Monte Carlo in Neutron Metrology and Dosimetry

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Training Course on: Neutron Dosimetry, Radiobiology and Instrumentation
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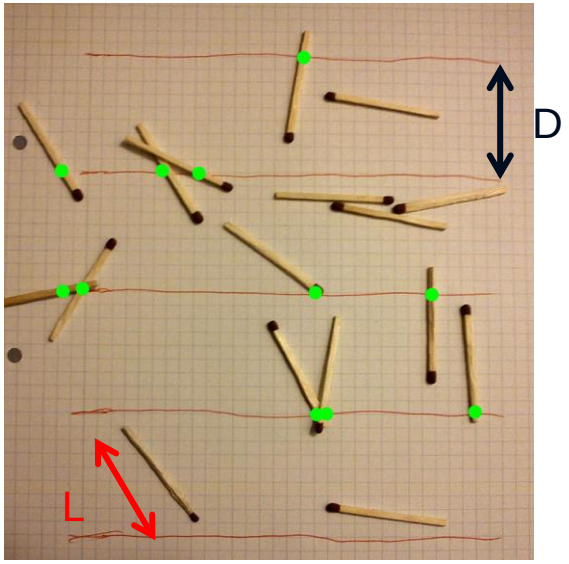
Outlook

- The Monte Carlo Method: short historical introduction
- MC for **particle transport:**
  - Random Numbers and central limit theorem
- Neutron interactions, nuclear data and Cross Sections
  - Thermal neutrons: free gas model
- Estimators and Tallies
  - Fluence & Lethargy example
  - Energy deposition and dose
- Variance Reduction Techniques
- Errors (statistical errors, systematic errors and mistakes)

Monte Carlo Method: Buffon‘s needle

George-Louis Leclerc, Comte de Buffon, in 1777 proposed that if needles or **sticks of length** L were dropped randomly on a plane surface that had parallel lines at **spacing** $\boldsymbol{D} \geq L$, then the probability P_{cut} that a needle would intersect one of the lines could be expressed as:

$$P_{cut} = \frac{2L}{\pi D}$$



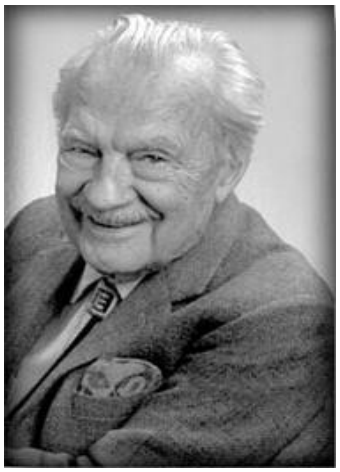
Pierre-Simon de Laplace in 1786 showed that such a procedure could be used to estimate the value of π since L and D are known and one can estimate P_{cut} from the number of success (needles cutting a line, n_c) over trials (needles dropped, n_d) :

$$\pi = \frac{2L}{P_{cut}D} \cong \frac{2L}{(n_c/n_d)D}$$

This problem is an excellent example of **analog Monte Carlo**, in which one phenomenon (dropping sticks) **„simulates“** another phenomenon (estimating the irrational number π)

The Monte Carlo method

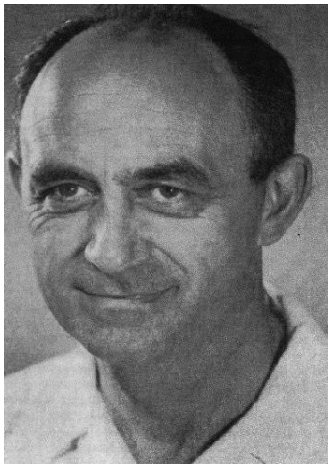
Invented by John von Neumann, Stanislaw Ulam and Nicholas Metropolis (who gave it its name), and independently by Enrico Fermi



N. Metropolis

S. Ulam

J. von Neumann



E. Fermi

1st Ref: N. Metropolis, S. Ulam, "The Monte Carlo Method", J. Am. Stat. Assoc. 1949

N. Metropolis, The Beginning of Monte Carlo Method, Los Alamos Science Special issue, 1987

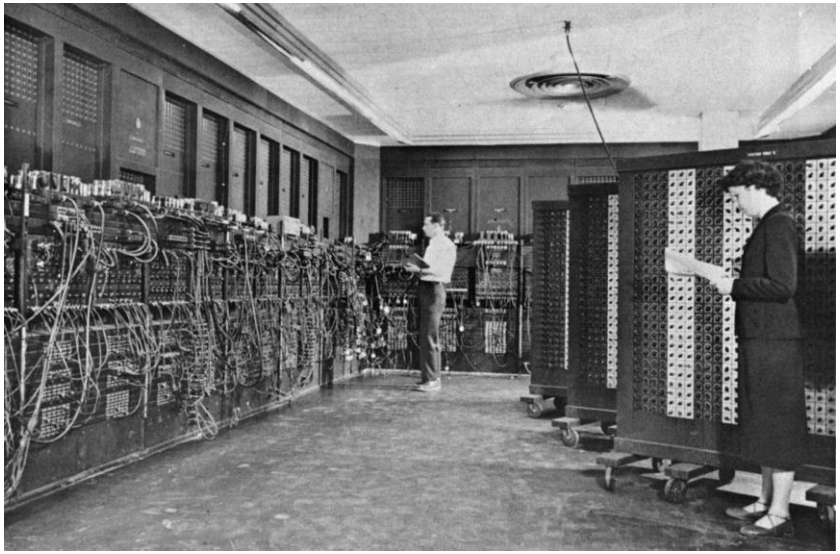
Stanislav M. Ulam, Adventures of a Mathematician, Univ. of California Press, 1991

Edward Teller, Memoirs: a twentieth Century journey in science and politics, Basic Books, 2009

Digital Programmable Computers

US

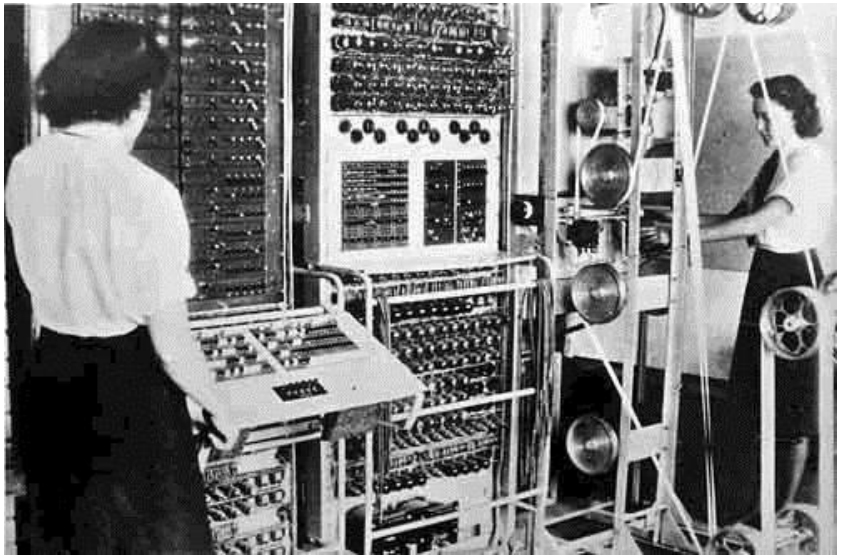
MARK1: 1939-1944, Harvard University
ENIAC: 1943-1945,Univ. of Pennsylvania



Manhattan Project: to calculate complex ballistics trajectories for the army and, later, study the implosion of the first atomic bomb and the hydrogen bomb

UK

Bombe: 1939-1940 UK Gov. Code & Cypher school
Colossus: 1943 Post Office research Station



Bletchey Park: used by cryptologists to decipher German Enigma machine-encrypted secret messages during WWII.

Computer programmers….and women

Ada Lovelace (1815–1852) was an analyst of Charles Babbage's analytical engine and considered the **"first computer programmer."**

At first, **"computers"** were actually people with amazing math skills able to make complex calculations for the army.

When programmable computers became available the process of calculation shifted from manual, paper-based calculations to machine calculations at first manipulating switches and cables rather than using programming language.

During WWII, women took the place of men who were engaged in the war effort or busy with the hardware to actually do the programming.
ENIAC's six primary programmers were women:
the "**ENIAC girls**".

Jennifer Light, When computers were women, Technology and Culture, 1999

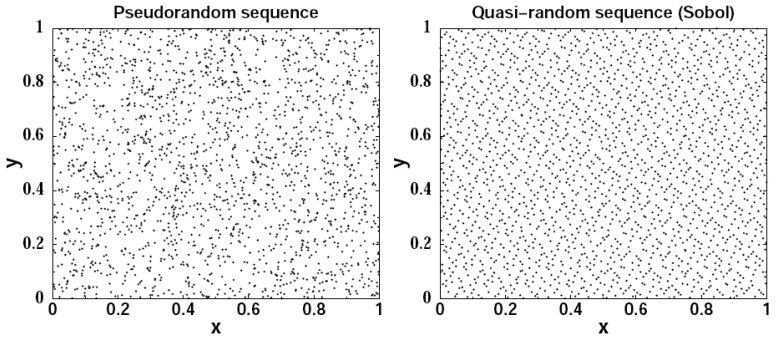
Monte Carlo codes for particle transport

There are many general purpose MC codes for radiation transport simulation: FLUKA, MCNP, GEANT4, PHITS, MARS…..etc. they differ in many ways and each one might be more useful for a specific kind a problem.

At the core of MC calculations there is some mechanism to produce a long sequence of **random numbers** uniformly distributed over the interval (0,1). But what's needed is a sequence of RN that is the same every time the program is run so that coded errors can be found and same results are reproduced when the same code is run on different computers. So, in reality a **pseudorandom number generator** is used. Such a generator is a deterministic algorithm that given the previous number in a sequence can efficiently calculate the next number. A **seed** is used to start the sequence.

Scatter random points on a plane generated with **pseudorandom sequence**:

For some specific problem also **quasi-random numbers** are used not so much to be random as to be extremely uniform over the interval and uniformly cover the plane



Note: When you embark on Monte Carlo investigations, be well aware of the goodness of the random number generator you are using and be sure that it has a long period to **avoid repetitions and hence false convergence**.

Monte Carlo method and deterministic method

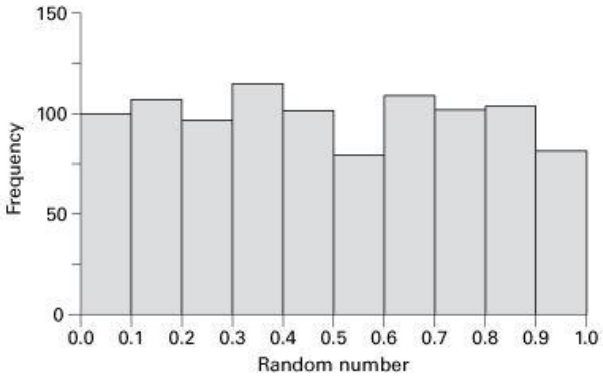
Neutron transport problems can generally be solved using **deterministic** or **stochastic** methods.

- **Deterministic methods** (the most common of which is the **discrete ordinate method**) solve the transport equation (or an approximation of it) for the average particle behavior.
- In **stochastic methods**, such as **Monte Carlo methods**, discrete particle histories are tracked and averaged in a random walk directed by **measured interaction probabilities**. The average behavior of particles in a physical system is then inferred (using the **central limit theorem**) from the average behavior of the simulated particles.

