An introduction to the Monte Carlo simulation of radiation transport

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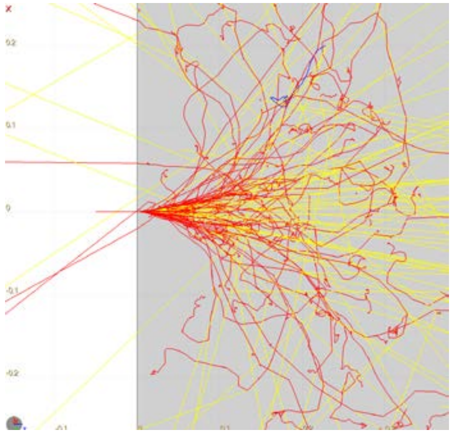
CERN Academic Training
Sep 12, 2022

Monte Carlo simulation tools for radiation transport problems in particle accelerators



Introduction
Mon Sep 12

Tue Sep 13

FLUKA

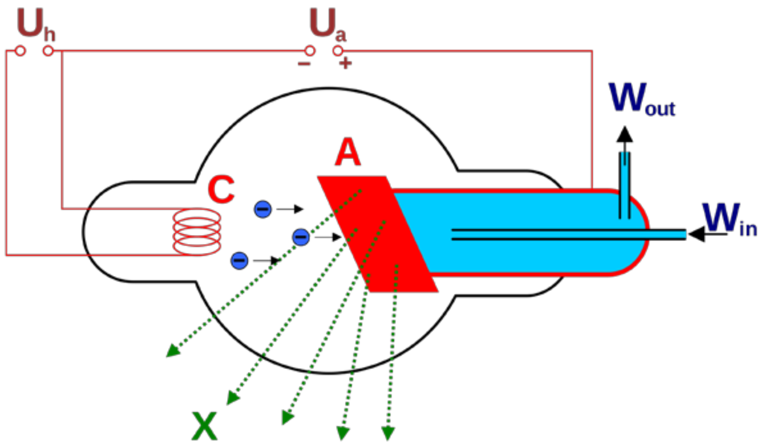
+ LIVE DEMO!

Wed Sep 14

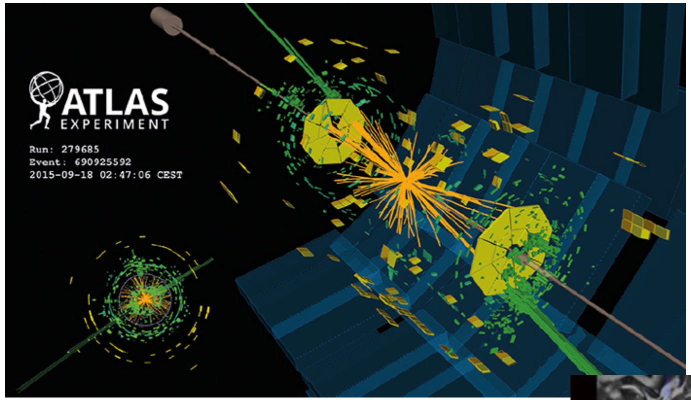
- Other codes exist, e.g. MCNP, PHITS, MARS, PENELOPE,…
- Aim is not to be exhaustive, but to show general capabilities

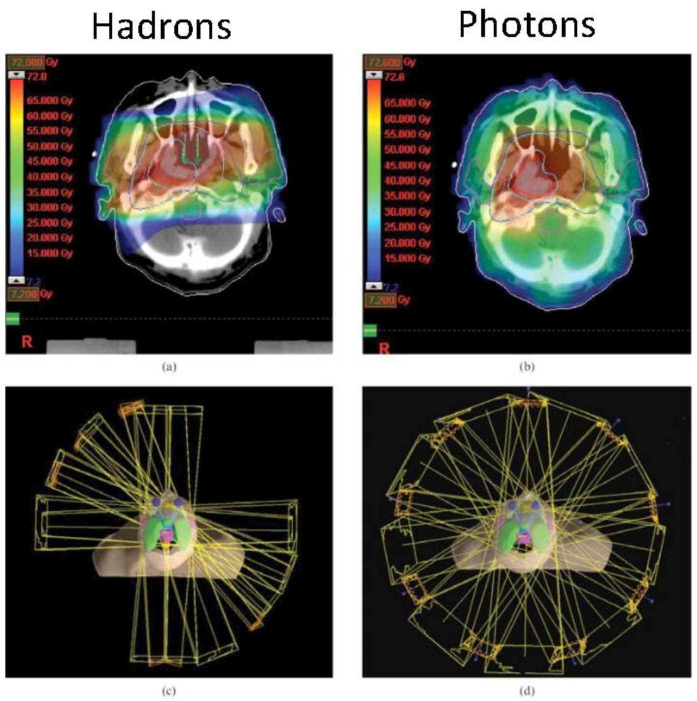
An introduction to the radiation transport problem

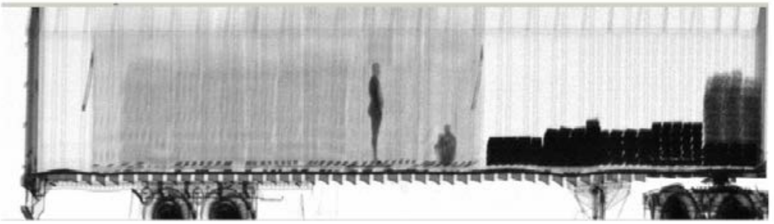
Radiation transport

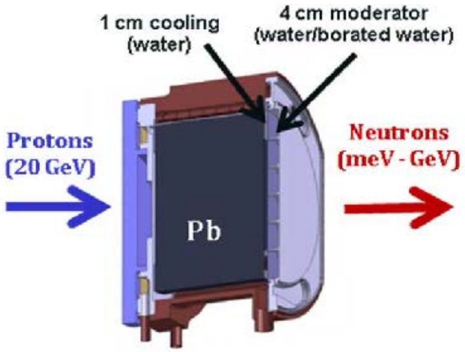


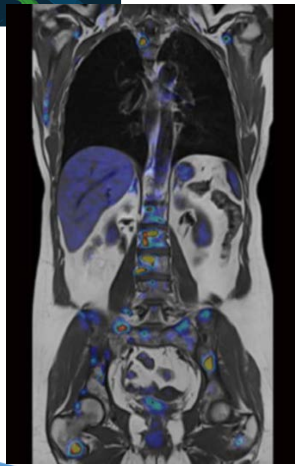
Source: Wikipedia







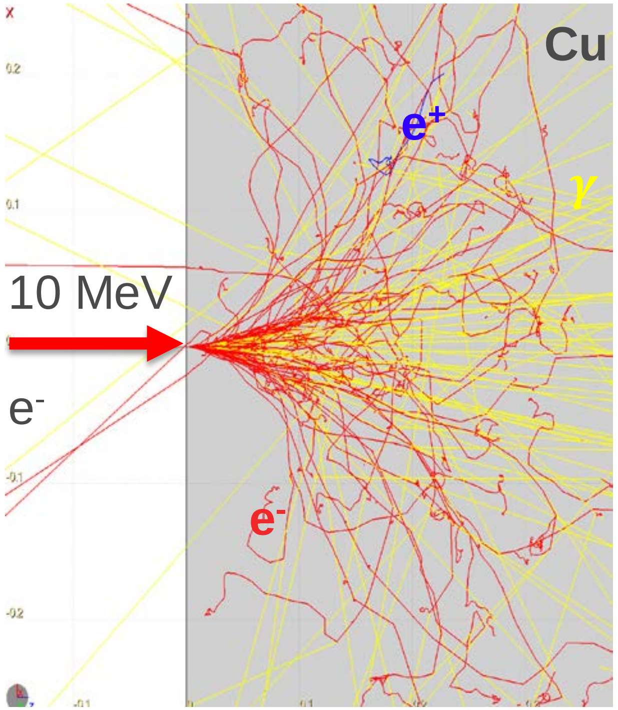




Radiation source → Propagation in matter → Detection

The physical picture

- **Radiation**: ensemble of particles (γ,e$^{\pm}$,$\mu^{\pm}$,ν_i,n,p,$\pi^{\pm}$,ions,…) propagating in matter, subject to a series of radiation-matter interaction mechanisms, leading to:
  - **Angular deflections** (target atom displacement)
  - **Energy losses** (energy transfer to material, heating up)
  - Generation of **secondary particles** (formation of a **radiation shower**)
  - Production of **residual nuclei,** possibly radioactive (emission of **prompt/delayed radiation**)

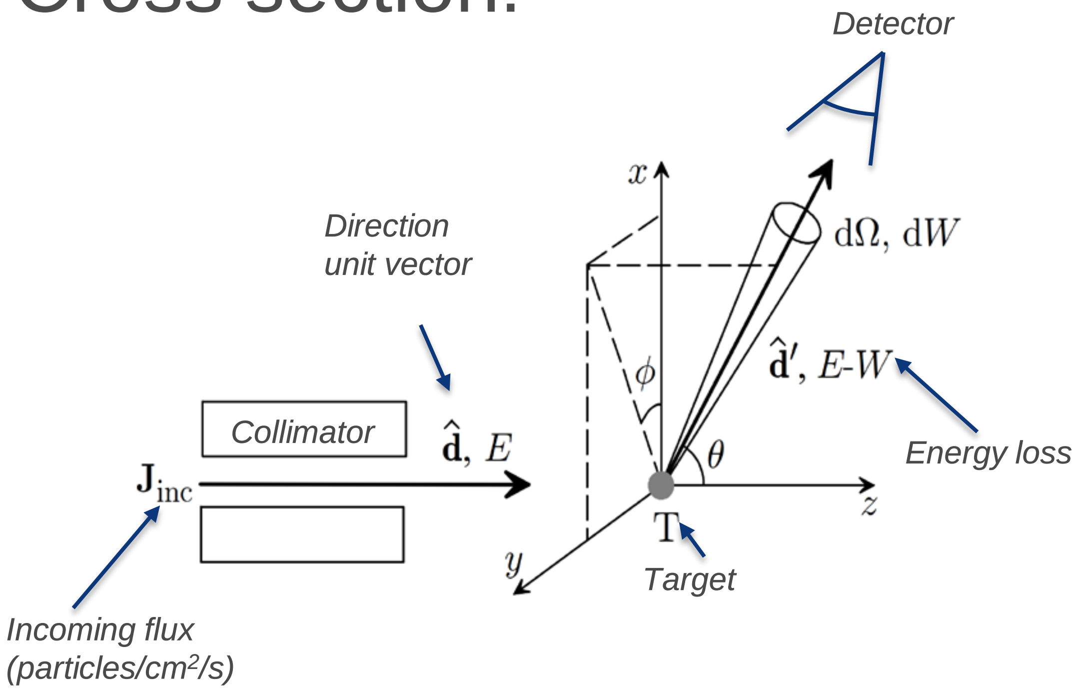


Example: Shower set up by 10-MeV e- in Cu

Basic quantities

species position energy direction time

- **Particle density** $n_i(\boldsymbol{r}, E, \Omega, t)$: number of particles of species i per unit volume, unit energy, unit solid angle, at a given time.
- Cross section:



Differential cross section

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}W} \equiv \frac{\dot{N}_{\text{count}}}{|\mathbf{J}_{\text{inc}}|\,\mathrm{d}\Omega\,\mathrm{d}W}$$

Dimensions: Area / Energy / Solid angle

~likelihood of being scattered into a direction Ω with an energy loss W

Cross section

$$\sigma \equiv \int\int \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}W}\,\mathrm{d}\Omega\,\mathrm{d}W$$

Dimensions: Area
Typical unit: 1 barn (=10^{-24} cm^2)

~likelihood of being scattered

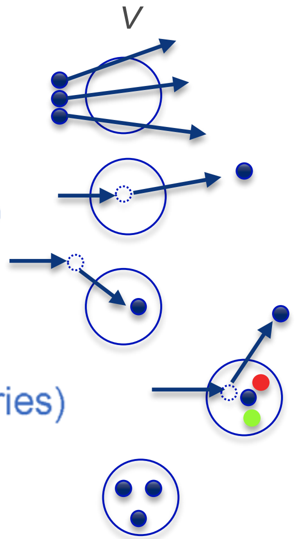
The transport equation

species position energy direction time

- Determine time evolution of particle density $n_i(\boldsymbol{r}, E, \Omega, t)$ in a small volume V
- Transport equation

$$
\begin{aligned}
\int_V \mathrm{d}\boldsymbol{r}\, \frac{\partial n_i(\boldsymbol{r},E,\Omega,t)}{\partial t} = & -\oint_S \mathrm{d}A\, \mathbf{j}(\boldsymbol{r},E,\Omega,t)\cdot\hat{\boldsymbol{a}} && \text{(unscattered particles)}\\
& - N \int_V \mathrm{d}\boldsymbol{r}\; n_i(\boldsymbol{r},E,\Omega,t) v(E)\sigma(E) && \text{(particles scattered out)}\\
& + N \int_V \mathrm{d}\boldsymbol{r} \int \mathrm{d}E' \int \mathrm{d}\Omega'\; n_i(\boldsymbol{r},E',\Omega',t) v(E') \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega''\mathrm{d}W''} && \text{(particles scattered in)}\\
& + N \int_V \mathrm{d}\boldsymbol{r} \int \mathrm{d}E' \int \mathrm{d}\Omega' \sum_j n_j(\boldsymbol{r},E',\Omega',t) v(E') \frac{\mathrm{d}\sigma_{\mathrm{sec},i}}{\mathrm{d}\Omega''\mathrm{d}W''} && \text{(production of secondaries)}\\
& + \int_V \mathrm{d}\boldsymbol{r}\; Q_{\mathrm{source}}(\boldsymbol{r},E,\Omega,t) && \text{(source)}
\end{aligned}
$$

Number of target atoms per unit volume



- **Integro-differential equation** (!)
- Analytical/closed solutions only for simplified scenarios (infinite medium, one/few interaction mechanisms, one/few particle species, etc.)

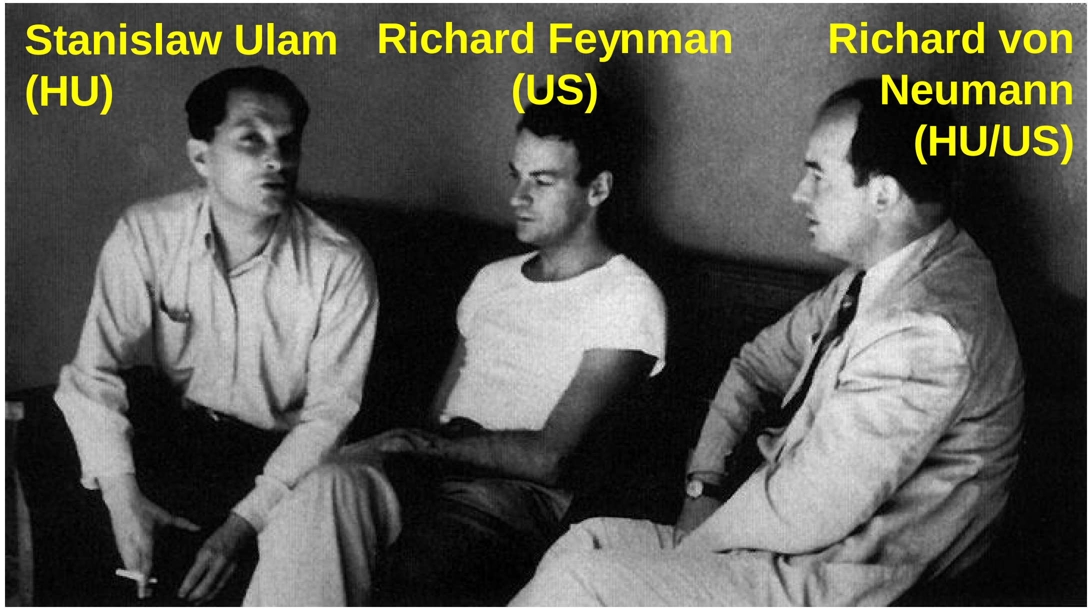
Buffon’s evaluation
of π using
random numbers
(dating back to the 1700s)

The Monte Carlo approach

Images source: Wikipedia

Monte Carlo (MC) method for radiation transport – The early days (1930s and 1940s)

