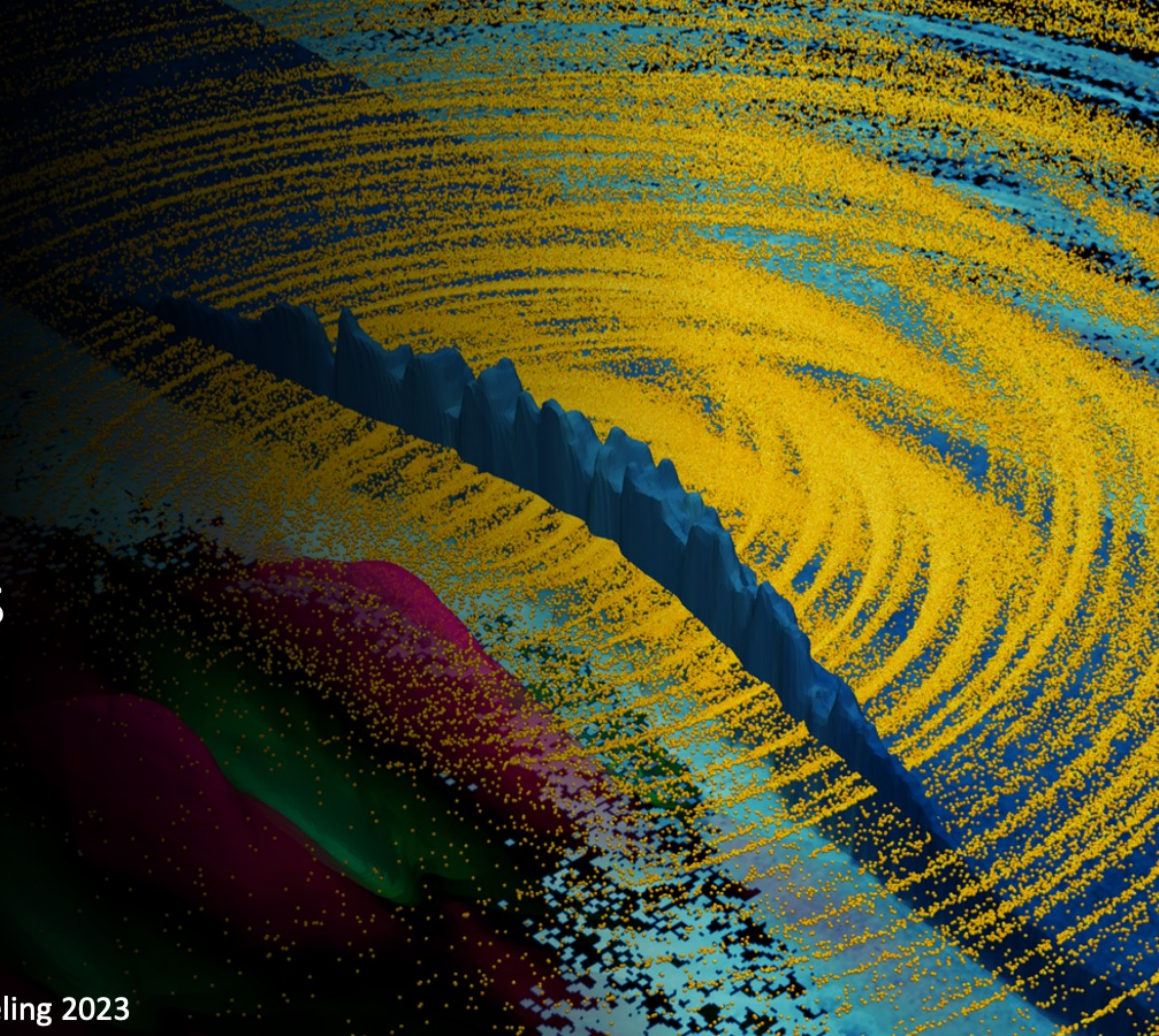
Monte Carlo simulations of particle transport relevant to laser produced plasmas



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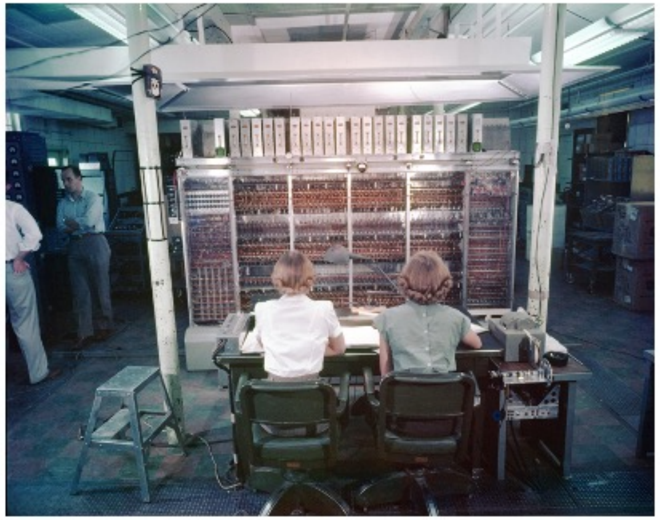
Simulation techniques in hot plasma modeling 2023

Monte Carlo simulations of particle transport relevant to laser produced plasmas

INTRODUCTION

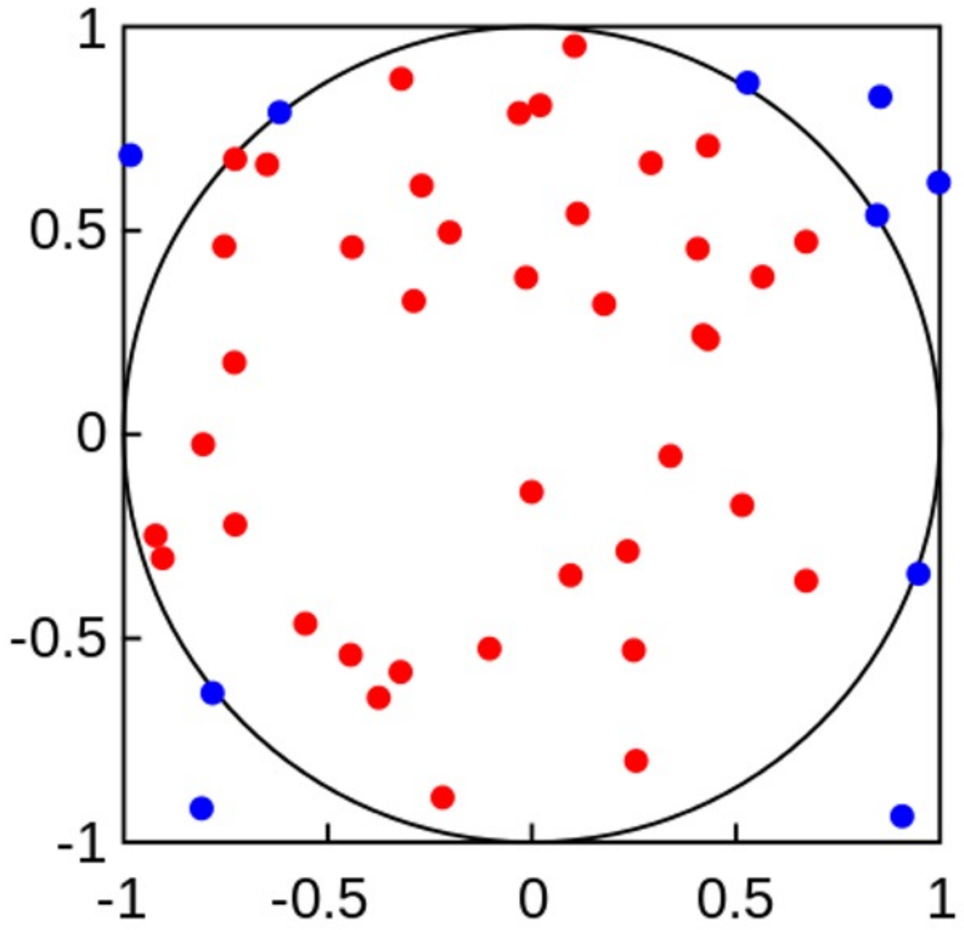
- **What is Monte Carlo (MC) method?**
  - Experimental mathematics – conclusions inferred from observations
  - A last resort when doing numerical integration (useful in cases when other numerical techniques become prohibitively inefficient)
  - A way to wastefully use CPU time – very slow "stochastic" convergence $O(n^{1/2})$
  - **A method to search for solutions to mathematical problem using a statistical sampling with random numbers**