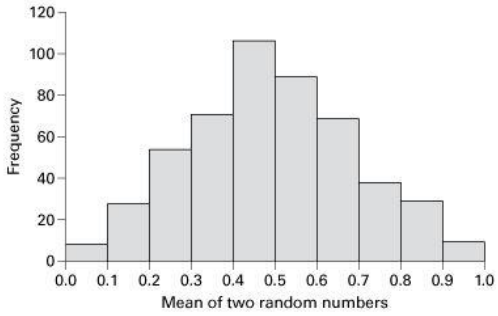
The central limit theorem states that given a population distribution with a finite mean **μ** and finite variance **σ^2** (or standard deviation **σ**), the sampling distribution of the means approaches a **normal distribution** with the same mean **μ** and a variance **σ^2/n** as **n**, the sample size increases.

Central Limit Theorem - 1

The amazing and counter-intuitive thing about the central limit theorem is that no matter what the shape of the original distribution, the **sampling distribution of the means** approaches a **normal distribution**. Furthermore, for most distributions, a normal distribution is approached very quickly as **n** increases.

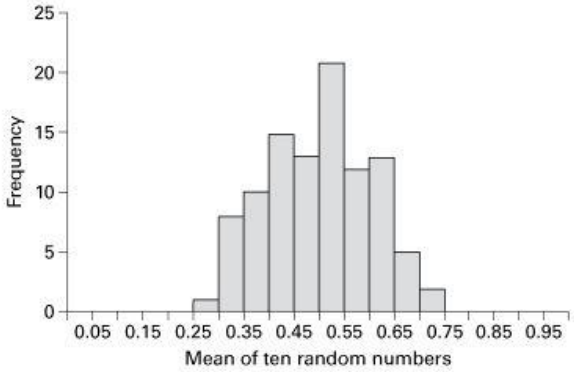


Distribution of 1000 random numbers



Distribution of 500 means of 2 random numbers

Sample size n=2



Distribution of 100 means of 10 random numbers

Sample size n=10

Les Kirkup, Data analysis for Physical Scientists, Cambridge Univ. Press, 2012

Central Limit Theorem – 2

Let the population mean of the raw data distribution be: **μ** which is the "**true mean**" (which we don't know)
and the population standard deviation be **σ** which is the "**true standard deviation**" (which we also don't know).

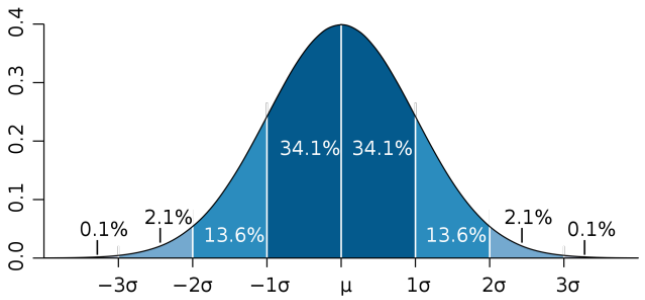
as **the number of histories, n → ∞**

- The deviation of the sample mean, **m**, from the true mean **μ** approach zero and
- the quantity $\mathbf{S = \frac{\sigma}{\sqrt{n}}}$ **provides a measure of the deviation of the sample mean from the population mean after n histories.**

Or, in other words, we can construct a confidence interval for the sample mean that has a specified probability of containing the true unknown mean and use the sample standard deviation to approximate the population standard deviation:

μ lies in the range of $m \pm k \frac{s}{\sqrt{n}}$ with a given confidence level

Where k is the **number of standard deviations** from the mean over which the normal distribution is integrated to obtain the **confidence level**



if k = 1 the confidence level is 68%, if k= 2 the confidence level 95% ……. etc.

Note: Inherent drawback of MC method: to halve the variance S four times the original number of histories must be calculated

Multidimensional Phase space

In reality, each particle is represented by a point in a phase space.

Each phase space dimension correspond to a particle degree of freedom:

- Position in space : **x, y, z**
- Momentum **p_x, p_y, p_z** (or energy and direction: **E, θ, φ**)
- More dimensions can be envisaged, corresponding to other degrees of freedom, such as quantum number: spin etc.

Time can also be considered as a coordinate or as independent variable: the **variation of the phase space coordinates as a function of time constitutes** a **particle „history“**

Note: When only one or two dimensions are considered Monte Carlo codes are NOT very efficient but they become more and more efficient at increasing dimensions

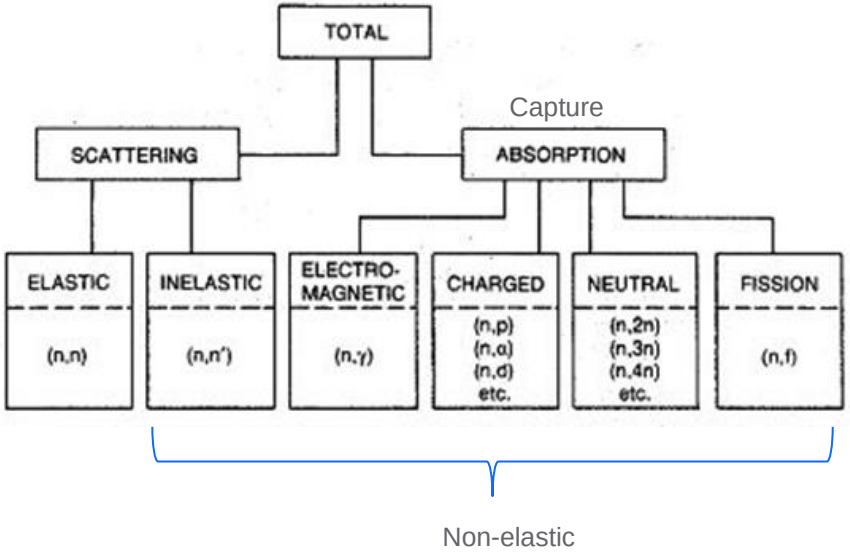
A. Fasso' , Simulation Calculations 2006

Neutron interactions (above thermal energies)

Two major types of neutron interactions with a nucleus : **scattering or absorption**:

When a neutron is **scattered by a nucleus**, its speed and direction change but the nucleus is left with the same number of protons and neutrons it had before the interaction. The nucleus will have some recoil velocity and it maybe left in an excited state that will lead to the eventual release of radiation. In general, **scattering moderates or reduces the energy of neutrons and provides the basis for some neutron detectors** (for example, proton recoil detectors).

When a neutron is **absorbed by a nucleus**, a wide range of radiations can be emitted or fission can be induced.



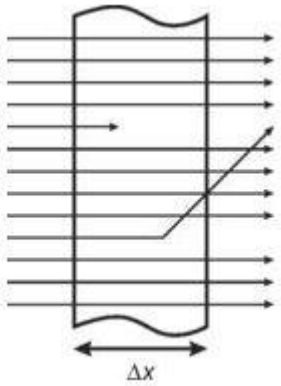
Elastic scattering is the most important process for neutron slowing down.
The total kinetic energy is conserved
A fraction of the neutron's kinetic energy is transferred to the recoiling nucleus.

Inelastic scattering the neutron is absorbed and re-emitted while the nucleus absorbs some energy and is left in an excited state eventually releasing s radiation.
In tissue, inelastic scatter reactions can occur in C, N and O

P. Rinard, Neutron Interaction with Matter, LA-UR-90-732

Cross Sections: Microscopic

The **probability** of a particular event occurring between a neutron and a nucleus is expressed with the concept of **cross section**.
If a large number of neutrons of the same energy are directed into a thin layer of material, some may pass through with no interaction, others may have interactions that change their directions and energies, and still others may fail to emerge from the sample. The **microscopic cross section σ describes the probability of neutron interaction with single nucleus divided by the areal atom density (the number of target atoms per unit area of the layer)** and has the dimension of an area ($1\ barn\ = 10^{-24}\ cm^2$).



The cross sections associated with the various interactions				
σ_t			=	**total** cross section ($\sigma_s + \sigma_a$)
σ_s			=	**total scattering** cross section ($\sigma_{el} + \sigma_i$)
σ_{el}	or	$\sigma_{n,n}$	=	**elastic scattering** cross section
σ_i	or	$\sigma_{n,n'}$	=	**inelastic scattering** cross section
σ_a	or	σ_c	=	**absorption** or capture cross section
σ_{ne}			=	**nonelastic** cross section, $\sigma_t - \sigma_{el}$
$\sigma_{n,g}$			=	**radiative capture** cross section
σ_f	or	$\sigma_{n,f}$	=	**fission** cross section
$\sigma_{n,p}$			=	(n,p) reaction cross section

Note: The probability of each type of event is independent on the probability of the others and the total probability is the sum of all of them

Energy- velocity relationship for neutrons

Cross sections are strongly dependent on neutron energy. The classical expression for kinetic energy, **$E = mv^2/2$**, is sufficiently accurate because even a kinetic energy of 100 MeV is still only about one-tenth of the rest-mass energy of a neutron (939.55 MeV). For velocity v in meters per second and kinetic energy, E in MeV,

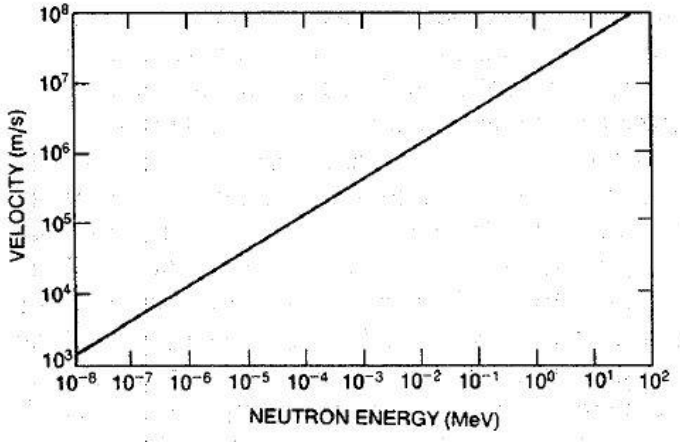
$$E = 5.227\ 10^{-15}\ v^2$$

and

$$v = 1.383\ 10^{7}\ \sqrt{E}$$

For example **a 1 MeV neutron** has a speed of 1.383 X 10^7 m/s and therefore will cross a **15-cm sample region** in a typical assay instrument in about **11 ns**.

A **thermal neutron** with an energy of 0.025 eV has a speed of 2187 m/s and will cross the same 15-cm region in about **70 µs**.

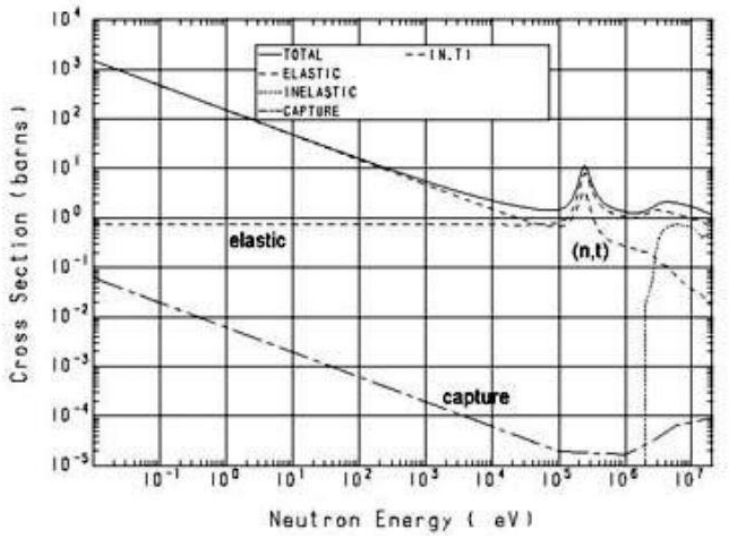


Energy dependence of cross section

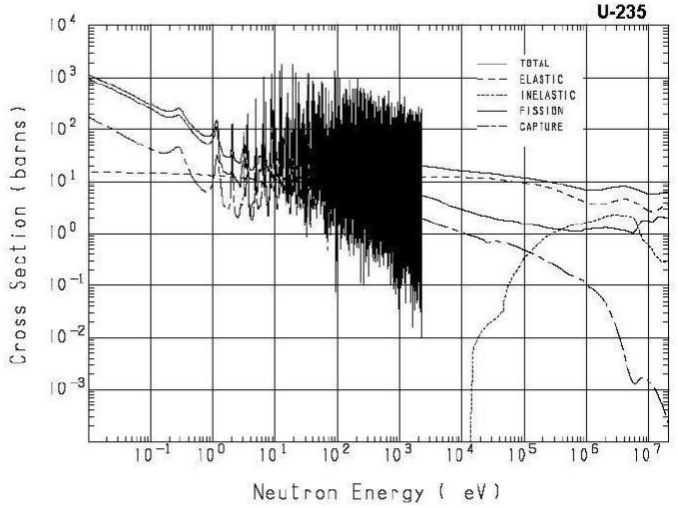
- Cross-section magnitudes are strong functions of neutron energy

As general rule the cross section decreases with increasing energy. At low energies, below 1 MeV, the elastic cross section is nearly constant, whereas the inelastic scattering cross section and absorption cross sections are proportional to 1/v.

