Introduction to Computational Dosimetry

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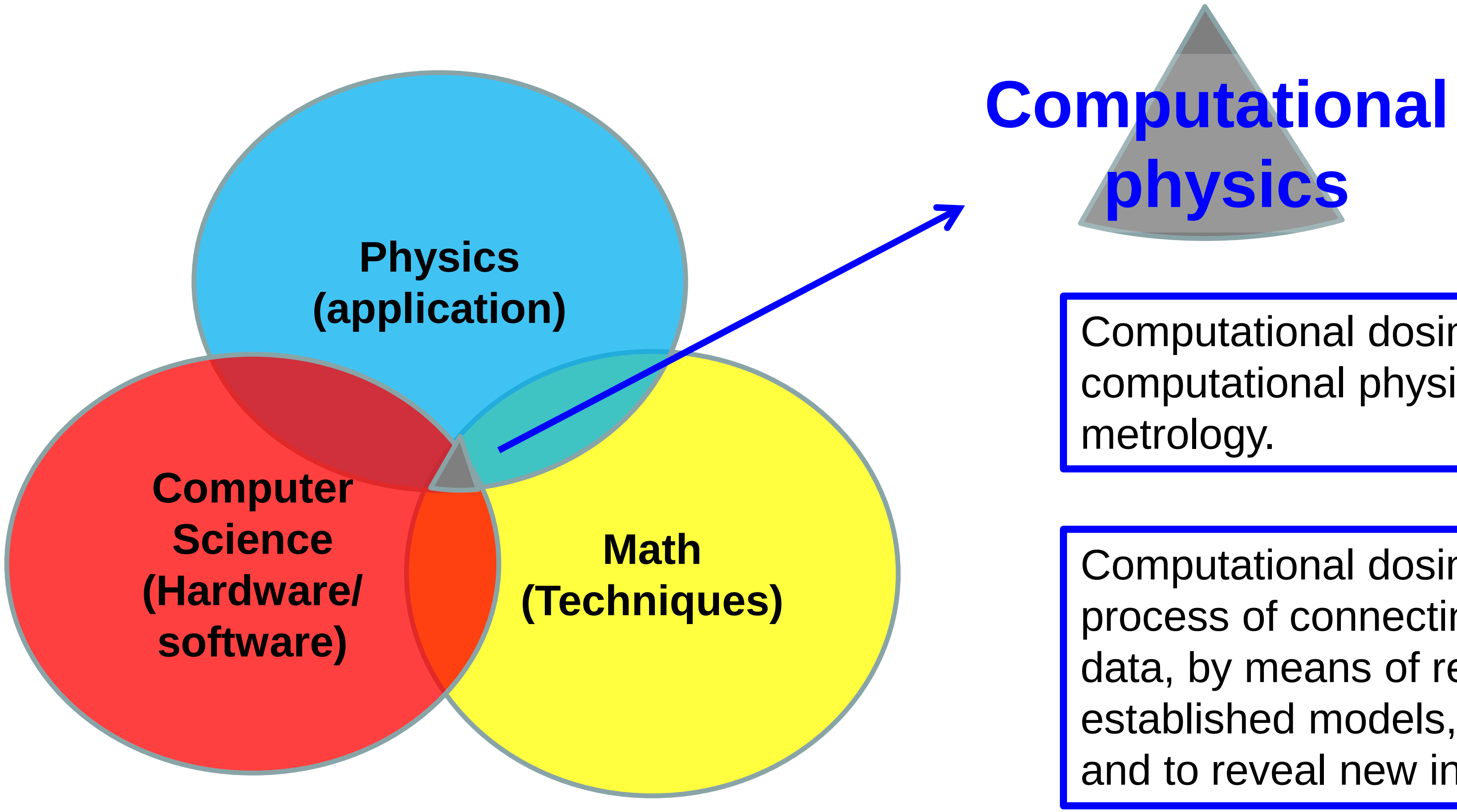
Definitions taken from B. Siebert and R. Thomas (RPD 1997)



Computational dosimetry is the sub-discipline of computational physics devoted to radiation metrology.

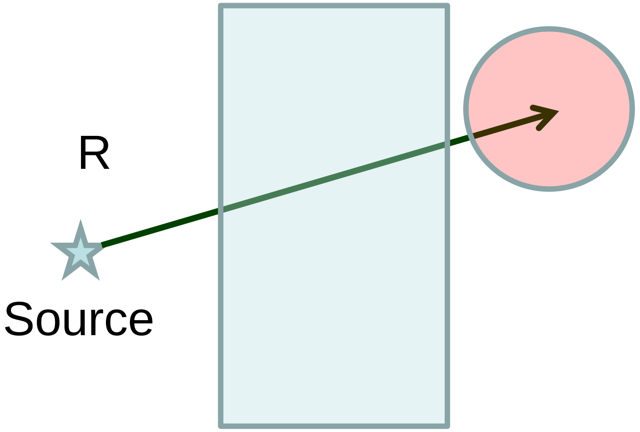
Computational dosimetry may be defined as the process of connecting and ordering of known data, by means of relations based on theory or established models, in order to create new data and to reveal new insight.

- ✓ **Computational dosimetry**
  - Analytical methods
  - Deterministic methods
  - Monte Carlo (MC) methods
- ✓ **MC calculation of fundamental radiological quantities**
- ✓ **MC simulation in complex geometries**
- ✓ **MC calculation of radiation protection quantities**
- ✓ **MC uncertainty and variance reduction**

Analytical methods

Only simple cases can be analytically treated (e.g.: attenuation in a semi-infinite media of an isotropically emitting gamma source homogeneously distributed on a surface):

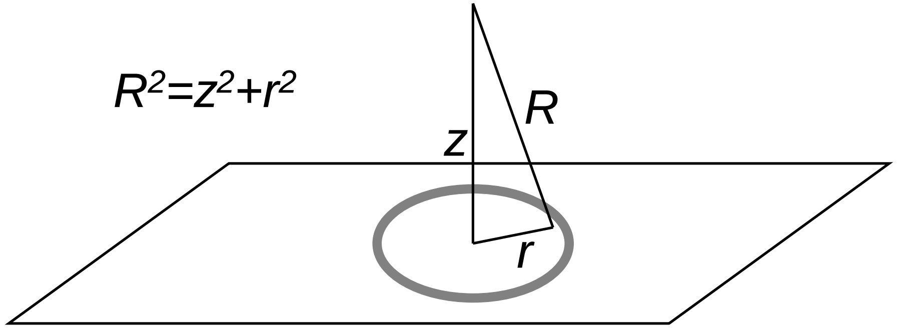
$$\dot{D} = \varphi . \frac{\mu_{en}}{\rho} . E = \left[\frac{1}{cm^2 . s}\right]\left[\frac{cm^2}{g}\right][MeV] . 1.6E^{-10} = \left[\frac{Gy}{s}\right]$$



$$\varphi = \frac{A}{4\pi R^2} = \left[\frac{Bq}{cm^2}\right]$$

$$\varphi = \frac{A}{4\pi R^2} e^{-\mu.d} = \left[\frac{Bq}{cm^2}\right]$$

$$d\varphi = \dot{N}_S \, 2\pi \, r \, dr \, \frac{e^{-\left(\mu/\rho\right)\rho R}}{4\pi R^2} B(\mu R)$$



with build-up factor, $B(\mu d)$

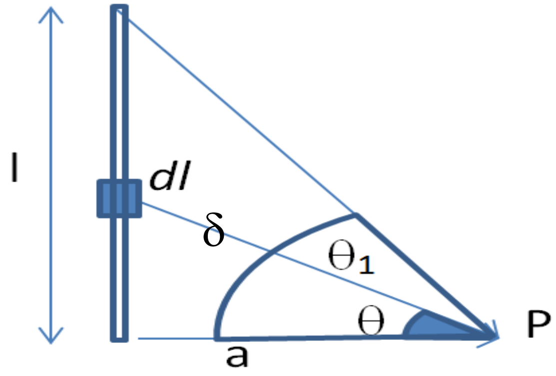
$$B(\mu d) = A' e^{-\alpha_1 \mu d} + (1 - A') e^{-\alpha_2 \mu d}$$

$$\varphi(z) = \dot{N}_S \, 2\pi \int_0^{+\infty} r \, \frac{e^{-\left(\mu/\rho\right)\rho R}}{4\pi R^2} B(\mu R) dr = \frac{\dot{N}_S}{2} \int_z^{+\infty} \frac{e^{-\left(\mu/\rho\right)\rho R}}{R} B(\mu R) dR =$$

$$= \frac{\dot{N}_S}{2} \left[A' E_1\left((1+\alpha_1)\mu z\right) + (1 - A') E_1\left((1+\alpha_2)\mu z\right) \right]$$

Where E_1 (the exponential integral function) can be solved numerically

(point kernel methods)



$$l = a.\tan(\vartheta)$$

$$dl = \frac{a}{\cos(\vartheta)^2} d\vartheta$$

$$d\varphi = \frac{S_l dl}{4\pi\delta^2}$$

$$\delta = \frac{a}{\cos(\delta)}$$

$$\varphi = \int_0^{\theta_1} \frac{S_l dl}{4\pi\delta^2} = \frac{S_l}{4\pi a}\theta_1$$

So the fluence decrease as 1/distance

Various type of sources (from: *Engineering compendium on radiation shielding*, Springer, 1968)

Rectangular surface sources

6.3.2. RECTANGULAR SOURCE [2]

6.3.2.1. RECTANGULAR SOURCE WITHOUT SHIELD

The flux from an unshielded rectangular surface source at a point P_1 directly above the corner of the rectangle (see Fig. 6.3.–4) can be represented by:

$$\phi = S_A \, \bar{\Phi}(m, n) \qquad (6.3.–5)$$

with $m = l/a$ and $n = h/l$. The function $\bar{\Phi}(m, n)$ is plotted in Fig. 6.3.–5.