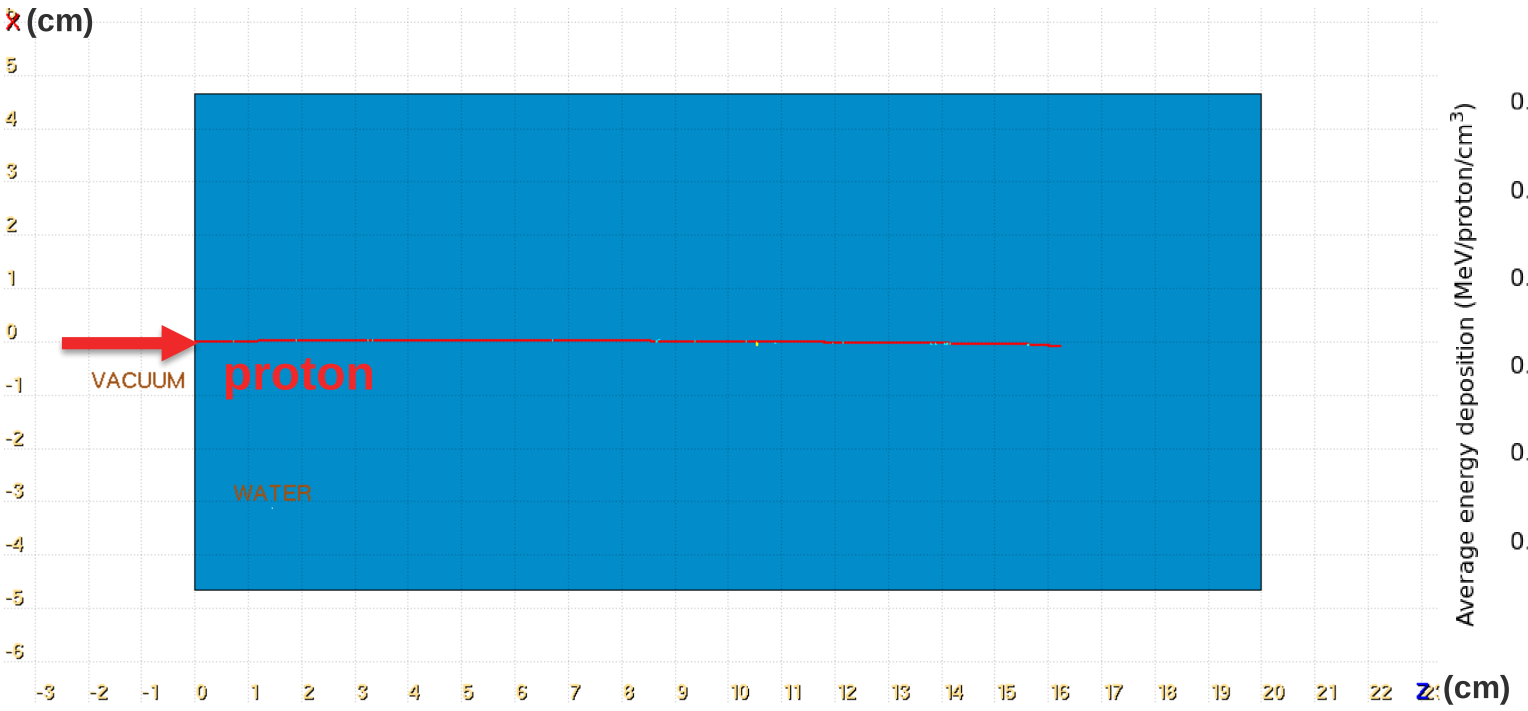
- Early ideas by Fermi took off during the Manhattan project effort:
  - Nicholas Metropolis
  - Stanislav Ulam
  - Richard von Neumann
  - Richard Feynman
  - ….

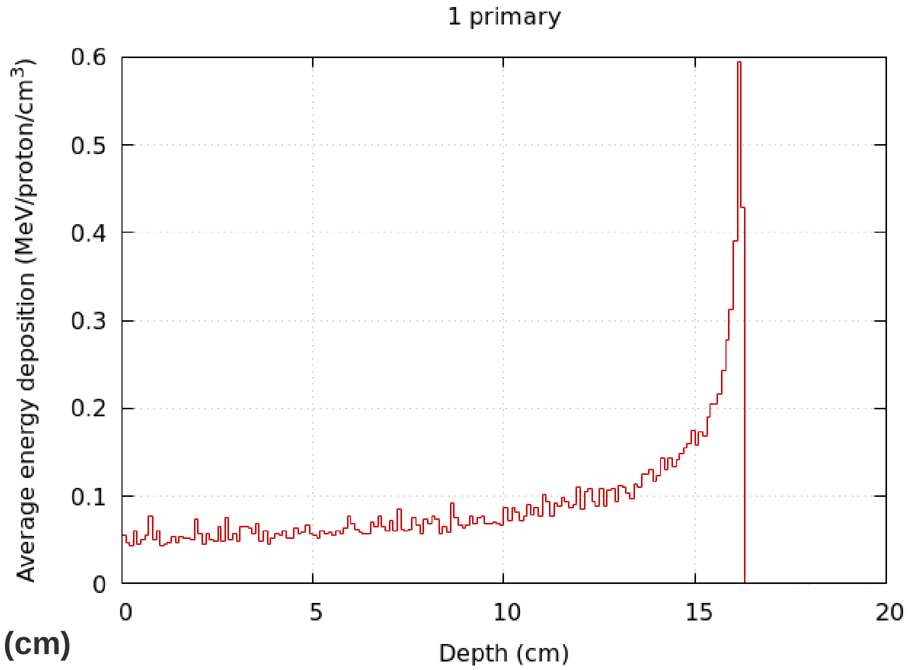


- Parallel to the development of the ENIAC
- *Ref: N. Metropolis "The beginning of the Monte Carlo method" (1987)*
  https://library.lanl.gov/cgi-bin/getfile?00326866.pdf
  See also: https://ieeexplore.ieee.org/document/6880250

Monte Carlo (MC) approach to radiation transport problems

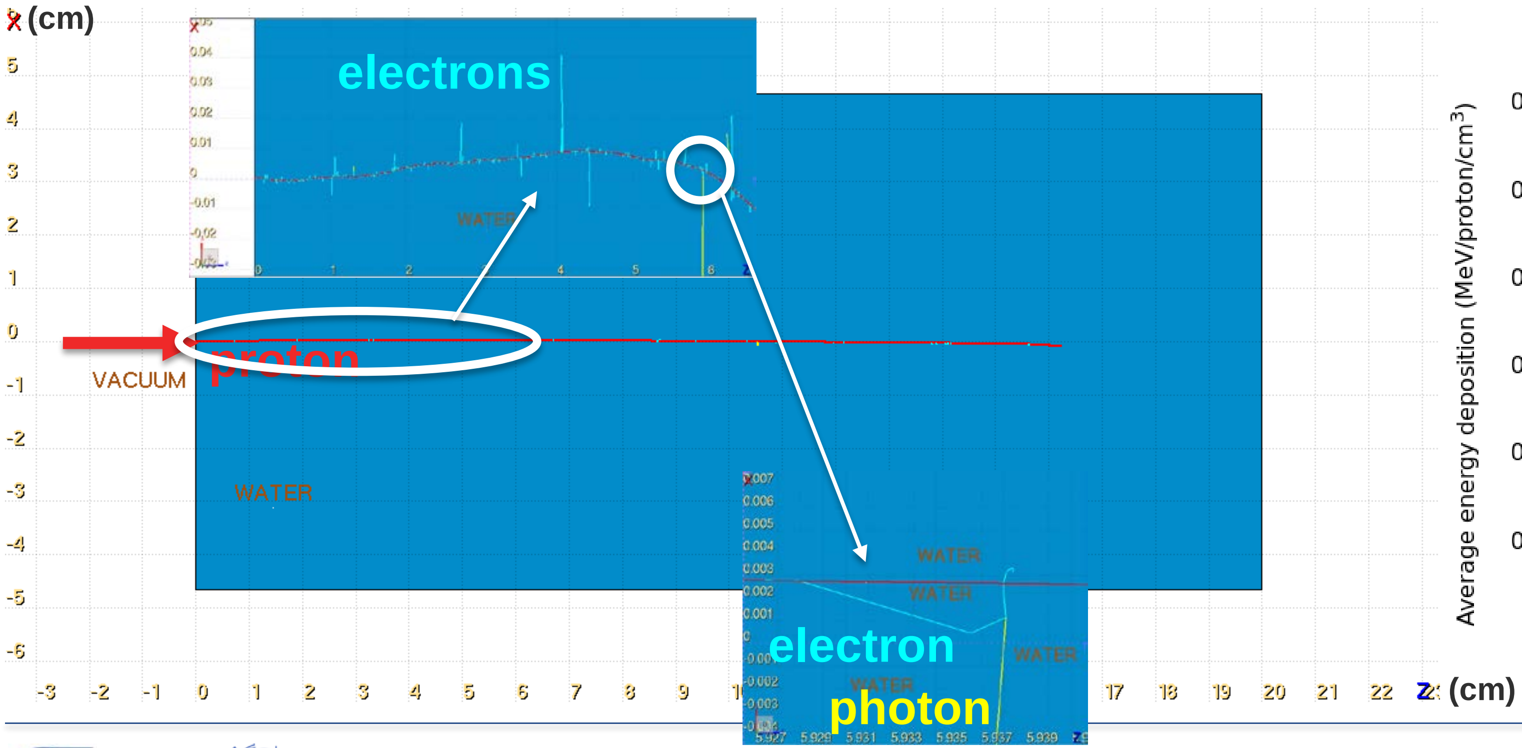
- **Numerically simulate** a large number of **random particle showers** with given interaction mechanisms
- Accumulate contributions of particle tracks to ***statistical estimator*** of observable
- Example: 150 MeV protons in water, *energy deposition histogram*

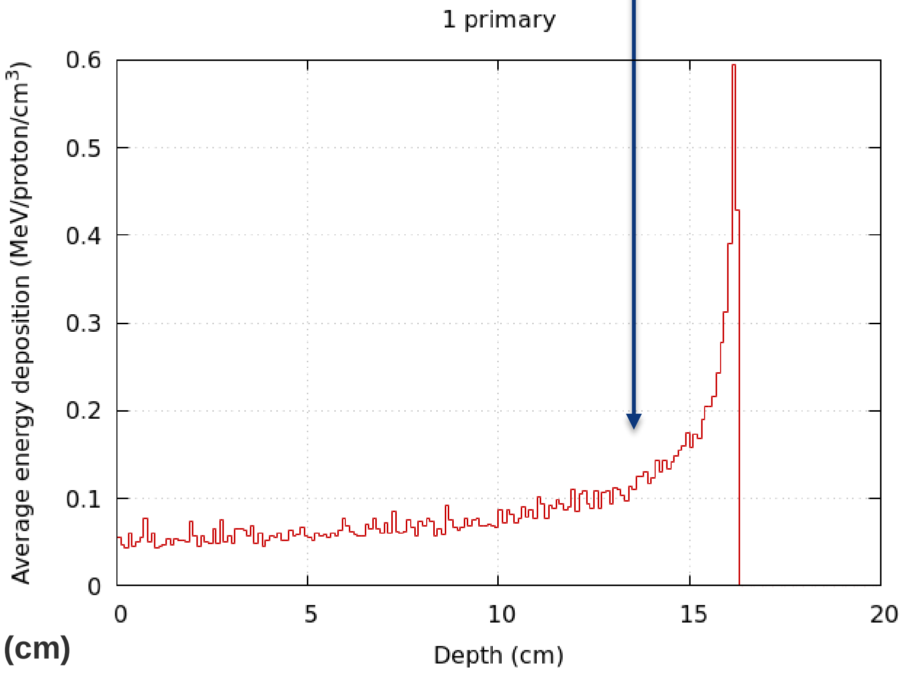




N=1 primary 150-MeV proton in H_2O

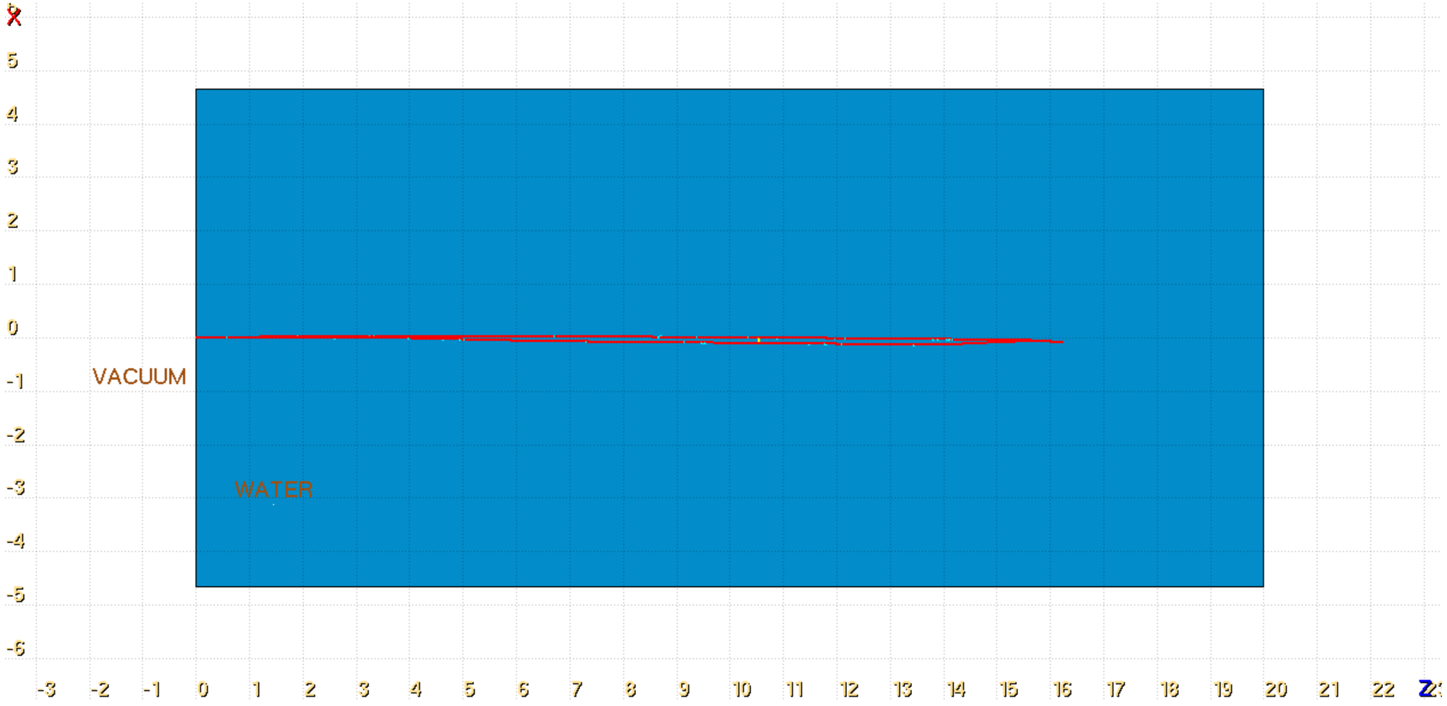
- Protons undergo frequent collisions with target e^-, leading to energy transfer and deposition throughout the depth of the target
- Energy deposition recorded in histogram
- Energetic e^- may radiate so-called Bremsstrahlung photons