So at low energies the total cross section can be nearly constant or decreasing with energy, depending on which type of event dominates. For high Z nuclei at higher energies large peaks (**resonances**) occur when neutron energy is close to an excited state of compound nucleus.



Reaction cross sections for trtium production in ^{6}Li



Reaction cross sections in ^{235}U

(Note: also seen as: slower neutron → greater wavelength→ longer time close to the atom→ greater the interaction probability)

Evaluated Nuclear Data Files and Transport Codes -1

Neutron interactions at energy higher than 20 MeV are handled by nuclear Models or a mix of models and libraries.

Below 20 MeV, where neutron cross sections are complicated and cannot be calculated by models, transport and interaction are handled by **dedicated libraries,** for example:

- **Evaluated Nuclear Data File (ENDF**) contain recommended, evaluated cross sections, spectra, angular distributions, fission product yields, photo-atomic, thermal scattering data; available at:
  IAEA : https://www-nds.iaea.org/exfor/endf.htm or NNDC: http://www.nndc.bnl.gov/sigma/index.jsp

- **Joint Evaluated Fission and Fusion data (JEFF)**
- **Japanese Evaluated Neutron Data Library (JENDL)**

General List and description : https://www.oecd-nea.org/dbdata/data/nds_eval_libs.htm

Note: No one is the absolute best and different cross sections can be better in one or another library

Evaluated Nuclear Data Files and Transport Codes -2

In neutron transport codes in general two approaches are used:

point-wise (“continuous” cross sections) and **group-wise** transport

- **Point-wise** follows cross section precisely but it can be time and memory consuming
- **Group-wise** approach is widely used in neutron transport codes because it is fast and gives good results for most application.

Complex programs such as the Nuclear Data Processing System (NJOY) or Pre-processing codes (PREPRO...) are used to **convert ENDF files to point-wise or group-wise cross sections** (including, for example, Doppler broadening in the thermal region at different temperatures)**.**

Group-wise cross sections

The energy range of interest is divided in a given number of discrete intervals ("**energy groups**").

Elastic and inelastic reactions are not simulated as exclusive processes, but by **group-to-group transfer probabilities** (downscattering matrix)

For example, for a neutron in a certain energy group (6) after scattering in a certain material :

0.4927 0.0148 0.0006 0.0012 0.0017 0.0023 0.0028 0.0033 0.0038 0.0045 0.0056 0.0070 0.0087 0.0104 0.0120 0.0134 0.0149 0.0163 0.0175
0.0184 0.0190 0.0193 0.0193 0.0190 0.0185 0.0178 0.0164 0.0329 0.0311 0.0278 0.0247 0.0219 0.0198 0.0158 0.0126 0.0101 0.0112 0.0070
0.0026 0.0008 0.0004 0.0002 0.0001 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 .....

the probability of getting a neutron in the same group (group 6) is 49.27%; to get a neutron in the following group (group 7) is 1.48%, in group 8 is 0.06% etc.

This matrix, normalised to 1, gives the relative probability of each neutron group

In the thermal region neutrons can gain energy.
This is taken into account by an up-scattering matrix, containing the transfer probability to a group of higher/lower energy. Each group i contains the **average σ_i** calculated weighting the cross section with the fluence Φ

$$<\sigma_i>=\frac{\int_{E_{i,low}}^{E_{i,high}}\sigma(E)\Phi(E)\,dE}{\int_{E_{i,low}}^{E_{i,high}}\Phi(E)\,dE}$$

Cross sections in MC

Different codes use different cross sections description, for example MCNP use pointwise while FLUKA use group-wise (260 groups for neutrons of approximately logarithmic width, 31 thermal groups and 42 for gammas)

WARNING : Pointwise does NOT mean correlated!

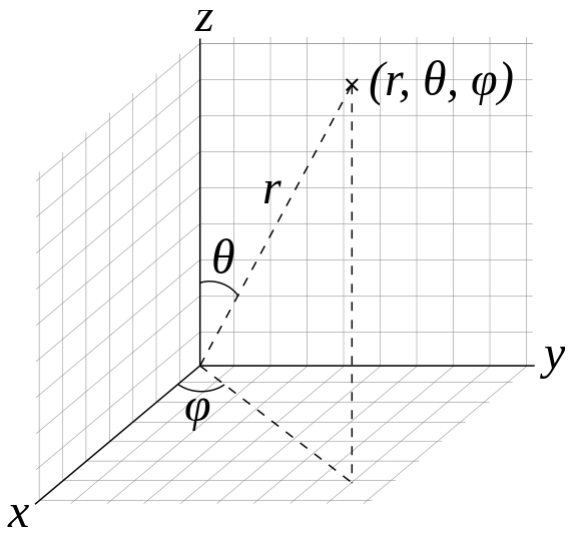
Both multigroup and pointwise codes use the international evaluated databases which contain only inclusive distributions of reaction products. To obtain exclusive (i.e. energy and momenta of all products), correlated final states ad-hoc models and algorithms have to be developed

Angular Probabilities:

In the center-of-mass system, generally neutron scattering is **rotationally invariant** → The probability of scattering from one direction into another is expressed as a probability distribution function of two **independent** angles:

Azimuthal angle, φ sampled from a uniform distribution, with any value between 0 and 2π equally likely

Polar angle, θ for which scattering angular probabilities are obtained by a discretization of a Legendre polynomial expansion (if P5 → **3 discrete polar angle cosines and 3 corresponding probabilities**)



Thermal neutrons: free gas scattering

A collision between a low energy neutron and an atom is affected by the **thermal motion of the atom**. This is taken into account in MC codes with the **free gas thermal treatment** to simulate the elastic scattering process on the basis of 3 assumptions:

1. The moderating and absorbing nuclei are unbound (so that any molecular and crystalline effects can be ignored)
2. The unbound nuclei have a distribution in energy which can be described by Maxwell-Boltzmann distribution
3. The scattering cross section (proportional to the probability of neutron scatter) is constant in the energy interval considered for the nuclide

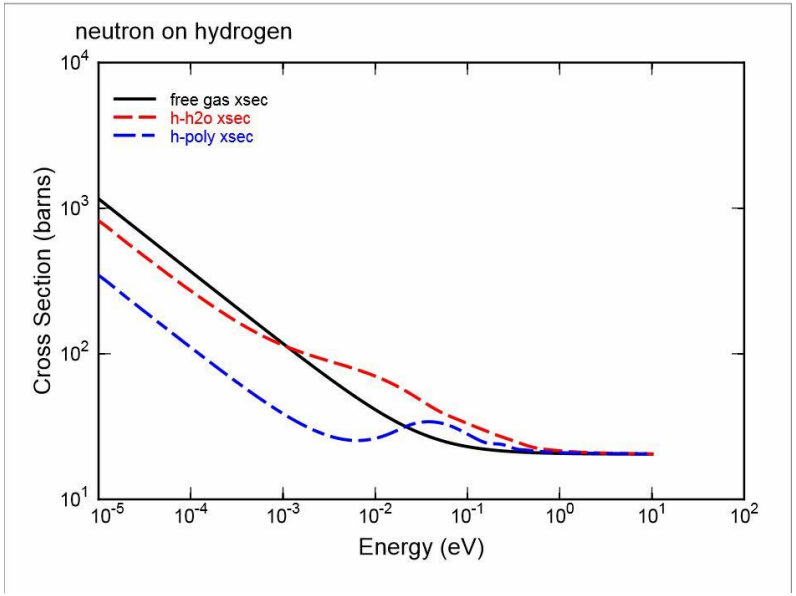
These assumptions are true at higher energy but at energies below the strength of the molecular bonds (a few eV) chemical binding and crystal structures have to be taken into account. Both elastic and inelastic scattering are modified with the use of preprocessing to produce **S(α,β)** tables for specific materials allowing the simulation of scattering also by multiatomic molecules.

R. E. MacFarlane, new thermal scattering files for ENDF/B-VI release 2, 1994

Thermal neutrons

Materials with same composition but different density or allotropic forms such as:
carbon (amorphous), graphite (crystalline) and diamond or
hydrogen in different compounds such as water (H2O) or Polyethylene (CH2)
can have different cross sections:

Thermal neutron scattering lengths and cross sections are available at:
http://webster.ncnr.nist.gov/resources/n-lengths/
and can be plotted with the Nuclear Data Viewer:
https://t2.lanl.gov/nis/data/ndviewer.html



At 293.6K from ENDF/B-VII.1 using pointwise cross sections

Note: In FLUKA with the card LOW-MAT it is possible to set the correspondence between a material and low-energy neutron cross section at different temperatures.
For example:
Free gas natural carbon (at 296, 87, 4 and 430 K)
Graphite bound natural Carbon (at 296 K)

Geometry

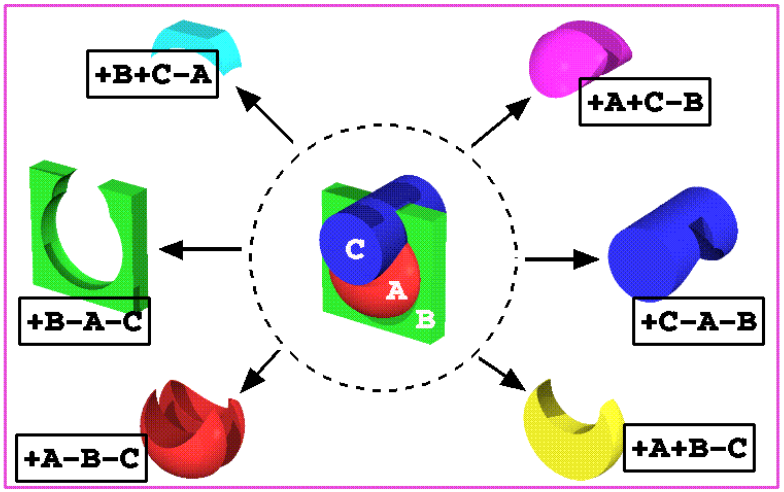
The algorithms to build a geometry and to track particles inside it differ from code to code.

In general:

- The geometry is built from basic **solids** and/or **surfaces:**
  - EGS: original CG, or user-defined
  - FLUKA (extended CG): solid “bodies” and surfaces
  - GEANT: solid “volumes”
  - MARS: 5 different geometries, including FLUKA and MCNP geometry
  - MCNP(X): originally surfaces, now also “macrobodies”
  - MORSE, SAM-CE (original Combinatorial Geometry, CG): solid “bodies”
  - PENELOPE: surfaces
  - PHITS: MCNP geometry
  - TRIPOLI: solid “bodies” and surfaces

- Defined by input cards (MCNP, FLUKA) or by user-written routines (GEANT)
- In some codes it can allow for repetition of structures (**lattice**)
- In some codes it can allow for “voxel” representation (**CT import**)

Combinatorial geometry



A. Fasso’ , Simulation Calculations 2006

Results from a MC calculation

- It is often said that Monte Carlo is a "mathematical experiment".

