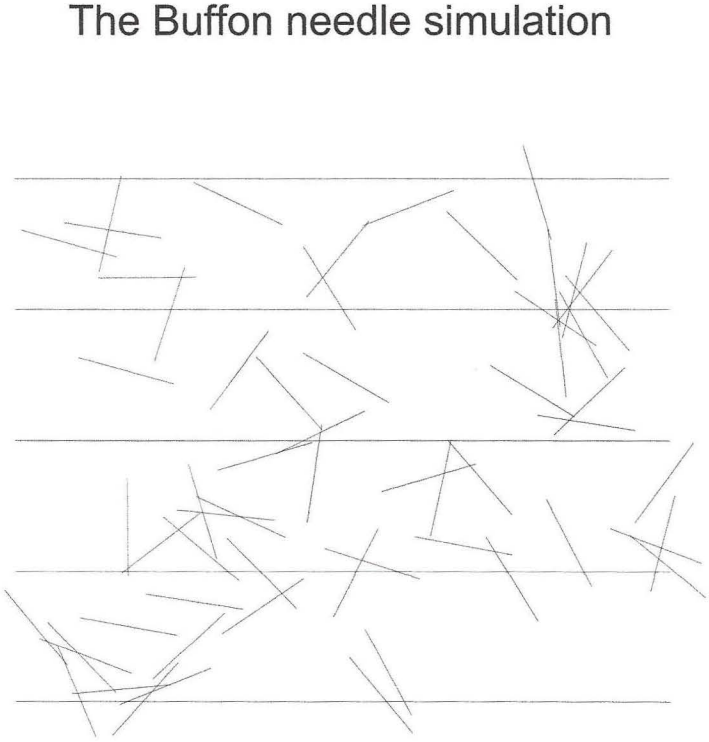


Figure 1.9: A computer simulation of the Buffon needle problem.

Later, Laplace [Lap86] suggested that this procedure could be employed to determine the value of π, albeit slowly. Several other historical uses of Monte Carlo predating computers

Stan Ulam [1909–1984] (Los Alamos)
is credited with the "modern" discovery
of Monte Carlo

Los Alamos
(LANL)

John von Neumann [1903–1957] (Los Alamos)
saw an automated way to do this
(computers)

MCNP

also Los Alamos
Nicholas Metropolis [1915–1999] did the
programming and published the
first book on the topic