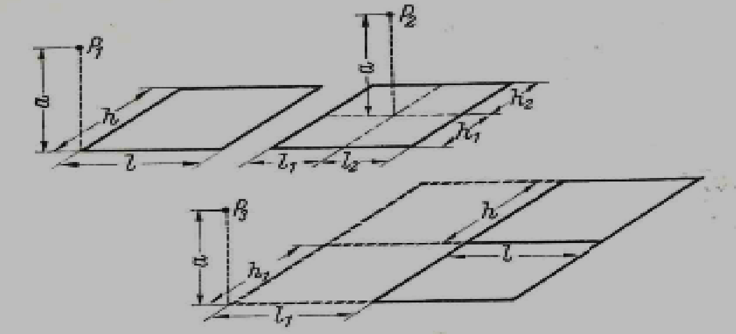


Fig. 6.3.–4. Geometry for rectangular source without shield.

Cylindrical surface sources

CALCULATED VALUES

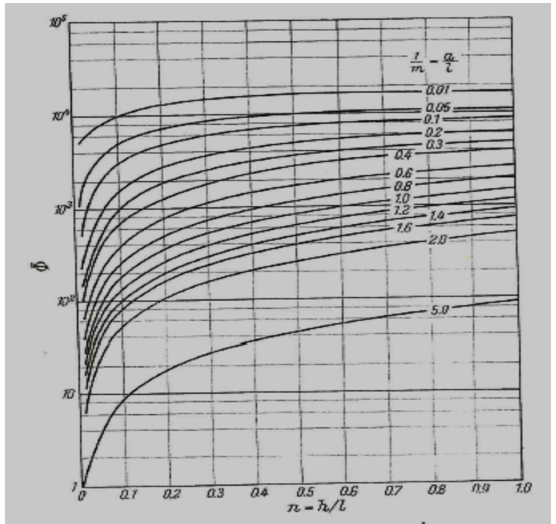


Fig. 6.3.–5. Rectangular source: $\bar{\Phi}$ vs. $n = \frac{h}{l}$ [3, p. 11].

$$F(\theta, b) = \int_0^{\theta} e^{-b.\sec(\theta')}\, d\theta'$$

Sievert Integral (tabulated)

Cylindrical volume sources

6.3.3. CYLINDRICAL SURFACE SOURCE [1]

6.3.3.1. CYLINDRICAL SURFACE SOURCE WITHOUT SHIELD

The fluxes at various points from an unshielded cylindrical surface source (see Fig. 6.3.–7) are as follows:

At P_1:

$$\phi = \frac{S_A R}{2(a+R)} F(\varphi, k),$$

$$\varphi = \arctan \frac{H}{a-R}, \quad k = \frac{2\sqrt{aR}}{a+R}; \qquad (6.3.–9)$$

at P_2:

$$\phi = \frac{S_A R}{2(a+R)} [F(\varphi_1, k) + F(\varphi_2, k)]; \qquad (6.3.–10)$$

at P_3:

$$\phi = \frac{S_A R}{2(a+R)} [F(\varphi_2, k) - F(\varphi_1, k)]; \qquad (6.3.–11)$$

at P_4:

$$\phi = \frac{S_A R}{2(R-a)} F(\varphi, k), \quad \varphi = \arctan \frac{H}{R-a}; \qquad (6.3.–12)$$

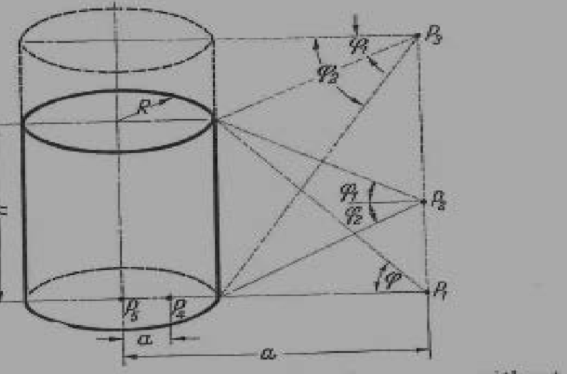


Fig. 6.3.–7. Geometry for cylindrical surface source without shield.

Deterministic methods

Solve by finite elements the Boltzmann's transport equation

Boltmann's transport equation

$$\varphi = n.v = \left[\frac{1}{cm^3}\right]\left[\frac{cm}{s}\right]$$

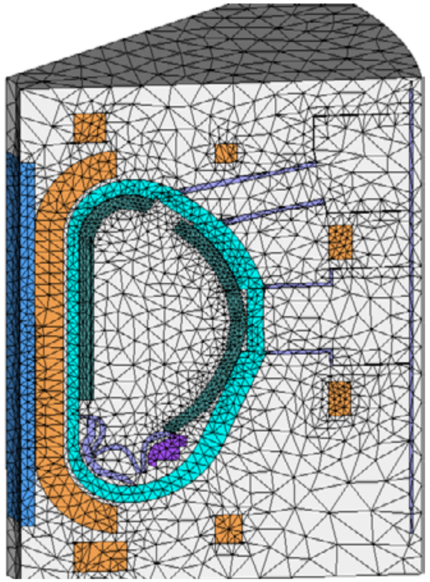
$$\frac{dn}{dt} = \frac{1}{v}\frac{d}{dt}n = production - absorption - leakage$$

$$\left(\frac{1}{v}\frac{\partial}{\partial t} + \vec{\Omega}\cdot\vec{\nabla} + \sigma_t\right)\varphi^{(i)}_{\Omega,E}(\vec{r},E,\vec{\Omega},t) =$$

$$= \int_0^{+\infty}\int_{4\pi} \sigma_s(\vec{r},E,E',\vec{\Omega},\vec{\Omega}')\varphi^{(i)}_{\Omega,E}(\vec{r},E,\vec{\Omega},t)\,d\Omega' dE + S(\vec{r},E,\vec{\Omega},t)$$

Vector energy fluence $\vec{\Psi}(\vec{r}) = \iiint E\,\vec{\Omega}\varphi_{\Omega,E}(\vec{r},E,\vec{\Omega},t)\,d\Omega\,dE\,dt$

Absorbed dose $D = Y - \frac{1}{\rho}\vec{\nabla}\cdot\vec{\Psi}$



Modelo simplificado para ITER
(ATTILA, 300.000 elementos)

FEM: finite elements method
FDM: finite difference method

Deterministic codes for computational dosimetry

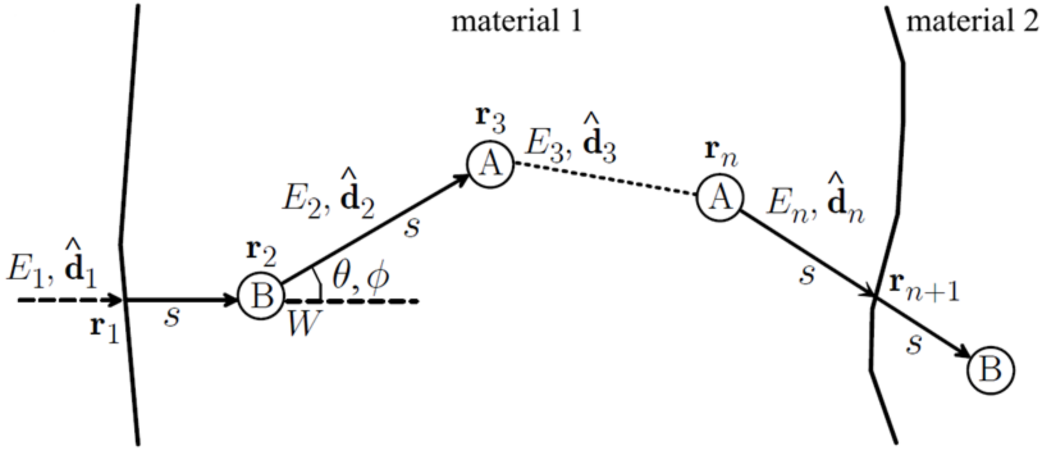
ANISN:	https://www.oecd-nea.org/tools/abstract/detail/ccc-0254	(NEA databank)
ATTILA:	https://silverfirsoftware.com/products/attila/	(Silver Fir Software)
DANTSYS:	https://www.oecd-nea.org/tools/abstract/detail/ccc-0547	(NEA databank)
DOORS:	https://www.oecd-nea.org/tools/abstract/detail/ccc-0650	(NEA databank)
SCEPTRE:	https://www.oecd-nea.org/tools/abstract/detail/ccc-0826/	(NEA databank)