- Each aspect of a real experiment has its MC equivalent

  - Experimental technique → Estimator
  - Instrument → Detector
  - Measurement → Score or tally
  - Result of an experiment → Monte Carlo result

- A score is obtained by sampling from a statistical distribution (as in real measurements)
- As an experimental result consists in an average of the measurements, a statistical error and a systematic error, a MC result is an average of scores, a statistical error (and a systematic error, generally unknown)
- There are often several different techniques to measure the same physical quantity: in the same way the same quantity can be calculated with different kinds of estimators

A. Fasso' , Simulation Calculations 2006

Estimators

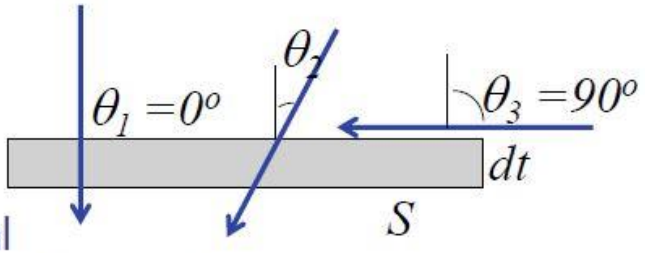
There are various types of estimators, depending on the quantity to be estimated and on the topology (phase space region over which the quantity is integrated)

- Boundary Crossing: used to estimate the fluence or the current of particles at a physical boundary between two space regions. Possible results are mono or multi-differential fluence spectra as a function of energy, angle, particle type, …
- Track length: calculate the fluence of particles in a region of real space. Possible results are fluence spectra as a function of particle energy , based on the path length of the particles within the region volume
- Pulse-height detector (e.g. simulation of a Ge spectrometer): estimate the quantity energy deposited in a region of real space and the result is the spectrum of deposited energy within the region volume
- Scalar integral estimator: used to predict scalar quantities such as deposited energy, inelastic interactions (stars), induced activity in a region of real space
- Mesh: special case of scalar estimator providing a 2- or 3-dimensional space distribution of scalar quantities (fluence, energy deposition, stars…) over a regular subdivision of a portion of real space in sub-volumes, generally independent from the tracking geometry

Estimator	Quantity	Detector
Tracklength est.	Fluence	A sphere of radius 10 cm centered at 0

Fluence estimation (2/2)

Surface crossing estimation



- Imagine a surface having an infinitesimal thickness dt
  A particle incident with an angle θ with respect to the normal of the surface S will travel a segment $dt/cos\theta$.
- Therefore, we can calculate an average surface fluence by adding $dt/cos\,\theta$ for each particle crossing the surface, and dividing by the volume $S\,dt$:

$$\Phi = \lim_{dt \to 0} \frac{\sum_i \frac{dt}{\cos\theta_i}}{S\,dt}$$

- While the current J will be to count the number of particles crossing the surface divided by the surface:

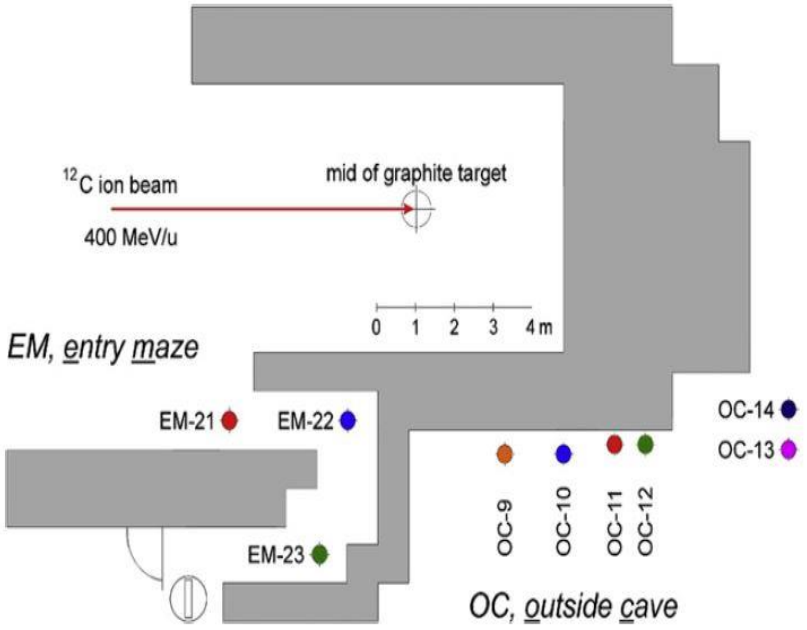
$$J = dN/dS$$

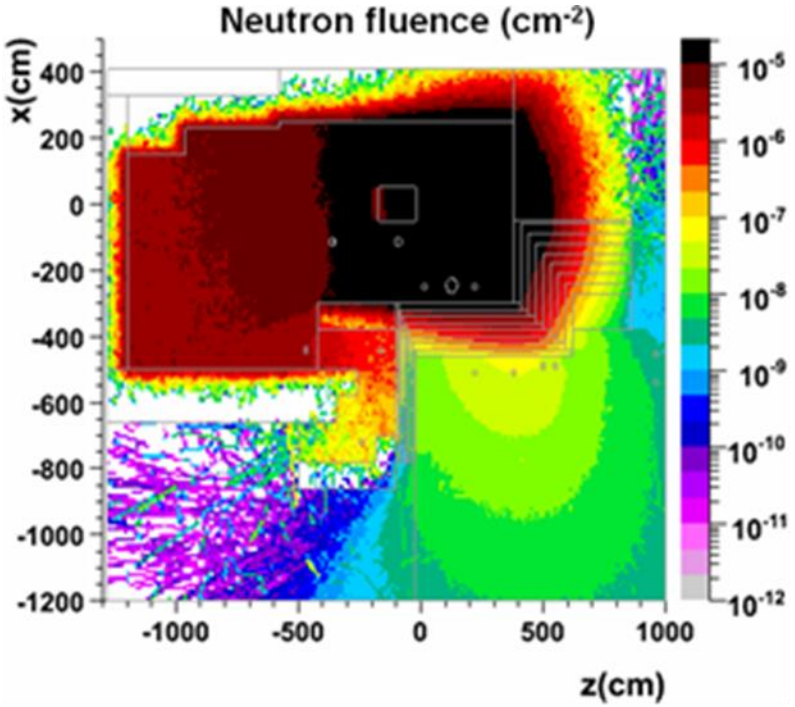
The fluence is independent from the orientation of surface S, while the current is NOT!

In an isotropic field can be easily seen that on a flat surface $J = \Phi/2$

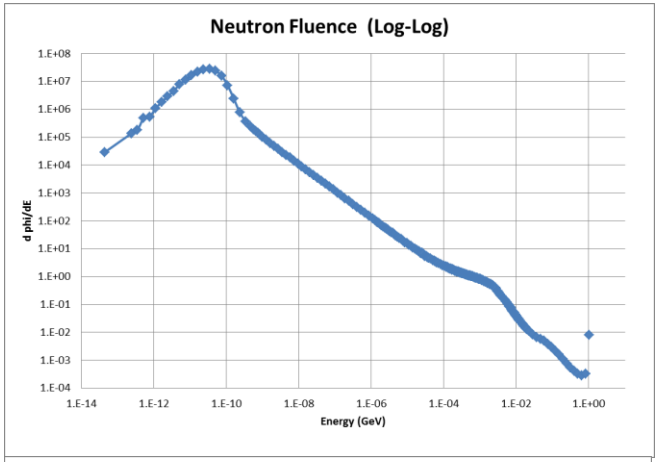
Example: Fluence and Lethargy outside shielding - 1

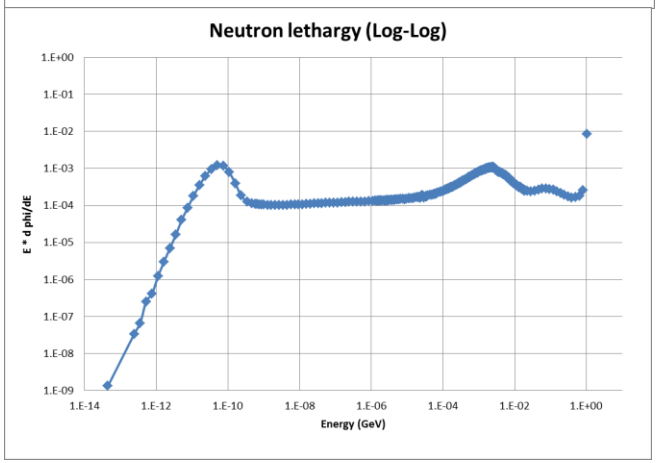
GSI – ^{12}C ions on graphite target





Example: Fluence and Lethargy outside shielding - 2



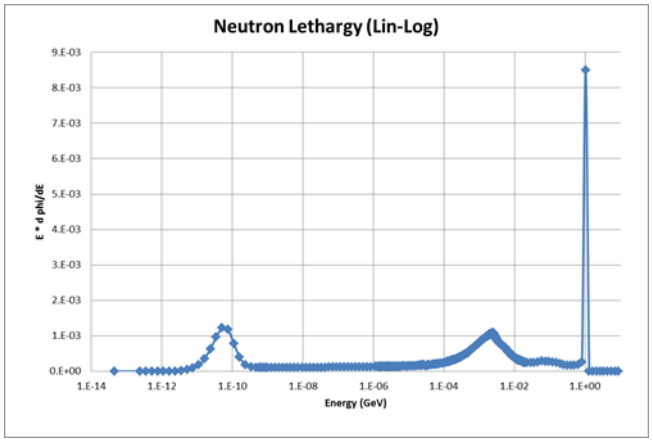


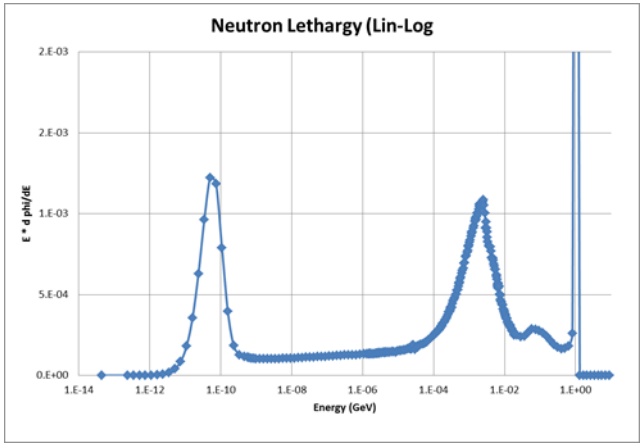
Fluence as the differential number of particles (neutrons) per each energy interval

The same data presented in the **lethargy representation**.

In this representation, the y axis displays the neutron fluence per lethargy unit $d\phi/d\ln(E/E_0) = d\phi/dE \cdot E$.

Example: Fluence and Lethargy outside shielding - 3





When this quantity is plotted linearly versus a log-energy scale, then equal areas below the curve correspond to equal fluences.

