Mathematical Challenges

in Linking Simulations of Nanodosimetric Track Structure and Radiation Transport

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Disclaimer:

This talk is **not** about

- *advanced methods*
- *smart solutions.*

It is about problems and challenges calling for this methodology to be developed.

Outline

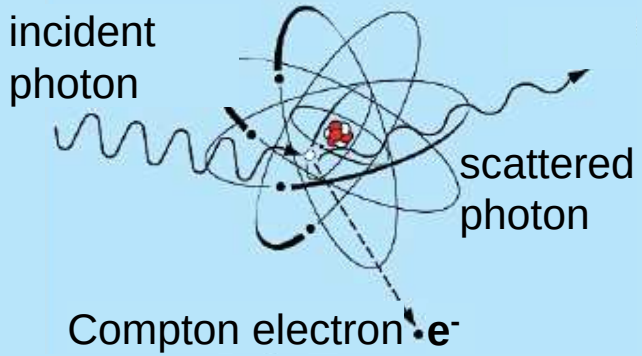
- Dosimetry of Ionizing Radiation
- Radiation Transport in Matter (Type A problems)
- Radiation Action in Matter (Type B problems)
- Challenges

Dosimetry of Ionizing Radiation

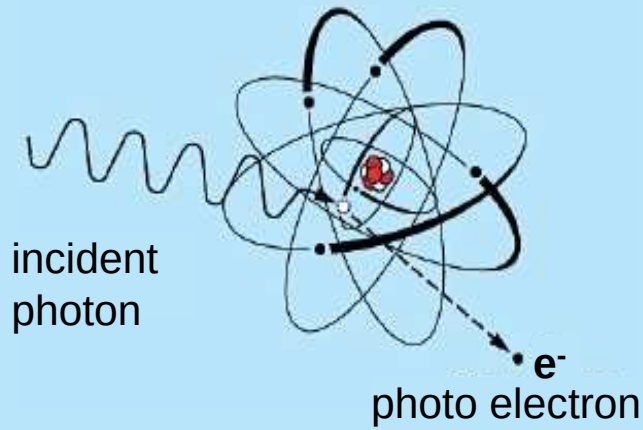
Ionizing radiation is different from optical radiation:

- *Inelastic interactions are always significant, often dominant*
- *Radiation energy is dissipated*
- *Matter state is changed*
- *Particle aspect is more appropriate than wave picture*

Compton scattering



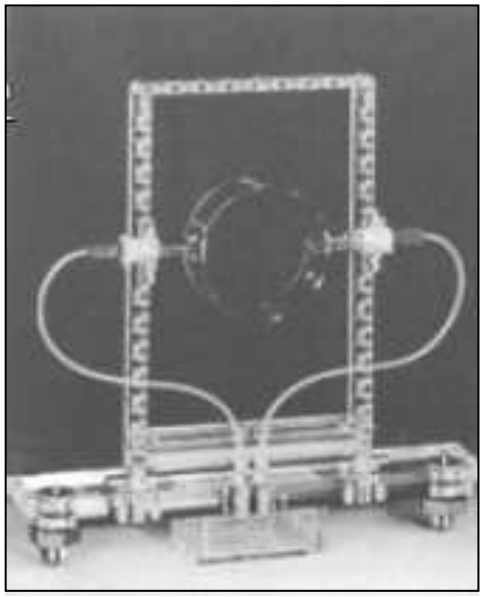
photoelectric absorption



Dosimetry of Ionizing Radiation

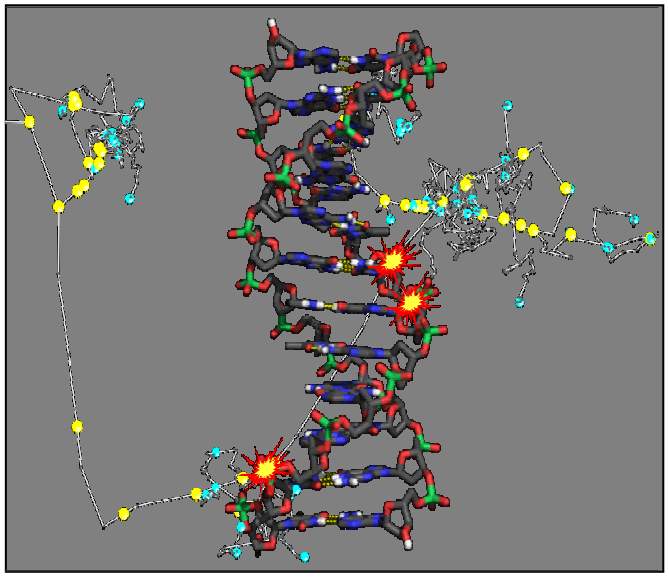
The traditional paradox of ionizing radiation metrology:

Dosimetric quantities are macroscopic averages



PTB water calorimeter

Radiation effects occur at the DNA level (Ø ≈ 2 nm)



DNA segment hit by electron track

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Radiation *Transport* in Matter (Type A problems)

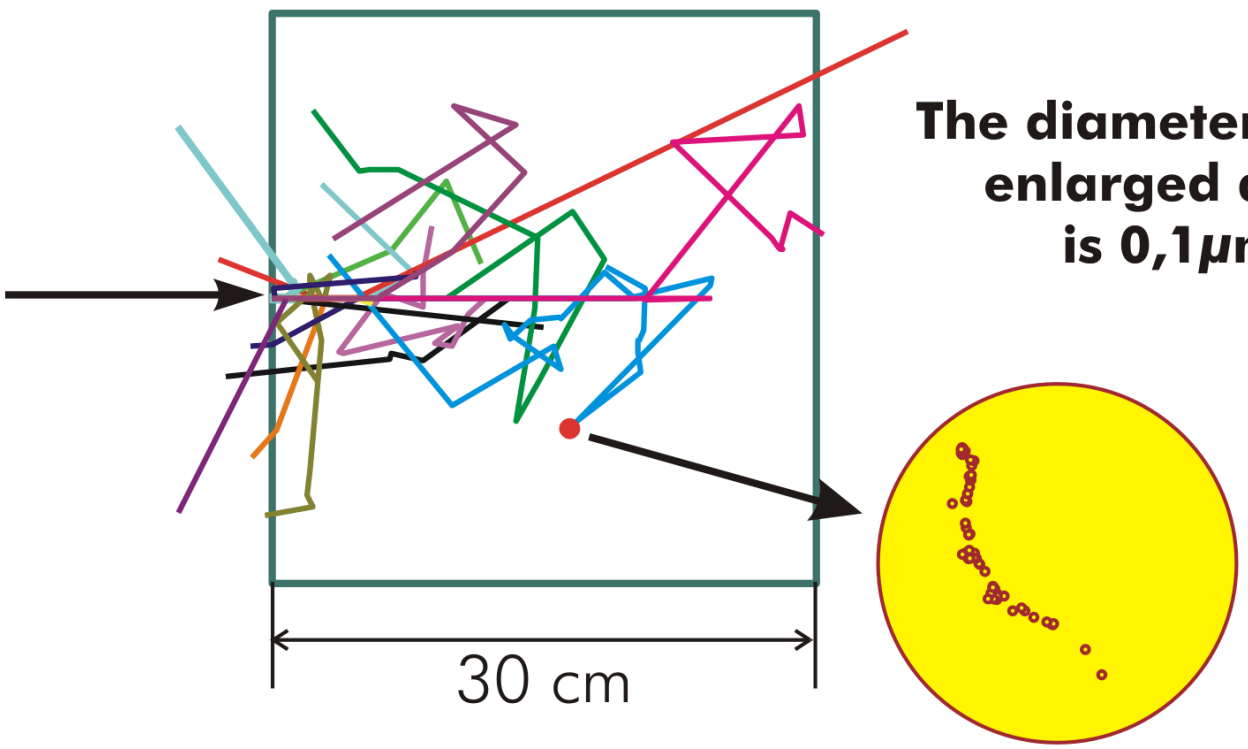
In principle, described by coupled Boltzmann equations

$$\vec{\Omega}\times\nabla\psi_\pi + \sigma_{tot}\,\psi_\pi = \sum_\nu \iint \sigma_T\left(\vec{r}\left|\begin{Bmatrix}\nu\\ E'\\ \vec{\Omega}'\end{Bmatrix}\rightarrow\begin{Bmatrix}\pi\\ E\\ \vec{\Omega}\end{Bmatrix}\right.\right)\psi_\nu\, d\vec{\Omega}'\, dE'$$

(+ source terms, if applicable)

$\psi_\pi = \psi_\pi\left(\vec{r}, t; E, \vec{\Omega}\right)$ (Probability) flux of particle type π