Monte Carlo (MC) simulation of radiation transport

MC method simulates the physical processes of radiation transport in matter by numerically sampling:

- distance between interactions
- interaction type
- angular distribution and energy loss
- production of secondary particles
- scoring of a physical quantity $(\vec{r}, \vec{p}, E)$

over a high number of histories

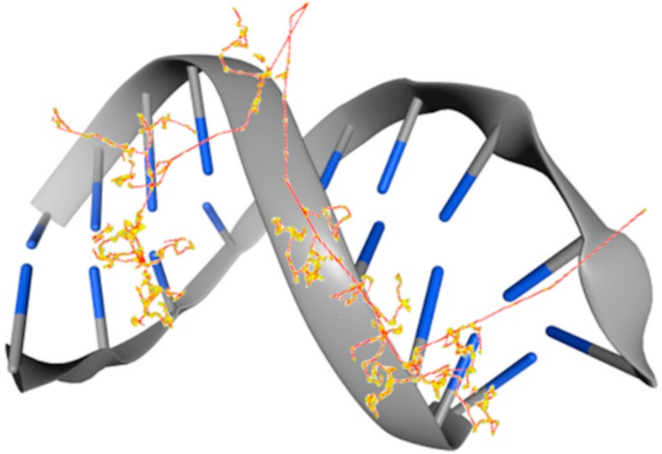


Monte Carlo codes for computational dosimetry

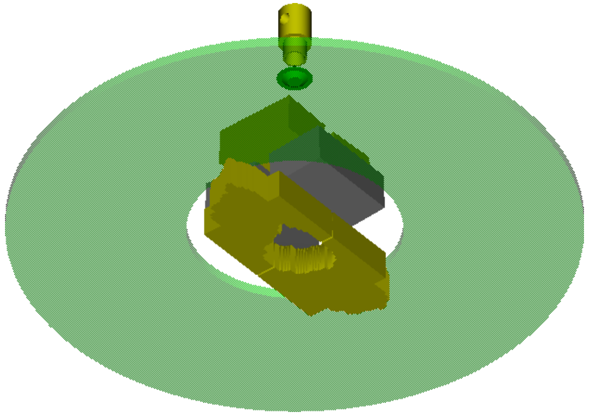
EGS5:	http://rcwww.kek.jp/research/egs/egs5.html	(KEK)
FLUKA:	http://www.fluka.org/fluka.php	(FLUKA website)
GEANT4:	http://geant4.cern.ch/	(CERN)
MCNP6:	https://mcnp.lanl.gov/	(LANL)
OpenMC:	https://docs.openmc.org/	(MIT)
PENELOPE:	http://www.nea.fr/abs/html/nea-1525.html	(NEA databank)
PHITS:	http://phits.jaea.go.jp/index.html	(JAEA)
TRIPOLI:	http://www.nea.fr/abs/html/nea-1716.html	(NEA databank)

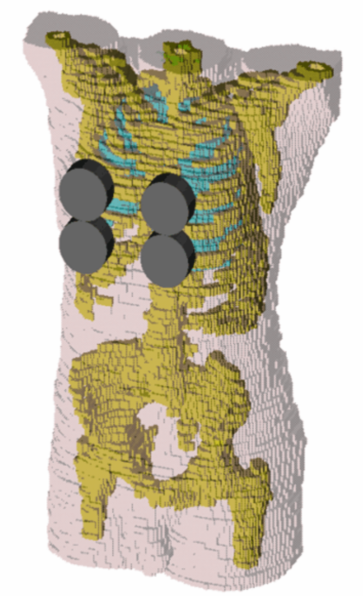
Monte Carlo codes for radiation transport simulation

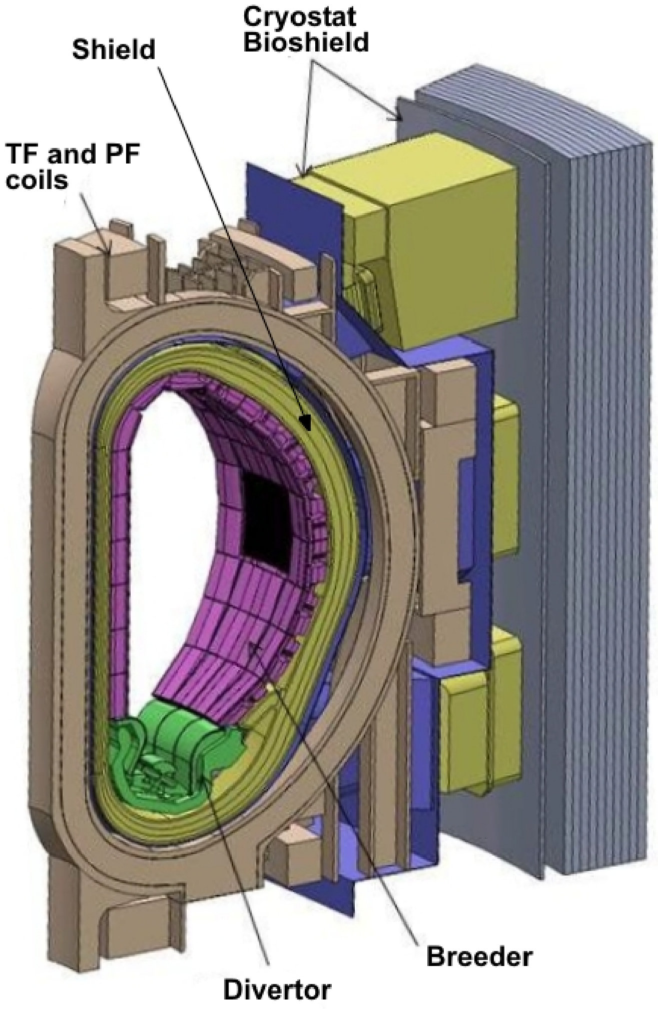
code	particles (energy range)
EGS5	photons (1 keV – 1 GeV) electrons (1 keV – 1 GeV)
FLUKA	*~ 60 different particles (up to 1 TeV, including nuclear models)*
GEANT4	~250 eV - 100 TeV [Nucl. Instrum. Meth. A 506, 250–303 (2003)]
MCNP6	photons (1 eV – 100 GeV) electrons (10 eV – 1 GeV) neutrons (0 - 150 MeV) protons (1 keV - 150 MeV) (+ 37 additional particles)
OpenMC	photons (1 keV – 20 MeV) [photoneutron reactions not yet implemented] neutrons (0 - 20 MeV)
PENELOPE	photons (50 eV – 1 GeV) electrons (50 eV – 1 GeV)
PHITS	photons, electrons (1 keV – 1 GeV; models up to 100 GeV) neutrons (thermal – 20 MeV, MCNP; models up to 200 GeV) protons, hadrons (models 1 MeV – 200 GeV) nuclei (models 10 MeV – 100 GeV)
TRIPOLI	photons (1 keV – 100 MeV) electrons (1 keV – 1 GeV) neutrons (0 – 150 MeV)



size ∼ nm (10^{-9} m)



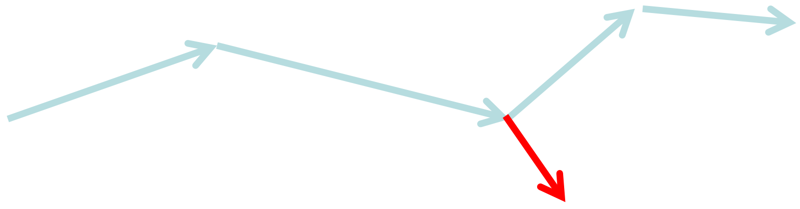




size ∼ (10^{2} m)