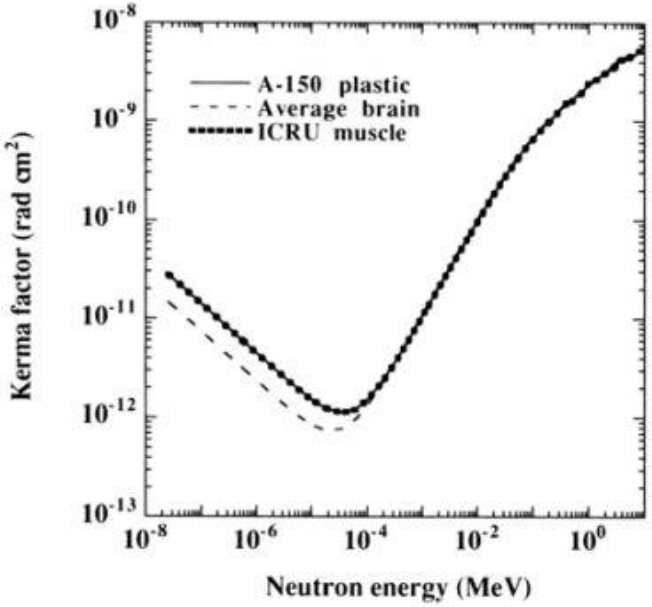
The mean spectral neutron flux distributions exhibit four typical features:

a) the Maxwell-Boltzmann peak that is due to thermalized neutrons,
b) a flat intermediate region with epithermal neutrons,
c) the MeV peak that is due to evaporation neutrons from highly excited residual nuclei, and
d) the 100 MeV peak that is due to a broad minimum in the corresponding neutron-air reaction cross-sections at high energies.

These four components are an example calculated outside the shielding of high-energy particle accelerators but they are also typical for secondary neutrons from cosmic radiation

Energy deposition and absorbed dose

Energy deposition by neutrons with energy < 20 MeV is estimated by means of fluence to Kerma factors

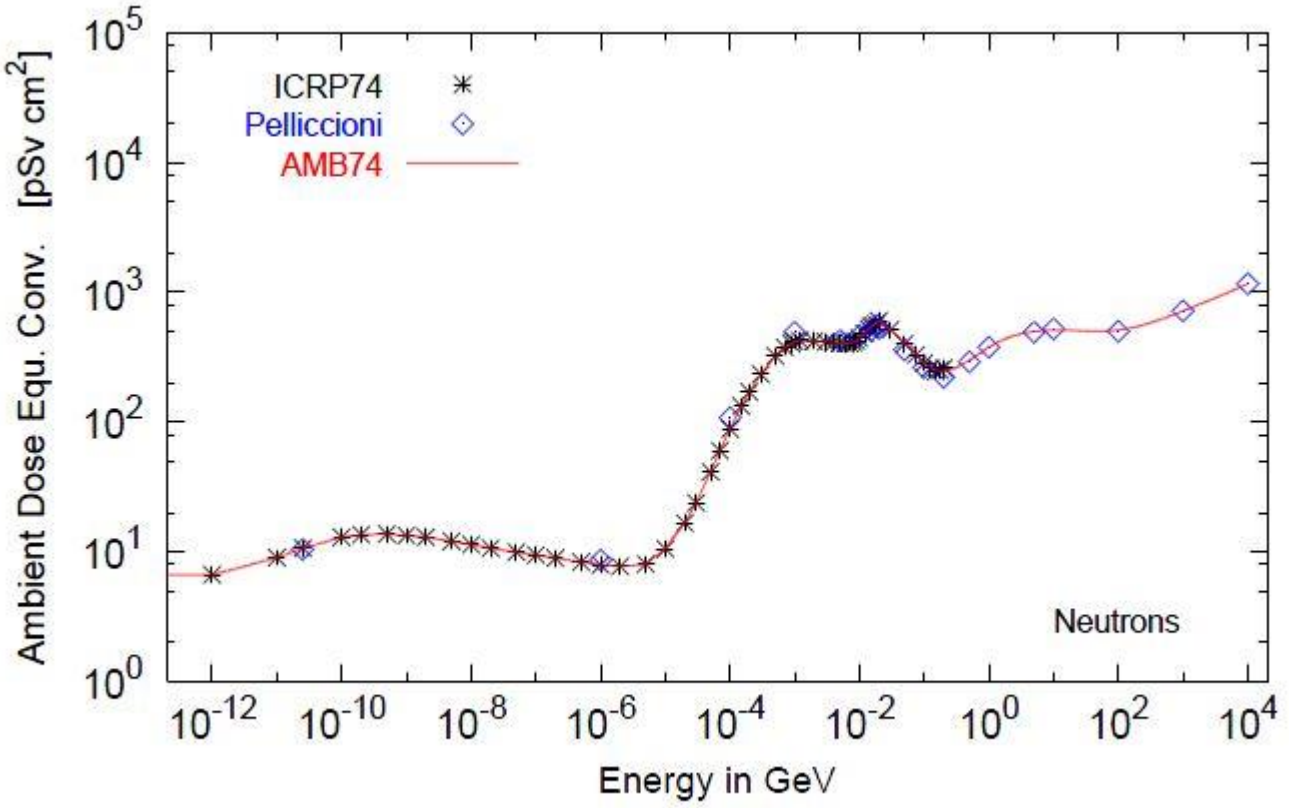


Example:
Below 100 eV the average brain has lower kerma factor than A-150 plastic because the brain has a lower nitrogen content.

Charged particles (p, alpha, C, N, O) generated in tissue by neutrons are important and it is through these secondary particles and the γ produced in (n,γ) reactions that nearly all the energy deposition and biological effects occur (especially important for thick target).

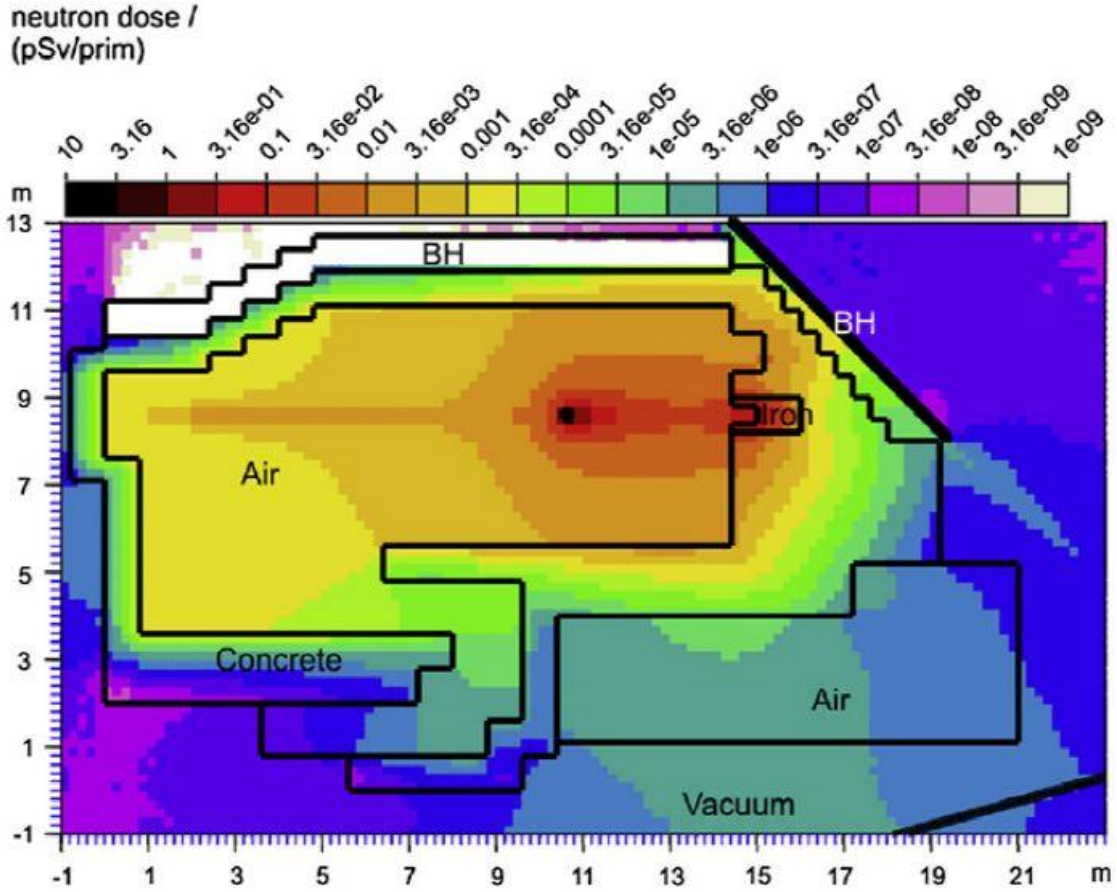
For applications in dosimetry or microdosimetry for which small tissue volume are considered secondary delta rays have to be taken into account and followed down to lower energies

Fluence to ambient dose equivalent



Maurizio Pelliccioni, Overview of Fluence-to-effective dose and fluence-to-ambient dose equivalent conversion coefficients for high energy radiation calculated using the FLUKA code, Rad. Protec. Dosim, Voll88, N.4 (2000)

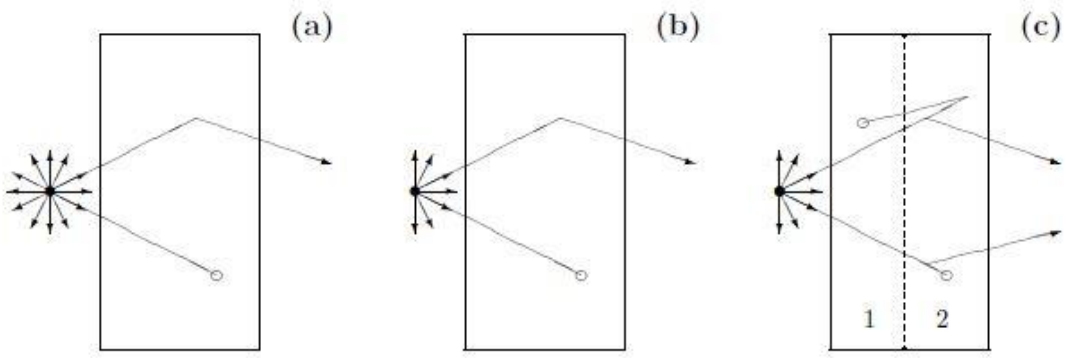
Ambient dose equivalent folding the fluence with the conversion coefficients



Non analog MC

Monte Carlo simulations that numerically mimic the actual physical processes involved are called analog Monte Carlo simulations.

In many problems an analog simulation is computationally impractical (for example in shielding and deep penetration problems) however MC can still be used effectively by introducing biases in the simulation. Such simulations no longer mimic nature and are called nonanalog Monte Carlo simulations.



Source biasing Splitting

For example, source neutrons can be forced to be emitted in direction toward the region of interest (b) and scattering particles could be biased so that they move preferentially toward the target (c) or killed if it has poor chance to contribute to the score.

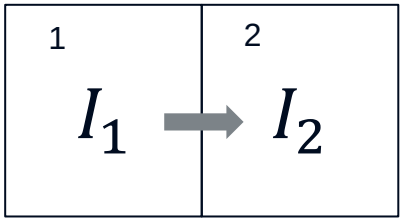
W. Dunn, KJ.K. Shultis, Exploring Monte Carlo Methods, Elsevier , 2012

Variance Reduction Techniques

1. Population Control Methods: artificially increase/decrease the number of particles in spatial or energy regions that are important/unimportant to the tally score.
   - Geometry splitting and Russian roulette (example: with importance I_2/I_1)
   - Energy splitting/roulette
   - Weight cutoff
   - Weight windows (example: with weight)
2. Modified Sampling Methods: These methods artificially increase the likelihood of events that increase the probability that a particle reaches the tally region.
   - Exponential transform
   - Implicit capture (example: with weight = $1 - \sigma_a / \sigma_t$)
   - Forced collision
   - Source direction and energy biasing
   - Neutron-induced photon production biasing
3. Partially deterministic Methods
   - Point and ring detectors
   - DXTRAN sphere
   - Correlated sampling

Importance Biasing (splitting + Russian roulette)

Importance biasing is the simplest, most safe and easy to use of all variance techniques.



When a particle leaves a cell with Importance I_1 and enters a cell of importance I_2 the particle is splitted/rouletted according to I_2/I_1

For example:

I_2/I_1 **= 3** the entering particle is split into 3 particles with a weight of 1/3
I_2/I_1 **= 0.6** the entering particle is killed with 40% probability and survive with 60% probability. If survive is weight is increased by a factor I_1/I_2

In each splitting or Russian roulette the weight of the remaining particles is adjusted to leave the tally unbiased and **the importance should be adjusted to keep the population of particles in a cell relatively constant**.