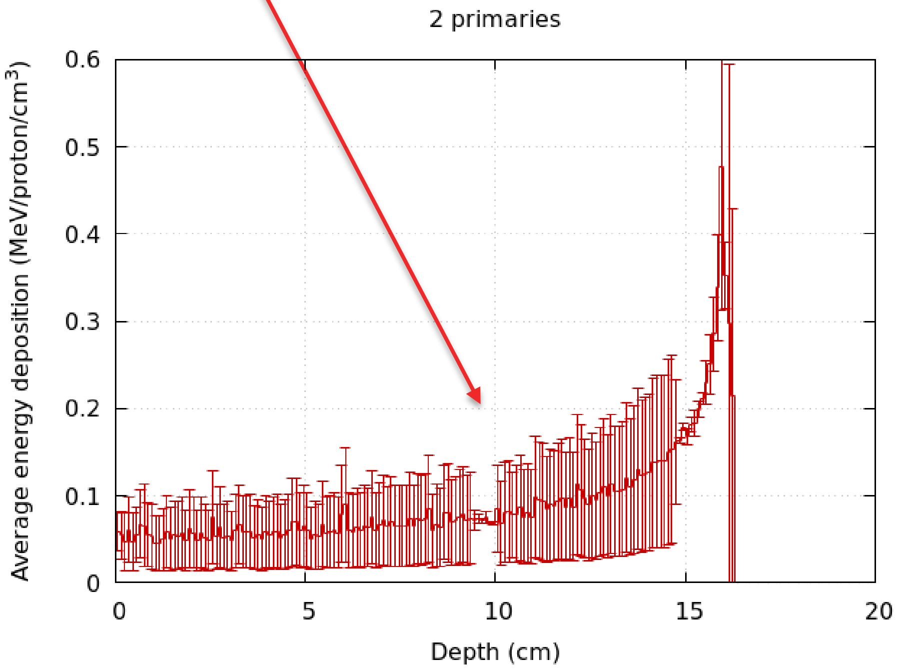




N=2 primary 150-MeV protons in H_2O

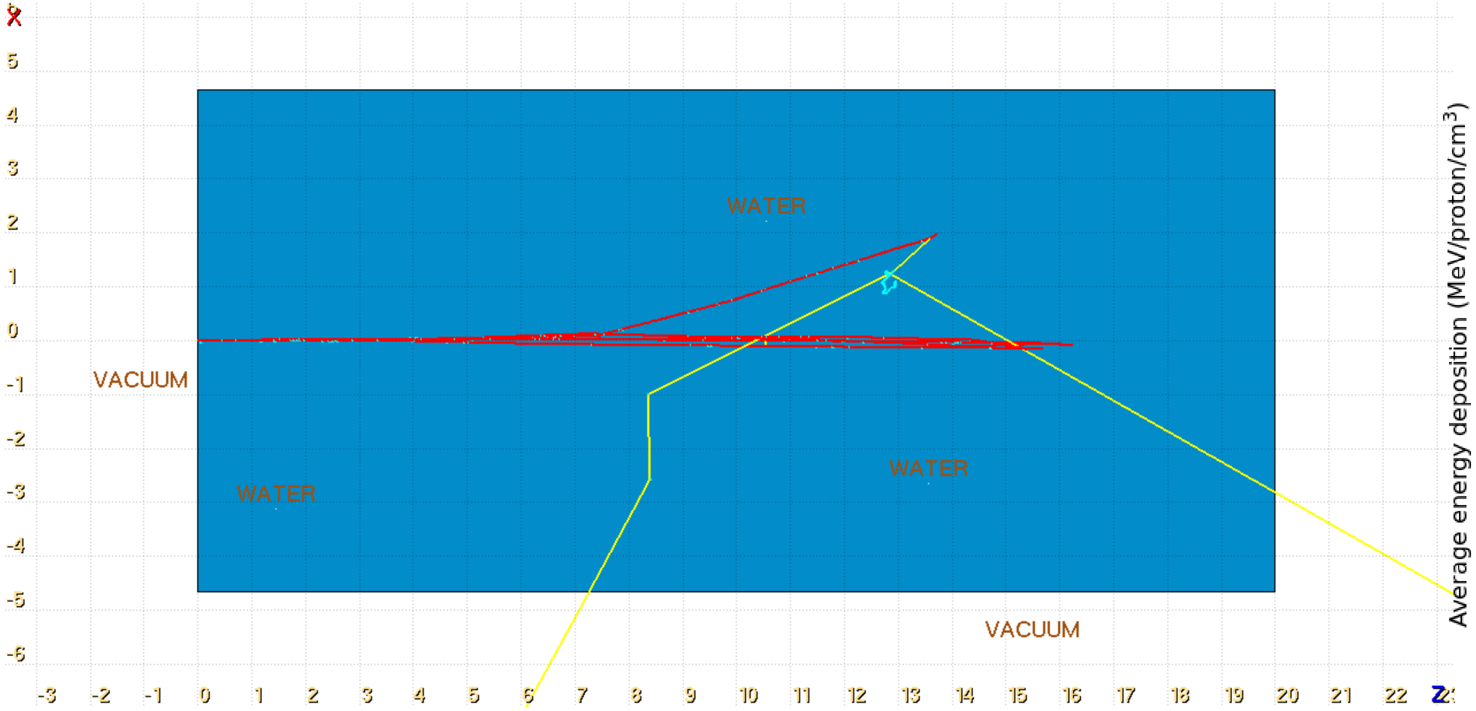
- MC simulation results are affected by **statistical uncertainty**:
- All MC results are accompanied by an error bar

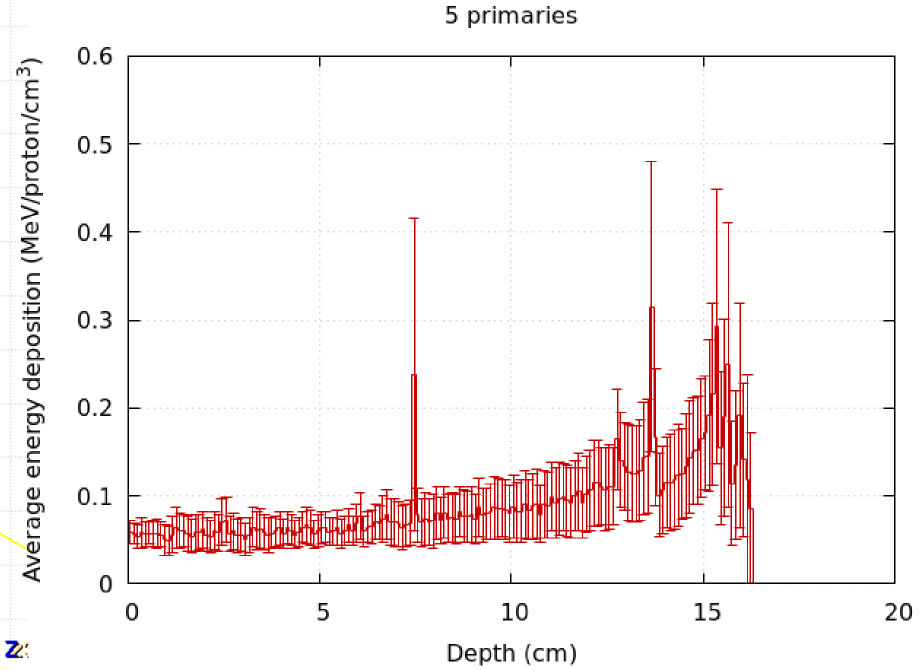




N=5 primary 150-MeV protons in H_2O

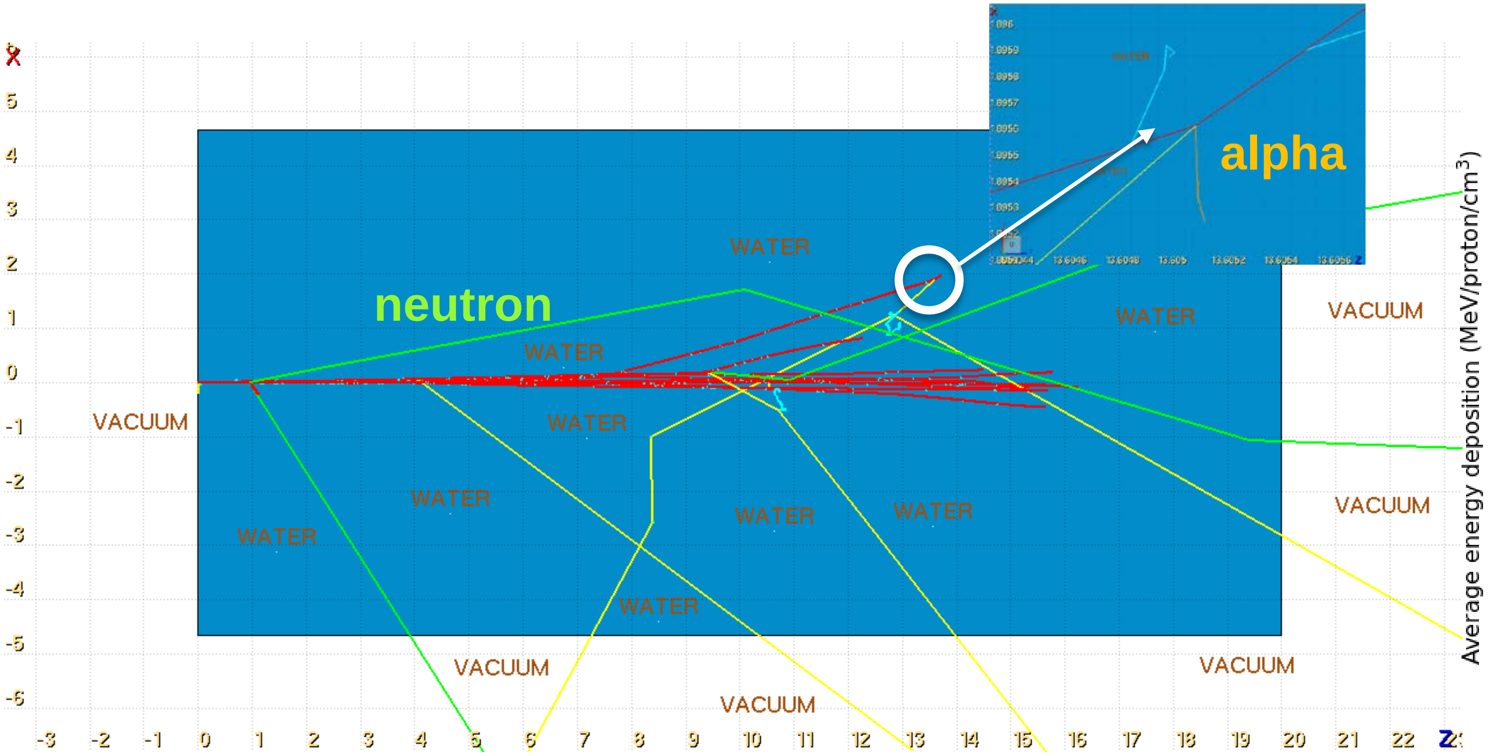
- Statistical uncertainty decreases with N
- Still considerable (~80%)

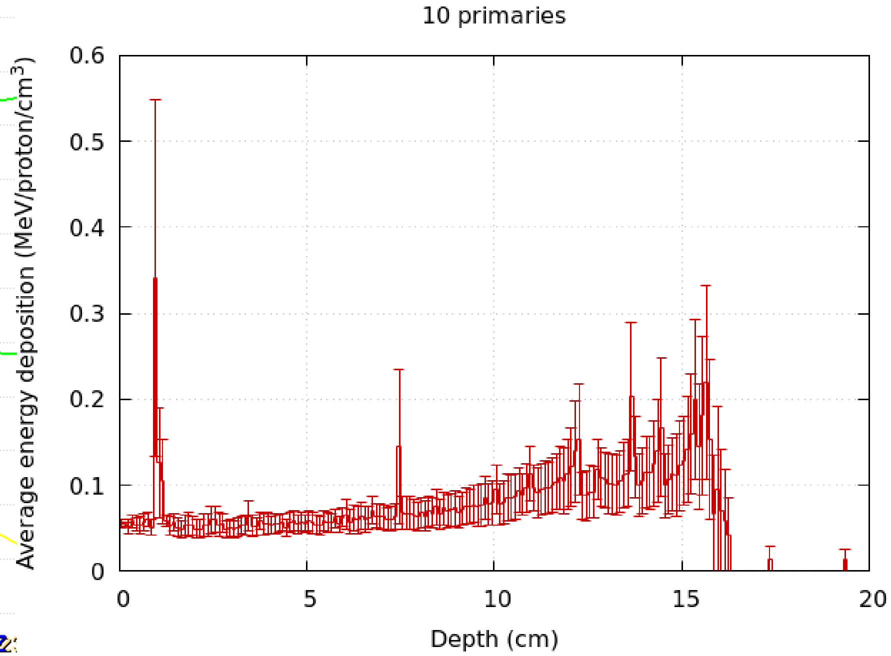




N=10 primary 150-MeV protons in H_2O

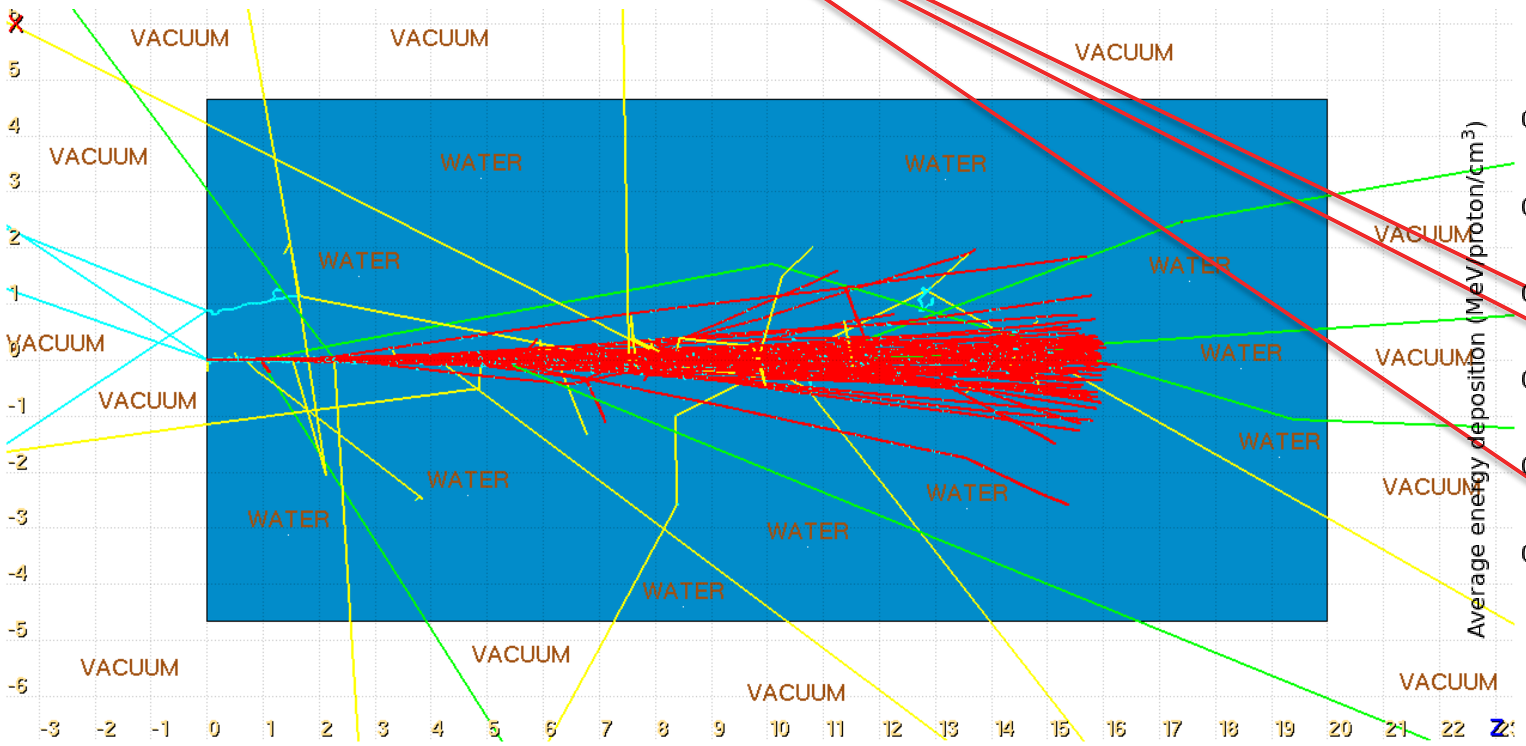
- Occasionally, p undergo nuclear inelastic interactions, producing γ,n,p,d,t,^{3}He,α,…, + (possibly unstable) residual nucleus