The MANIAC I at Los Alamos in 1952. Photo courtesy of LANL.
https://www.atomicheritage.org/history/computing-and-manhattan-project



- **Basic facts about MC particle transport method?**
  - MC method was developed by Stanislaw Ulam during the H-bomb project at Los Alamos Laboratory after Word War II.
  - MC is often intuitive – direct physical intuition used to get the algorithm
  - MC has a sound mathematical basis

INTEGRATION

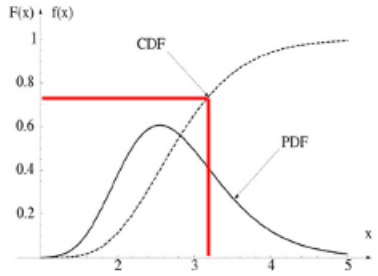


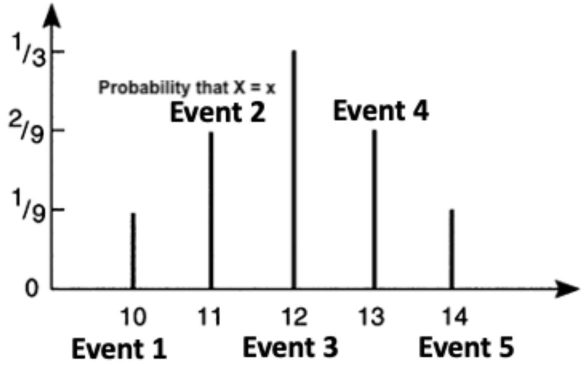
https://en.wikipedia.org/wiki/Monte_Carlo_integration

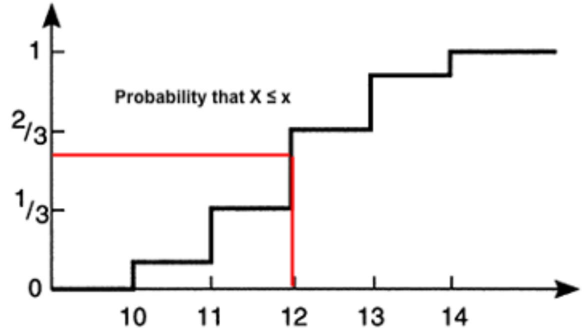
BASIC CONCEPT

- **Using a computer to generate random events:**
  - Uniformly distributed random numbers - $U_{[0,1]}$
  - General random numbers are obtained using $U_{[0,1]}$ with various methods – e.g.
    - inversion
    - rejection
  - Need to generate random numbers X with any probability distribution function (PDF) - $f_X(x)$ or probability mass function (PMF) in the discrete case
  - A cumulative distribution function (CDF) (or cumulative mass function - CMF) is often used – inversion method

$$F_X(x) = \int_{-\infty}^{x} f_X(t)\mathrm{d}t$$







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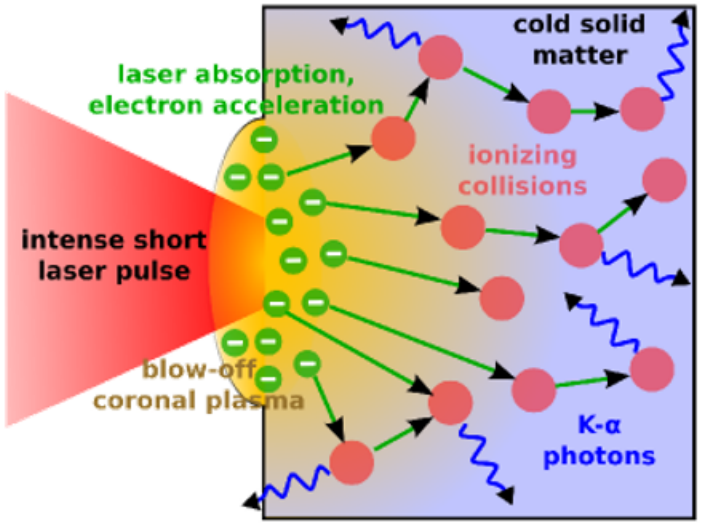
APPLICATIONS

- **Transport of energetic particles in particular in solid matter** (examples)
- **Electrons**
  - characteristic radiation – e.g. K-α source
  - Bremsstrahlung radiation – γ-ray source
- **Ions**
  - Isochoric heating (Warm Dense Matter)
  - Energy deposition in matter (hadron therapy)
  - Nuclear activation (nuclear reaction, ion diagnostics)
- **Photons**
  - Nuclear activation (nuclear reaction, photon diagnostics)
  - Attenuation (filtering/shielding)
  - Secondary e^- production (e.g. detector design)
  - Positron production - Bethe-Heitler (e^+ source)



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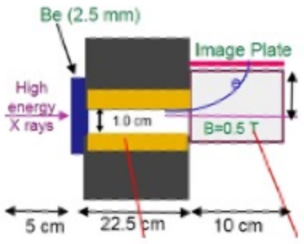
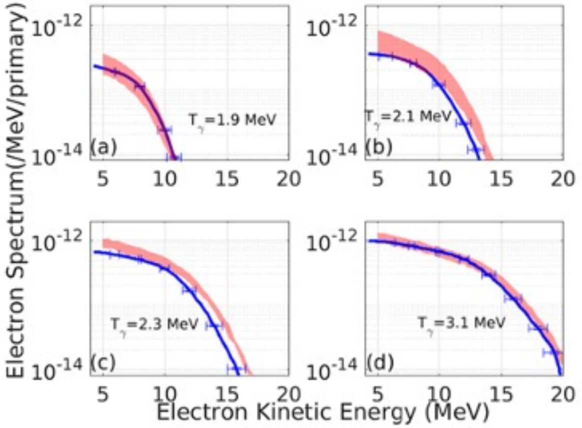
APPLICATIONS

- Example: **Gamma detector design** – FLUKA simulation of production of Compton electrons

  S. Singh et al., Rev. Sci. Instrum. 89, 085118 (2018), Compact high energy x-ray spectrometer based on forward Compton scattering for high intensity laser plasma experiments





