Monte Carlo simulation of radiation transport

EUTEMPE-RX module 03

Monte Carlo simulation of x-ray imaging and dosimetry

Barcelona, June 2017

Monte Carlo simulation of radiation transport

"Imitates" on a computer the propagation of radiation in matter, by numerically sampling

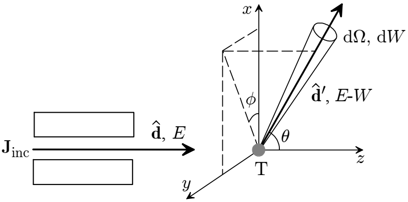
1. Distance between physical interactions
2. Kind of interaction
3. Angular deflection and/or energy loss
4. Generation of secondary radiation

Advantages of MC methods

- Ability to deal with arbitrary geometries
- Accurate interaction models are easily implemented

Differential & total cross section

Target: one atom or molecule



DDCS

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

Energy-loss DCS

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

Total (i.e. integrated) cross section

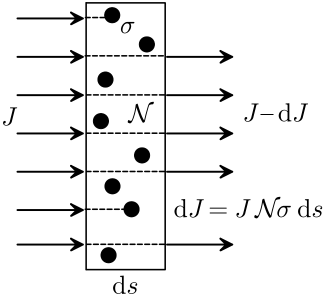
$$\sigma \equiv \int_0^E \frac{\mathrm{d}\sigma}{\mathrm{d}W}\,\mathrm{d}W$$

Interaction probability per unit path length

Imagine each target as a sphere of radius r_s such that $\pi r_\mathrm{s}^2 = \sigma$

Number of atoms or molecules per unit volume

$$\mathcal{N} = \mathrm{N_A} \frac{\rho}{A_\mathrm{w}}$$



$\mathcal{N}\sigma\,\mathrm{d}s =$ fractional area covered by the spheres

Interaction probability per unit path length

$$\frac{\mathrm{d}J/J}{\mathrm{d}s} = \mathcal{N}\sigma \equiv \mu \equiv \lambda^{-1}$$

PDF of s

Probability to travel a path length s without interacting

$$P_0(s) = 1 - \int_0^s p(s')\,\mathrm{d}s' = \int_s^\infty p(s')\,\mathrm{d}s'$$

Probability of having the next interaction in the interval $(s, s + \mathrm{d}s)$

$$p(s)\,\mathrm{d}s = P_0(s)\,\mu\,\mathrm{d}s \quad \Rightarrow \quad p(s) = \mu \int_s^\infty p(s')\,\mathrm{d}s'$$

Solving this equation with the boundary condition $p(\infty) = 0$ yields

$$p(s) = \mu\,\mathrm{e}^{-\mu s} = \lambda^{-1}\,\mathrm{e}^{-s/\lambda}$$

Mean free path

$$\langle s \rangle = \int_0^\infty s\,p(s)\,\mathrm{d}s = \mu^{-1} = \lambda$$

Scattering model & PDFs

Consider a particle with energy E
moving in an infinite, homogeneous and isotropic medium

Various interaction mechanisms i are possible,
giving angular deflections θ and/or energy losses W

DDCSs (per target)

$$\frac{\mathrm{d}^2\sigma_i(E;W,\theta)}{\mathrm{d}W\,\mathrm{d}\Omega}$$

Targets randomly oriented & unpolarized beams
$\Rightarrow$ DDCSs independent of ϕ

Total cross sections (per target)

$$\sigma_i(E) = \int_0^E \mathrm{d}W \int_0^\pi 2\pi \sin\theta\,\mathrm{d}\theta\ \frac{\mathrm{d}^2\sigma_i(E;W,\theta)}{\mathrm{d}W\,\mathrm{d}\Omega}$$

Total interaction cross section

$$\sigma_{\mathrm{T}}(E) = \sum_i \sigma_i(E)$$

Total interaction probability per unit path length

$$\lambda_{\mathrm{T}}^{-1} = \sum_i \lambda_i^{-1} = \mathcal{N}\sigma_{\mathrm{T}}$$

PDFs

For each E

$$\begin{aligned} p(s) &= \lambda_{\mathrm{T}}^{-1}\,\mathrm{e}^{-s/\lambda_{\mathrm{T}}} \\ p_i &= \sigma_i/\sigma_{\mathrm{T}} \\ p_i(W,\theta) &= \frac{1}{\sigma_i}\,2\pi\sin\theta\,\frac{\mathrm{d}^2\sigma_i}{\mathrm{d}W\,\mathrm{d}\Omega} \\ p(\phi) &= 1/2\pi \quad \forall\, i \end{aligned}$$