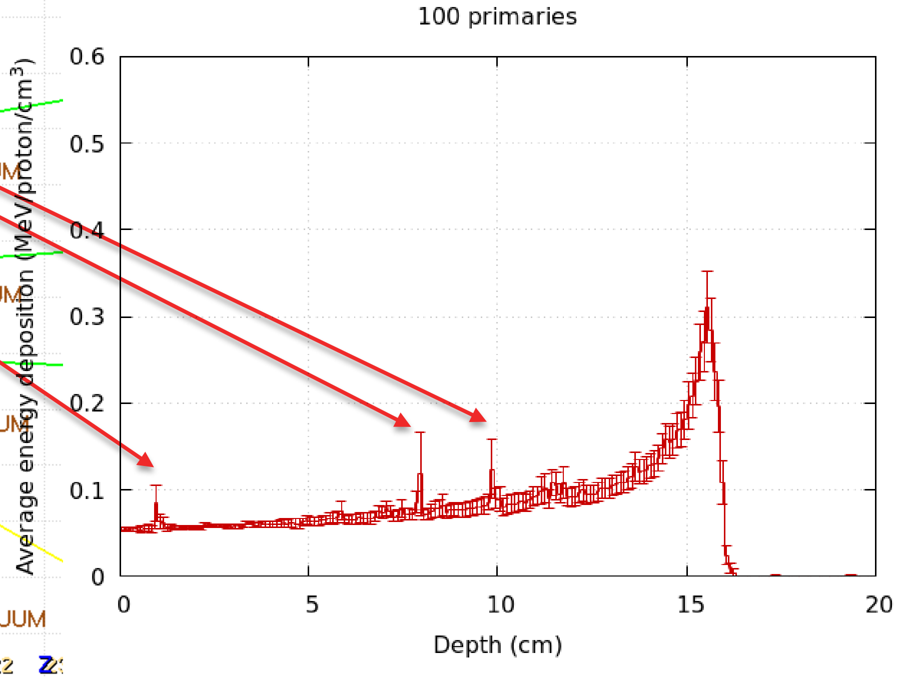




N=100 primary 150-MeV protons in H_20

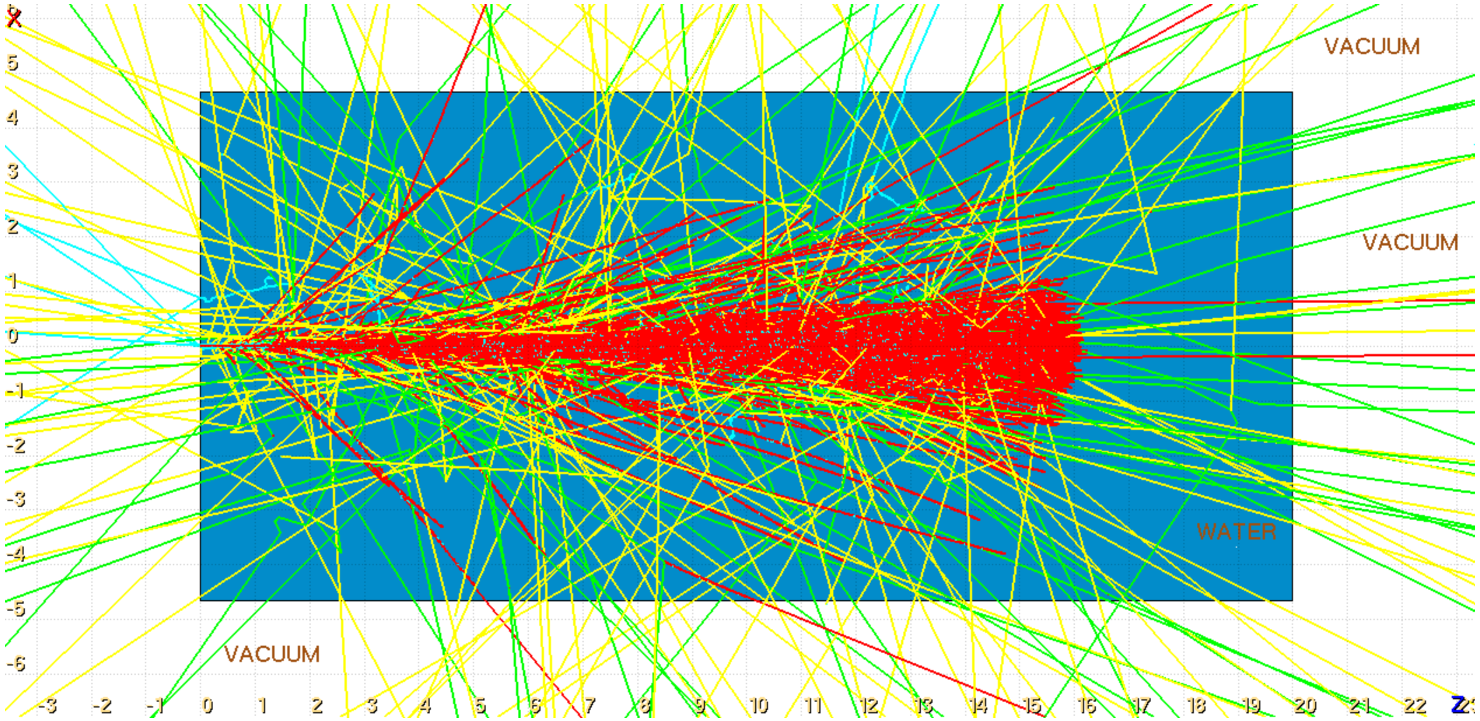
- Statistical uncertainty is gradually decreasing (~20-25%), but there are still fluctuations

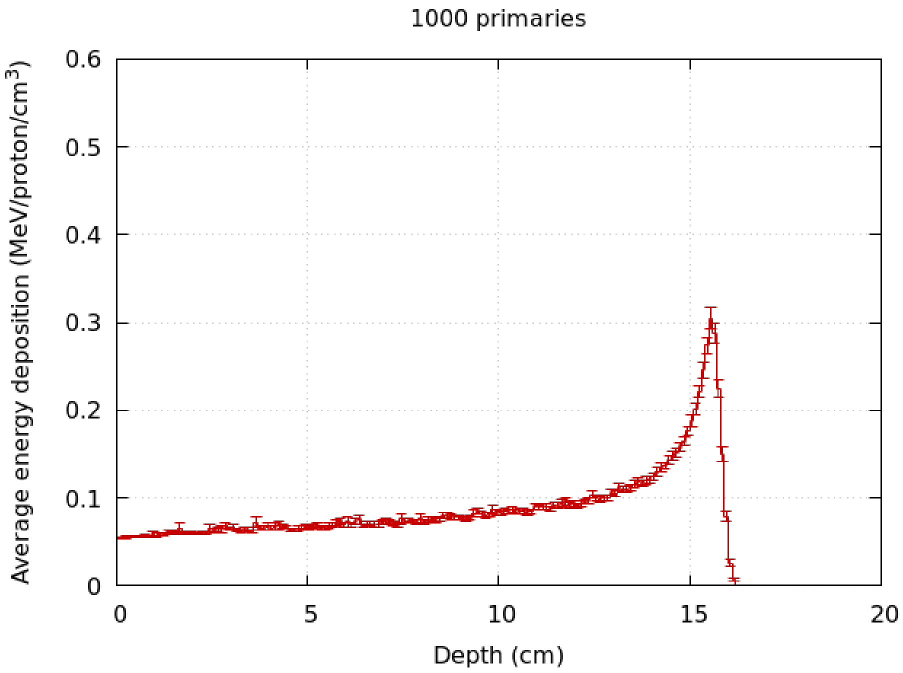




N=1000 primary 150-MeV protons in H_20

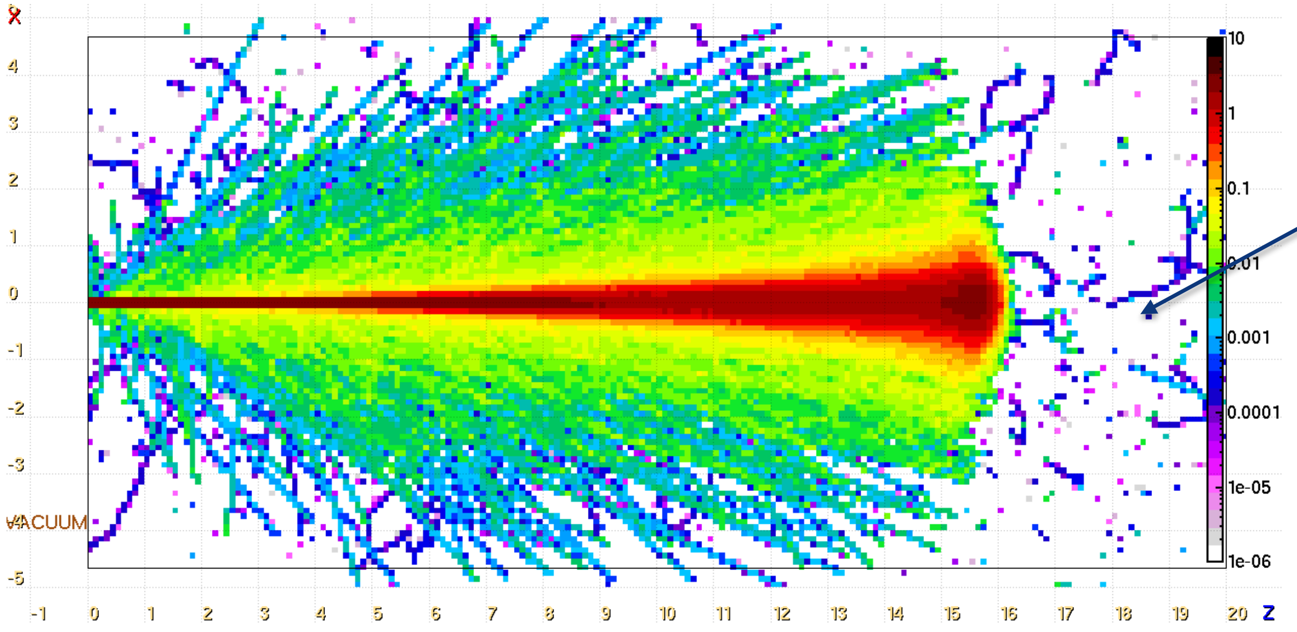
- Convergence is typically approached when statistical uncertainty is below ~10%

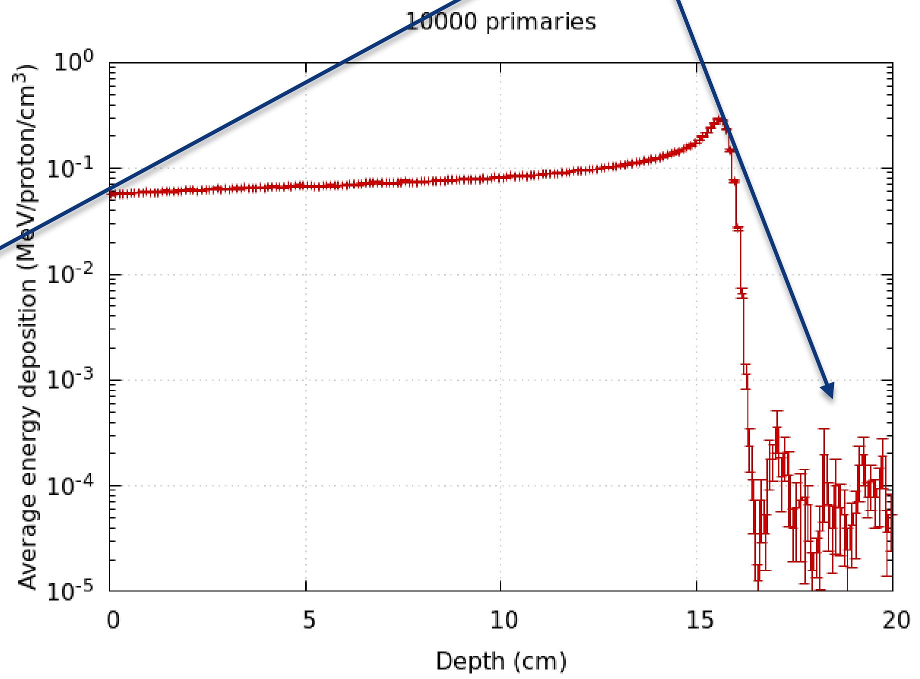




N=10000 primary 150-MeV protons in H_20

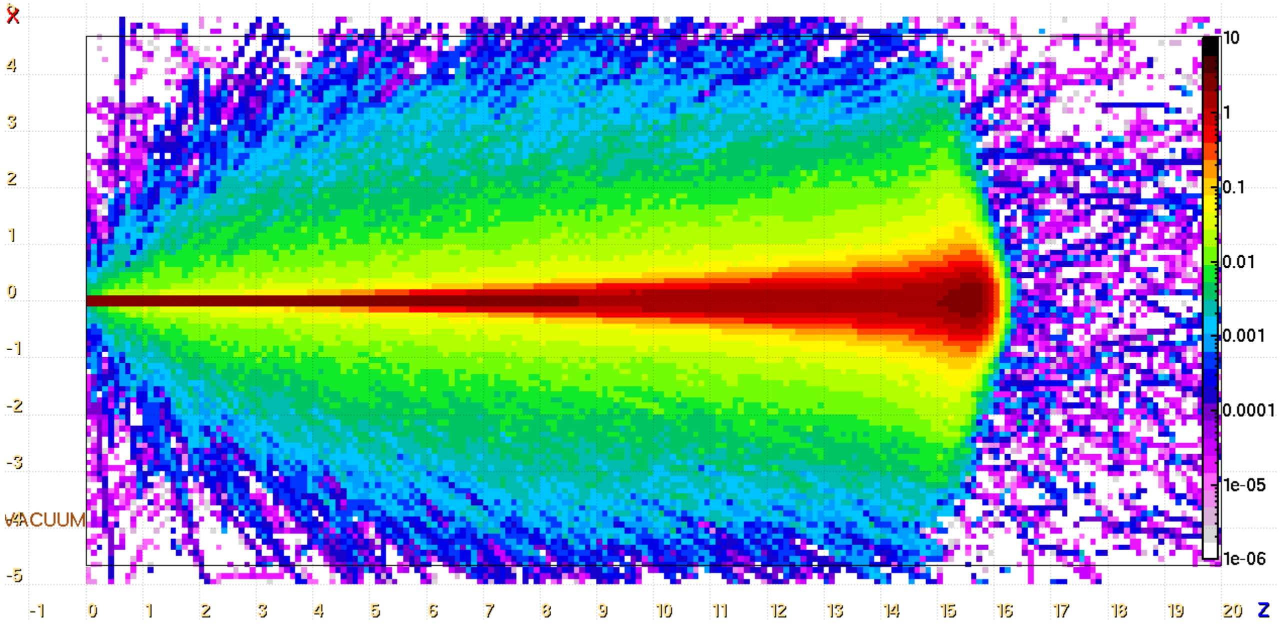
- One does not look at tracks, but rather 2D/1D distributions
- Switching now to log scale to see details
- Neutrons and photons contribute to tails of distribution

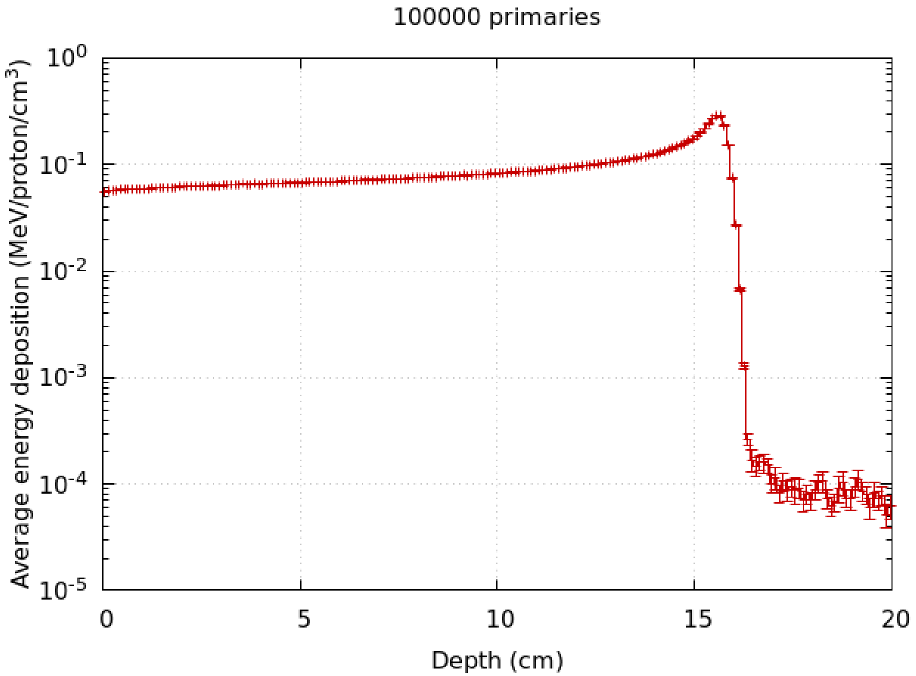




N=100000 primary 150-MeV p in H_20

- Convergence of suppressed features requires further primaries
- There exists a series of tricks to address slow convergence (biasing / variance reduction techniques)
  See: https://www.frontiersin.org/articles/10.3389/fphy.2021.718873/full