Note1: The ratio of importances should not be too big (<5-6)
Note2**: splitting reduces σ but increases t (more particles to follow) while RR decreases t but increase σ (less particles to follow)**

Variance Reduction Techniques

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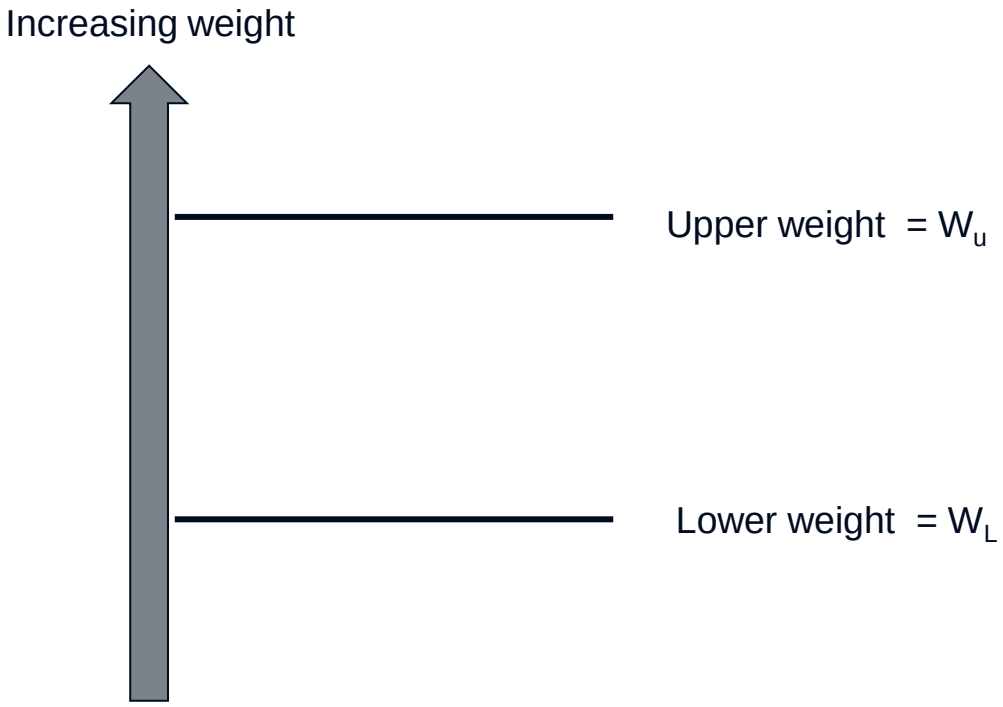
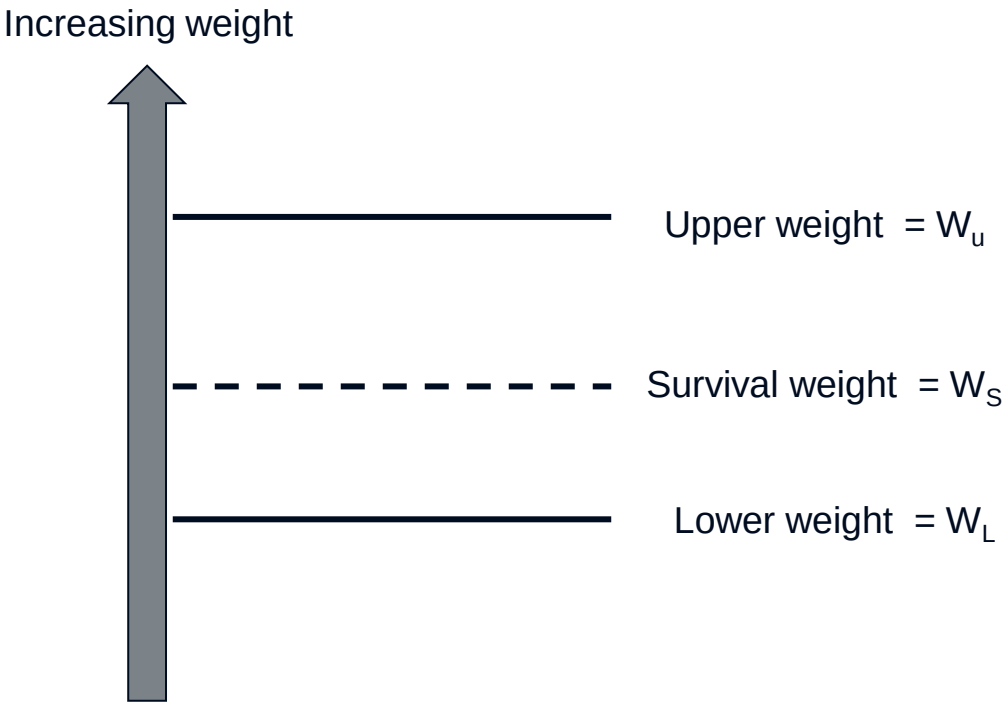
Weight Windows (Space and/or Energy)

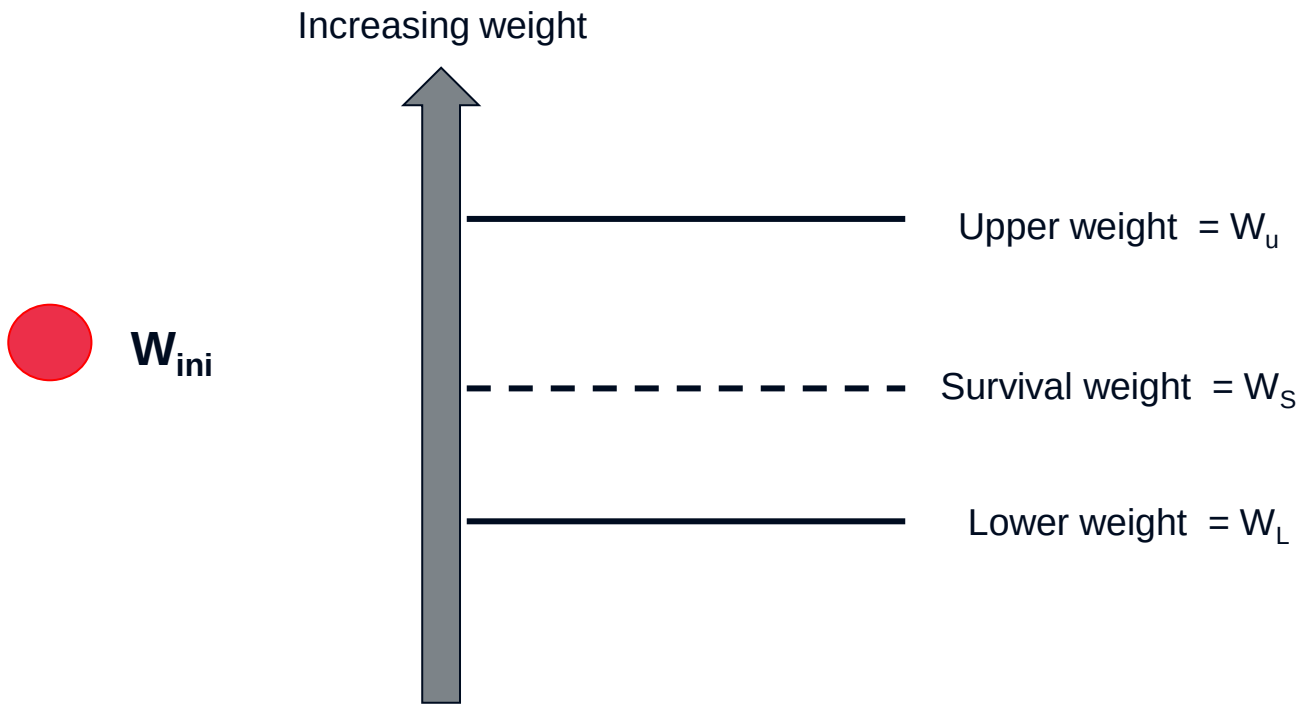


Based on absolute weight of each individual particle rather than relative region importance