most popular
code in
Nuc Eng

First public conference was given in 1949,
and spread to all sciences

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

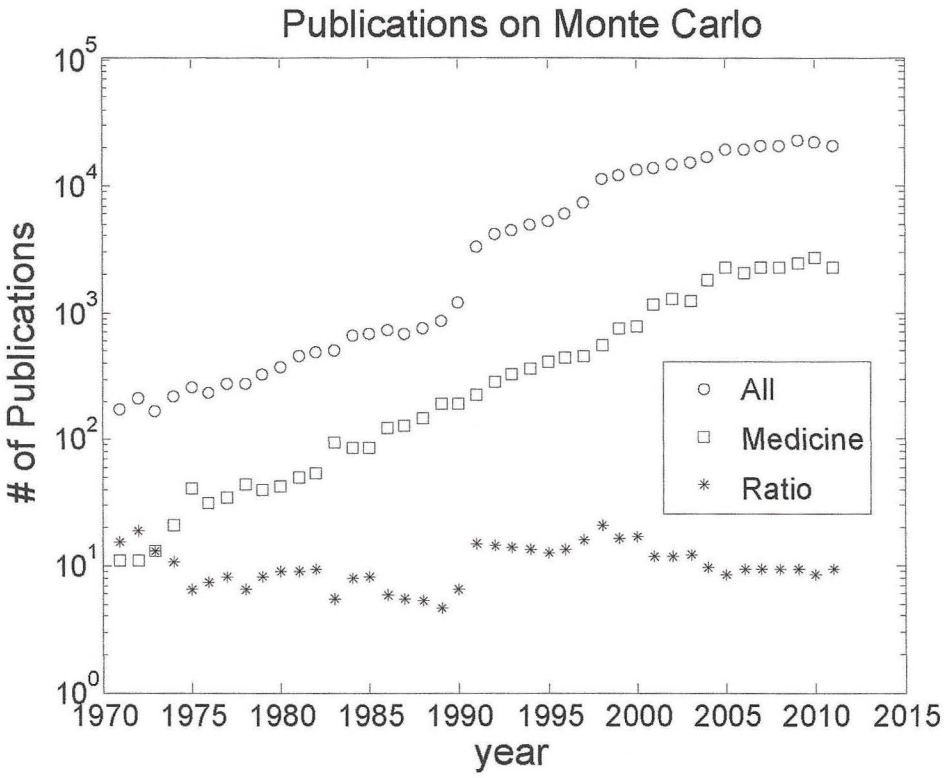


Figure 2: The number of papers published per year garnered from the Web of Knowledge ('All') and MedLine ('Medicine').

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].

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.

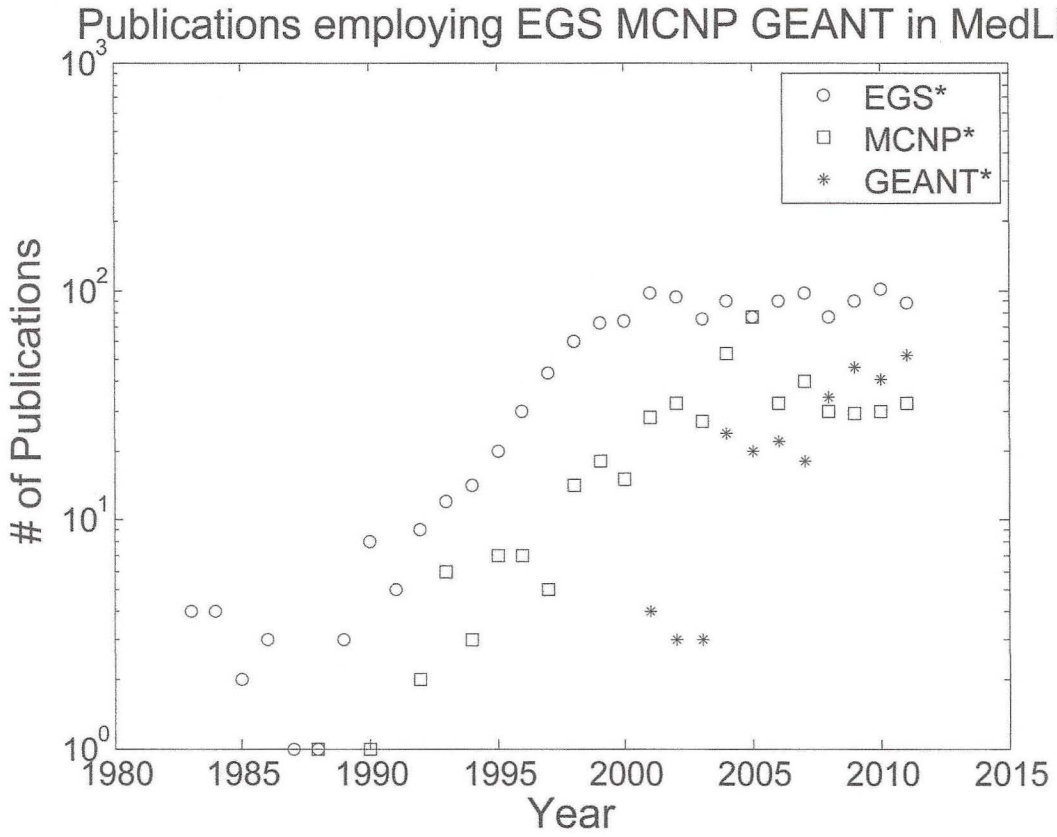


Figure 3: Papers using EGSx, MCNPx, and GEANTx, as captured on MedLine.