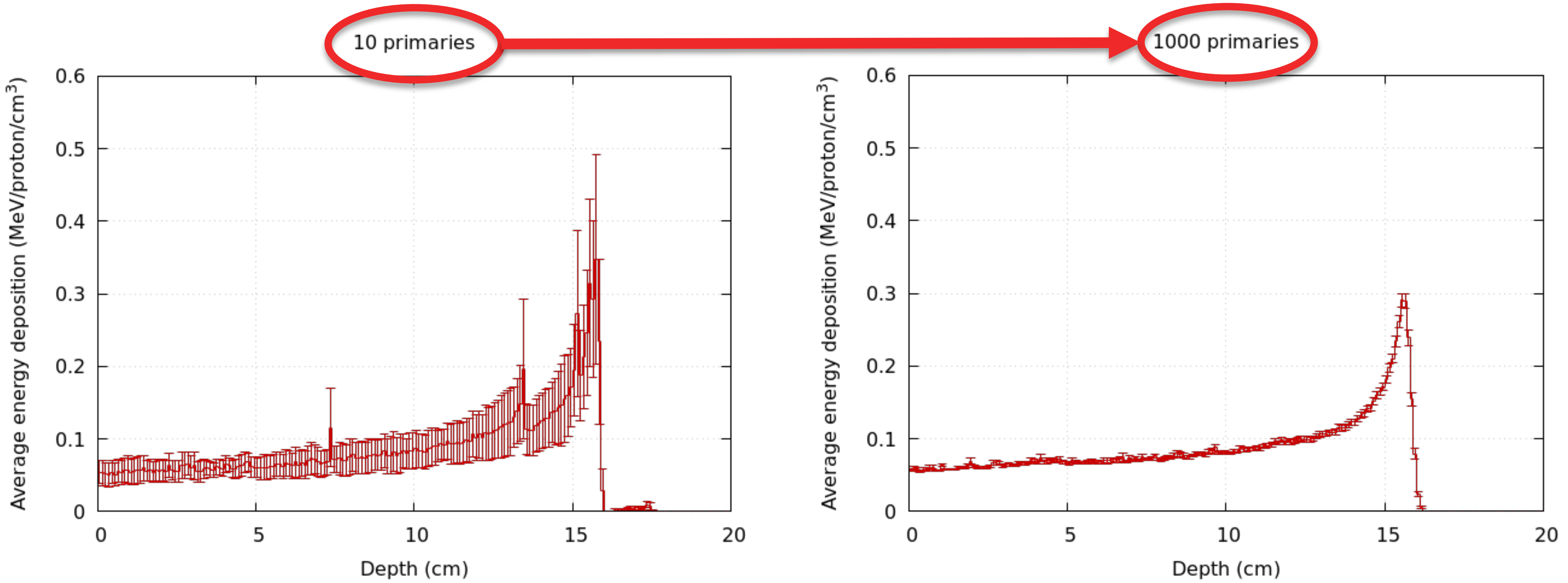


Statistical uncertainty

- Statistical uncertainty in a MC simulation σ drops like

$$\boldsymbol{\sigma = \frac{1}{\sqrt{N}}}$$

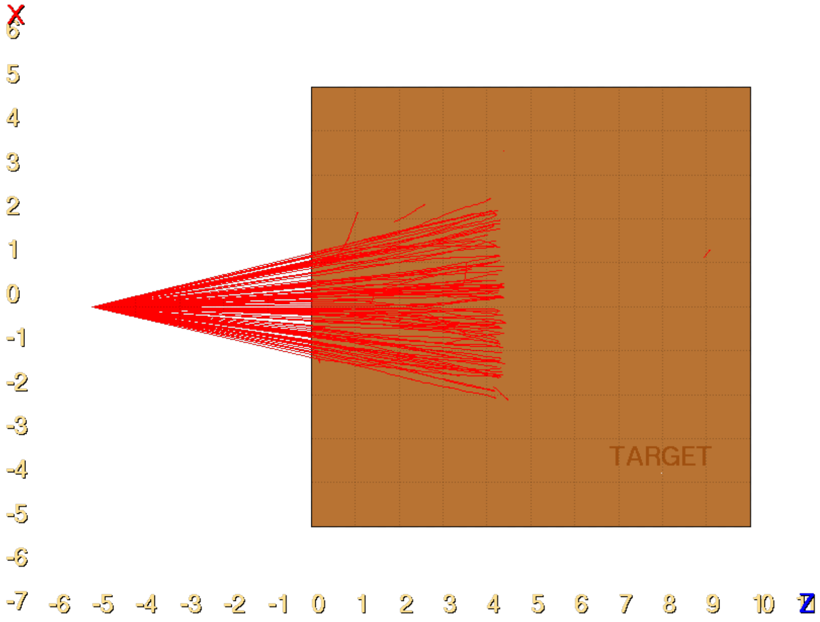
i.e. to lower error bars by a factor 10 one needs 100 times more primaries:



Basic ingredients for a MC code: 1 – Radiation sources

Radiation sources

- Particle beam:
  - Angular divergence
  - Energy spectrum…
- Radioactive isotopes
- Particle-particle collision



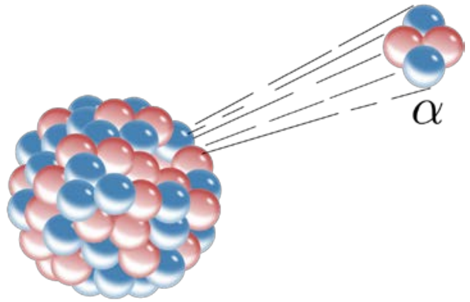
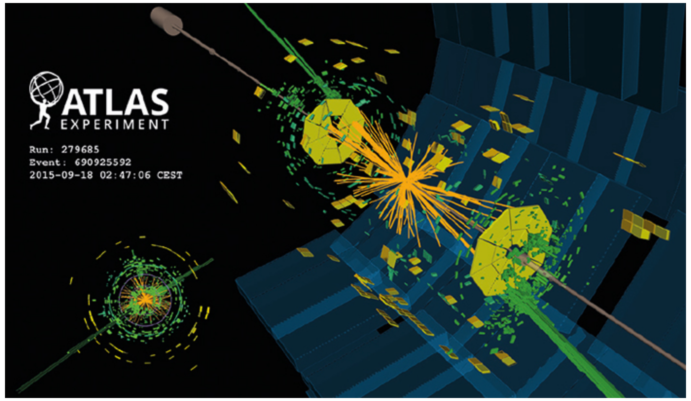
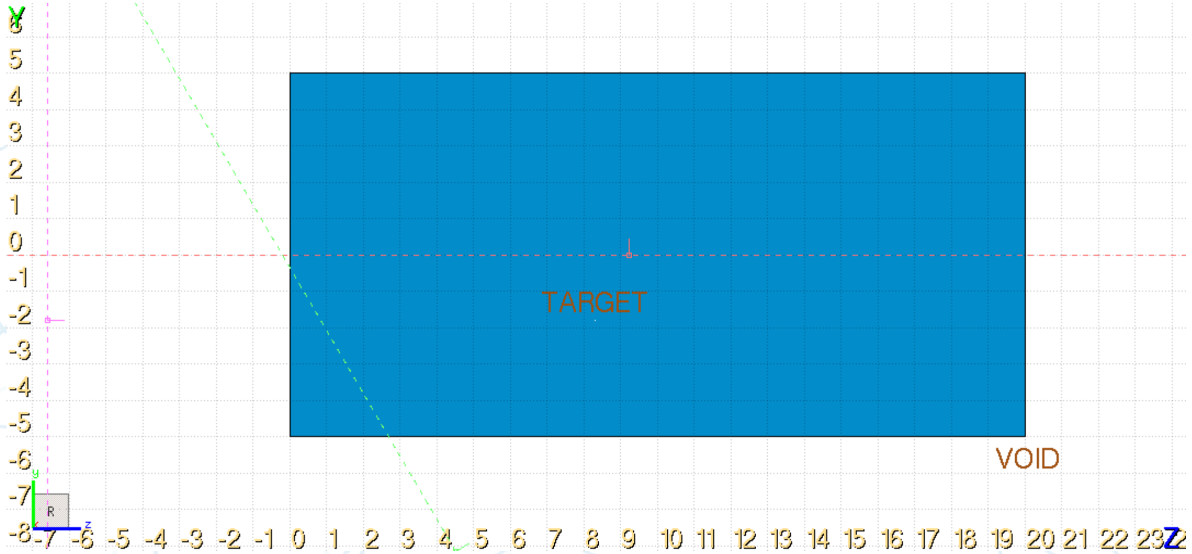
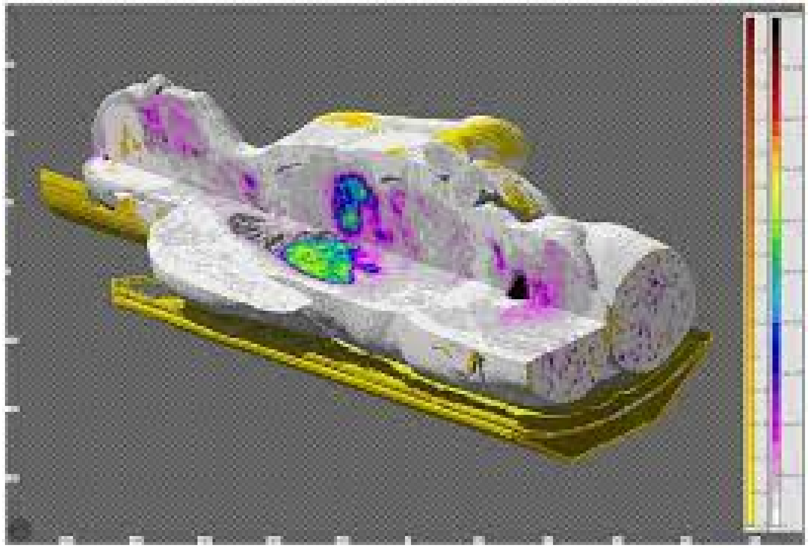
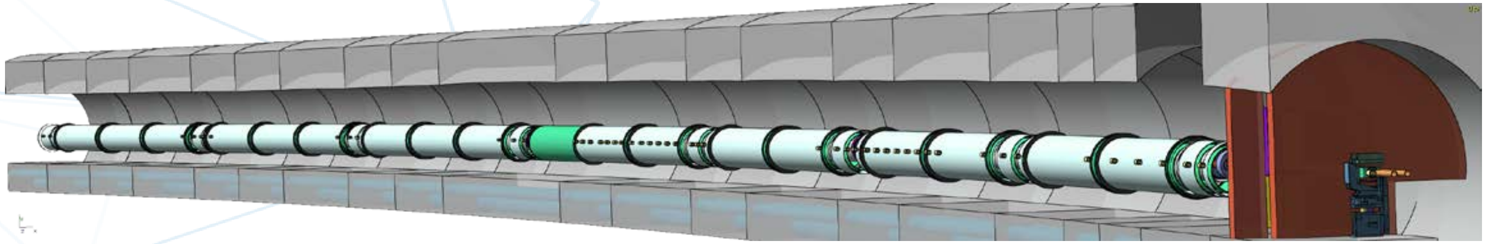


Image source: Wikipedia









Basic ingredients for a MC code: 2 - Geometry

Combinatorial geometry package

- Basic objects (bodies): spheres, cylinders, parallelepipeds, planes…
- Combined to form complex regions via Boolean operations:
  - Union
  - Intersection
  - Subtraction
- Ability to clone/replicate regions
- Build macroscopic geometry to the desired degree of accuracy using these basic objects and operations

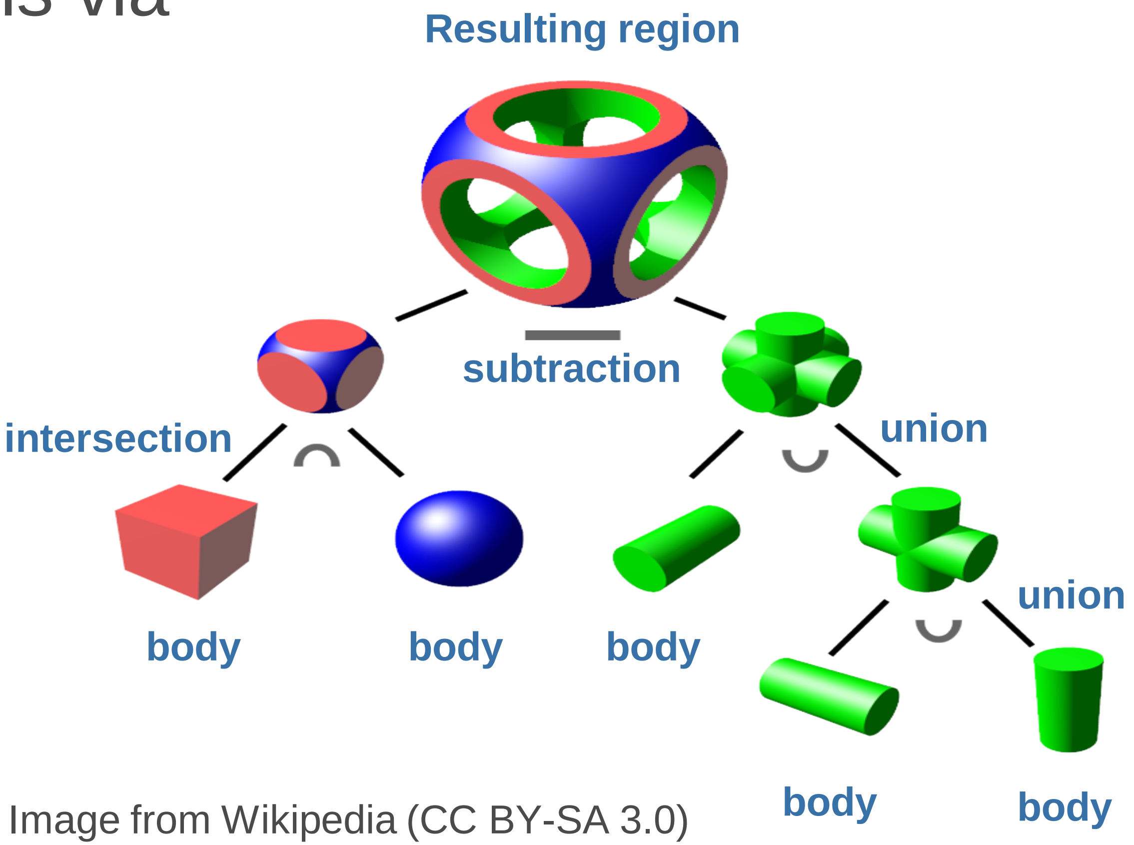
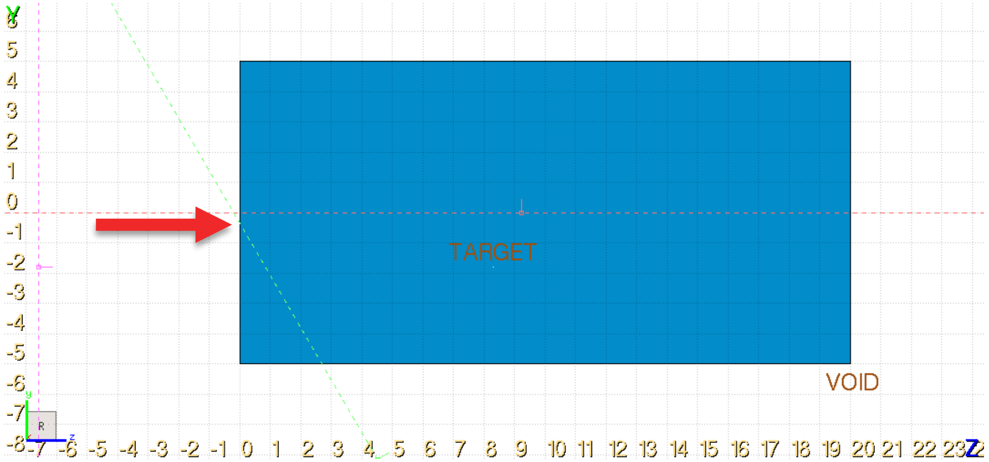


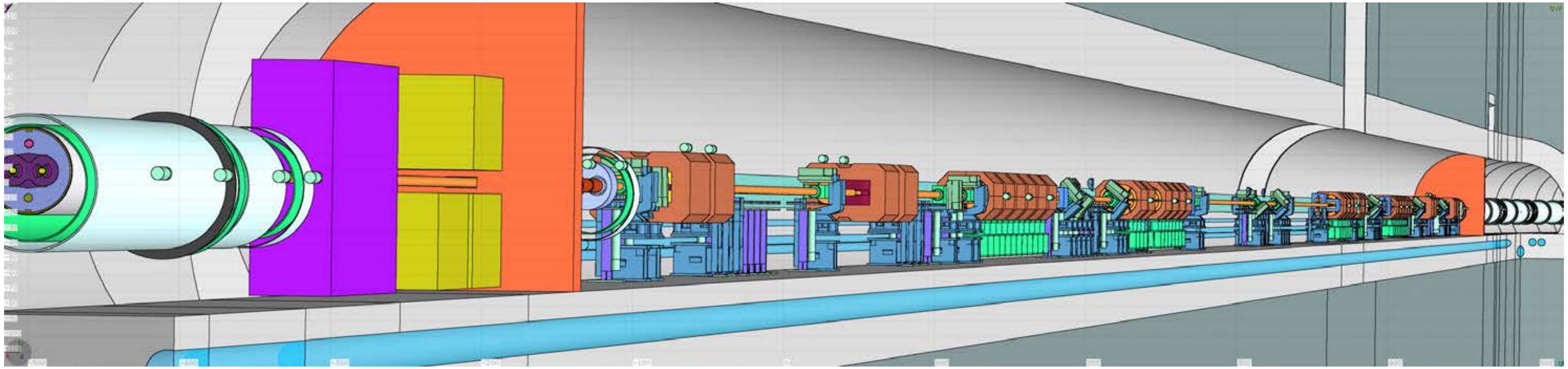
Image from Wikipedia (CC BY-SA 3.0)