Ingredients

1. The theoretical «life» of a particle, a model of interactions

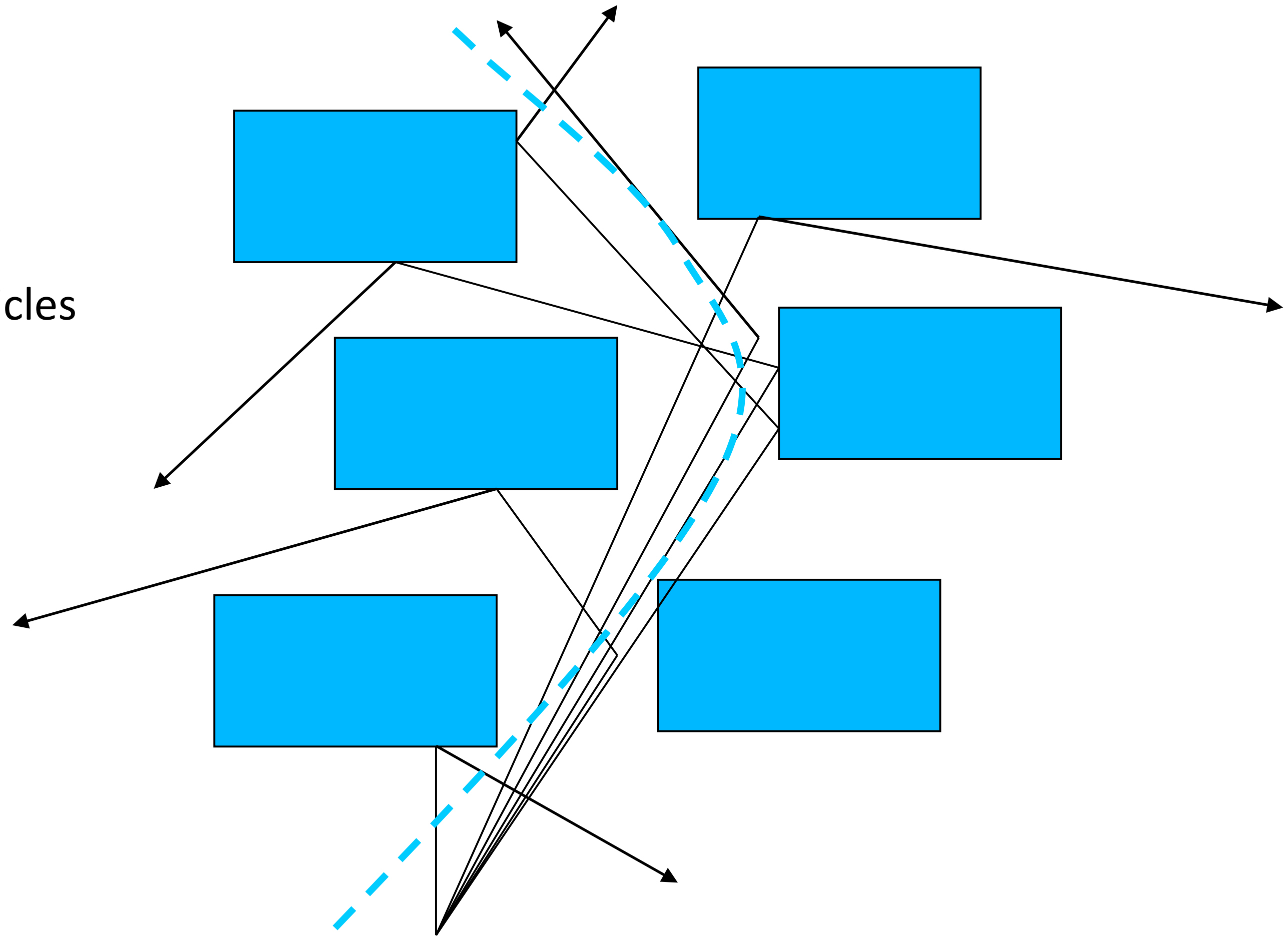


2. Practical methodology: Monte Carlo (mean of the particles «lives»).

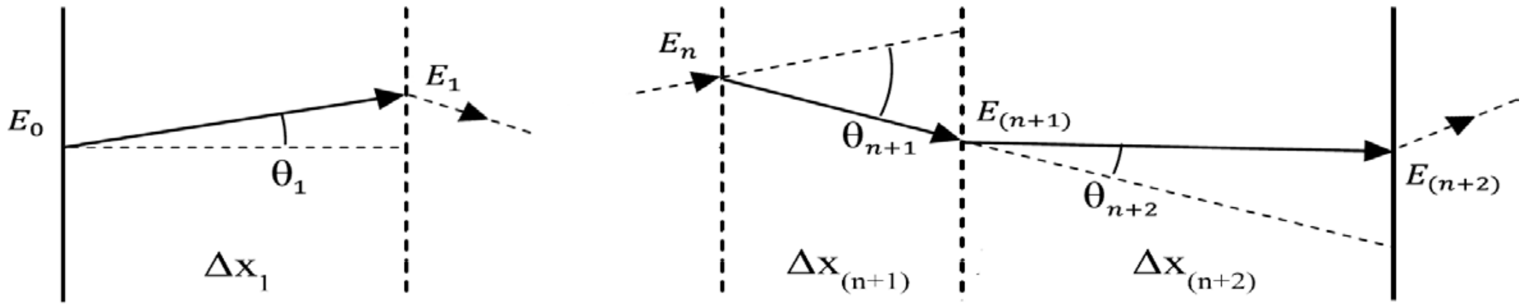
3. Random numbers generator from 0 to 1.

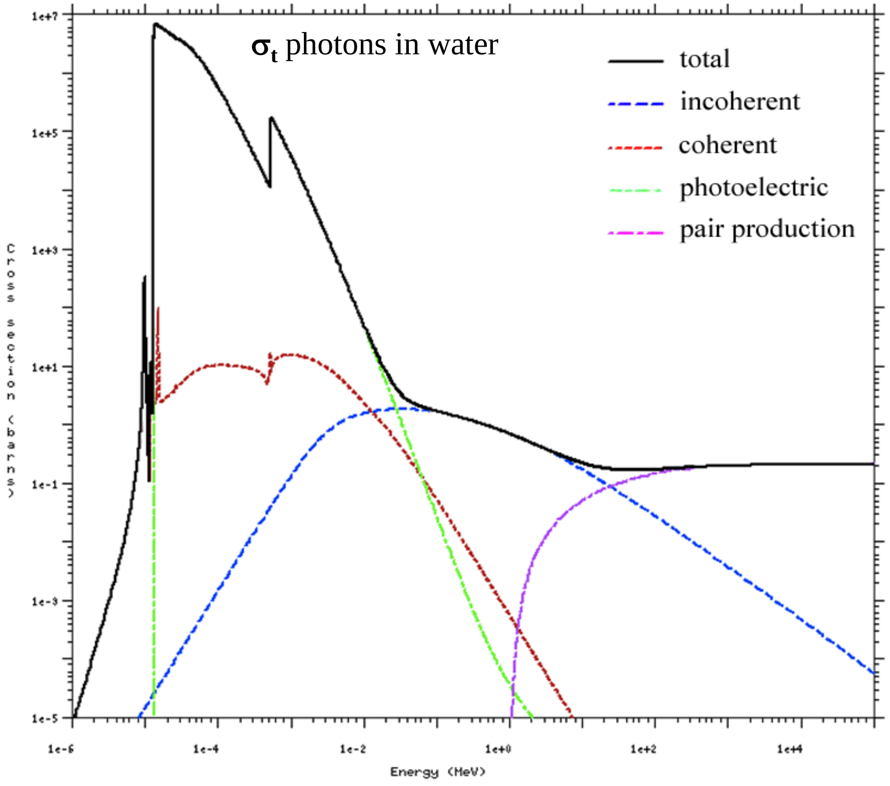
Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin.
John von Neumann (1951)

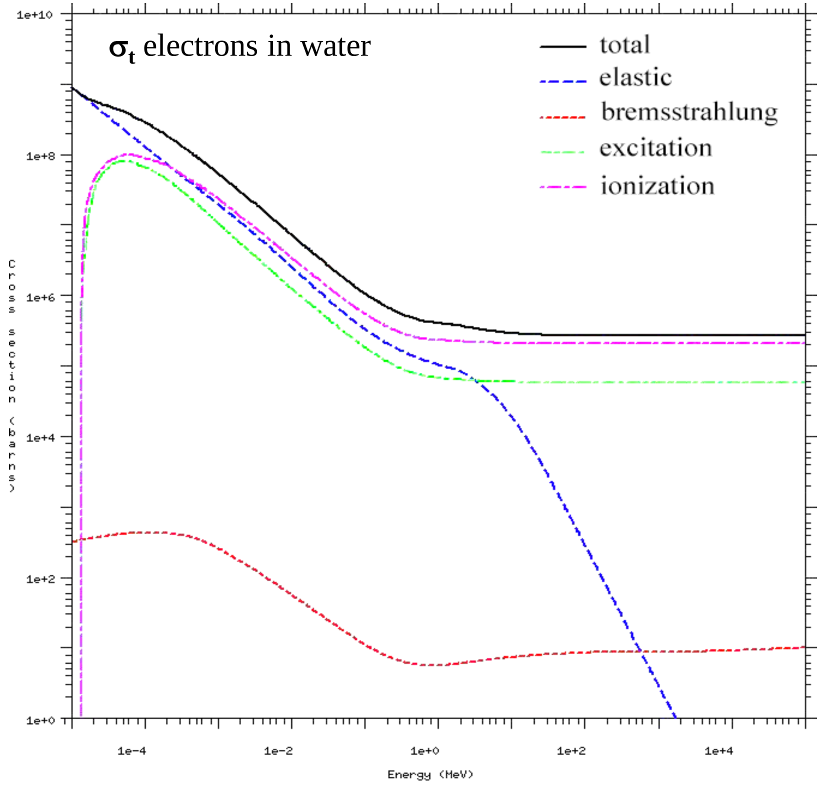
4. Data libraries associated to interactions probabilities.