- **Transport of energetic particles in particular in solid matter** (examples)
- **Neutrons as secondary particles**
  - Nuclear activation – decay (diagnostics)
  - Fusion (neutron source)
- **Sources, detectors and safety/filtering/shielding**
- **Other processes in particle simulations** (e.g. PIC) Monte Carlo approach:
  - Binary Coulomb collisions
  - Ionization
  - γ-radiation emission due to Bremsstrahlung or non-linear Compton scattering
  - e^+e^- production

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DRUNK WALK

- **The question is: How far will a drunk pedestrian be from the beginning $(\mathbf{0}, \mathbf{0})$ after doing N steps of the same length but in random directions?**
- At each step, the starting point is at the same time the end point of the previous step.
- The direction of the next step is given by the random angle (with respect to the previous direction given by angle θ_O)

$$\theta_W = 2\pi \cdot U_{[0,1]}$$

O – old angle in the lab frame
W – new angle in the walker frame
N – new angle in the lab frame

- Transformation to the laboratory frame using the previous direction as

$$\begin{pmatrix} \cos\theta_O & -\sin\theta_O \\ \sin\theta_O & \cos\theta_O \end{pmatrix} \begin{pmatrix} \cos\theta_W \\ \sin\theta_W \end{pmatrix} = \begin{pmatrix} \cos\theta_N \\ \sin\theta_N \end{pmatrix}$$

- The end point coordinates are thus

$$x_n = x_{n-1} + step \cdot \cos\theta_N$$
$$y_n = y_{n-1} + step \cdot \sin\theta_N$$

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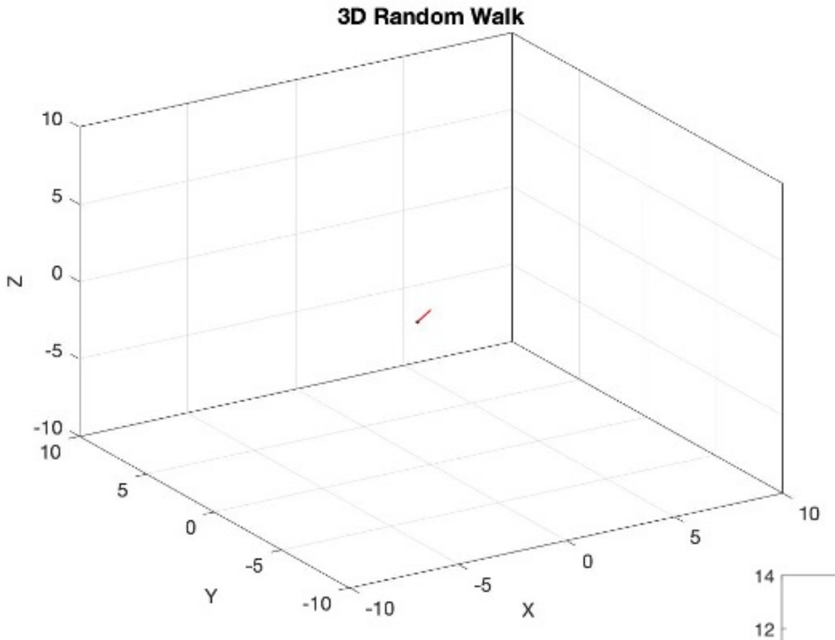
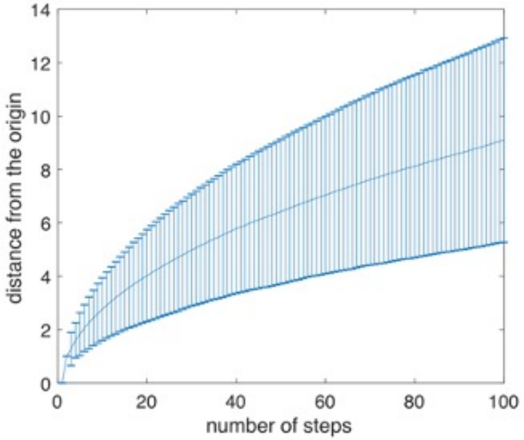
DRUNK WALK

- **Intuitive - basic algorithm for particle transport:**

1. Start at $(x_0 = 0, y_0 = 0), n = 0$
2. Sample initial direction - θ_N
3. $n = n + 1, \theta_O = \theta_N$
4. Sample new direction - θ_W
5. Transform to the lab frame – calculate θ_N
6. Calculate new coordinates (x_n, y_n)
7. Measure the distance from the origin $s = \sqrt{x_n^2 + y_n^2}$
8. Go to step 2. and repeat





- Simulate for N pedestrians to get mean and standard deviation (variance)

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PARTICLE TRANSPORT

- **What is different in particle transport:**
  - Step length is changing and has a given probability distribution
  - 3D transport – 2 scattering angles – polar and azimuthal
  - Particle loses energy
  - Particle may cross the boundary between objects from with different properties
  - Different events may occur at the end point (ionization, photon emission, nuclear excitation, absorption of the particle)
  - Secondary particles may emerge
  - Different quantities are measured during the transport

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- **Intuitive - basic algorithm for particle transport:**
  1. Sample the source for a particle - $(E, \boldsymbol{\Omega})$
  2. Calculate the mean free path (MFP) - λ_{mfp}
  3. Sample the exponential distribution to get new coordinates
  4. Sample the event at new coordinates
  5. Calculate energy loss and new direction of propagation $(E, \boldsymbol{\Omega}) \rightarrow (E', \boldsymbol{\Omega}')$
  6. Go to step 2. and repeat until particle absorbed or leaves the region of interest

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MATH BACKGROUND

- **Continuous path processes**
  - Diffusion process e.g. Brownian motion
  - Transport equation – e.g. Fokker-Planck equation

$$\frac{\partial}{\partial t} f(x,t) = -\frac{\partial}{\partial x}[D_1(x,t)f(x,t)] + \frac{\partial^2}{\partial x^2}[D_2(x,t)f(x,t)]$$

$f(x,t)$ - distribution function

D_1 and D_2 are the drift and diffusion coefficients.

  - Appropriate e.g. for charged particle transport in plasmas – transport dominated by many small angle Coulomb collisions

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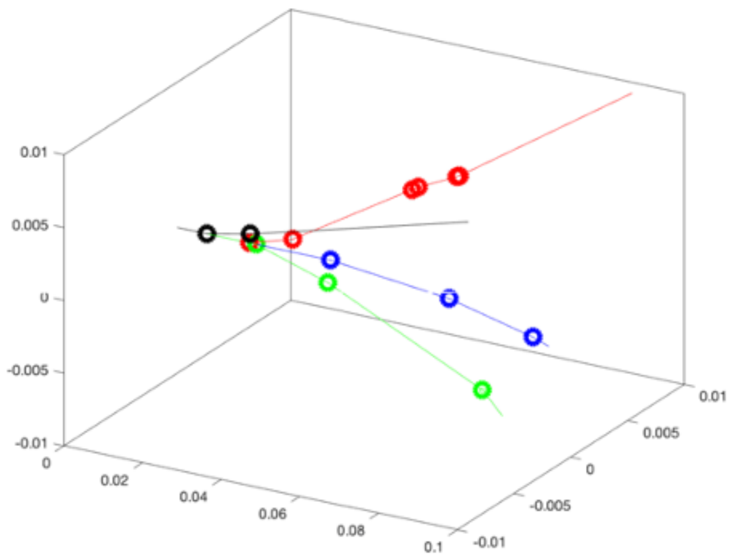
MATH BACKGROUND



- **Jump process** – discrete path
  - Can be described as Markov chain process (current state depends only on the previous one) and simulated using Monte Carlo method.
  - Transport equation – Fredholm integral equation of the second kind

$$\psi(\boldsymbol{p}) = S(\boldsymbol{p}) + \int \mathrm{d}\boldsymbol{p}' K(\boldsymbol{p}' \to \boldsymbol{p})\, \psi(\boldsymbol{p}')$$

$\boldsymbol{p}$ - phase space coordinate
$\psi(\boldsymbol{p})$ - probability density of finding the particle at the phase space coordinate
$S(\boldsymbol{p})$ - external source
The integral accounts for transition of particles from other parts of the phase space.