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

Elementary Probability Theory (Chapter 2) – as it is used in Monte Carlo

2.1 Continuous random variables

2.1.1 1D probability distributions

A probability distribution function (pdf) must have the following properties

1) $p(x) \geq 0 \quad \forall \; x_{min} \leq x \leq x_{max}$ (pdf is a fn of x; x: some independent variable)

e.g. $p(t) = A e^{-\lambda t}$ (1) $\quad 0 \leq t < \infty$

t = time, λ = decay constant (units T^{-1}), A = normalisation constant

Interpretation: $p(t)$ is the probability of decay of a single nuclide at time t in an interval dt about t.

i.e. $p(t)dt = A e^{-\lambda t} dt$ (2) $\quad 0 \leq t < \infty$

2) $p(x)$ must be normalizable...

$$\int_{x_{min}}^{x_{max}} p(x)\,dx = 1 \qquad (3)$$

In this example

$$1 = \int_0^\infty dt\, p(t) = A \int_0^\infty dt\, e^{-\lambda t} \qquad (4)$$

$$= \frac{A}{\lambda} \underbrace{\int_0^\infty dx\, e^{-x}}_{=1} \qquad \text{let } x = \lambda t$$

$$1 = \frac{A}{\lambda} \Rightarrow A = \lambda$$

So, our example pdf is

$$(5) \qquad p(t)\,dt = \lambda e^{-\lambda t}\, dt \qquad 0 \le t < \infty$$

3) $-\infty < x_{min} < x_{max} < \infty$,

satisfied in this example.