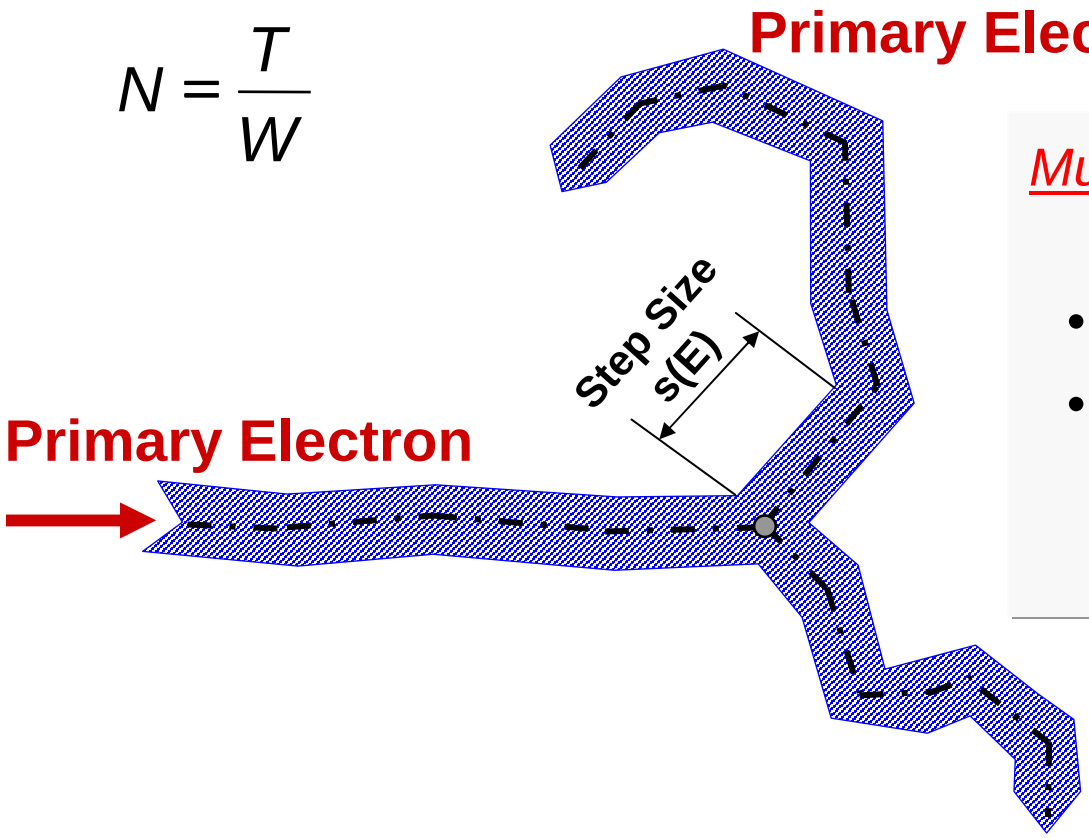
Monte Carlo Simulation of Radiation Transport
Example: Photons Entering a Water Phantom