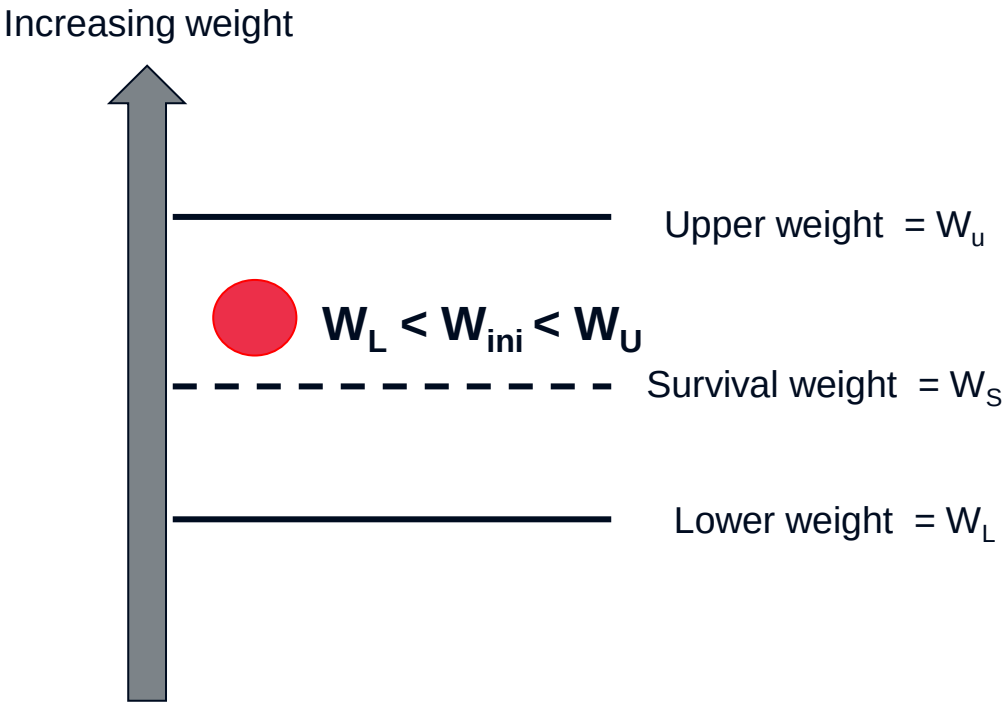
Weight Windows



Weight Windows

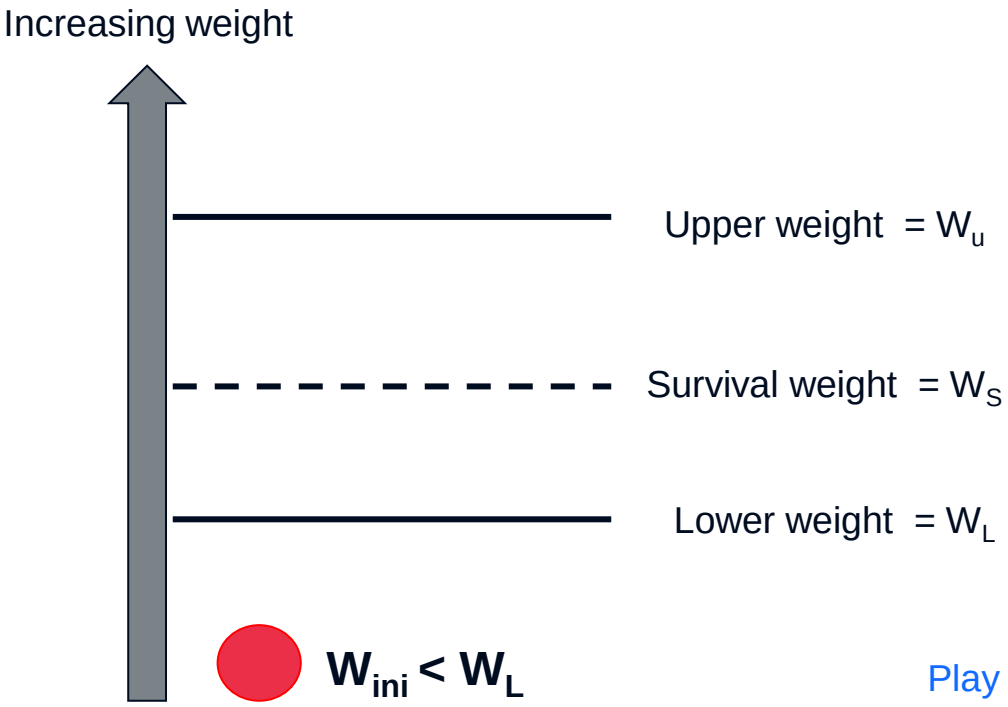


Weight Windows



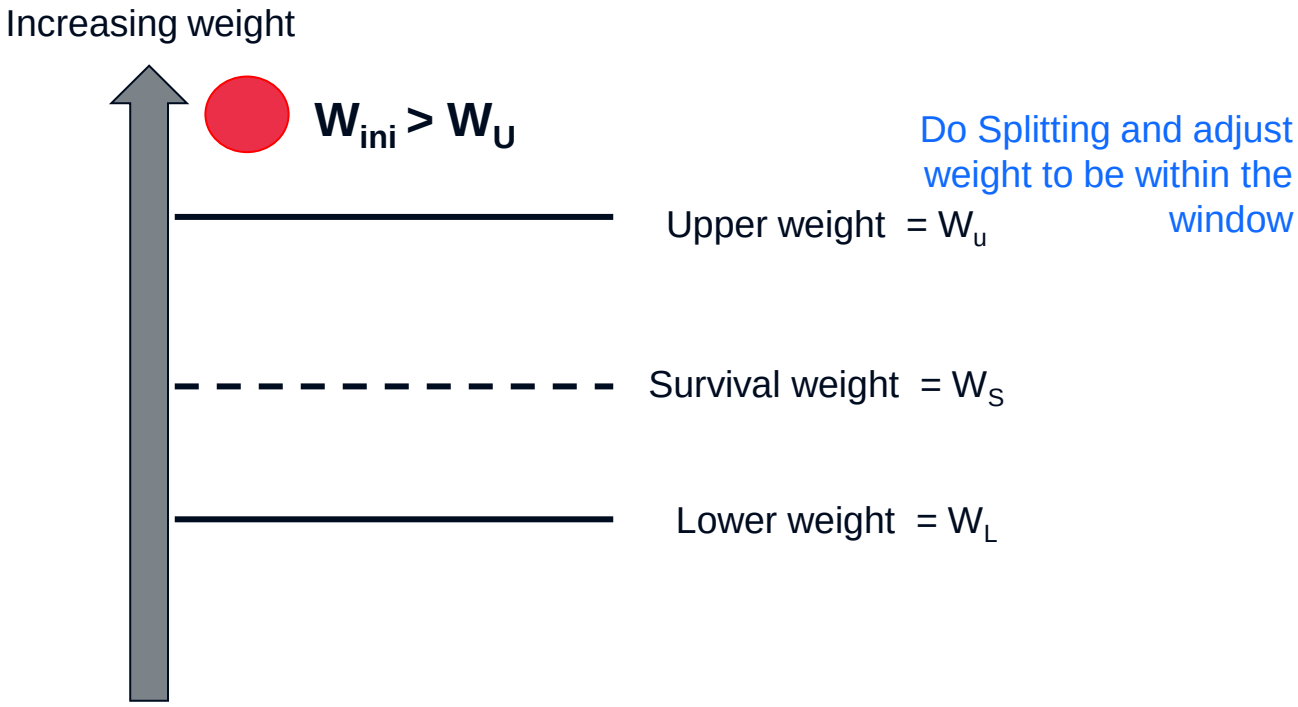
Do nothing

Weight Windows



Play Russian Roulette:
Kill or move to Ws

Weight Windows



WW is more powerful but require more experience and patience to set it up correctly
WW is essential when other biasing techniques generate excessive weight fluctuations in a given space region (large weight fluctuations → large σ

Variance Reduction Techniques

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   - Correlated sampling

Implicit capture

A particle absorbed before to reach the tally might be a waste of computing time

- In analog capture at a collision site a particle is killed with probability

$$\sigma_a / \sigma_t$$

Where σ_a is the absorption cross section (= 1/ λ)

And σ_t is the total cross section (absorption+scattering)

And hence $(1 - \sigma_a / \sigma_t)$ is the survival probability

- In implicit capture the particle is allowed to continue its trajectory as no interaction has occurred but with a new weight:

$$W_{new} = W_{in} (1 - \sigma_a / \sigma_t)$$

Note: to avoid endless thermal neutron scattering in materials with low thermal neutron absorption cross section the survival probability can be set < 1

Variance Reduction Techniques

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   - DXTRAN sphere
   - Correlated sampling

The key for biased simulations is to adjust the tally to undo the biases introduced into the physical models to obtain a correct score.→ **the (probability x weight) should be conserved!**

Figure of Merit

Variance Reduction Techniques are used to modify the sampling and scoring procedures of Monte Carlo **without changing the sample mean** but **do change the sample variance**.

Some biasing techniques reduce σ^2 while others reduce the time

$$\sigma^2 \propto \frac{1}{n} \quad \text{while} \quad t \propto n$$

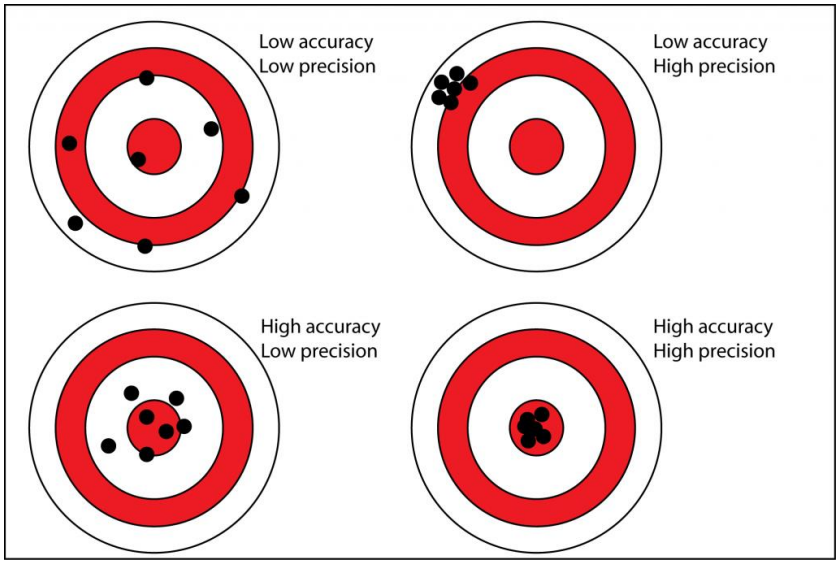
Therefore minimizing $\sigma^2 \cdot t$ means reducing the variance faster than t increase and viceversa.

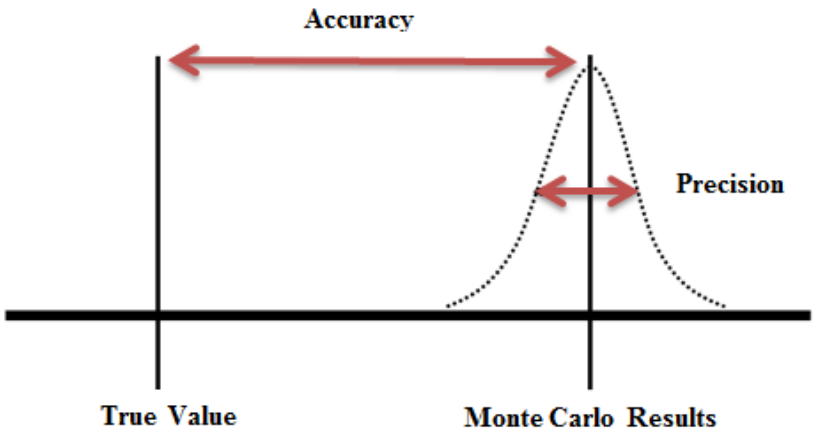
This product can be considered a **Figure of Merit** of the problem and can be used to estimate which variance reduction method is better

If carefully implemented variance reduction schemes can significantly reduce the sample variance but cannot be applied blindly or automatically. Sometimes combining different techniques or misusing a single scheme can produce totally wrong results.

The effective implementation of variance reduction for a particular problem is part of the "art" of using Monte Carlo.

Precision & Accuracy





P. Saidi, et al. variance reduction of MC simulation in Nuclear Energy Field, Theory and Applications of Monte Carlo Simulations, DOI: 10.5772/53384.

Precision & Accuracy

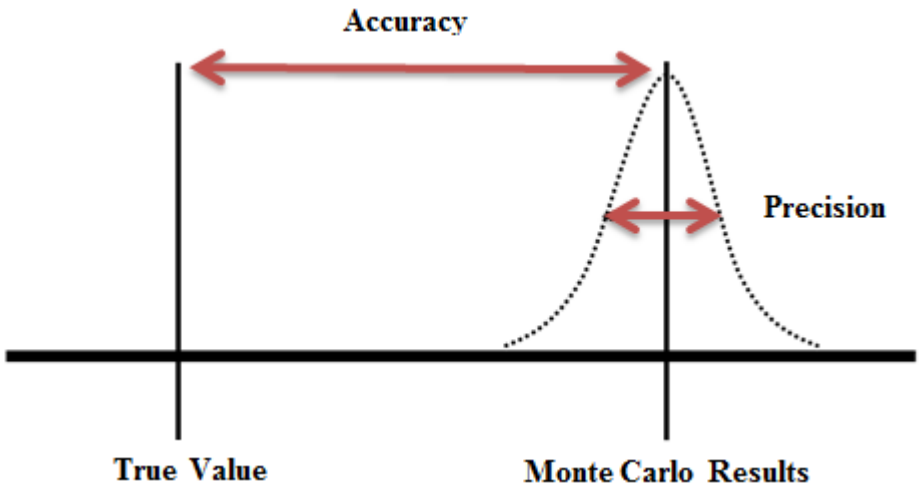
Factors Affecting Accuracy (systematic errors) :

- Physics/mathematical models
- Uncertainties in nuclear/atomic data including **cross sections**, atomic weights etc
- Improper modelling of source energy and angular distribution
- Poor representation of geometry
- Errors in material compositions

Factors Affecting Precision:

(statistical errors)

- Forward versus adjoint calculations (extended sources and tally in small region)
- Tally type
- **Variance reduction**
- Number of histories