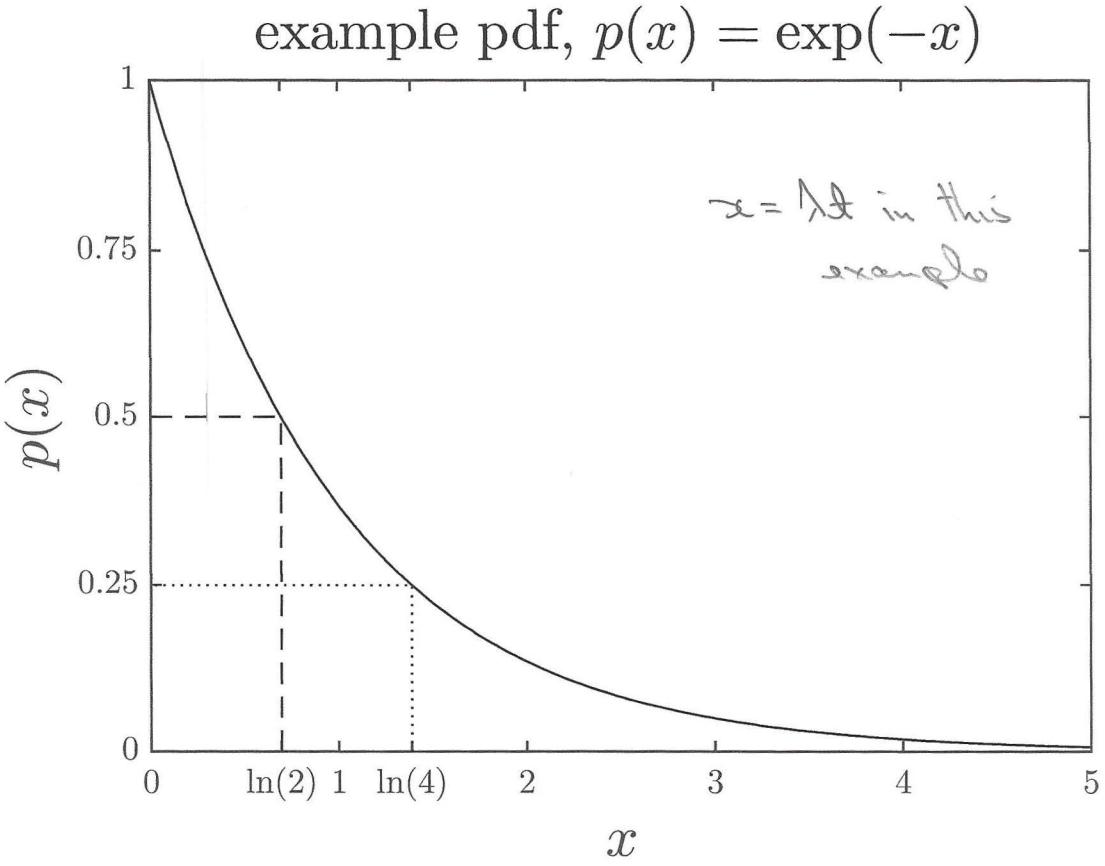


Figure 2.1: The pdf $p(x) = \exp(-x)$. $p(\ln 2) = 2p(\ln 4)$

These are the only restrictions on $p(x)$. Note that the statement of normalization above implies that $p(x)$ is integrable over its range of definition. The pdf may be discontinuous and even infinite. For example, $p(x) = a\delta(x - x_1) + (1 - a)\delta(x - x_2)\ \forall\ |x| < \infty$, where $\delta()$ is the Dirac delta function, is an example of a properly defined pdf.

Cumulative distribution functions

Associated with every pdf, is its cumulative distribution function, $c(x)$, also known as the "cdf", or "CDF" The cdf is computed below:

$$c(x) = \int_{x_{\min}}^{x} \mathrm{d}x\ p(x)\ , \tag{2.2}$$

and has the property:

$$c'(x) = p(x)\ . \tag{2.3}$$

Some notes:

1) $p(x)$ can be infinite ($+\infty$) at any x_0, so long as

$$\int_{x_0-\delta}^{x_0+\delta} p(x)\,dx \text{ is finite}$$

$\Rightarrow$ $p(x)$ is normalizable.

e.g. $p(x) = \dfrac{1}{2\sqrt{x}} \qquad 0 \le x \le 1$

$\lim_{x\to 0} p(x) \to +\infty$

yet $$\int_0^1 dx\, p(x) = \frac{1}{2}\int_0^1 dx\, \frac{1}{x^{1/2}} = \frac{1}{2}\, 2x^{1/2}\Big|_0^1 = 1 \checkmark$$

This is a pdf.

2) a pdf does not need to be continuous, nor does its derivatives need to be continuous

Cumulative probability distributions

Every pdf has associated with it, a "cumulative probability distribution function (aka "cdf") defined by

$$c(x) = \int_{x_{min}}^{x} dx\, p(x) \qquad (5)$$

↑ conventional symbol for a cdf

Note that, by definition

$$\left.\begin{aligned} c(x_{max}) &= 1 \\ c'(x) &= p(x) \end{aligned}\right\} (6)$$

↑ derivative wrt x

In our example, $p(t)\,dt = \lambda e^{-\lambda t}\,dt$

$$c(t) = \int_0^t \lambda\, dt\, e^{-\lambda t} = \int_0^{\lambda t} dx\, e^{-x}$$

$$c(t) = 1 - e^{-\lambda t}$$

$$c'(t) = \lambda e^{-\lambda t} \quad \checkmark$$

$$c(\infty) \longrightarrow 1 \quad \checkmark$$

Moments of pdfs

pdfs are characterized by their integral moments.

(7) $\langle x^n \rangle = \int_{x_{min}}^{x_{max}} dx\, x^n\, p(x)$, where

$n \geq 0$ $\wedge$ ("and") $n \in \mathbb{N}$ (n is an element of the natural numbers)

$n = 1, 2, 3 \ldots$

sometimes 0

i.e. non-negative integers

aside

$\mu \equiv \langle x^1 \rangle$ is common nomenclature for the "mean" of a pdf

By definition

$\langle x^0 \rangle = 1$ (if $p(x)$ is a pdf)

Note that $\langle x^n \rangle$ for $n \geq 1$ is not guaranteed to exist

example $p(x) = \frac{1}{x^2}$

$\langle x^0 \rangle = 1$

$\langle x^1 \rangle = \int_1^\infty dx\, x \frac{1}{x^2} = \int_1^\infty dx\, \frac{1}{x} = \log x \Big|_1^{+\infty} \to +\infty$

$\langle x^1 \rangle$ does not exist

Variance

The variance of a pdf is defined as

$$\underbrace{\sigma_x^2 = \mathrm{var}\{x\}}_{\text{equivalent nomenclature}} \equiv \langle x^2 \rangle - \langle x \rangle^2 \qquad (9)$$

$\mathrm{var}\{x\} \geq 0$ for all pdfs

σ_x is the "width" of a pdf.