The diameter of the enlarged area is 0,1µm

Charged Particle Track Simulation Based on Condensed Histories

$$N = \frac{T}{W}$$

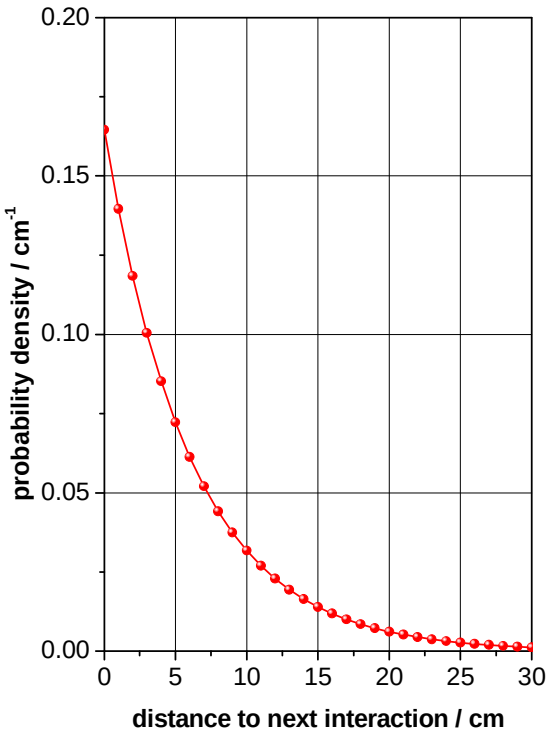


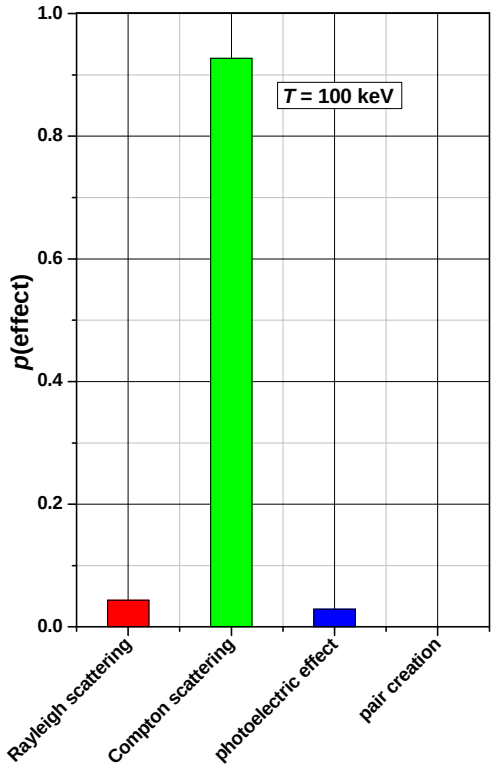
Multiple scattering theories

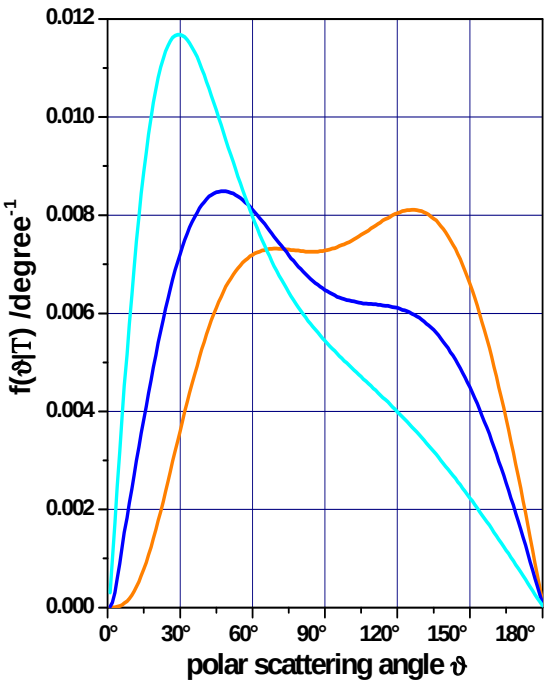
- *Energy-loss straggling*
- *Angular scattering*
  (Molière; Goudsmit and Saunderson)

Monte Carlo Simulation of a Particle Track: Sequence in Each Individual Step

Distance to the next interaction point → Type of particle interaction → New particle direction → Energy loss







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Radiation *Action* in Matter (Type B problems)