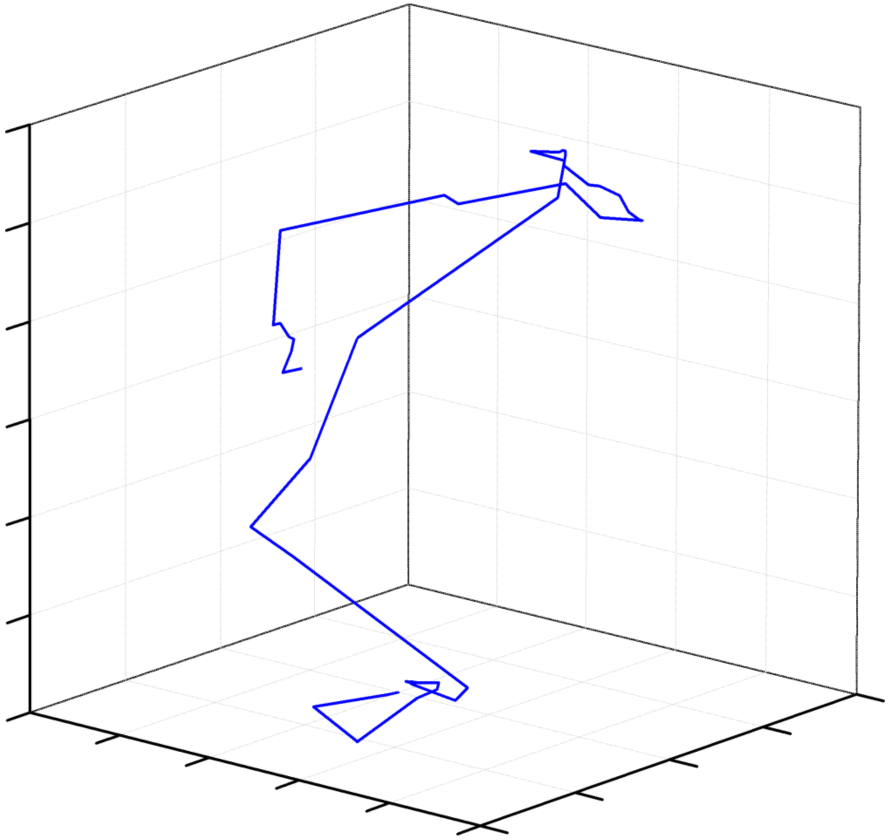
MC simulation of radiation transport



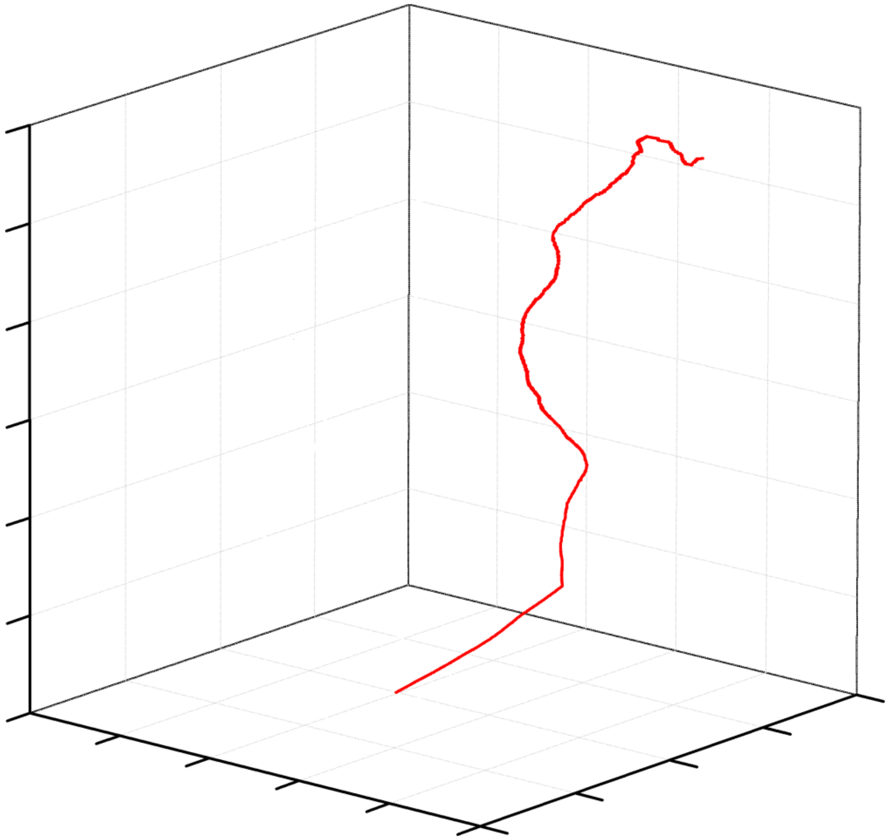




MC simulation of radiation transport

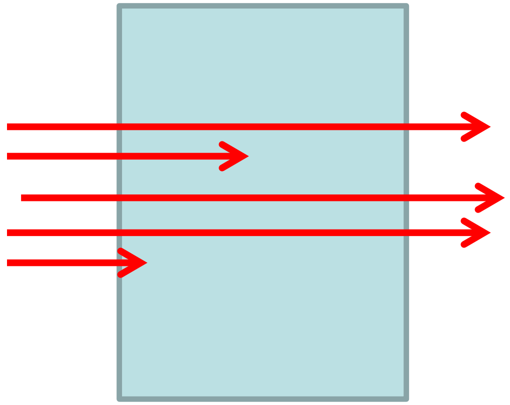


10 MeV photon in water
down to 1 keV: ∼ 20 collisions
down to 1 eV: ∼ 50 collisions



10 MeV electron in water
down to 1 keV: ∼ 90 000 collisions
down to 20 eV: ∼ 200 000 collisions

How to simulate the interaction of a photon (?)



$$\frac{I}{I_0} = e^{-\mu x}$$

Is the «surviving beam fraction»

$$P(x) = 1 - e^{-\mu x}$$

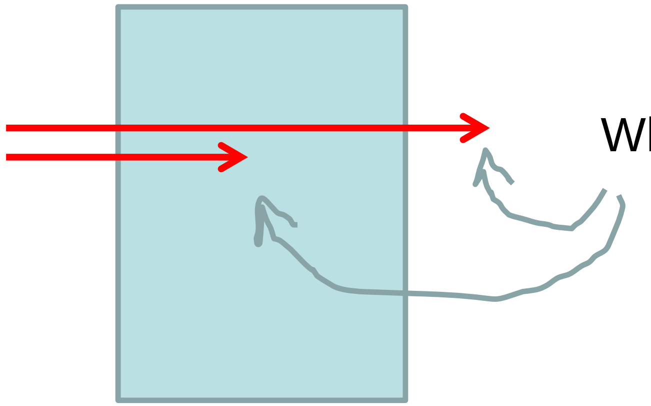
Represents the fraction of the beam that had an interaction with the material

$$r^* = 1 - e^{-\mu x}$$

r^* is extracted in the range between 0 and 1 (uniformly distributed)

$$x^* = -\frac{1}{\mu} ln(1 - r^*)$$

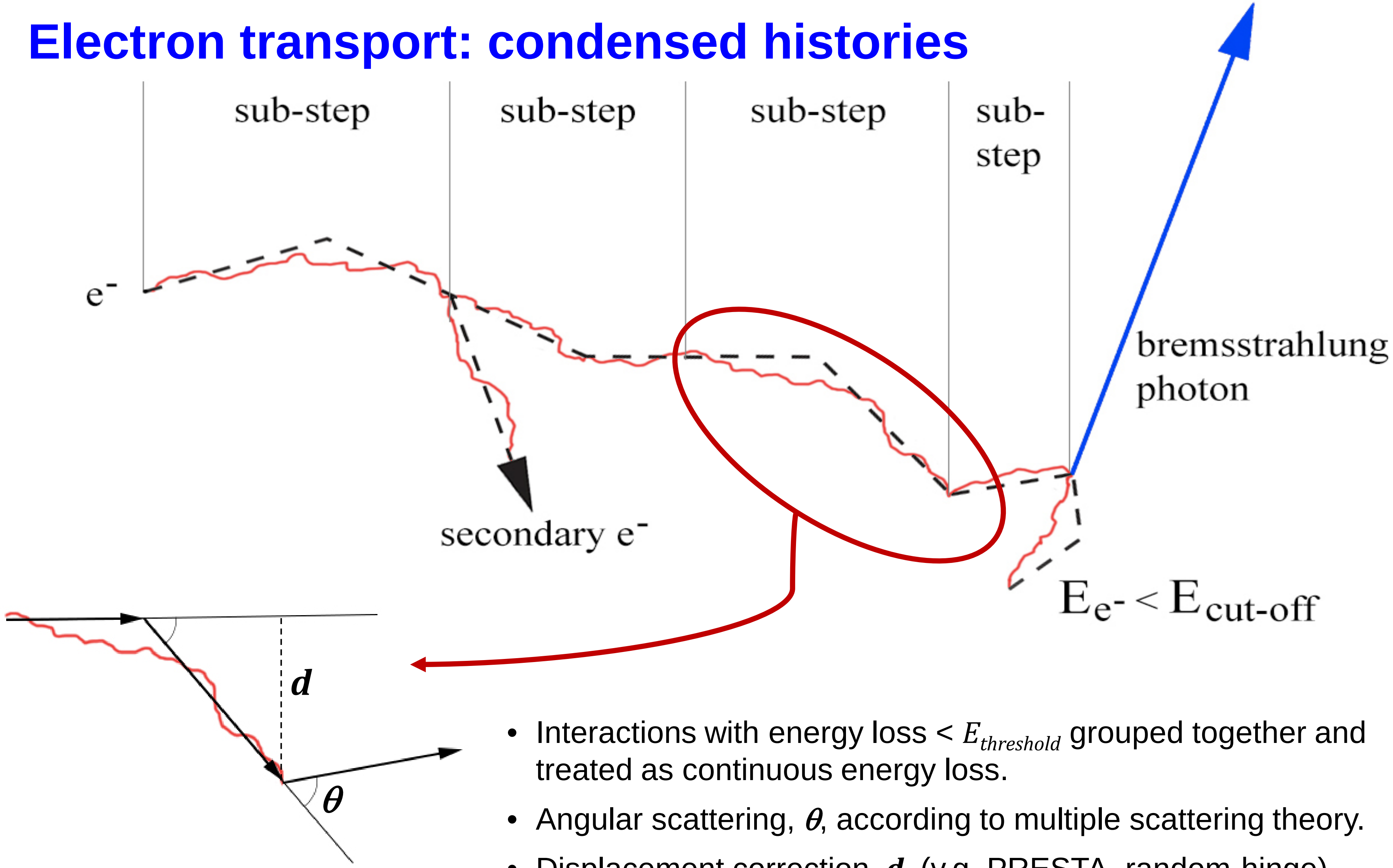
x* is the possible intersection point



Where is x*? Is it inside the material?