The existence of σ_x is not guaranteed (We shall see examples)

Examples of some common pdfs seen in radiation transport

The δ-function

Aside

The δ-function is more an "idea" than a true mathematical function.
It's definition is:

(9) $$\int_a^b dx\, \delta(x-x_0) = 1 \quad \text{when } a < x_0 < b$$
note $a < b$

(10) $$\int_a^b dx\, f(x)\, \delta(x-x_0) = f(x_0)$$
$f(x)$: any function

Consider the pdf

For (11) $p(x) = \delta(x-x_0) \quad \forall \; |x| < \infty$
i.e. $-\infty < x < \infty$

(11a) $$\int_{-\infty}^{\infty} dx\, p(x) = 1$$ ✓ qualifies as a pdf

(11b) $\langle x^n \rangle = x_0^n$

(11c) $\mathrm{var}\{x\} = 0$

(11d) $c(x) = \Theta(x-x_0)$

$\Theta(x)$ is the "Heavyside step function"

(12)
$$\begin{cases} \Theta(x) = 0 & \text{for } x<0 \\ \Theta(x) = 1 & \text{for } x>1 \\ \Theta(0) & \text{is undefined (one of the quirks of } \delta\text{-non functions!)} \end{cases}$$

(show picture)

The "true or false" distribution

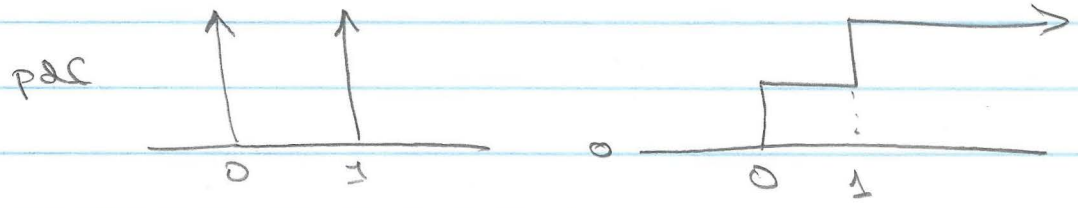
(13) $$p(x) = \frac{1}{2}\left[\delta(x) + \delta(x-1)\right] \quad \forall \; |x|<\infty$$

ICBS...

(13a) $$\int_{-\infty}^{\infty} dx\, p(x) = 1 \quad \checkmark$$

(13b) $$\langle x^n \rangle = \frac{1}{2} \quad \forall \; n>0$$

(13c) $$c(x) = \frac{1}{2}\left[\Theta(x) + \Theta(x-1)\right]$$



(13d) $$\mu = \sigma = \frac{1}{2}$$

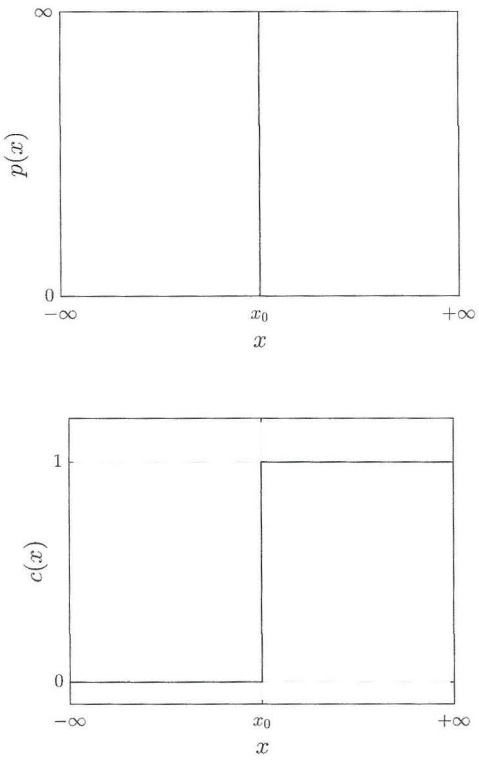


Figure 2.2: The pdf $p(x) = \delta(x - x_0)$ and its associated cdf.