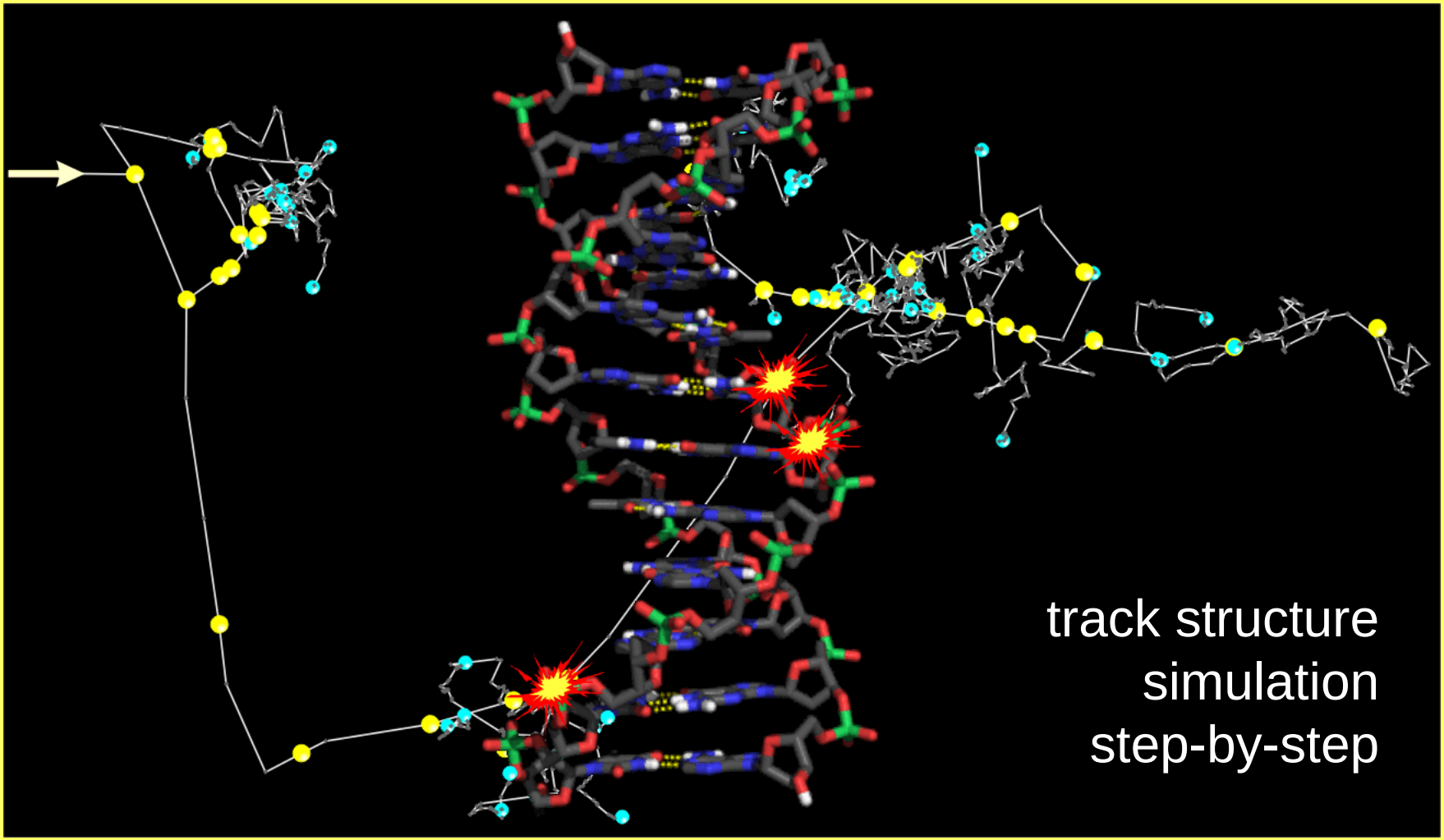
In principle, described by

$$\dot{\varepsilon}(\vec{\boldsymbol{r}},\boldsymbol{t};\mathrm{E})+\mathrm{K}[\varepsilon]=\sum_{\pi}\iiint\sigma_{\mathrm{A}}\left(\vec{\boldsymbol{r}},\boldsymbol{t}-\boldsymbol{t'};\mathrm{E}\left\|\begin{Bmatrix}\nu\\ \boldsymbol{E'}\\ \vec{\Omega}'\end{Bmatrix}\rightarrow\begin{Bmatrix}\pi\\ \boldsymbol{E}\\ \vec{\Omega}\end{Bmatrix}\right.\right)\psi_{\pi}\,\boldsymbol{d}\vec{\Omega}'\,\boldsymbol{dE'}\,\boldsymbol{dt'}$$

(chemistry & biological effects included)

$\psi_{\pi}=\psi_{\pi}(\vec{\boldsymbol{r}},\boldsymbol{t};\boldsymbol{E},\vec{\Omega})$ (Probability) flux of particle type π