Generation of random tracks: detailed simulation

State of a particle <u>after</u> the n-th interaction

$$\vec{\mathbf{r}}_n = (x, y, z), \quad \hat{\mathbf{d}}_n = (u, v, w) = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta), \quad E_n$$

i) Sample the path length to the next interaction

$$s = -\lambda_{\mathrm{T}} \ln \xi$$

New position $\vec{\mathbf{r}}_{n+1} = \vec{\mathbf{r}}_n + s\,\hat{\mathbf{d}}_n$

ii) Sample the interaction mechanism
i is the index that fulfills

$$\mathcal{P}_i < \xi \leqslant \mathcal{P}_{i+1}$$

where

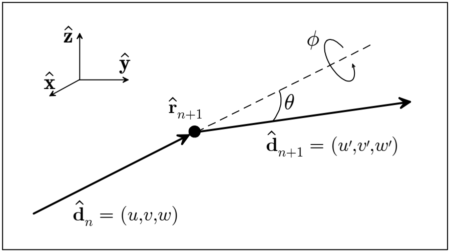
$$\mathcal{P}_1 = 0, \quad \mathcal{P}_2 = p_1, \quad \mathcal{P}_3 = p_1 + p_2, \quad \ldots, \quad \mathcal{P}_{N+1} = \sum_{i=1}^{N} p_i = 1$$

Generation of random tracks (cont'd)

iii) Sample the energy loss and the angular deflection
W and θ are sampled from $p_i(W,\theta)$, whereas $\phi = 2\pi\xi$

New energy $E_{n+1} = E_n - W$

New direction $\hat{\mathbf{d}}_{n+1} = \mathcal{R}(\theta,\phi)\,\hat{\mathbf{d}}_n$



iv) Store the initial state of secondary particles, if any

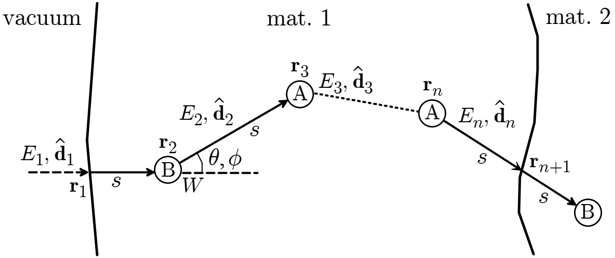
▷ The simulation of the track proceeds by repeating steps **i–iv**

Generation of random tracks (cont'd)

Conditions to finish a track

- The particle leaves the material system
- $E < E_{\text{abs}}$

▷ Generate a large number N of histories



Statistical averages & type A uncertainties

i) Scalar quantities

In a formal sense $Q = \int q\, p(q)\, \mathrm{d}q$

MC estimate of Q after a (large) number of histories N

$$\overline{q} = \frac{1}{N} \sum_{i=1}^{N} q_i$$

Statistical uncertainty (standard deviation) of the MC estimate

$$\sigma(\overline{q}) = \frac{\sigma(q)}{\sqrt{N}} \approx \sqrt{\frac{1}{N} \left[\frac{1}{N} \sum_{i=1}^{N} q_i^2 - \overline{q}^2 \right]}$$

- MC result: $Q_{\mathrm{MC}} = \overline{q} \pm \kappa\, \sigma(\overline{q})$, typically $\kappa = 2$ (95% confidence)

▷ We have to score q_i and q_i^2

Statistical averages & type A uncertainties (cont'd)

ii) Continuous distributions

▷ Distributions are tallied as histograms

Example: depth-dose distribution $D(z)$ in $(z_{\text{min}}, z_{\text{max}})$

The interval is partitioned into M depth bins (z_{k-1}, z_k) with $z_{\text{min}} = z_0 < z_1 < \ldots < z_M = z_{\text{max}}$

$e_{ij,k}$ denotes the amount of energy deposited into the k-th bin by the j-th particle of the i-th history

Average energy deposited into the k-th bin (per history) and corresponding statistical uncertainty

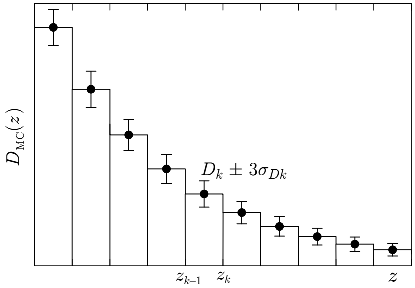
$$\overline{E}_k = \frac{1}{N} \sum_{i=1}^{N} e_{i,k} \qquad \sigma(\overline{E}_k) = \sqrt{\frac{1}{N} \left[\frac{1}{N} \sum_{i=1}^{N} e_{i,k}^2 - \overline{E}_k^2 \right]} \qquad e_{i,k} \equiv \sum_j e_{ij,k}$$

Statistical averages & type A uncertainties (cont'd)

$$\overline{D}_k \equiv \frac{\overline{E}_k}{z_k - z_{k-1}} \qquad \sigma(\overline{D}_k) \equiv \frac{\sigma(\overline{E}_k)}{z_k - z_{k-1}}$$

- MC result:

$$D_{\mathrm{MC}}(z) = \overline{D}_k \pm \kappa\,\sigma(\overline{D}_k) \qquad \text{for } z_{k-1} < z < z_k$$



Type B uncertainties

Sources of “systematic” uncertainties

- Geometry
- Material composition
- Interaction models (cross sections)
- Transport mechanics for charged particles