  - Appropriate e.g. for neutron transport, electron transport in solid target, fast ion transport – straight path between individual discrete collisions

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NEUTRON TRANSPORT

- Fredholm equation is a **Boltzmann** type transport **equation**
- **Simplifying assumptions – derivation for neutrons**
  - neutrons – point particles
  - neutrons – neutral particles – trajectory between interactions straight line
  - neutron-neutron interactions neglected
  - collisions are instantaneous
  - material properties are isotropic, known and time independent
  - expected or mean value of the neutron density distribution is considered
- **Quantities used to describe the transport**
  - <u>Neutron angular density</u> - $n(\boldsymbol{r}, E, \boldsymbol{\Omega}, t)$ - expected number of neutrons at position $\boldsymbol{r}$ with direction $\boldsymbol{\Omega}$ and energy E at time t per unit volume per unit solid angle per unit energy
  - <u>Neutron angular flux</u> - $\phi(\boldsymbol{r}, E, \boldsymbol{\Omega}, t)$ - product $n(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) \cdot v$ - neutron angular density n and neutron velocity v

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NEUTRON TRANSPORT

- **Transport equation**

$$\frac{\partial n}{\partial t} = \frac{1}{v}\frac{\partial \phi}{\partial t} = Production\ rate\ \boldsymbol{Q}\ - Leakage\ rate\ \boldsymbol{L}\ - Removal\ rate\ \boldsymbol{R}$$

- **Production rate** – three source terms
  - fission source - Q_f
  - independent external source - S
  - scattering source - Q_s - incident neutrons scatter from $(E', \boldsymbol{\Omega}')$ to $(E, \boldsymbol{\Omega})$

$$Q_s = \int_0^\infty \mathrm{d}E' \int \Sigma_s(\boldsymbol{r}, E') C(\boldsymbol{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}) \cdot \phi(\boldsymbol{r}, E', \boldsymbol{\Omega}', t) \mathrm{d}\boldsymbol{\Omega}'$$

C – probability of scattering from $(E', \boldsymbol{\Omega}')$ to $(E, \boldsymbol{\Omega})$

Σ_s – macroscopic scattering cross section

- **Leakage rate**
  - Difference between the number of neutrons exiting the volume $\mathrm{d}V$ and the number of neutrons entering the volume $\mathrm{d}V$ per unit time

$$L = \boldsymbol{\Omega} \cdot \nabla\phi$$

Y. Wu, Fusion Neutronics, Springer, 2017

- **Removal rate**
  - neutrons absorbed in $\mathrm{d}V$
  - neutrons scattered out from $(E, \boldsymbol{\Omega})$ in $\mathrm{d}V$

$$\mathrm{R} = (\Sigma_s + \Sigma_a)\,\phi(\boldsymbol{r}, E, \boldsymbol{\Omega}, t) = \Sigma_t\,\phi(\boldsymbol{r}, E, \boldsymbol{\Omega}, t)$$

Σ_s - macroscopic scattering cross section, Σ_a - macroscopic absorption cross section

- **In total**

$$\frac{1}{v}\frac{\partial \phi}{\partial t} + \boldsymbol{\Omega}\cdot\nabla\phi + \Sigma_t\phi = S + \int_0^\infty \mathrm{d}E' \int \mathrm{d}\boldsymbol{\Omega}'\,\Sigma_s(\boldsymbol{r}, E')C(\boldsymbol{r}, E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})\cdot\phi(\boldsymbol{r}, E', \boldsymbol{\Omega}', t)$$

- **Further simplification**
  - Stationary solution - $\frac{\partial \phi}{\partial t} = 0$, no absorption - $\Sigma_a = 0, \Sigma_t = \Sigma_s$
  - $\psi = \Sigma_s\phi$ – particle collision density - average number of collisions
  - Integration along characteristics

$$\psi(\boldsymbol{r}, E, \boldsymbol{\Omega}) = \int \mathrm{d}\boldsymbol{r}' \left[S + \int_0^\infty \mathrm{d}E' \int \mathrm{d}\boldsymbol{\Omega}'\psi(\boldsymbol{r}', E', \boldsymbol{\Omega}')C(\boldsymbol{r}', E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})\right] T(\boldsymbol{r}' \to \boldsymbol{r}, E, \boldsymbol{\Omega})$$

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MC SOLUTION

- The equation to be solved by MC approach
  - Let $\boldsymbol{p} = (\boldsymbol{r}, E, \boldsymbol{\Omega})$ and $K(\boldsymbol{p}' \to \boldsymbol{p}) = C(\boldsymbol{r}', E' \to E, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}) T(\boldsymbol{r}' \to \boldsymbol{r}, E, \boldsymbol{\Omega})$

$$\psi(\boldsymbol{p}) = \int S(\boldsymbol{r}')\, T(\boldsymbol{r}' \to \boldsymbol{r}, E, \boldsymbol{\Omega}) \mathrm{d}\boldsymbol{r}' + \int \psi(\boldsymbol{p}')\, K(\boldsymbol{p}' \to \boldsymbol{p}) \mathrm{d}\boldsymbol{p}'$$

  - ψ – particle collision density
  - S – source term
  - C – collision kernel
  - T – transport kernel

W. L. Dunn, J. K. Shultis, Exploring Monte Carlo Methods, Academic Press 2012

- Summary of assumptions
  - Static (time independent) homogeneous medium
  - Markovian
  - Particles transport independent of each other
  - Straight trajectories between collisions (no long-range forces)
- **Superposition principle applicable**

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MC SOLUTION

- Expantion of ψ into components after $0,1,2,\ldots,k$ collisions

$$\psi(\boldsymbol{p}) = \sum_{k=0}^{\infty} \psi_k(\boldsymbol{p}), \quad \text{with} \quad \psi_0(\boldsymbol{p}) = \int S(\boldsymbol{r}')\, T(\boldsymbol{r}' \rightarrow \boldsymbol{r}, E, \boldsymbol{\Omega})\mathrm{d}\boldsymbol{r}'$$

- As the process is Markovian

$$\psi_k(\boldsymbol{p}) = \int \psi_{k-1}(\boldsymbol{p}')K(\boldsymbol{p}' \rightarrow \boldsymbol{p})\mathrm{d}\boldsymbol{p}'$$

  - $\psi_{k-1}(\boldsymbol{p}')$ - probability density of $(k-1)$ collision at $\boldsymbol{p}'$
  - $K(\boldsymbol{p}' \rightarrow \boldsymbol{p})$ - conditional probability of (k) collision at $\boldsymbol{p}$ provided that the $(k-1)$ collision was at $\boldsymbol{p}'$