The "true or false" probability distribution

Consider the "true or false" probability distribution,

$$p(x) = (1/2)[\delta(x) + \delta(x-1)] \; \forall \; |x| < \infty. \tag{2.7}$$

This could describe a coin-flip experiment where a result of zero (or false) corresponds to "tails" and a result of one (or true) correspondes to "heads".

By definition of the delta function,

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}x \, p(x) &= 1 \; , \\ \int_{-\infty}^{\infty} \mathrm{d}x \, x^n \, p(x) &= \frac{1}{2} \; \forall \; n > 0 \; , \\ c(x) &= \frac{1}{2}[\Theta(x) + \Theta(x-1)] \; . \end{aligned}$$

Note that $\mu = \frac{1}{2}$ and $\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \frac{1}{2}$ in this case. The pdf and cdf are shown in 2.3.

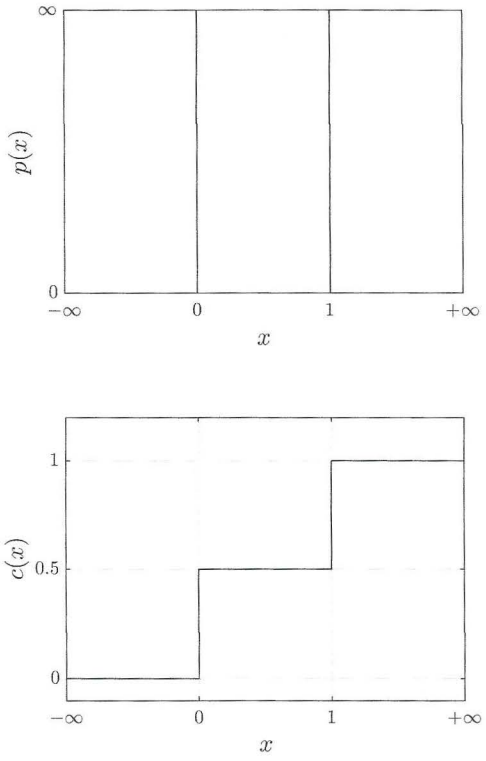


Figure 2.3: The pdf $p(x) = (1/2)[\delta(x) + \delta(x-1)]$ and its associated cdf.

The exponential probability distribution

Consider the exponential probability distribution,

$$p(x) = \Sigma \exp(-\Sigma x) \text{ for } 0 \leq x < \infty \; . \tag{2.8}$$

This probability distribution is used in the decay of nuclides and determination of pathlength distributions in particle interactions in matter. For interaction pathlength distributions, Σ is the macroscopic cross section in an attenuating material.

Computing the characteristics of this distribution,

$$\begin{aligned} \int_0^\infty \mathrm{d}x \, p(x) &= 1 \; , \\ \int_0^\infty \mathrm{d}x \, x^n \, p(x) &= \frac{n!}{\Sigma^n} \; \forall \; n \geq 0 \; , \\ c(x) &= 1 - \exp(-\Sigma x) \; . \end{aligned}$$

Note that $\mu = \sigma = \Sigma^{-1}$ in this case. The pdf and cdf are shown in 2.4.