Yes, it is → determine the interaction and the products, check the energy
No, it isn't → the photon leaves the material unaltered.

Electron transport: condensed histories



- Interactions with energy loss < $E_{threshold}$ grouped together and treated as continuous energy loss.
- Angular scattering, θ, according to multiple scattering theory.
- Displacement correction, d, (v.g. PRESTA, random-hinge).
- “Catastrophic events” explicitly simulated.

Track length estimator of fluence, Φ

Fluence, Φ, is the quotient of dN by da, where dN is the number of particles incident on a sphere of cross sectional area da, thus (ICRU report 85, 2011):

$$\Phi = \frac{dN}{da}$$

This definition is equivalent to say that fluence is the quotient of dl by dV where dl is the sum of the lengths of particle trajectories in the volume dV:

$$\Phi = \frac{dl}{dV}$$

$$\int_V dV \Phi(\vec{r}) = V\bar{\Phi}$$

$\Phi(\vec{r})$ = fluence in $\vec{r}$

$\bar{\Phi}$ = averaged fluence in a volume V

$\bar{\Phi}(E)$ = averaged fluence between E and $E+\Delta E$ in a volume V

$$\bar{\Phi} = \frac{1}{V}\sum_j s_j$$

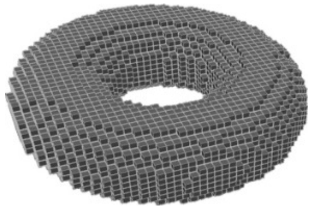
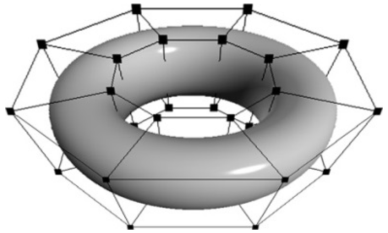
$$\bar{\Phi}(E)\Delta E \simeq \int_E^{E+\Delta E} dE' \bar{\Phi}(E') = \frac{1}{V}\sum_j s_j(E,\Delta E)$$

s_j = path length of particle j within volume V

$s_j(E,\Delta E)$ = path length of particle j within volume V and energy between E and $E+\Delta E$ (excluding rest energy)

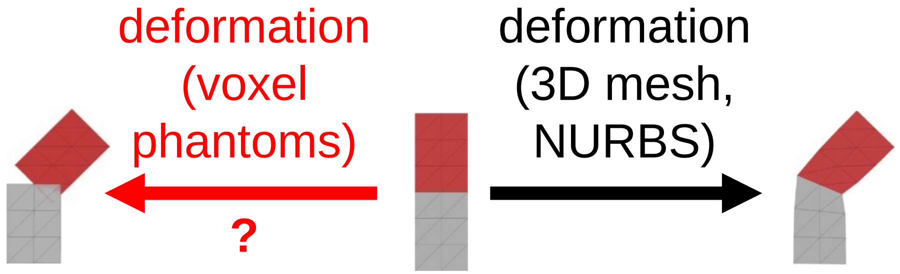
MC simulation in complex geometries

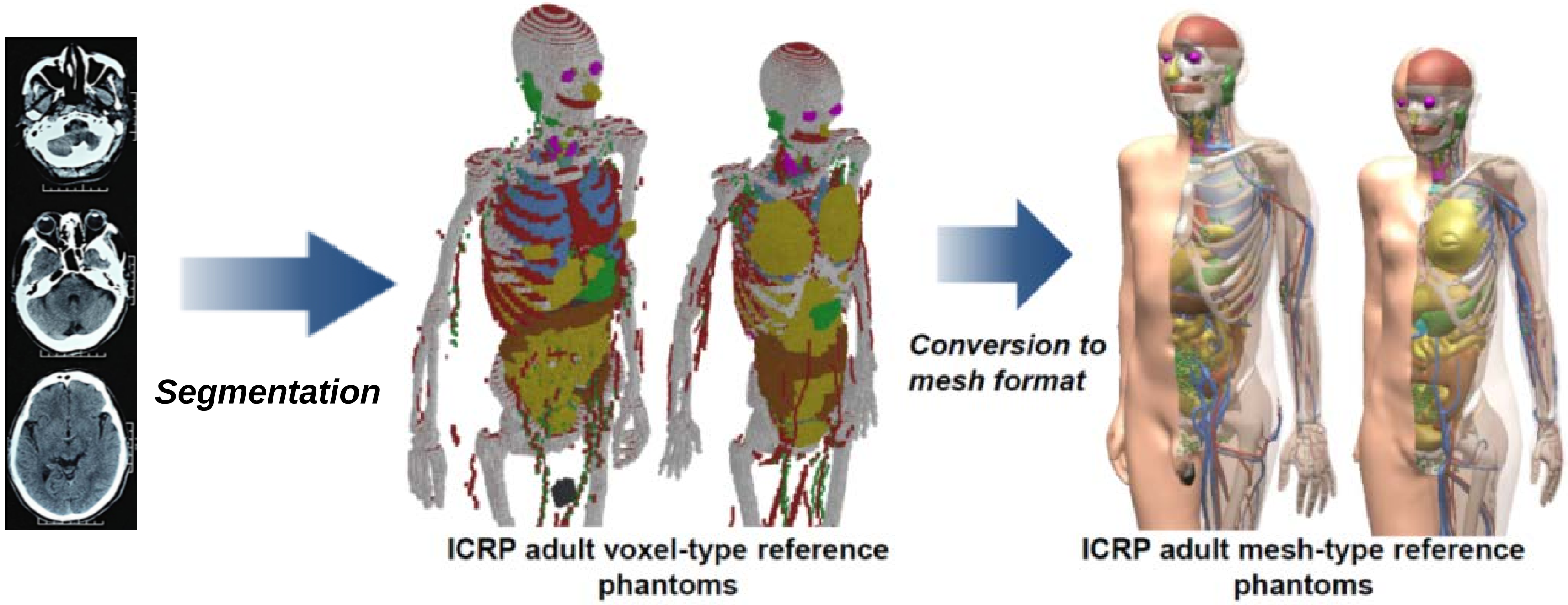
geometric model

geometrical object e.g. torus	**voxel geometry**	**3D mesh**	**NURBS**
			
$\left(R-\sqrt{x^2+y^2}\right)^2+z^2=r^2$	$N_x + N_y + N_z$ planes $x=x_i;\ y=y_j;\ z=z_k$	N tetrahedra $\leq 4N$ vértices	control points weights

Accuracy:	moderate	good	good
Complexity:	moderate	complex	complex
MC tracking:	easy	complex	?

MC simulation in complex geometries
(Ref. 13, 15, 17)





- Some organs (e.g. skin) NOT accurately represented.
- Rotations and deformations NOT allowed.

- Accurate anatomical detail.
- Rotations and deformations allowed.

Calculation of radiation protection quantities (using conversion coefficients)

$$\int f(E)\Phi_E \, dE$$

OPERATIONAL QUANTITIES (ICRU 47, ICRU 51)
- **Ambient dose equivalent, *H*(d)***
- **Personal dose quivalent, $H_p(d)$**
- **Directional dose quivalent, $H'(d,\Omega)$**

$$H^*(10) = \int \left(H^*(10)/\Phi\right)\Phi_E \, dE$$

$$H_P(10,\alpha) = \int \left(H_P(10,\alpha)/\Phi\right)\Phi_E \, dE$$

$$H'(10,\alpha) = \int \left(H'(10,\alpha)/\Phi\right)\Phi_E \, dE$$

LIMITING QUANTITIES (ICRP 103)
- **Organ equivalent dose, H_T**
- **Effective dose, *E***

$$H_T = \int \left(H_T/\Phi\right)\Phi_E \, dE$$

$$E = \int \left(E/\Phi\right)\Phi_E \, dE$$

NEW OPERATIONAL QUANTITIES (ICRU 95)
- **Ambient dose, *H****
- **Directional absorbed dose, $D'(\Omega)$**
- **Personal dose, H_P**
- **Personal absorbed dose, D_P**

$$H^* = \int h^*(E)\, \Phi_E \, dE \qquad H_p = \iint h_p(E,\Omega)\, \Phi_{E,\Omega} \, dE \, d\Omega$$