……and Mistakes

“Your best teacher is your last mistake ! “

Ralph Nader

Acknowledgment

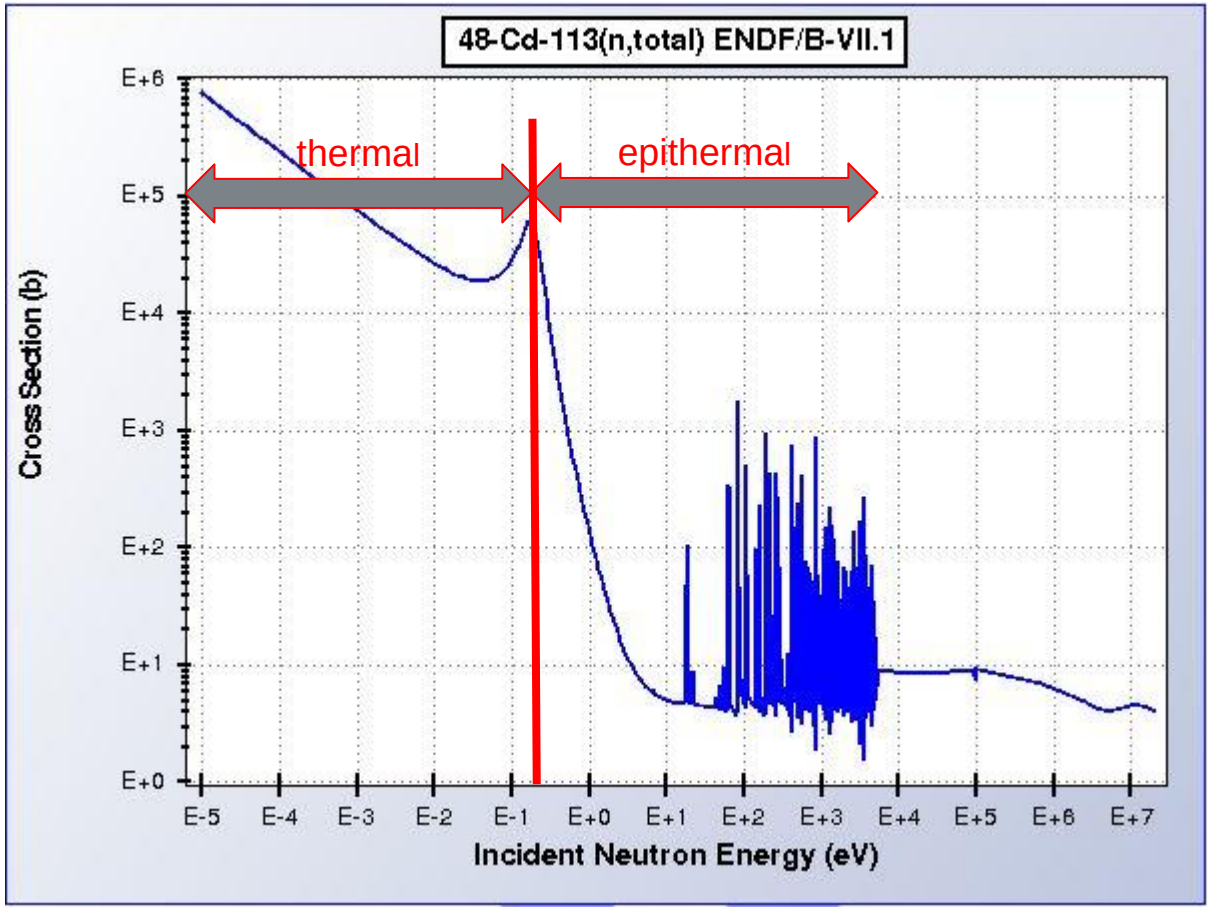
I especially acknowledge Alberto Fasso' huge and impressive experience in Monte Carlo codes, thanks him for teaching me FLUKA and for his precious suggestions during all these years

FLUKA Courses & Manual (also written by Alberto)

MCNP Manual (I am not aware of any Alberto's contribution here but I would not excluded the possibility there might also be some!)

Additional slides

Thermal Cross Section



Gamma generation (for FLUKA)

- Gamma generation from (n,xγ) reactions is possible only for those elements for which data are available in the evaluated nuclear data files
- Gamma generation is performed by a multigroup scheme as well
- Number of gamma groups: 42, different from neutron groups (Energy range: 1keV - 50 MeV)
- The actual energy of the generated photon is sampled randomly in the energy interval corresponding to its gamma group
- Exception: 2.2 MeV from H(n, γ)**2**H reaction, 478 keV photon from **10**B(n, γ) and gamma cascades from Cd(n, γ) and Xe(n, γ)
- Capture gammas as well as gammas from inelastic reactions like (n,n') are included

- The neutron library only creates gammas, the transport is done by the EMF module (like all other gammas in FLUKA)

Thermal neutrons

- At thermal neutron energies, the binding of the scattering nucleus in a solid, liquid or gas, affects the cross section and the distribution of secondary neutrons. In practice, the scattering of neutrons from a system of N particles with a random distribution of spins or isotopes types can be expressed as the sum of a **coherent part** and an **incoherent part**. The coherent scattering includes the effects from waves that are able to interfere with each other and the incoherent part depends on a simple sum of noninterfering waves from all the N particles. The cross sections for coherent and incoherent scattering can be considered to be characteristic properties of the materials.
- As examples, the scattering from hydrogen is almost completely incoherent and the scattering from carbon and oxygen is almost completely coherent. Furthermore, the coherent and incoherent scattering included both elastic and inelastic parts. The elastic scattering takes place with no energy change. It should not be confused with the elastic scattering from a single particle that is familiar for higher neutron energies where the neutron loses energy; thermal elastic scattering can be considered to be scattering from the entire lattice; thus the effective mass of the target is very large, and the neutron does not lose energy in the scattering process.
- Thermal inelastic scattering results in an energy loss (gain) for the neutron with a corresponding excitation (deexcitation) of the target. The excitation may correspond to the production of one or more phonons in a crystalline material, to the production of rotations or vibrations in molecules, or to the initiation of atomic or molecular recoil motions in a liquid gas.

Therefore, we can usually divide the thermal scattering cross section in three different parts:

- Coherent elastic: important for crystalline solids like graphite or beryllium
- Incoherent elastic: important for hydrogenous solids like solid methane, polyethylene and zirconium hydride
- Inelastic: important for all materials (this category includes both incoherent and coherent inelastic)

Can be seen as the resolution is linked to the wavelength (as in a microscope) and therefore can interact with a part or all the atom or the lattice

R. E. Mac Farlane, New thermal neutron scattering files for ENDF/B-VI release 2, 1994

Cross Sections: Macroscopic

The **macroscopic cross section** derived from the transmission of a parallel beam of neutrons through a thick sample considered to be a series of atomic layers; for each layer we can apply the results found with the microscopic cross-section. By integrating through enough atomic layers to reach a depth x in the sample, the intensity $I(x)$ of the uncollided neutron beam is

$$I(x) = I_0\, e^{-N\sigma_t x}$$

where $\mathbf{I_0}$ is the **intensity of the beam** before it enters the sample, **N** is the **atom density** and $\boldsymbol{\sigma_t}$ is the **total microscopic cross section**. The **total macroscopic cross section** is $\boldsymbol{\Sigma_t = N\,\sigma_t}$ has dimension of cm^{-1} (and is analogous to the linear attenuation coefficient for gamma rays).

When traveling with a speed v, a neutron has an average time between interactions of λ/v. The **reaction rate** is the frequency with which interactions occur: **v/λ**, or $\mathbf{v\,\Sigma_t}$.

The **mean-free-path** length is the mean distance a neutron travels between interactions and the reciprocal of the macroscopic cross section:

$$\lambda = \frac{1}{\Sigma_t} = \frac{1}{N\,\sigma_t}$$

The probability of a first collision for a particle between $l\ and\ l + dl$ along its line of flight is

$$p(l)dl = e^{-\Sigma l}\,\Sigma\,dl \quad \text{Setting the random Number } \xi = \int_0^1 e^{-\Sigma s}\,\Sigma\,ds = 1 - e^{-\Sigma l}\,\Sigma$$

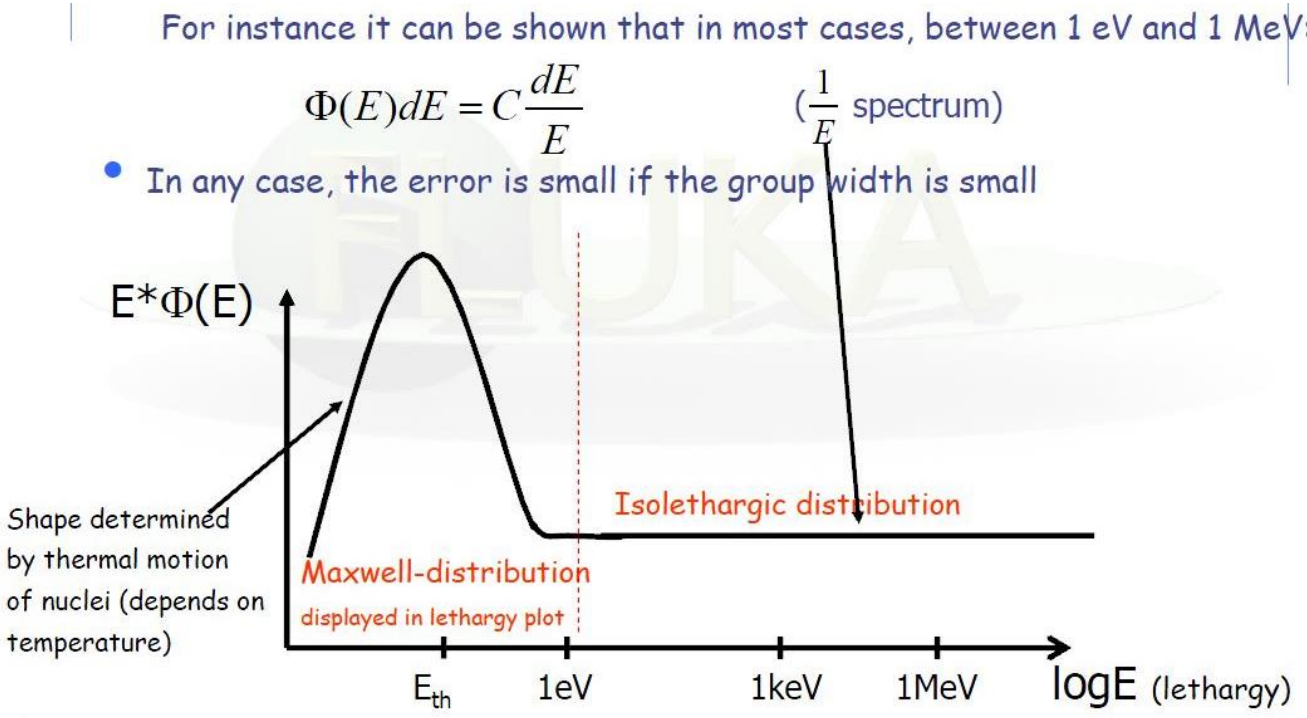
$$l = -\frac{1}{\Sigma}\ln(1-\xi) \rightarrow l = -\frac{1}{\Sigma}\ln(\xi)$$

Tallies/Scores/Edits (Results) …

Tallies	MCNPX	GEANT4	FLUKA	MARS	PHITS
Standard					
Flux					
Volume	Yes	Yes	Yes	Yes	Yes
Surface	Yes	Limited	Yes	Yes	Yes
Point/ring	Yes	No	No	Yes (neutrons)	No
Current	Yes	Limited	Yes	Yes	Yes
Charge	Yes	Yes	Yes	Yes	Yes
Kinetic energy	Yes	Yes	Yes	Yes	Yes
Particle density	Yes	Yes	No	No	No
Reaction rates	Yes	No	Star (inelastic)	Yes	Yes
Energy deposition	Yes	Yes	Yes	Yes	Yes
Rapidity	No	Yes	Yes	Yes.	No
DPA	HTAPE3X	No (user)	Yes	Yes	Yes
Momentum	No	Yes	Yes	Yes	No
Pulse-height	Yes	User input	Yes	No	Yes
Termination	Partial	??	Yes	Partial	Yes
Modifiers	9	2	2	2	2
Special					
Mesh	rec, cyl, sph	rec, cyl	rec, cyl	rec, cyl, sph	rec,cyl
Coincidence	Yes	No	Yes	Yes	Yes
Residuals	Yes	No	Yes	Yes	Yes
Activation	2.5.D	??	Yes	Yes	No
Event logs	Yes	Yes	Yes	Yes	Yes

Thermal neutrons - 2

An assumption is needed about the neutron spectrum to be used as a weighting function for calculating the average cross section on each group



P. Sala –FLUKA course