Ability to construct geometries, from trivial to complex

Trivial example: a simple material slab

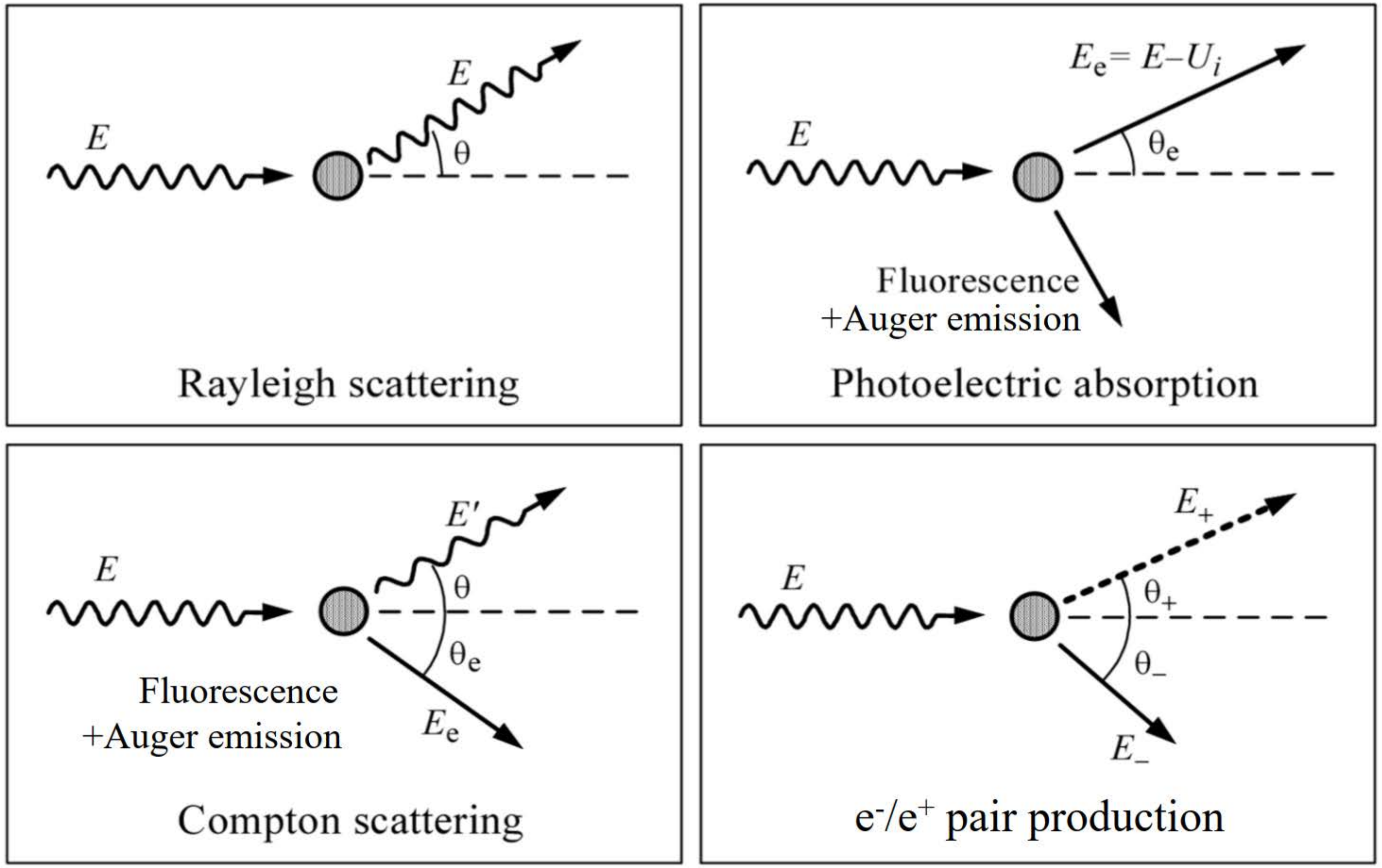


Complex example: LHC collimation insertion region (~100 m) built from the combination of **planes**, **cylinders**, **cuboids**, ...:



Basic ingredients for a MC code: 3 – Radiation-matter interactions

Basic interaction mechanisms of photons

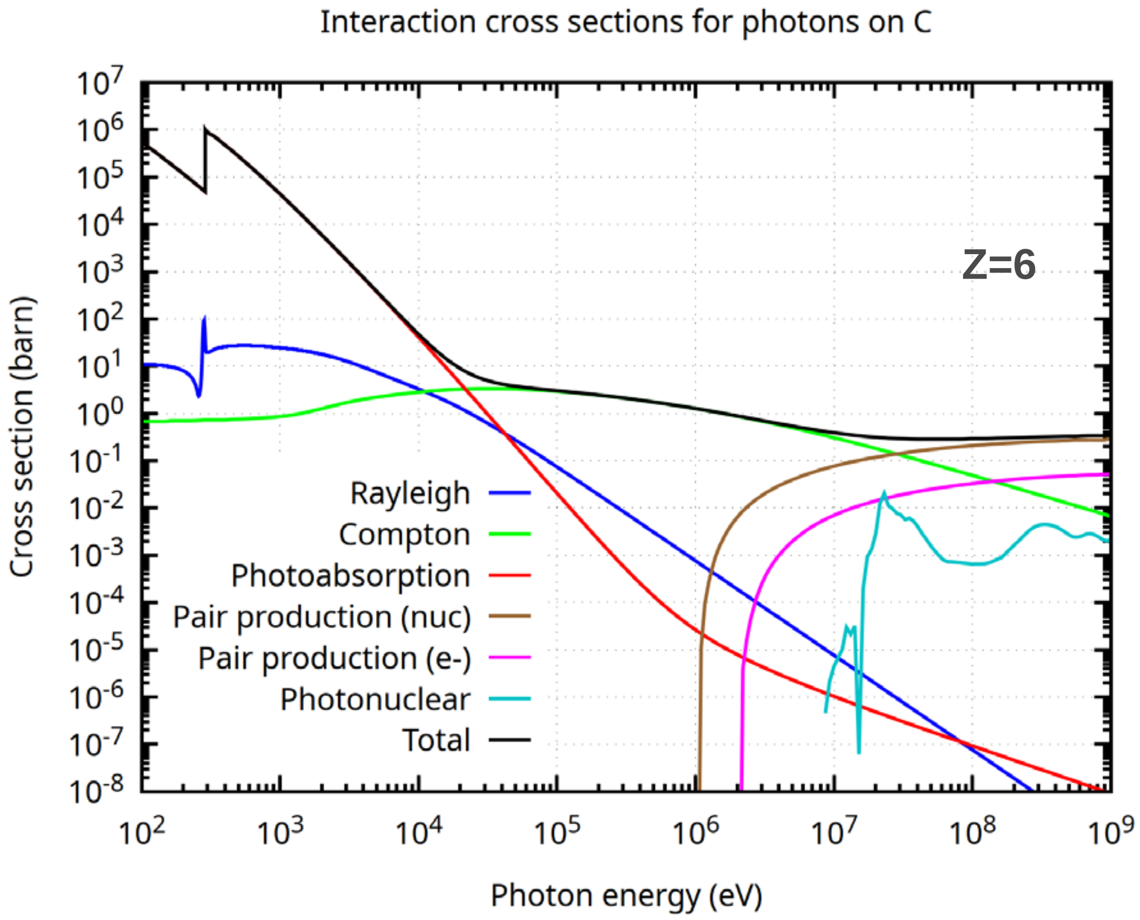


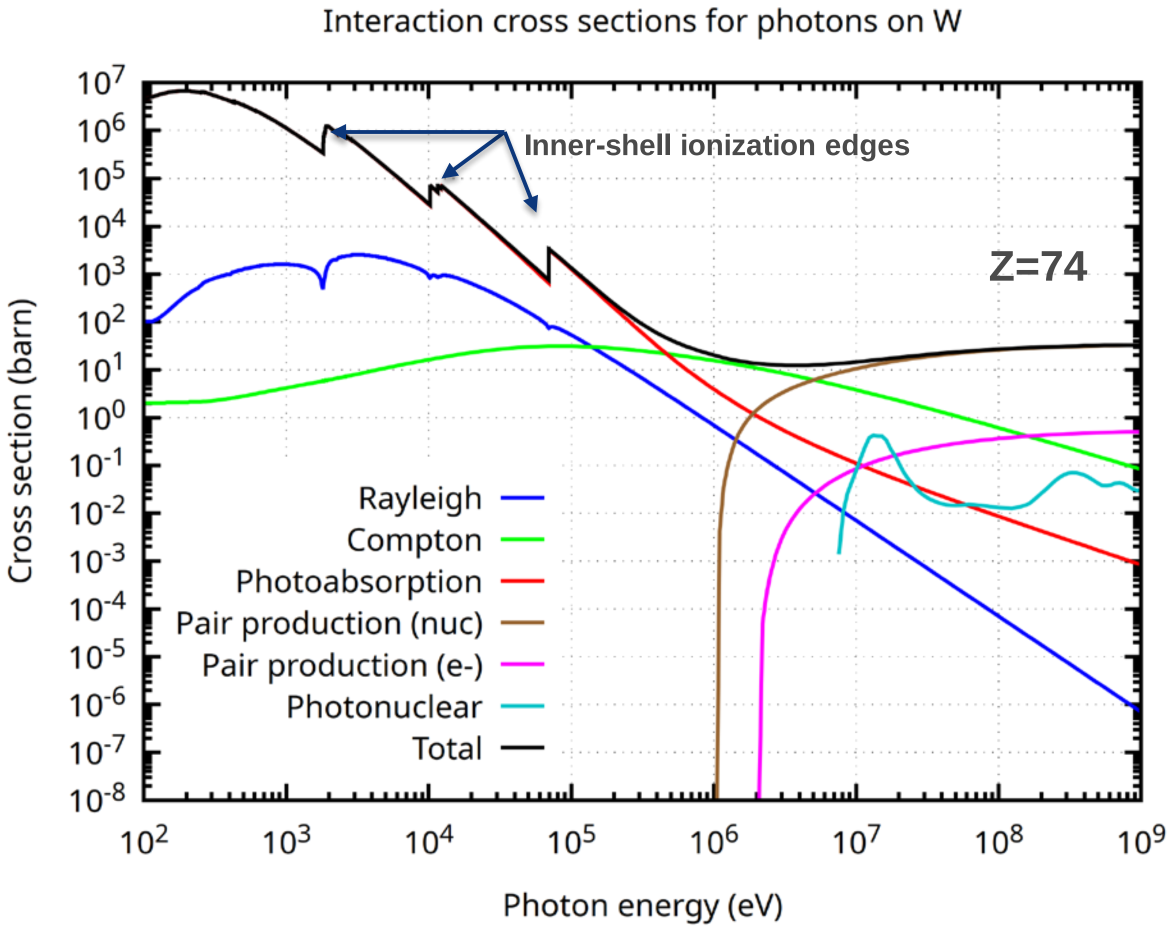
- Photonuclear reactions:
  - (γ,n), $(\gamma,2n)$,…
- $\mu^\pm$ pair production

- At least 2 particles in the final state (except for Rayleigh scattering)
- Rapid increase of particles in the shower

Image source: PENELOPE manual

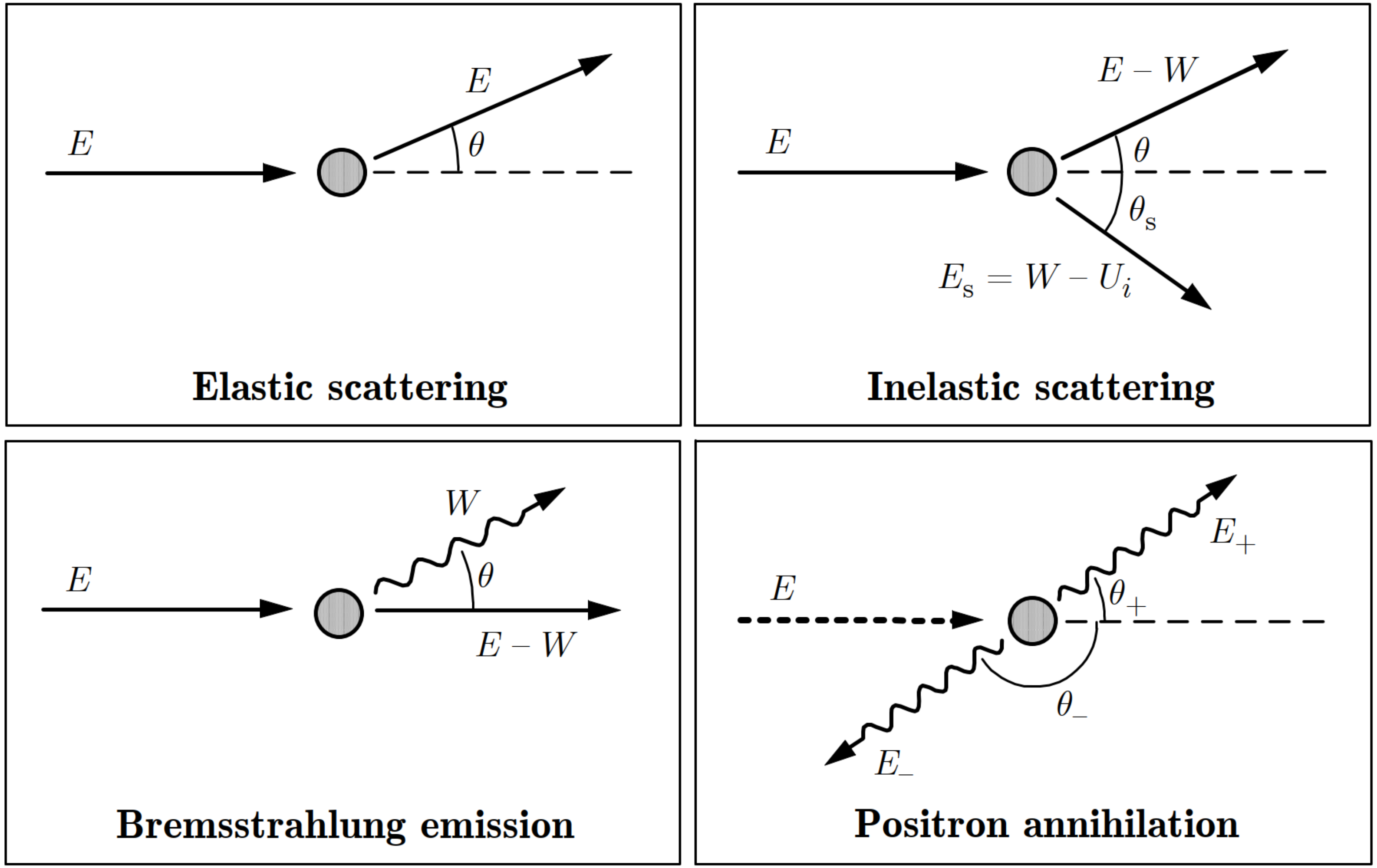
Photon cross sections





Basic interaction mechanisms of $e^{\pm}$

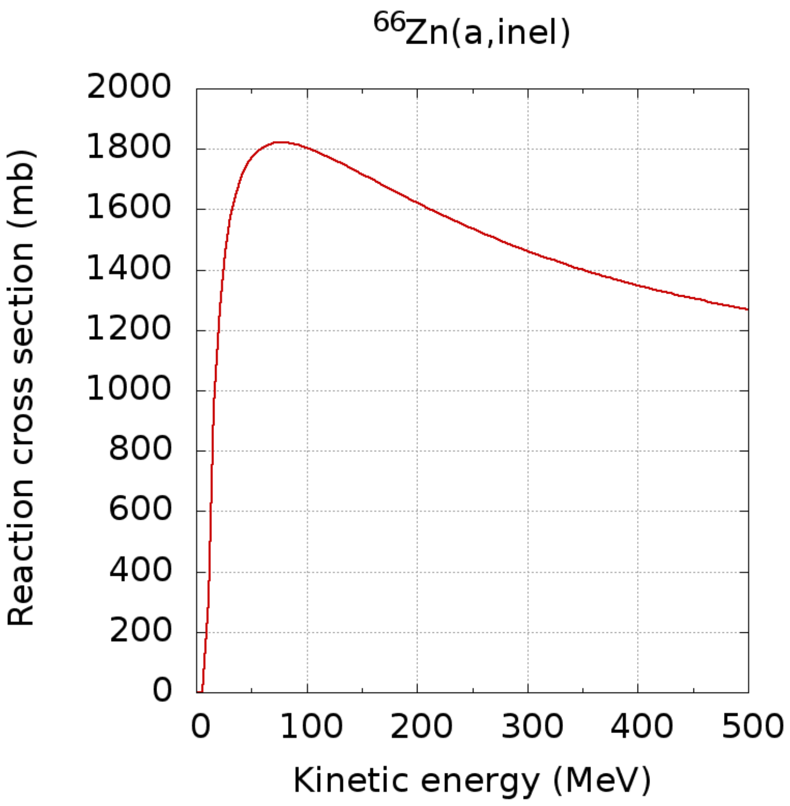
(Multiple scattering algorithms)