- **Monte Carlo solution**

1. Randomly sample $\boldsymbol{p}'$ from $\psi_{k-1}(\boldsymbol{p}')$
2. Randomly sample $\boldsymbol{p}$ from $K(\boldsymbol{p}' \rightarrow \boldsymbol{p})$
3. If $\boldsymbol{p} \in (\boldsymbol{p}_i - \mathrm{d}\boldsymbol{p}_i, \boldsymbol{p}_i + \mathrm{d}\boldsymbol{p}_i)$ then $\psi_k(\boldsymbol{p}_i) = \psi_k(\boldsymbol{p}_i)$+1
4. Repeat steps 1,2,3 N - times
5. Monte Carlo solution is $\psi_k(\boldsymbol{p}_i) = \psi_k(\boldsymbol{p}_i)/N$

P. Vaz, Neutron transport simulation, Radiation Physics and Chemistry 78, 829-842 (2009).

MC SOLUTION

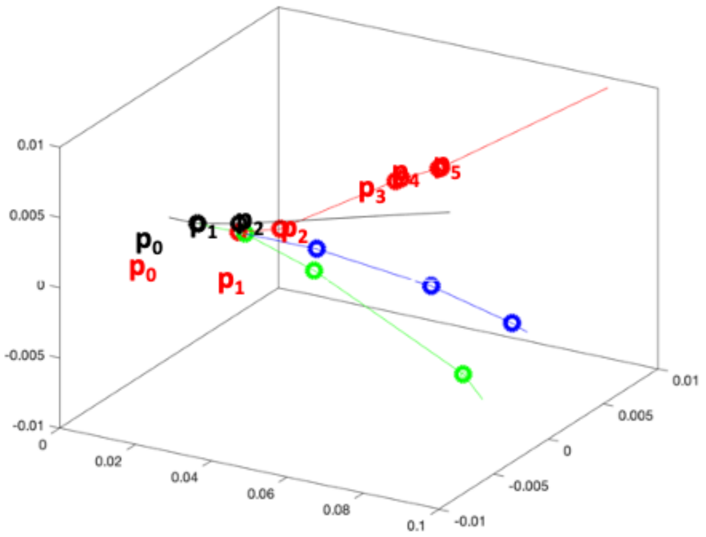
- A better approach – **Histories**

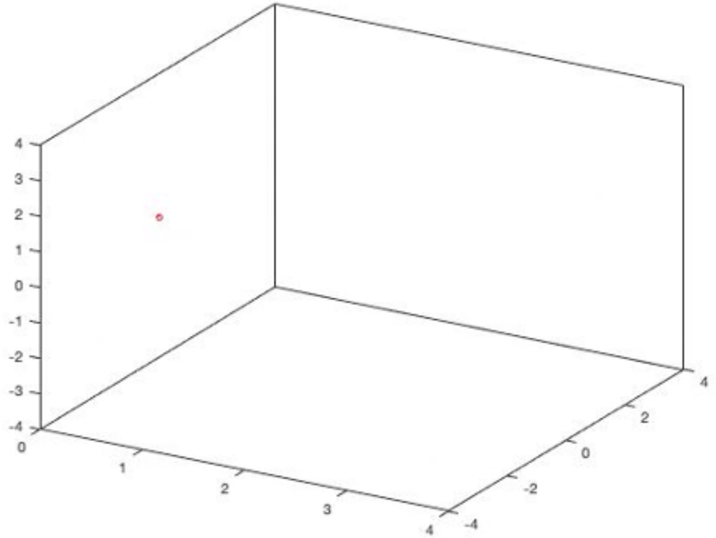
$$\psi_k(\boldsymbol{p}) = \int \psi_{k-1}(\boldsymbol{p}')K(\boldsymbol{p}' \to \boldsymbol{p})\mathrm{d}\boldsymbol{p}'$$

$$= \int \dots \int \psi_0(\boldsymbol{p}_0)K(\boldsymbol{p}_0 \to \boldsymbol{p}_1) \dots K(\boldsymbol{p}_{k-1} \to \boldsymbol{p})\mathrm{d}\boldsymbol{p}_0 \dots \mathrm{d}\boldsymbol{p}_{k-1}$$

- History - a sequence of states going from the source up to the „absorption“ state

Sample histories – 4 fast electrons propagating in Al target





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MC SOLUTION

- The **histories** are generated as follows
  - Randomly sample source with PDF - $\psi_0(\boldsymbol{p}_0)$
  - Randomly sample the k^{th} transition with PDF - $K(\boldsymbol{p}' \to \boldsymbol{p})$
- Having ***M* histories** – phase space density – measurements are possible

$$A = \int A(\boldsymbol{p})\,\psi(\boldsymbol{p})\mathrm{d}\boldsymbol{p} = \frac{1}{M}\sum_{m=1}^{M}\left(\sum_{k=1}^{\infty} A(\boldsymbol{p}_{k,m})\right)$$

- Measurable quantities are for example:
  - linear energy transfer (similar to dose) - amount of energy ionizing particle transfers to the material per unit distance (action of radiation into matter)
  - ionizing events – characteristic radiation emission
  - hard collisions – bremsstrahlung emission, etc.

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ELECTRON SCATTERING

- Individual scattering events modelled – **single scattering** model
- Scattering events
  - **Elastic** – no energy loss – scattering angle can be large – different analytical formulas exist – for electrons in the keV screened Rurherford cross section
    cross sections for a wider range of energies (Mott and Massey, The Theory of Atomic Collisions 1965)
  - **Inelastic** – energy loss due to excitation or ionization (events with large scattering angle are unlikely as $\theta \sim \Delta E / E$ - relative energy loss in collision)
    for cross sections see e.g. manual of the PENELOPE code
- Inelastic scattering not accounted for (not interested in ionization) – energy loss calculated differently
- Screened Rutherford elastic scattering cross section

$$\sigma_R = 5210 \frac{Z^2}{E^2} \frac{4\pi}{\alpha(1+\alpha)} \left(\frac{E+511}{E+1024}\right)^2 \ \left[{}^{\text{barn}}/_{\text{atom}}\right]$$

electron kinetic energy E is in keV, Z – atomic number and α – screening parameter

D.C. Joy, Monte Carlo Modeling for Electron Microscopy and Microanalysis, Oxford, 1995

- Total cross section integrated over all scattering angles, can be used to calculate the mean free path

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MEAN FREE PATH

- **Mean free path** - average distance travelled by a moving particle between successive collisions, which modify its properties $(E, \boldsymbol{\Omega})$
- **The exponential law**:
  - $P(x)$ - probability of not having an interaction after a distance x
  - $w\,\mathrm{d}x$ - probability to having an interaction between x and $x + \mathrm{d}x$
  - $w = \sigma \times N$
    - N - number of target particles per unit volume
    - σ – microscopic interaction cross section

$$P(x + \mathrm{d}x) = P(x) \times (1 - w\,\mathrm{d}x)$$

Probability of no-interaction up to x [$P(x)$]; Probability of no-interaction in $\mathrm{d}x$ [$(1 - w\,\mathrm{d}x)$]

- Poisson process - exponential distribution describes the time (distance) between events in a Poisson point process in probability theory and statistics
- Solution - exponential distribution. $P(x) = \exp(-w \cdot x),\ P(0) = 1$
- **Mean free path** between interactions $\lambda_{mfp} = {}^{1}/_{w}$