The exponential probability distribution

Let

(14) $p(x) = \Sigma e^{-\Sigma x}$ for $0 \le x < \infty$

This is the same example as before.
In this notation it represents the distance, x, to an interaction of a particle

Σ is the "macroscopic" cross section

$$\Sigma = \rho \frac{N_A}{A} \sigma$$

ρ ← mass density
N_A ← Avogadro's number
σ ← single atom cross section
A ← atomic mass

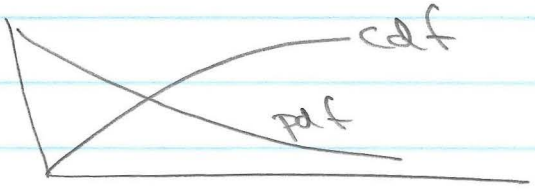
(14a) $\int_0^\infty dx\, p(x) = 1$

(14b) $\langle x^n \rangle = \frac{n!}{\Sigma^n}$

(14c) $\mu = \frac{1}{\Sigma}$

(14d) $\sigma^2 = \frac{2}{\Sigma^2} - \frac{1}{\Sigma^2} = \frac{1}{\Sigma^2}$

(14e) $\mu = \sigma = \frac{1}{\Sigma}$



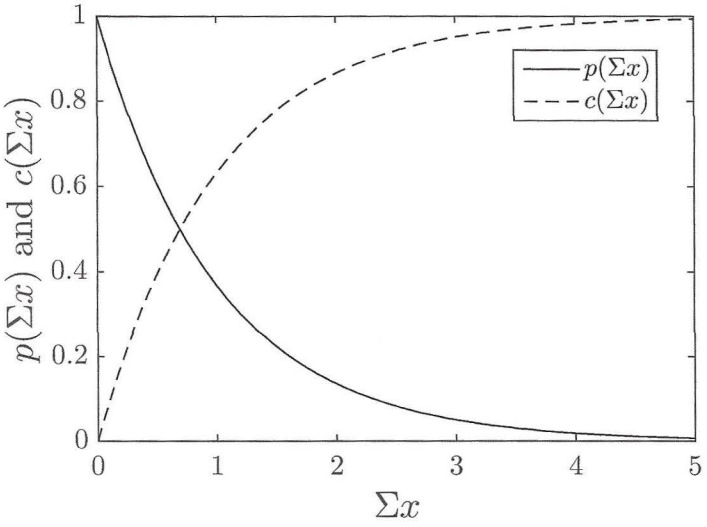


Figure 2.4: The pdf $p(\Sigma x) = \exp(-\Sigma x)$ and its associated cdf.

The Cauchy probability distribution

An example of a probability distribution function that has no moments is the Cauchy probability distribution, also known as the Lorentz, or Breit-Wigner distribution. In our context, this distribution arises from an interesting application—the intrinsic probability distribution of the energy of a quantum from an excited atomic state of finite lifetime.

The Cauchy probability distribution is

$$p(x) = \frac{1}{\pi} \frac{\gamma}{\gamma^2 + (x - x_0)^2} \; \forall \; |x| < \infty \; . \tag{2.9}$$

The Cauchy distribution has no moments, but its mode and median are x_0. The parameter γ is the half width at half maximum, since $p(x_0 \pm \gamma) = \frac{1}{2} p(x_0)$, and serves as a measure of the width of the pdf.

The mean value of the Cauchy/Lorentz distribution can be made to be x_0 if the "principle value" of the first moment is obtained in the following way:

$$\begin{aligned} \langle x \rangle &= \frac{\gamma}{\pi} \lim_{a \longrightarrow \infty} \int_{-a-x_0}^{a-x_0} \mathrm{d}x \, \frac{x}{\gamma^2 + (x - x_0)^2} \\ &= \frac{\gamma}{\pi} \lim_{a \longrightarrow \infty} \int_{-a-x_0}^{a-x_0} \mathrm{d}x \, \frac{x_0 + (x - x_0)}{\gamma^2 + (x - x_0)^2} \\ &= x_0 + \frac{\gamma}{\pi} \lim_{a \longrightarrow \infty} \int_{-a}^{a} \mathrm{d}u \, \frac{1}{1 + u^2} \; \to 0 \text{ (by antisymmetry)} \end{aligned} \tag{2.10}$$

The Cauchy pdf

is defined by

(15) $$p(x) = \frac{1}{\pi}\frac{\gamma}{\gamma^2 + (x-x_0)^2} \qquad \forall\ |x| < \infty$$

Note
$p(x_0 \pm \gamma) = \frac{1}{2}p(x_0)$
γ is called the half width at half maximum