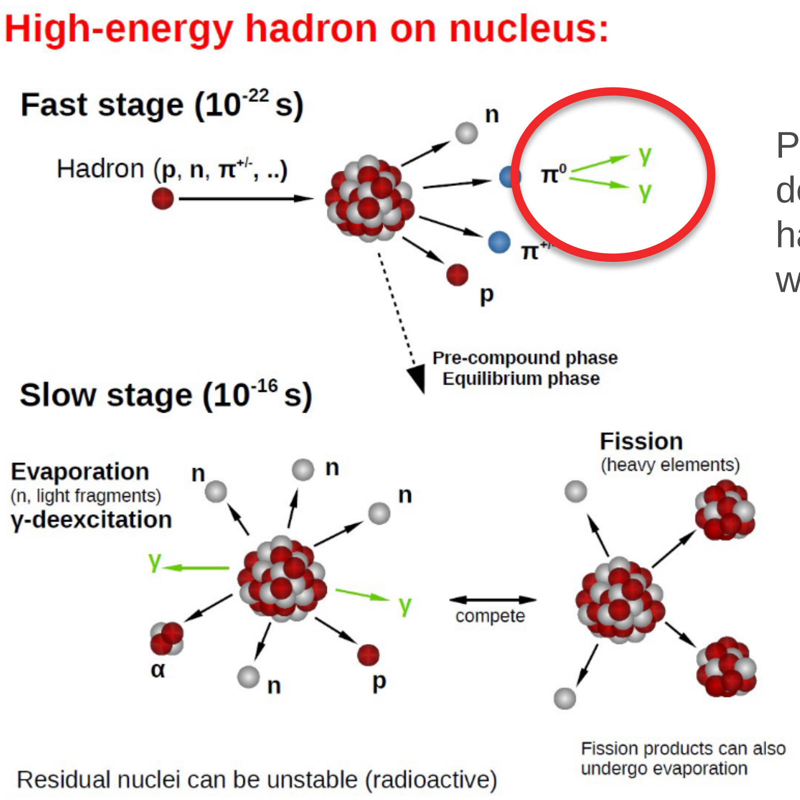
(Aggregate energy loss along particle step via stopping power. See backup slide)

Hadronic interactions

Reaction cross section (typically parametrized)



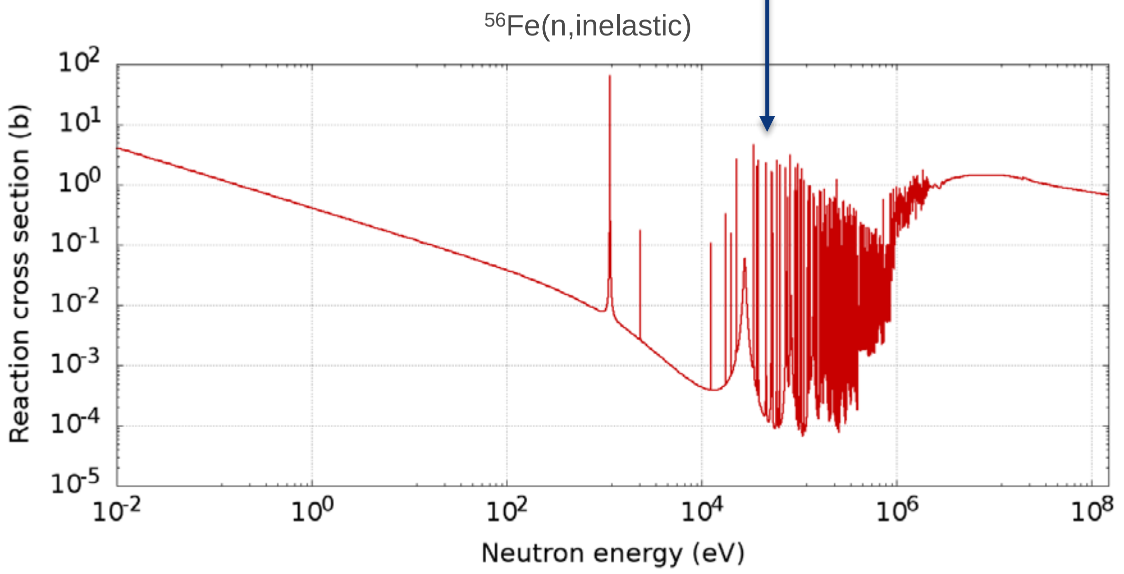
Interaction model



Photons from π^0 decay couple hadronic shower with EM shower

Low-energy neutron interactions

- Neutron energy degrades quickly (elastic scattering or lower energy n secondaries)
- Low energies: **neutron capture** has high cross section and leads to MeV photons + production of residual nuclei. Relevant for radiation protection and shielding aspects
- Neutron cross sections have **rich resonant structure:**



- No model available to effectively reproduce all resonant details

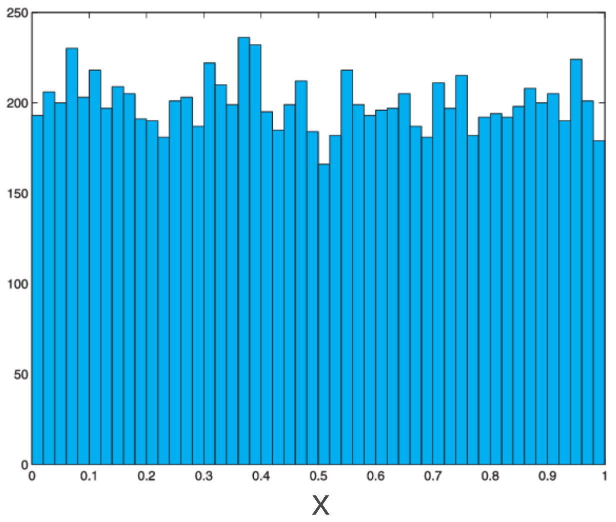
Low-energy neutron interactions - Approaches

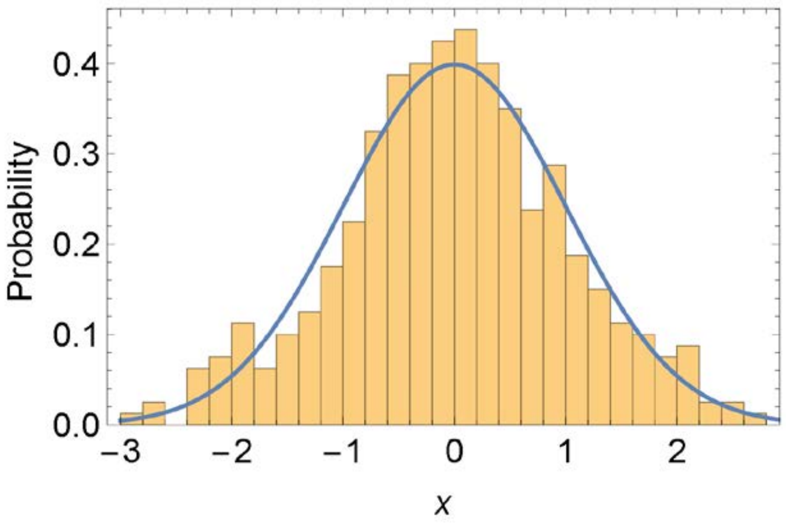
- Either relying on a coarse-grained version of neutron cross sections (***group-wise** neutron interactions*) or retaining as many details as possible (***point-wise** neutron interactions*).
- Both rely on evaluated nuclear data libraries, e.g.:
  - Joint Evaluated Fission and Fusion (JEFF) https://www.oecd-nea.org/jcms/pl_27365/the-jeff-nuclear-data-library
  - Evaluated Nuclear Data Files (ENDF) https://www-nds.iaea.org/exfor/endf.htm
  - Japanese Evaluated Nuclear Data Library (JENDL) https://wwwndc.jaea.go.jp/jendl/jendl.html
  - etc
- Covering: elastic scattering, capture, fission, and explicit inelastic channels e.g. (n,p), (n,a), etc.

Basic ingredients for a MC code:
4 – Random sampling

(Pseudo-)Random number generator (PRNG)

- Function returning homogeneously sampled values from 0 to 1
- **Sampling techniques**: exploit PRNG values to sample from arbitrary distributions (e.g. angular distribution of secondaries)





https://www.researchgate.net/publication/230860021_An_introduction_to_the_numerical_analysis_of_the_Boltzmann_equation

https://www.researchgate.net/publication/360098338_Optimisation_of_Thimble_Simulations_and_Quantum_Dynamics_of_Multiple_Fields_in_Real_Time

Basic flow diagram of a Monte Carlo simulation of radiation transport

Mean free path

- Cross section (slide 6):

Cross section

$$\sigma \equiv \int\int \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}W}\,\mathrm{d}\Omega\,\mathrm{d}W$$

~likelihood of being scattered

Dimensions: Area
Typical unit: 1 barn (=10^{-24} cm^2)

- Consider a medium with $\mathcal{N}$ atoms per unit volume
- The mean free path

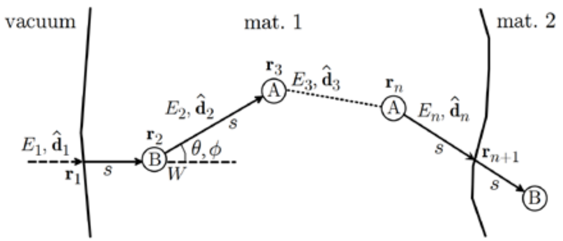
$$\lambda = \frac{1}{\mathcal{N}\sigma}$$

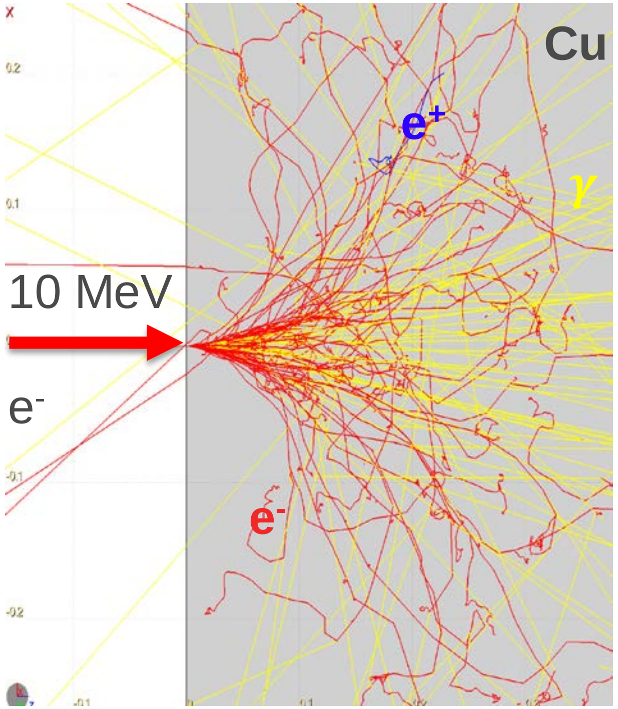
is a quantity with units of length that gives the average distance to the next interaction

- One can see (backup slides) that it follows an exponential distribution

Simplified flowchart of a MC simulation of particle transport

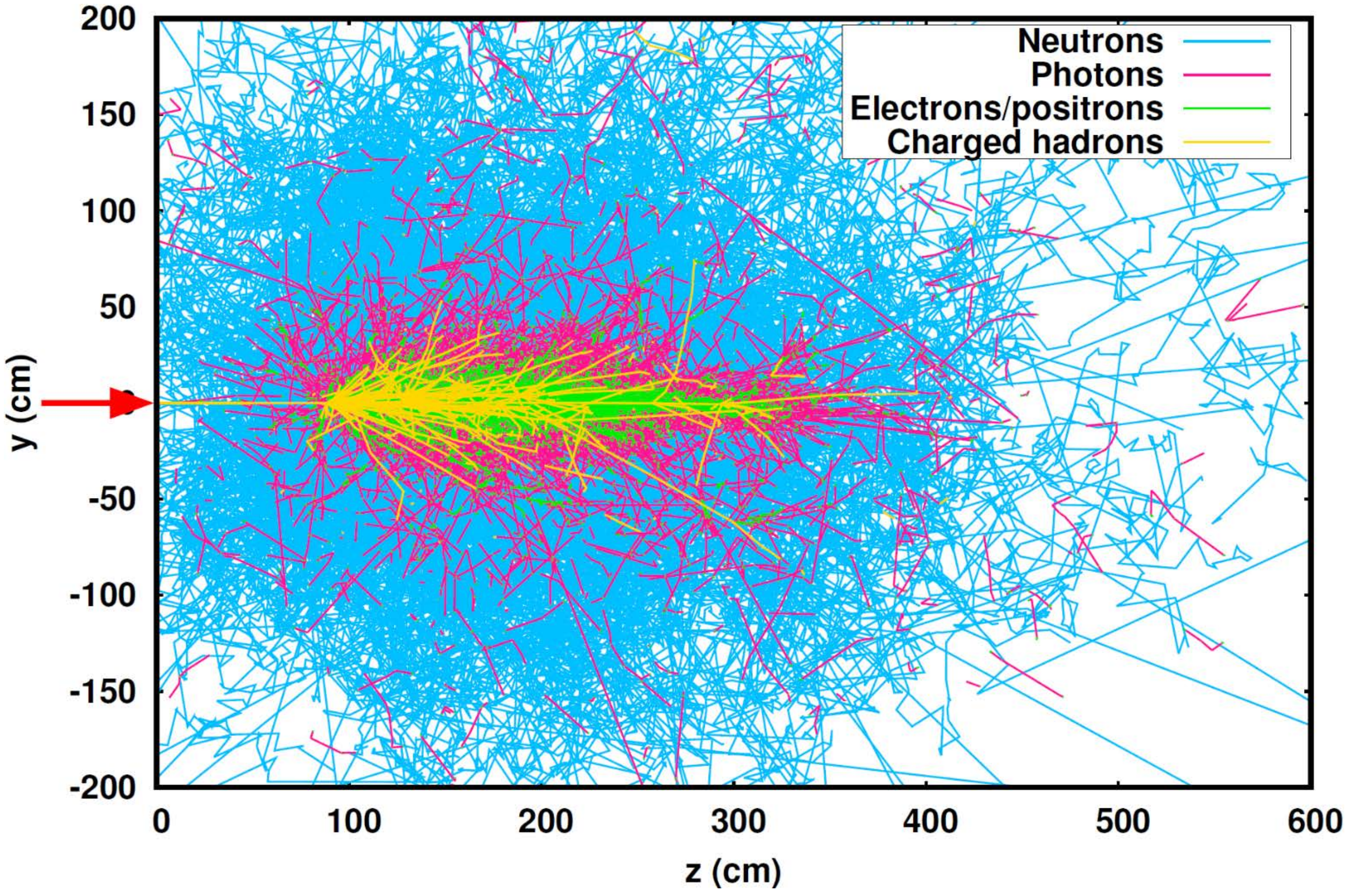
- Define radiation source and material geometry
- Do for a sufficiently large number N of primary particles:
  1. New primary event: add 1 (or more!) particles to stack
  2. Pick up particle from stack, advance to next material medium (score contribution of this step to observables)
  3. Evaluate mean free path $\lambda(E)$
  4. Sample random step length to next interaction
  5. Accumulate contribution of step to statistical estimators
  6. Decide kind of interaction that takes place
  7. Sample final state (add possible secondaries to particle stack)
  8. Accumulate contribution of interaction to statistical estimators
  9. If primary particle survives, update energy/direction, go to 3. Otherwise, go to 2 (or go to 1 if no more particles in stack).