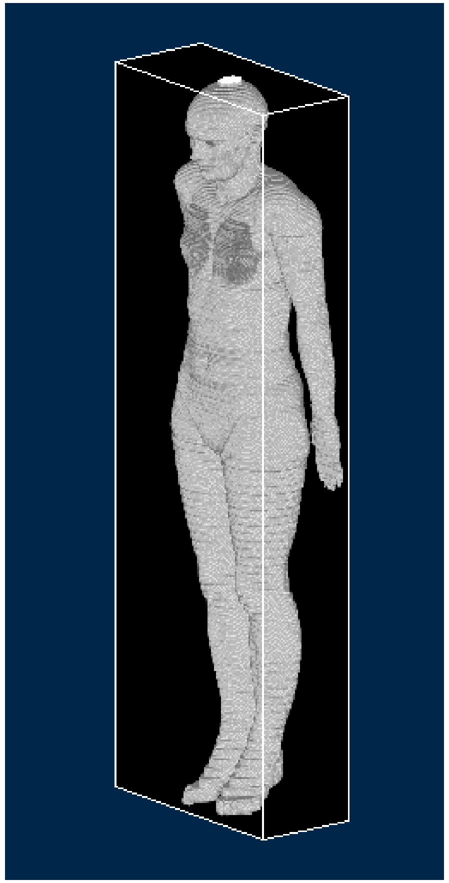
$$D'(\Omega) = \int d'(E,\Omega)\, \Phi_E(\Omega) \, dE \qquad D_p = \iint d_p(E,\Omega)\, \Phi_{E,\Omega} \, dE \, d\Omega$$

MC calculation of limiting quantities H_T and E

Equivalent dose in an organ or tissue, H_T:

$$H_T = \sum_R w_R \cdot D_{T,R}$$

$D_{T,R}$ = absorbed dose in organ T due to radiation R
w_R = weighting factor of radiation R
w_T = weighting factor of organ T



Effective dose, E:

$$E = \sum_T w_T \cdot H_T$$

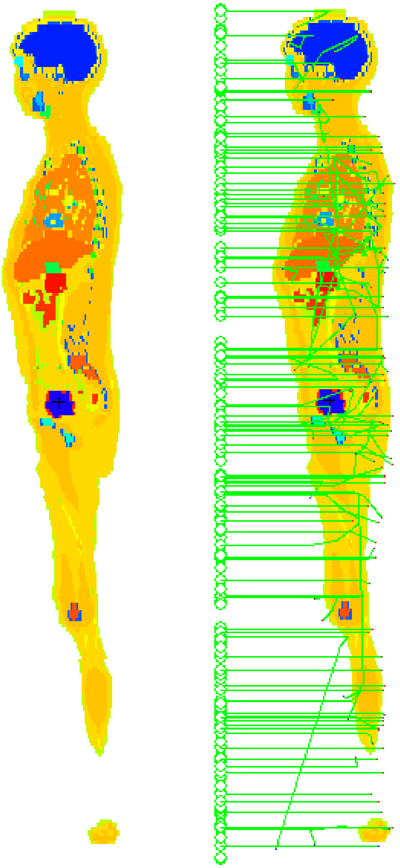
$$E = \frac{1}{2}\left\{\left(\sum_T w_T \cdot H_T\right)_{male} + \left(\sum_T w_T \cdot H_T\right)_{female}\right\}$$

AM (adult male) phantom (ICRP 110)

- Height: 1.76 m; Mass: 73.0 kg
- Number of tissue voxels: 1 946 375
- Slice thickness (voxel height): 8.0 mm
- Voxel in-plane resolution: 2.137 mm

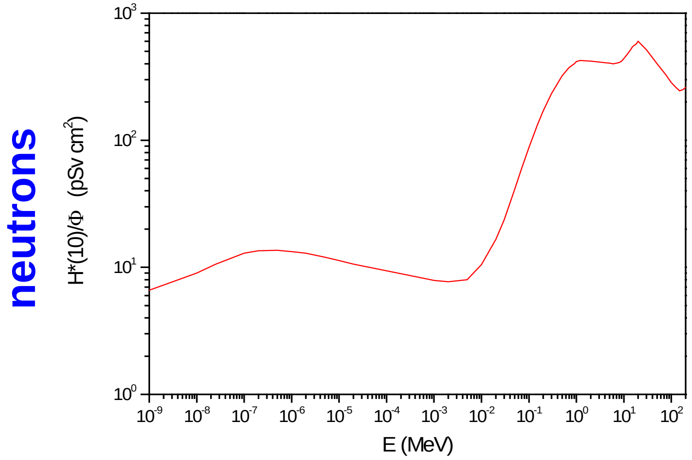
AF (adult female) phantom (ICRP 110)

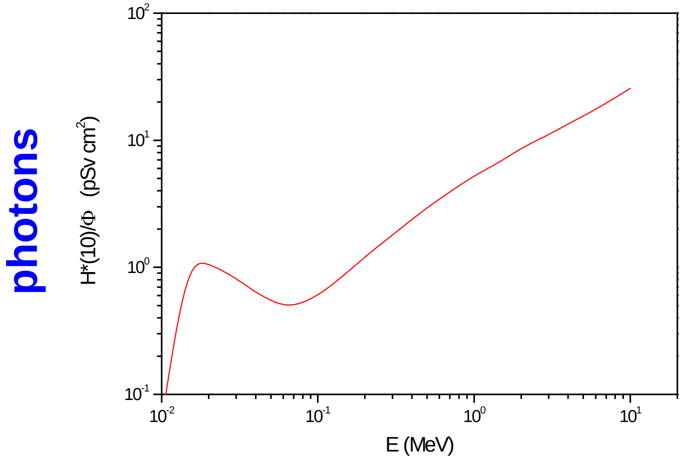
- Height: 1.63 m; Mass: 60.0 kg
- Number of tissue voxels: 3 886 020
- Slice thickness (voxel height): 4.84 mm
- Voxel in-plane resolution: 1.775 mm

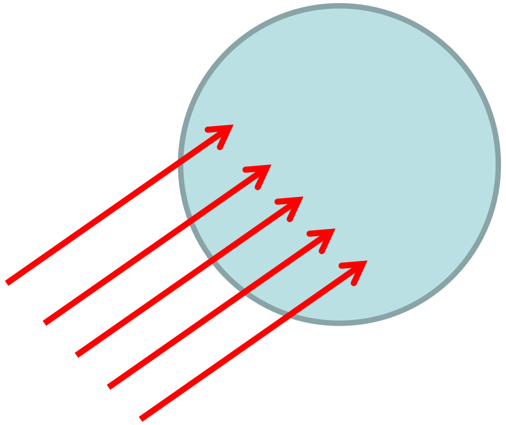


H(10)* calculation:

$$H^*(10) = \int \left(H^*(10)/\Phi \right) \Phi_E \, dE$$

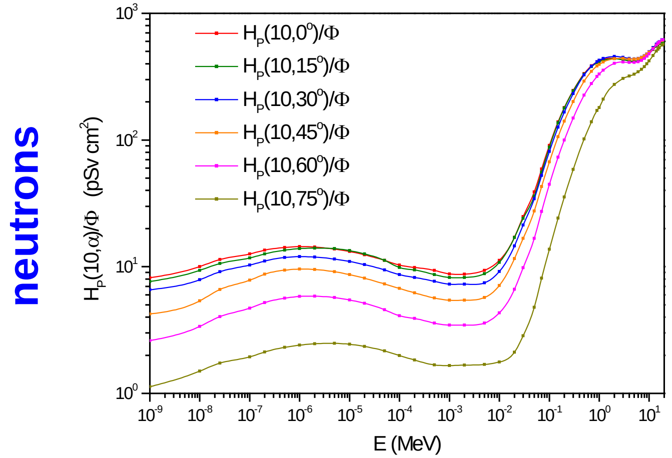


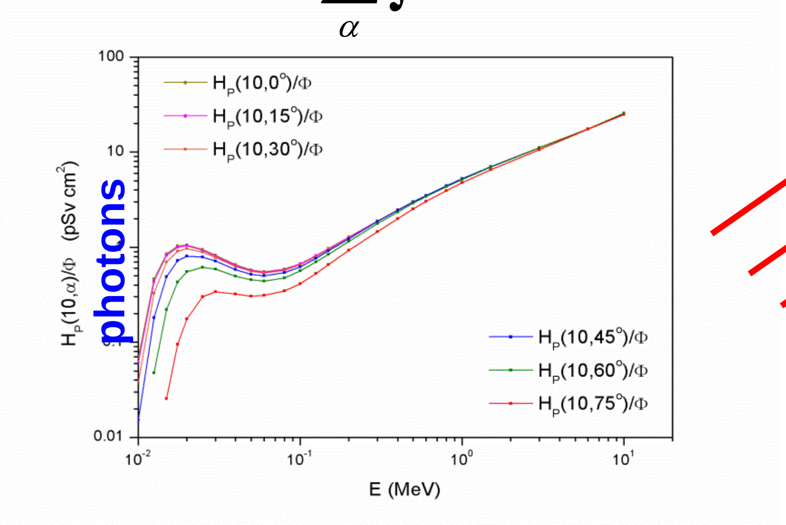


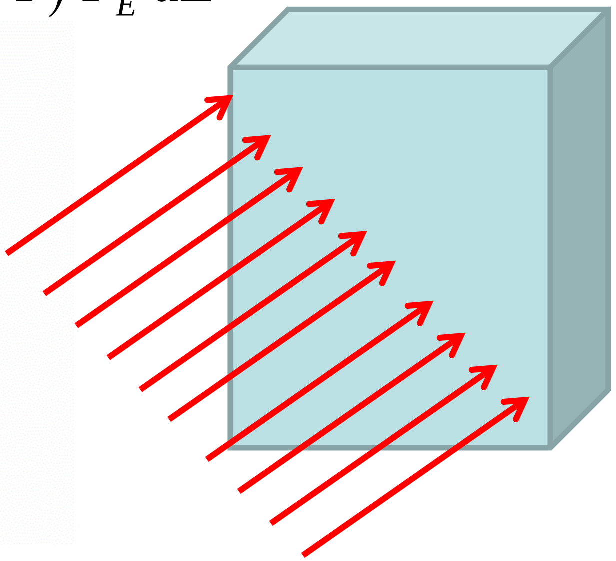


H$_p$(10) calculation:

$$H_P(10) = \sum_{\alpha} \int \left(H_P(10,\alpha)/\Phi \right) \Phi_E \, dE$$



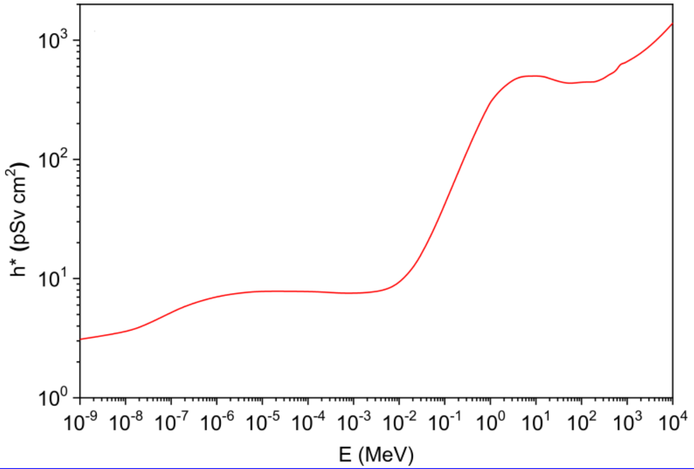




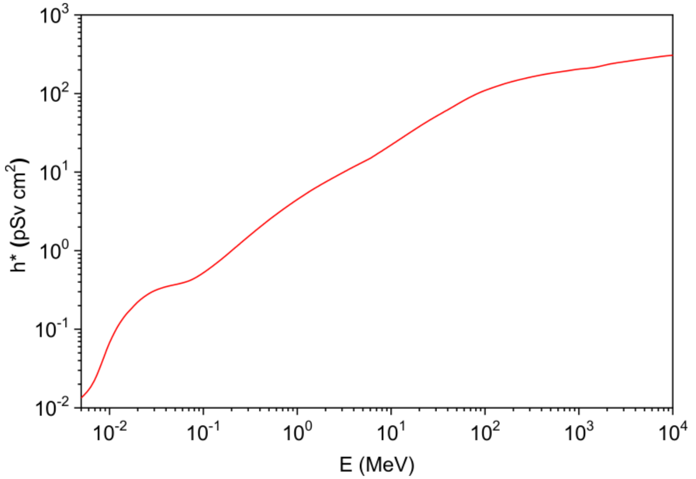
*H** calculation:

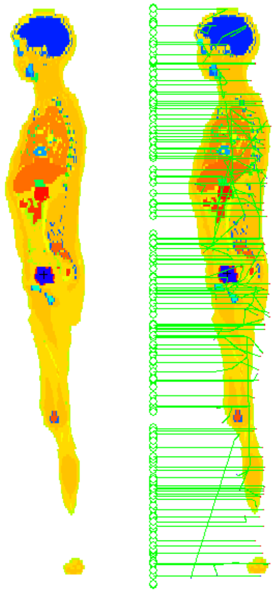
$$H^* = \int h^*(E)\, \Phi_E \, dE$$

neutrons



photons

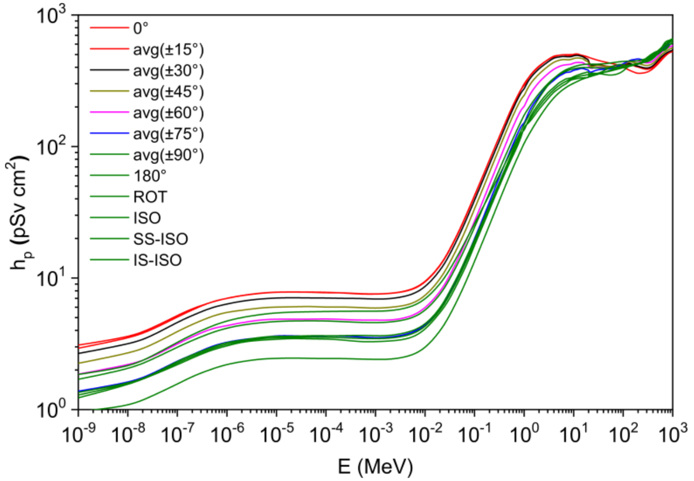




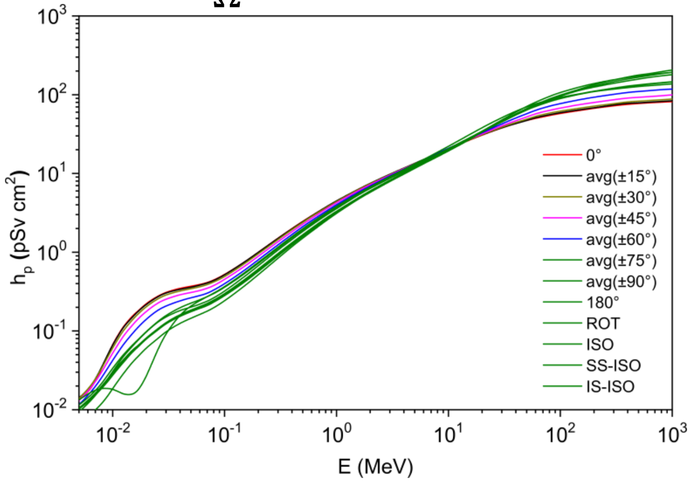
H$_p$ calculation:

$$H_p = \sum_{\Omega} \int h_p(E,\Omega)\, \Phi_E \, dE$$

neutrons



photons



MC uncertainty and variance reduction

Mean:

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

Variance:

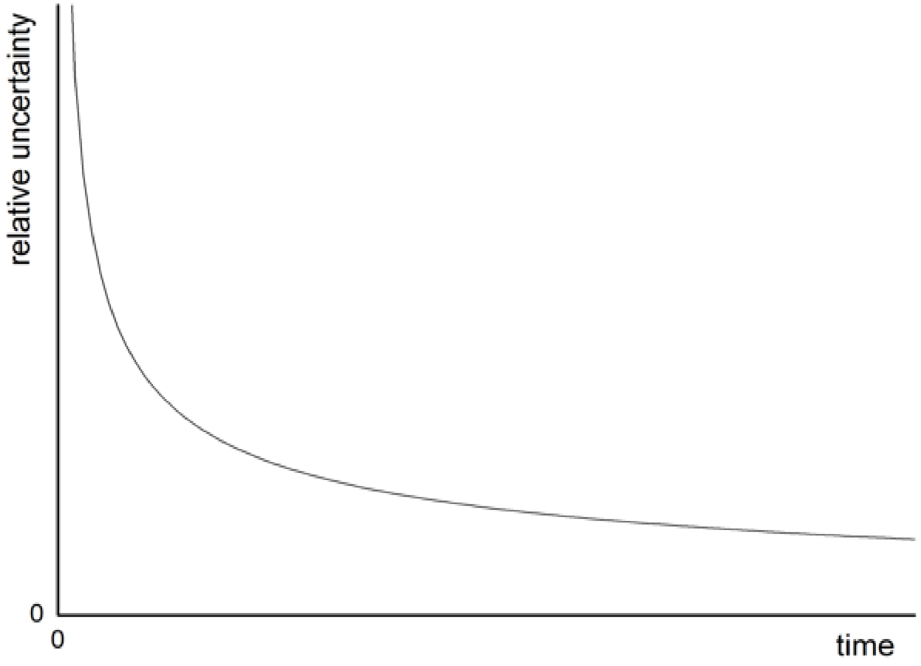
$$S_{\bar{x}}^2 = \frac{1}{N(N-1)}\sum_{i=1}^{N}(x_i - \bar{x})^2 = \frac{1}{N-1}\left[\overline{x^2} - \bar{x}^2\right]$$

Relative uncertainty (R):

$$R = \frac{S_{\bar{x}}}{\bar{x}} = \sqrt{\frac{1}{N}\left(\frac{\overline{x^2}}{\bar{x}^2} - 1\right)} \propto \frac{1}{\sqrt{N}}$$

Computing time $\propto N$

Relative uncertainty $\propto \frac{1}{\sqrt{N}}$



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