$p(x)$ has moments, although by symmetrizing the integrand, as shown in the text, about x_0, one can show that it should be x_0

$$\langle x \rangle = \frac{\gamma}{\pi}\lim_{a\to\infty}\int_{-a-x_0}^{a-x_0} dx\ \frac{x}{\gamma^2 + (x-x_0)^2}$$

$$= \frac{\gamma}{\pi}\lim_{a\to\infty}\int_{-a-x_0}^{a-x_0} dx\ \frac{x_0 + (x-x_0)}{\gamma^2 + (x-x_0)^2}$$

$$= x_0 + \lim_{a\to\infty}\int_{-a}^{a} du\ \frac{u}{1+u^2}$$ by anti-symmetry

$$\langle x^2 \rangle \to \infty$$

This distribution is employed in the energetics of quantum level decay

For this pdf

$$C(x) = \frac{1}{2} + \frac{1}{\pi}\arctan\left(\frac{x-x_0}{\gamma}\right)$$

but the second moment and hence the variance can not be defined in any fashion.

Of course, this procedure would cause a mathematician to have conniptions! However, infinities in physical applications can usually be rationalized by physical argument.

The Cauchy pdf, being a proper probaility function, has the cdf:

$$c(x) = \frac{1}{2} + \frac{\arctan(\frac{x-x_0}{\gamma})}{\pi} \ . \tag{2.11}$$

The Cauchy pdf and cdf for $x_0 = 0$ and $\gamma = 1$ are shown in 2.5. The pdf was denormalized for display purposes.

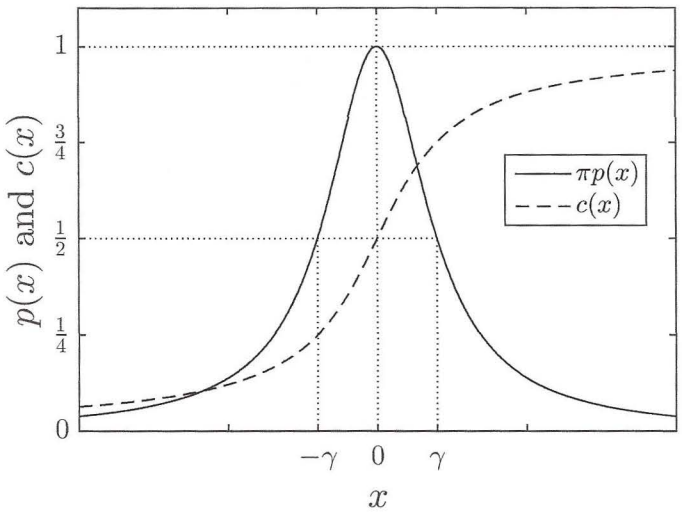


Figure 2.5: The Cauchy pdf and its associated cdf for $x_0 = 0$ and $\gamma = 1$.

A generalized Cauchy probability distribution

A generalized Cauchy probability distribution[1] is

$$\begin{aligned} p_m(x) &= \frac{\Gamma(m)}{\gamma\sqrt{\pi}\,\Gamma(m-1/2)}\left[\frac{\gamma^2}{\gamma^2+(x-x_0)^2}\right]^m \ \forall\ |x|<\infty \wedge m > \frac{1}{2} \\ c_m(x) &= \frac{1}{2} + \frac{\Gamma(m)}{\sqrt{\pi}\,\Gamma(m-1/2)}\left(\frac{x-x_0}{\gamma}\right) {}_2F_1\left[\frac{1}{2}, m; \frac{3}{2}; -\left(\frac{x-x_0}{\gamma}\right)^2\right] , \end{aligned} \tag{2.12}$$

[1] A standard version of the generalized Cauchy distribution does not yet exist, though there is some literature to be found on this topic. For this book, we will consider this form, and exploit it to illustrate aspects of moments.

The generalized Cauchy distribution
- not covered here (unless we redit)

The Rutherford pdfs
- will figure prominently later and will be investigated in Assignment 1

Two-dimensional probability distribution
will be covered later (at least partially)