Ref: W.R. Leo, "Techniques for Nuclear and Particle Physics Experiments"

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MEAN FREE PATH

- **Mean free path** between interactions $\lambda_{mfp} = \frac{1}{w} = \frac{1}{\sigma N}$
- E.g. in solids, λ_{mfp} is of the order of tens nm for 100 keV electron and 10 times smaller for 10 keV electron
- How to sample **MFP** – using cumulative distribution function (CDF) and inversion method - CDF is monotonic function increasing from 0 to 1

$$F(x) = \frac{\int_0^d P(x)\mathrm{d}x}{\int_0^\infty P(x)\mathrm{d}x} = \frac{\int_0^d \exp(-x/\lambda_{mfp})\mathrm{d}x}{\int_0^\infty \exp(-x/\lambda_{mfp})\mathrm{d}x} = 1 - \exp\left(-\frac{s}{\lambda_{mfp}}\right)$$

- Sampling of the distance traveled s

$$s = -\lambda_{mfp} \ln\left(1 - F(x)\right) = -\lambda_{mfp} \ln\left(U_{[0,1]}\right).$$

If $F(x)$ is $U_{[0,1]}$ then $(1 - F(x))$ is too.

- **Different interactions**
  - Different cross sections – different mean free path e.g. $\lambda_A \sim 1/\sigma_A$, $\lambda_B \sim 1/\sigma_B$
  - Total mean free path - $\sigma_T = \sigma_A + \sigma_B \implies \frac{1}{\lambda_T} = \frac{1}{\lambda_A} + \frac{1}{\lambda_B}$

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SCATTERING ANGLE

- Scattering angle is given by the cross section differential in scattering angle

$$\sigma_R{}' = \frac{\mathrm{d}\sigma_R}{\mathrm{d}\Omega} = 5210\,\frac{Z^2}{E^2}\left(\frac{E+511}{E+1024}\right)^2 \frac{1}{(\sin^2(\vartheta/2)+\alpha)^2}$$

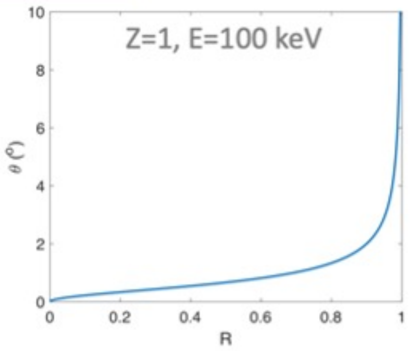
$$\sigma_R = \int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \mathrm{d}\vartheta \sin\vartheta\, \sigma_R{}'$$

- Polar scattering angle is obtained as

$$U_{[0,1]} = \int_0^{2\pi} \mathrm{d}\varphi \int_0^{\theta} \mathrm{d}\vartheta \sin\vartheta\, \frac{\sigma_R{}'}{\sigma_R}$$

- Using the inversion method

$$\cos\theta = 1 - \frac{2\alpha R}{(1+\alpha-R)}, R = U_{[0,1]}$$



- Azimuthal scattering angle is random, rotational symmetry of the collision frame

$$\varphi = 2\pi \cdot U_{[0,1]}$$

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ENERGY LOSS

- Energy loss
  - Inelastic collisions – dominates for lower E and lower Z
  - Bremsstrahlung emission – emission of photon during elastic collision
- Simulation of all energy loss events very complicated and time consuming
- Energy loss in individual collisions usually low – so called soft events
- Energy loss averaged per unit path – so called stopping power
- For solid targets and electrons – **Bethe stopping power**
- For electron in keV range

$$\frac{\mathrm{d}E}{\mathrm{d}S} = -78500 \cdot \frac{Z}{AE} \cdot \ln\left(\frac{1.166E}{J}\right), \qquad S = s \cdot \rho$$

where s is the distance traveled in cm, ρ is the density in g/cm^3, A is the atomic weight a both E and the mean ionization potential J are in keV (only for $E \gg J$)

- Stopping powers and range tables can be found in Estar database of NIST, not now

NOTICE: Due to a lapse in government funding, this and almost all NIST-affiliated websites will be unavailable until further notice. Learn more
NIST websites for programs using non-appropriated funds (NVLAP and PSCR) or those that are excepted from the shutdown (such as NVD) will continue to be available and updated.

https://pml.nist.gov/PhysRefData/Star/Text/ESTAR.html

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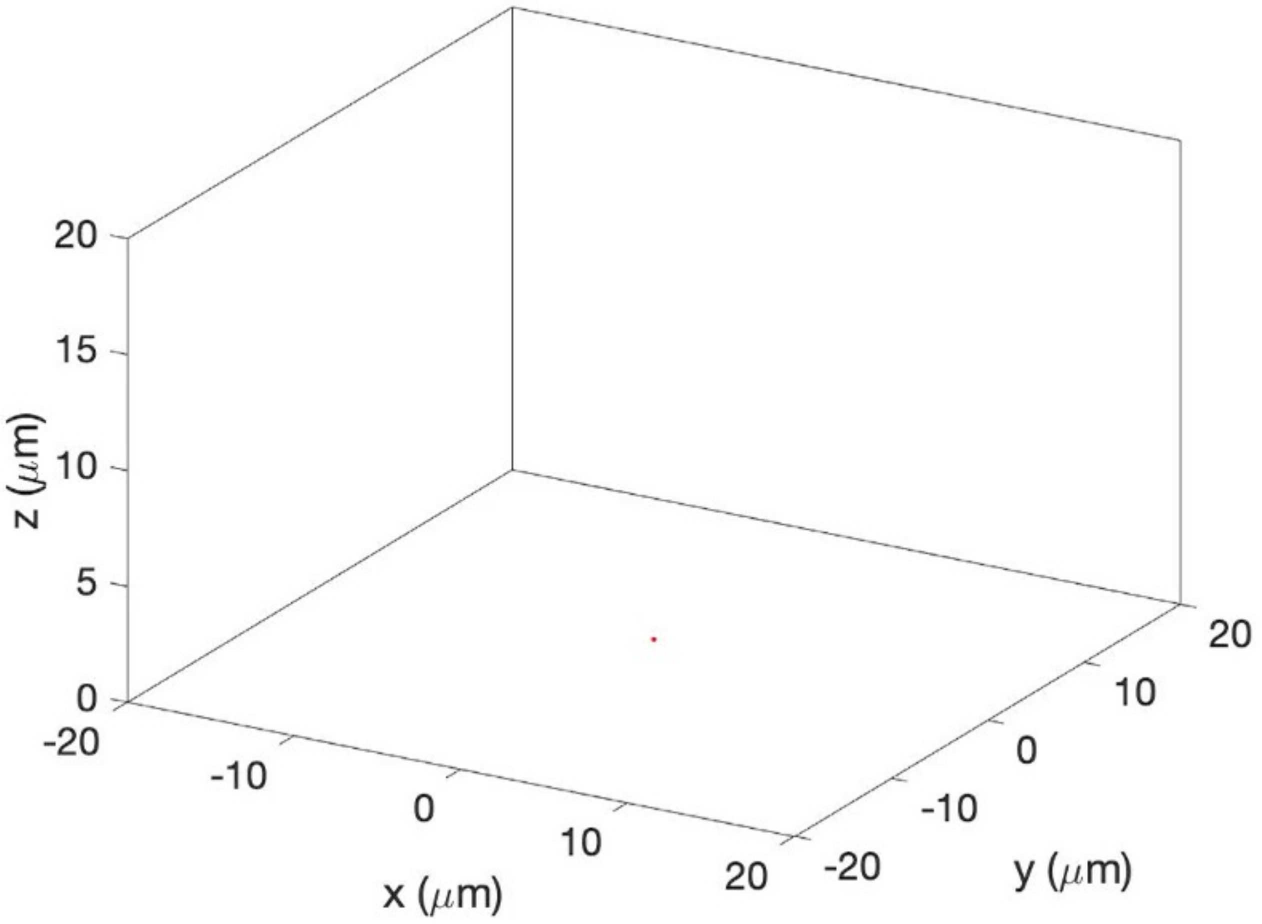
SINGLE SCATTERING