Radiation Action at DNA level

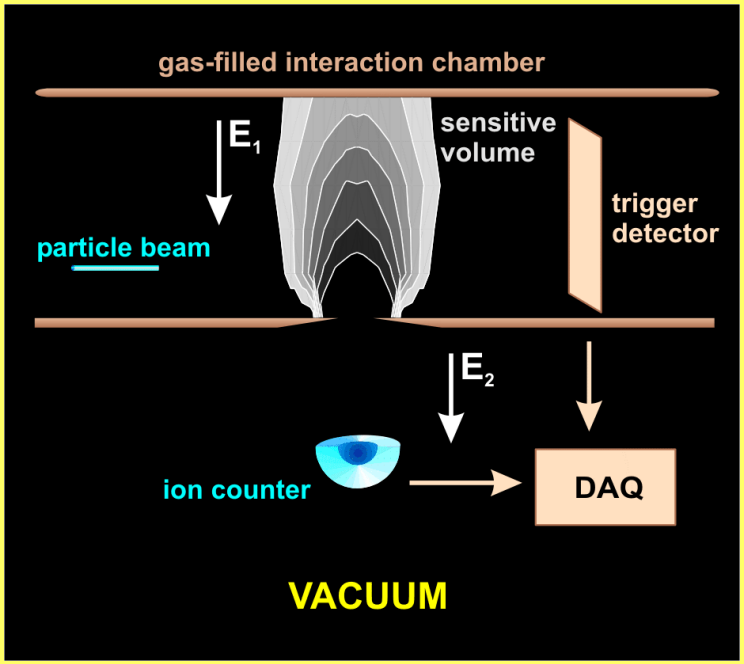


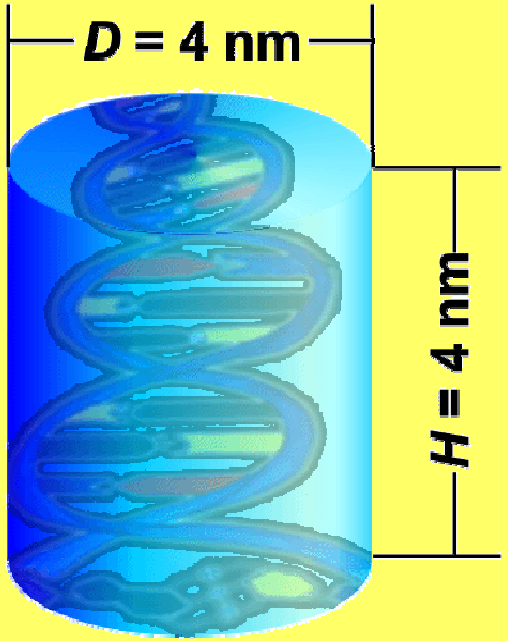
A First Step Towards a Novel Dosimetry Concept

Nanodosimetry

Measurement of track structure parameters in macroscopic gas targets

Monte-Carlo simulation for nanometric volumes („biological targets“)





Status of Nanodosimetry

- Evidence that characteristics of track structure derived from nanodosimetric probability distributions „behave“ like biological effectiveness

Missing links …

- … to macroscopic radiation transport
- … to interaction dynamics

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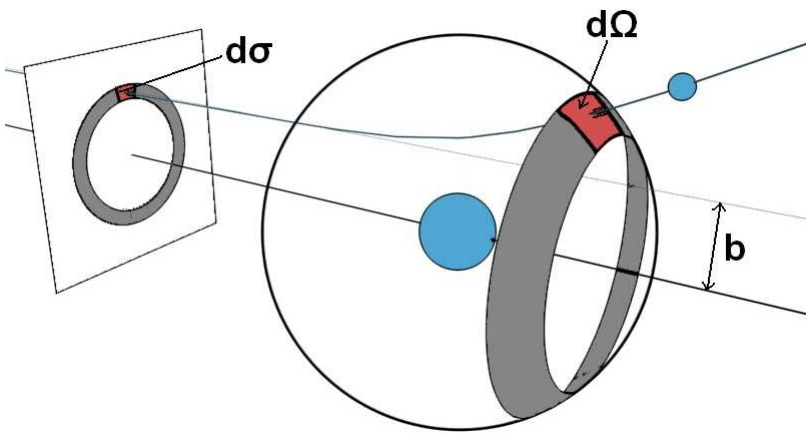
Challenges 1

- How to combine modelling of large-scale radiation transport and nanometric track structure of physical interactions?
- Interfacing Monte Carlo simulation schemes is inhibited by CPU constraints
- Is Monte Carlo the appropriate approach?

Challenges 2

- How to include femtosecond dynamics which cannot be accurately described by the interaction cross section concept.



Interaction cross-section $= \frac{d\sigma}{d\Omega}$

Outlook

- Probably both challenges can be addressed by advanced mathematical approaches
- Proposal for developing nanodosimetry-based traceability in ion beam therapy is planned for the next EMRP call “Health” that ***could need mathematical support***.