MC simulation of hadronic and electromagnetic radiation showers

- Coupled hadronic and electromagnetic shower set up by a **single** 450 GeV proton in Al



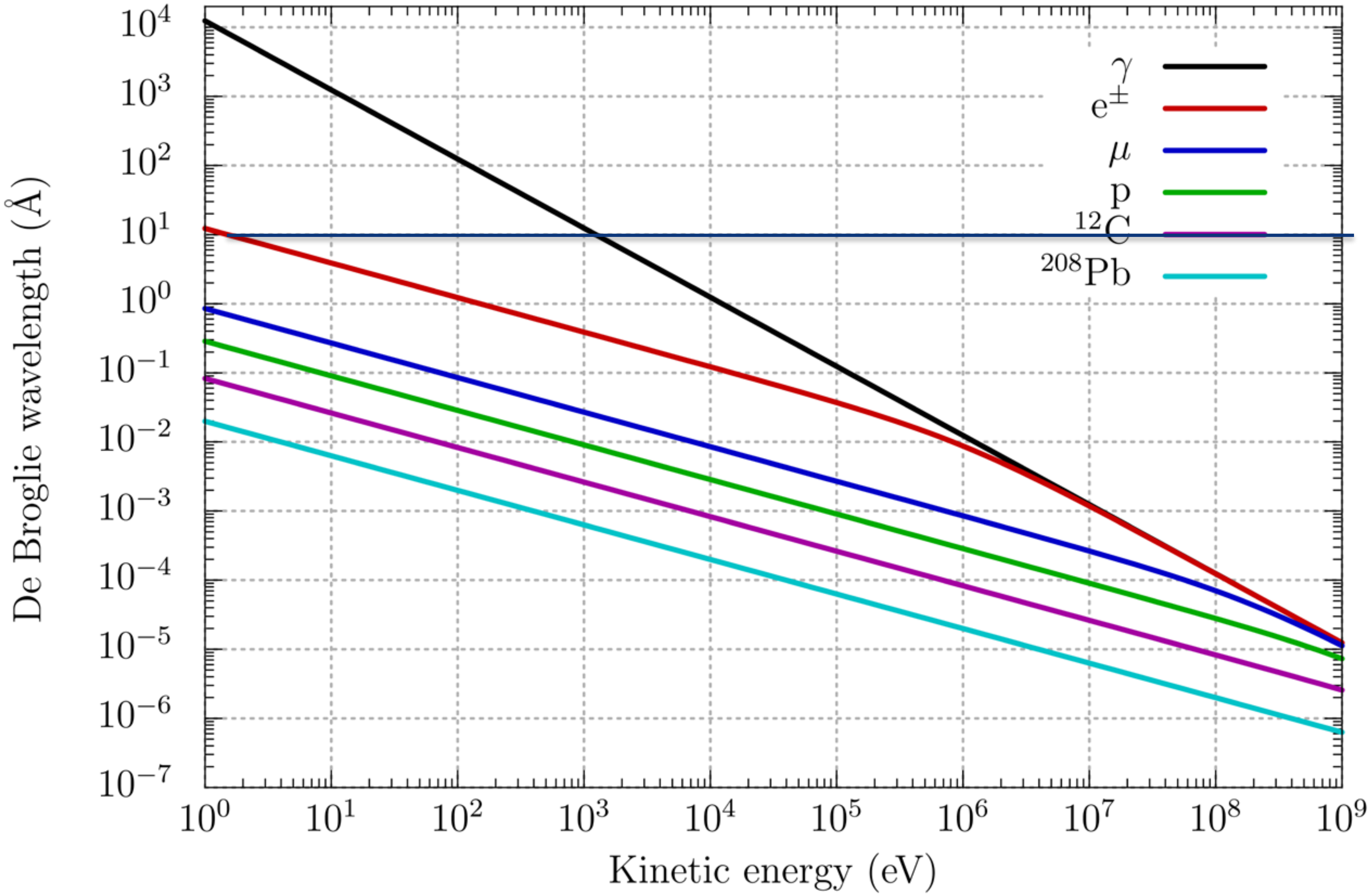
Limitations

Assumptions underlying MC simulation of radiation transport

- Medium is **amorphous** and **isotropic**:
  - No diffraction effects out of the box
  - Small subset: e.g. channeled charged particles in bent crystals (FLUKA,Geant4)
- **Material is not affected** by previous particles
- Shower particles do not interact with each other
- Transport is assumed to be Markovian: fate of a particle does not depend on its past history
- Particles interact on an individual atom/nucleus

De Broglie wavelength vs typical interatomic distance

- At low energies, wavelength extends to several interatomic distance
- Picture of a particle interacting on a single atom breaks down



General-purpose MC codes for particle interaction simulations

Capabilities of general-purpose MC codes

- Transport e-,e+,γ as well as muons, hadrons, and ions
- Allow for particle beams, particle-particle collision, or radioactive isotope as radiation source
- Cover a broad energy range:
  - Up to TeV for accelerator physics
  - Down to 1 keV for e-,e+,gamma
  - Down to meV for neutrons
- Offer up-to-date and thoroughly benchmarked physics
- Offer a flexible and efficient geometry package
- Capability to score physical observables of interest: energy deposition, particle spectra, radioactive inventories, etc.
- Capability to run in parallel / distributed

General-purpose codes for MC simulation of radiation transport

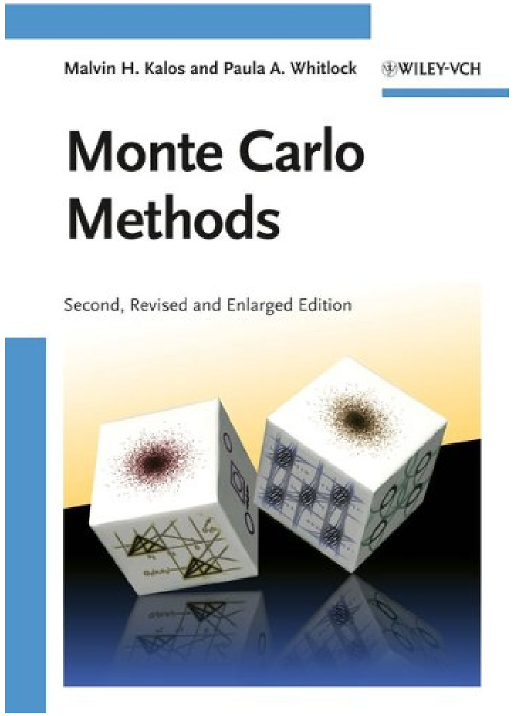
- Geant4
- FLUKA
- PHITS
- MARS
- MCNP
- PENELOPE
- EGS
- Tripoli
- …

General-purpose codes (hadrons, leptons, photons)

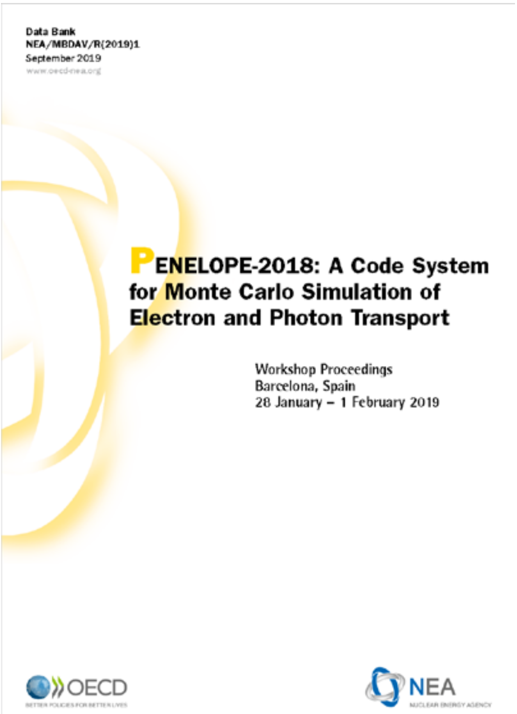
$e^{\pm},\gamma$

Reactor physics

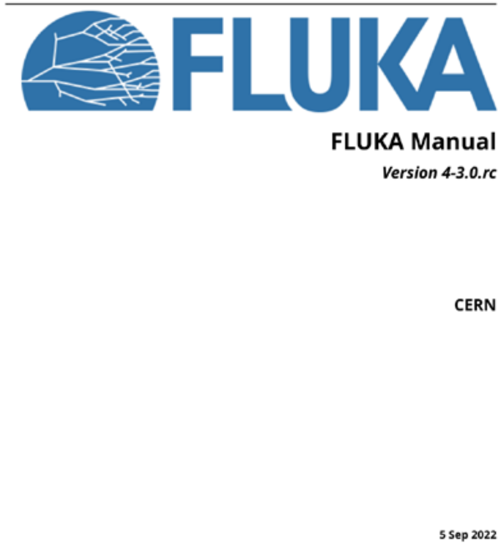
References



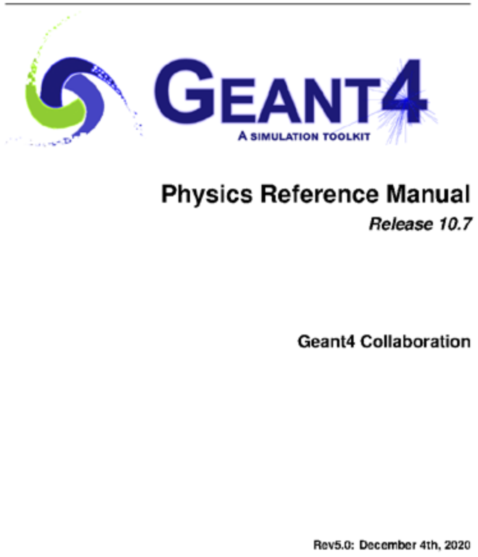
Malvin H. Kalos and Paula A. Whitlock
WILEY-VCH
Monte Carlo Methods
Second, Revised and Enlarged Edition



Data Bank
NEA/MBDAV/R(2019)1
September 2019
PENELOPE-2018: A Code System for Monte Carlo Simulation of Electron and Photon Transport
Workshop Proceedings
Barcelona, Spain
28 January – 1 February 2019
OECD
NEA



FLUKA
FLUKA Manual
Version 4-3.0.rc
CERN
5 Sep 2022

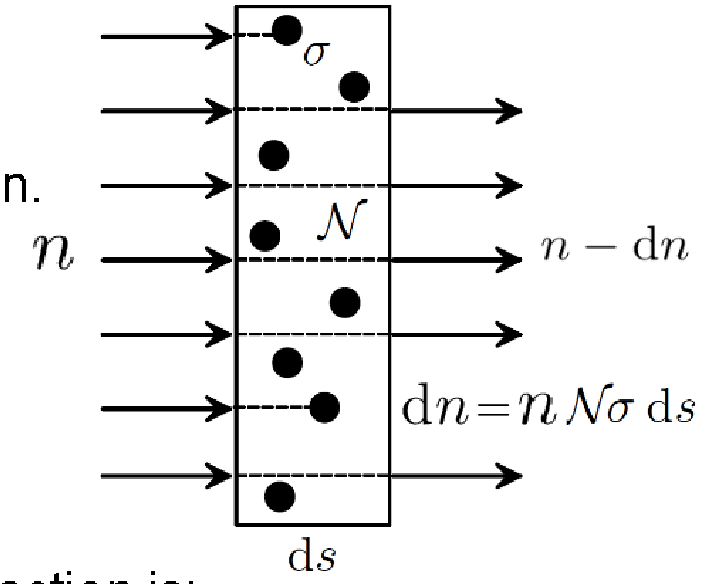


GEANT4
A SIMULATION TOOLKIT
Physics Reference Manual
Release 10.7
Geant4 Collaboration
Rev5.0: December 4th, 2020

Thank you very much
for your attention!

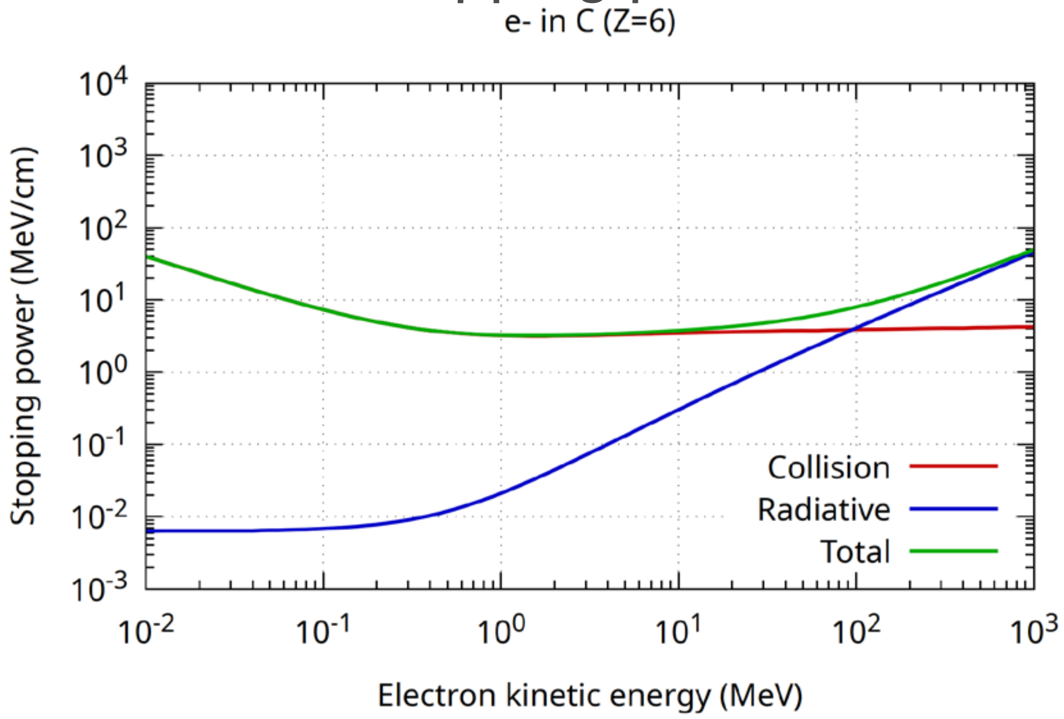
The exponential distribution of path lengths

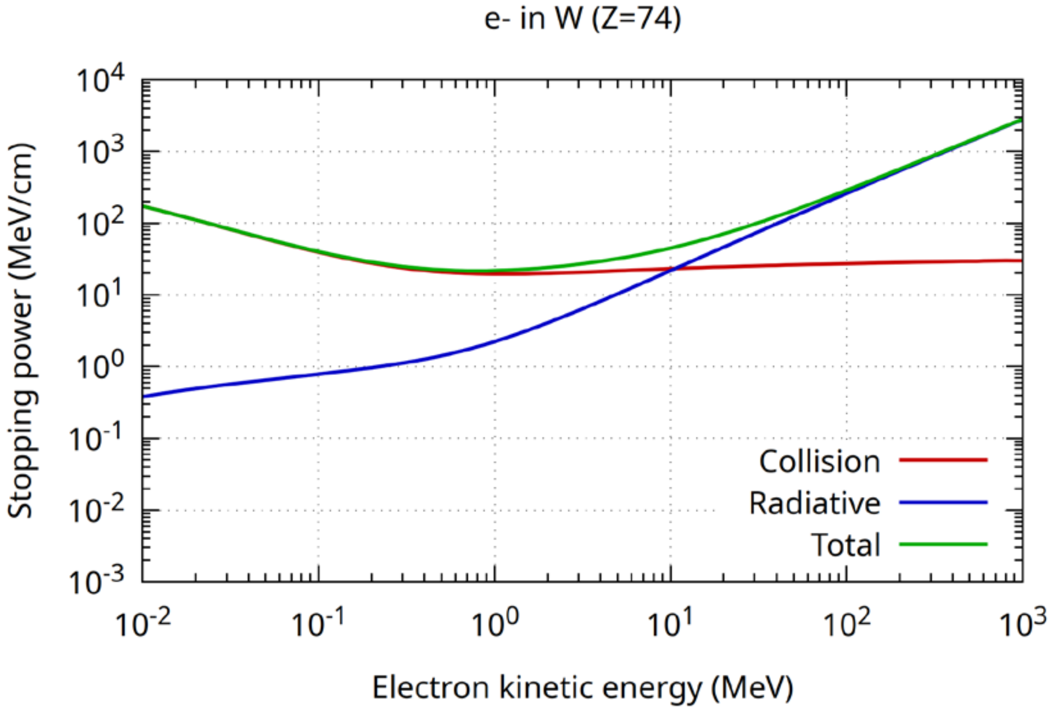
- Let n particles per unit time and surface impinge normally on a thin material slab of width ds with a density of N scattering centers per unit volume, each having a cross sectional area σ.
- Number of particles that interacted: $dn = n N\sigma\, ds$.
- The interaction probability in ds: $dn/n = N \sigma\, ds$
- Let $p(s)$ be the distribution of path lengths to the next interaction.
- The probability that the next interaction is within ds of s is
  $p(s) = [1 - \int_0^s ds'\, p(s')]\ (N\sigma) = \int_s^{inf} p(s')\,(N\sigma)\, ds'$
- The solution of this diff eq is
  $p(s) = (N\sigma)\, e^{-s(N\sigma)}$
- Thus the path length to the next interaction follows an exponential distribution. The average distance to the next interaction is:
  $\langle s \rangle = 1/(N\sigma) = \lambda$,
  i.e., we recover the expression of the mean free path given above.



Stopping power of charged particles in matter

- **Stopping power**: energy loss per unit path length
  - **Collision** stopping power: due to collisions with target e^-
  - **Radiative** stopping power: due to the emission of Bremsstrahlung photons





See: https://physics.nist.gov/PhysRefData/Star/Text/intro.html