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CONDENSED HISTORY

- With stopping power – **Continuous Slowing Down Approximation** (CSDA) – step size related only to events, where electron is deflected
- Simulating all elastic scattering events (**single scattering**) very inefficient – many small angle deflections and only few large angle ones
- Condensed history technique (**plural** or **multiple scattering**) – deflection events grouped together
- Multiple scattering – step size not related λ_{MFP}
- Popular choice – constant fractional energy loss per step, i.e. $\frac{\Delta E}{E} = \text{const.}$ e.g. 4%
- **Condensed history Class II scheme**
  - Bremsstrahlung photon creation directly above an energy threshold E_γ
  - Knock-on electrons above energy threshold E_δ treated by creation and transport
  - Sub-threshold processes accounted for in CSDA model and multiple scattering
- Depending on the application, condensed history "outperforms" single-scattering by a factor $10^3 – 10^5$
- Radiation transport - random process, energy loss fluctuations called "energy straggling" may be important

e.g. O. N. Vassiliev, Monte Carlo Methods for Radiation Transport Fundamentals and Advanced Topics, Springer, 2017

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VARIANCE REDUCTION

- The classical (so called) analog MC method works well if the probability of the situation of interest occurring is not very low
- Otherwise too time consuming and bad statistics
- **Variance reduction** techniques help to make it more efficient by
  - **PDF biasing**
  - **Particle splitting**
- **Biasing** – PDF of unlikely events of interest is increased. Each particle is assigned with a statistical weight w to obtain unbiased results

$$w_{biased} = w_{unbiased} \frac{PDF_{unbiased}}{PDF_{biased}}$$

- If PDF_{biased} is increased, w_{biased} is decreased proportionally so the averaged outcome of the unbiased PDF is preserved. Examples are:
- <u>Implicit capture</u> (survival)
  - Instead of "absorption" the particle is forced to continue and w_{biased} is reduced
  - If w_{biased} too low – Russian roulette – either termination or increase of weight

Monte Carlo simulations of particle transport relevant to laser produced plasmas

VARIANCE REDUCTION

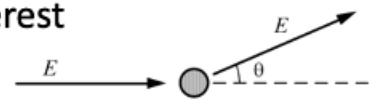
- Forced collision in a small volume – particle is split into 2
  - First one passes through, $w_1 = \exp(-s/\lambda_{mfp})$
  - Second one is forced to collide, $w_2 = (1 - w_1)$
- **Particle splitting** - different particles contribute differently to the objective
- Increase the survivability of the "important" particles and eliminate "less important" ones. For example:
- Geometric splitting with Russian roulette - volume partitioned into regions with different importance
- Particle moves:
  - From region of lower importance to higher importance - splitting
  - From region of higher importance to lower importance - Russian roulette decides whether the particle is killed

e.g. A. Haghighat, Monte Carlo Methods for Particle Transport, CRC Press, 2015

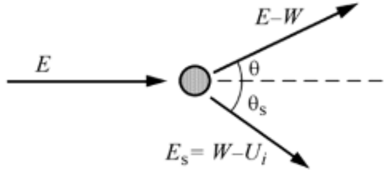
Monte Carlo simulations of particle transport relevant to laser produced plasmas

e^+/e^- INTERACTIONS

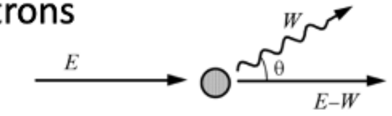
- Possible interactions of electrons with matter in the range of interest
- **Elastic scattering**
  - Initial and final quantum states of target atom same
  - Responsible for angular deflections
  - Target recoil neglected
- **Inelastic scattering**
  - Produce electronic excitations and ionizations in the medium
  - Dominant energy loss mechanism for lower energies
  - Relaxation to ground state by emitting X-rays and Auger electrons
- **Bremsstrahlung emission**
  - Result of acceleration by the electrostatic field of atoms
  - Angular deflection accounted by elastic collision
  - Photon energy in the range 0 to E
- **Positron annihilation**
  - Annihilation with the electrons in the medium by emission of two photons



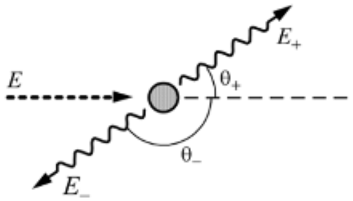
Elastic scattering



Inelastic scattering



Bremsstrahlung emission

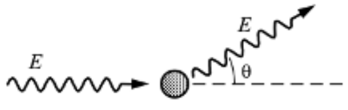


Positron annihilation

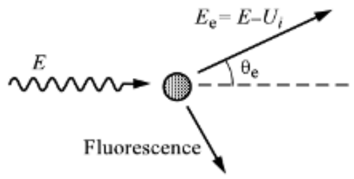
F. Salvat, J. Fernández-Vera, J. Sempau,
PENELOPE-A code system for Monte Carlo simulation of electron and photon transport, OECD/NEA Data Bank. (2006).

PHOTON INTERACTIONS

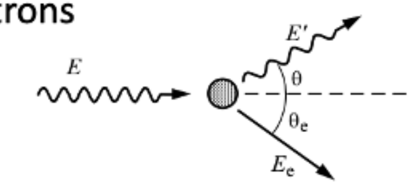
- Dominant interactions in the energy range 0.1 keV – 1 GeV
- **Rayleigh (coherent) scattering**
  - By bound electrons without excitation – elastic scattering
  - Cross section related to Thomson scattering by free electron and atomic form factor
- **Photoelectric effect**
  - Photon absorbed by target atom, transition to excited state
  - Photon energy > ionization energy – photoionization
  - Relaxation to ground state by emitting X-rays and Auger electrons
- **Compton scattering**
  - Photon absorbed by atomic electron and re-emited
  - Active target electron ejected with finite kinetic energy
- **Pair production**
  - Absorption of photon in vicinity of a nucleus – Bethe Heitler
  - Threshold process – 2 $m_e c^2$



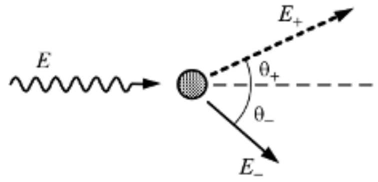
Rayleigh scattering



Photoelectric absorption



Compton scattering



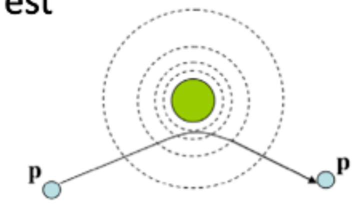
Pair production

F. Salvat, J. Fernández-Vera, J. Sempau,
PENELOPE-A code system for Monte Carlo simulation of electron and photon transport, OECD/NEA Data Bank. (2006).

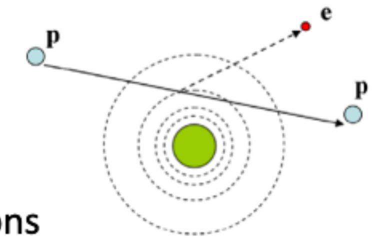
Monte Carlo simulations of particle transport relevant to laser produced plasmas

PROTON INTERACTIONS

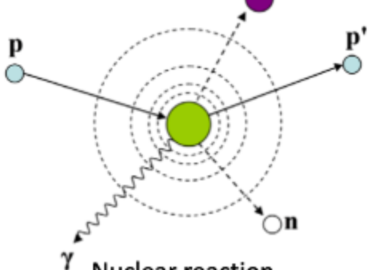
- Important interactions of protons with matter in the range of interest
- **Elastic scattering**
  - Pure electromagnetic - point-like nucleus and proton
  - Residual - includes strong interaction due to nucleus size effect
  - Recoil important
- **Inelastic scattering**
  - Produce electronic excitations and ionizations in the medium
  - Dominant energy loss mechanism
  - Relaxation to ground state by emitting X-rays and Auger electrons
- **Nuclear reaction**
  - Less frequent but have more profound effect.
  - Projectile proton enters the nucleus, which emits a proton, deuteron, triton, heavier ion or one or more neutrons
- **Bremsstrahlung emission**
  - Small effect on stopping of protons - radiated power small
  - Dosimetry simulations - bremsstrahlung often neglected



Elastic scattering



Inelastic scattering



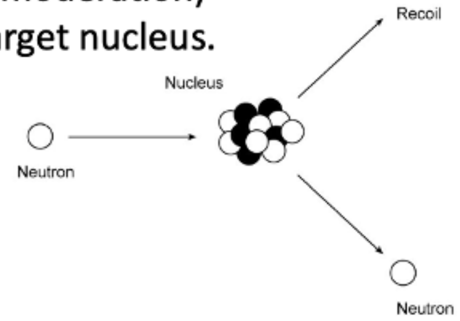
Nuclear reaction

L. Hult, Interaction Models for Proton Transport Monte Carlo Simulations based on the PENELOPE code, thesis at KTH 2015
W. D. Newhauser, R. Zhang, The physics of proton therapy ,Phys. Med. Biol. 60, R155 (2015)

Monte Carlo simulations of particle transport relevant to laser produced plasmas

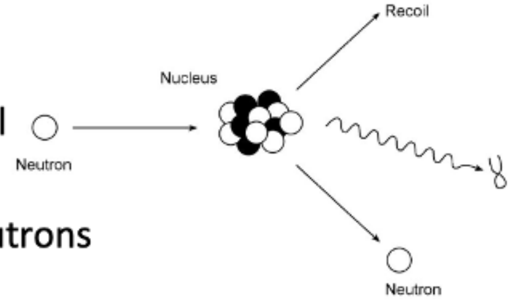
NEUTRON INTERACTIONS

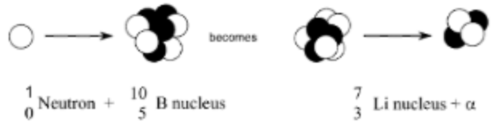
- Neutrons are born fast, they slow down due to scattering (moderation) until they reach thermal energies and are absorbed by a target nucleus.



- **Neutron energies**
  - Fast (>100 keV)
  - Intermediate (10 eV – 100 keV)
  - Slow (< 10 eV)
  - Thermal (0.025 eV)

- **Interactions with atomic nuclei**
  - **Elastic Scattering** - most likely interaction, nuclear recoil
  - **Inelastic Scattering** – excitation of the nucleus (emission of gamma rays), higher Z and high energy neutrons
  - **Capture/absorption** by the nucleus - nuclear reaction
    - Unstable nucleus created - deexcitation by emission of p, α, nucleus fragments





E. Malinen, E. Waldeland, Neutron interactions and dosimetry, Univ. of Oslo

CANDU Fundamentals, canteach.candu.org

Monte Carlo simulations of particle transport relevant to laser produced plasmas

MC CODES

- **EGSnrc** https://nrc-cnrc.github.io/EGSnrc/
  - Particle interactions - photons, electrons and positrons with kinetic energies between 1 keV and 10 GeV
  - Software toolkit - set of functions and subroutines for the simulation of coupled electron/photon transport
  - Applications based on EGSnrc
    - BEAMnrc - used to model medical linear accelerators
    - DOSXYZnrc - dose distributions including geometries defined via CT images, incorporated into a number of clinical treatment planning codes
- **GEANT4** http://geant4.web.cern.ch
  - Particle interactions - electron, ion, muon, gamma ray, electromagnetic (EM), hadronic, and optical photons (many kinds of particles) very wide energy range
  - Toolkit for simulation of passage of particles through matter with applications in high energy, nuclear and accelerator physics, medical and space science
    - MULASSES - used to analyze radiation shielding for space missions
    - OpenGATE - used for tomography applications

Monte Carlo simulations of particle transport relevant to laser produced plasmas

MC CODES

- **MCNP** https://mcnp.lanl.gov
  - Particle interactions - neutrons up to 20 MeV for all isotopes and up to 150 MeV for some, photons from 1 keV to 100 GeV and electrons from 1 keV to 1 GeV.
  - Applications include radiation protection and dosimetry, shielding, radiography, medical physics, nuclear criticality safety, detector design and analysis, accelerator target design, fission and fusion reactor design, decontamination and decommissioning.
- **PENELOPE** https://www.oecd-nea.org/tools/abstract/detail/nea-1525
  - Particle interactions – electron/positron-photon transport in energy range between 50 eV and 1 GeV.
  - Applications include electron backscattering, electron probe microanalysis and X-ray generators, response of radiation detectors, dosimetry and characterization of ionization chambers, radio-therapy and simulation of medical electron accelerators and cobalt units, and synchrotron radiation.

Monte Carlo simulations of particle transport relevant to laser produced plasmas

MC CODES

- **FLUKA** http://www.fluka.org/fluka.php
  - Particle interactions

	Secondary particles	Primary particles
charged hadrons	1 keV – 20 TeV	100 keV – 20 TeV
neutrons	thermal – 20 TeV	thermal – 20 TeV
electrons	1 keV – 1000 TeV	70 keV - 1000 TeV (low-Z material)
		150 keV - 1000 TeV (high-Z material)
photons	1 keV – 1000 TeV	7 keV – 1000 TeV
heavy ions	10 MeV/n – 10000 TeV/n	100 MeV/n – 10000 TeV/n

  - Applications in high energy experimental physics and engineering, shielding, detector and telescope design, cosmic ray studies, dosimetry, medical physics and radio-biology.

Particle methods for laser-produced plasmas

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Simulation techniques in hot plasma modeling 2023

What was not covered here?

- Particle-in-cell simulation method for macroscopic degenerate plasmas
  https://doi.org/10.1103/PhysRevE.102.033312
- The Pretty Efficient Parallel Coulomb Solver
  https://www.fz-juelich.de/en/ias/jsc/about-us/structure/simulation-and-data-labs/sdl-plasma-physics/pepc

Thank you for attention