Monte Carlo Tutorial
- a hands-on 4 week course

- Outline:
  - Lecture: Introduction to MC methods
  - Lecture: Practical MC
  - Exercises set 1: FLUKA basics
  - Exercises set 2: Advanced FLUKA
  - Exercises set 3: SHIELD-HIT12A basics
  - Exercises set 4: Catch-up, SHIELD-HIT12A + TRiP98

  Requirements:

  - Laptop (ideally with some Linux distribution) registered on network
  - Plotting capabilities *(use your own favourite tool, this is course is not about data processing :)*

Monte Carlo Tutorial

Part 1 - Introduction to Monte Carlo Methods

IFJ-PAN, Cracow, May 2014

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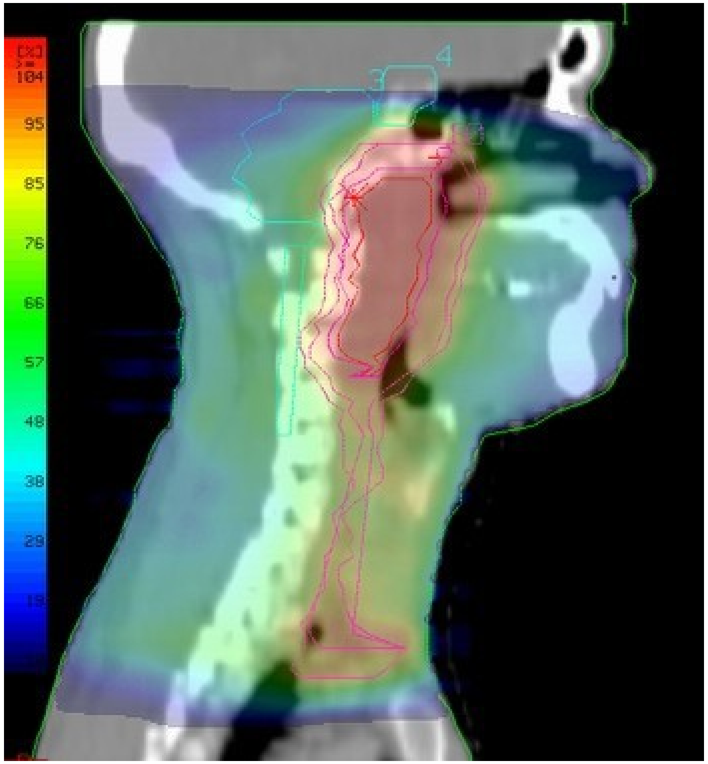
Treatment Planning

Radiation transport equation (see below) can ***only*** be solved analytically for ***simple geometries*** (paper+pencil method)

A treatment plan is not a simple geometry.

Photon, electron and ion calculation algorithms are mostly based on simple superposition of **pre-calculated dose kernels.**

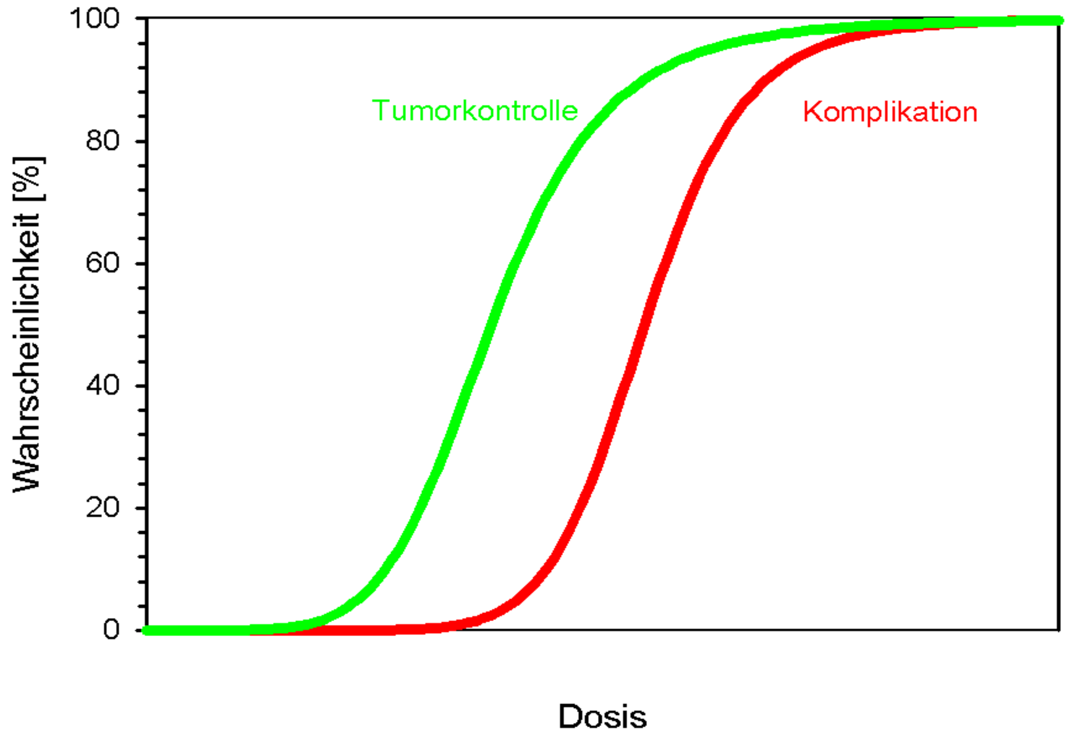
Problems:
• Dose at ***steep density gradients*** are not well simulated, due to incorrect treatment of scattering (air cavities, metal implants)
• Dose to water is calculated, which is different from the actual ***dose to medium***
• Some algorithms fail when (T)CPE cannot be applied



$\nabla \cdot \vec{\Phi}$ =net flow out

$$\nabla\cdot\dot{\vec{\Phi}} = -\int_{4\pi} d\Omega \int_{T_{cut}}^{\infty} dT\, \mu(T,\vec{\Omega})\,\Phi_{T,\Omega} + \int_{4\pi} d\Omega \int_{T_{cut}}^{\infty} dT \int_{4\pi} d\Omega' \int_{T_{cut}}^{\infty} dT'\, \mu_{T,\Omega}(T',\Omega';T,\Omega)\,\Phi_{T',\Omega'} + \int_{4\pi} d\Omega \int_{T_{cut}}^{\infty} dT\, S_{T,\Omega}$$

The need for Precision and Accuracy



TCP = Tumour Control Probability

NTCP = Normal Tissue Complication Probability

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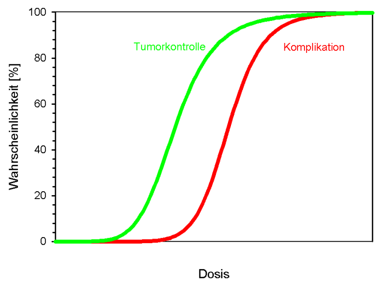
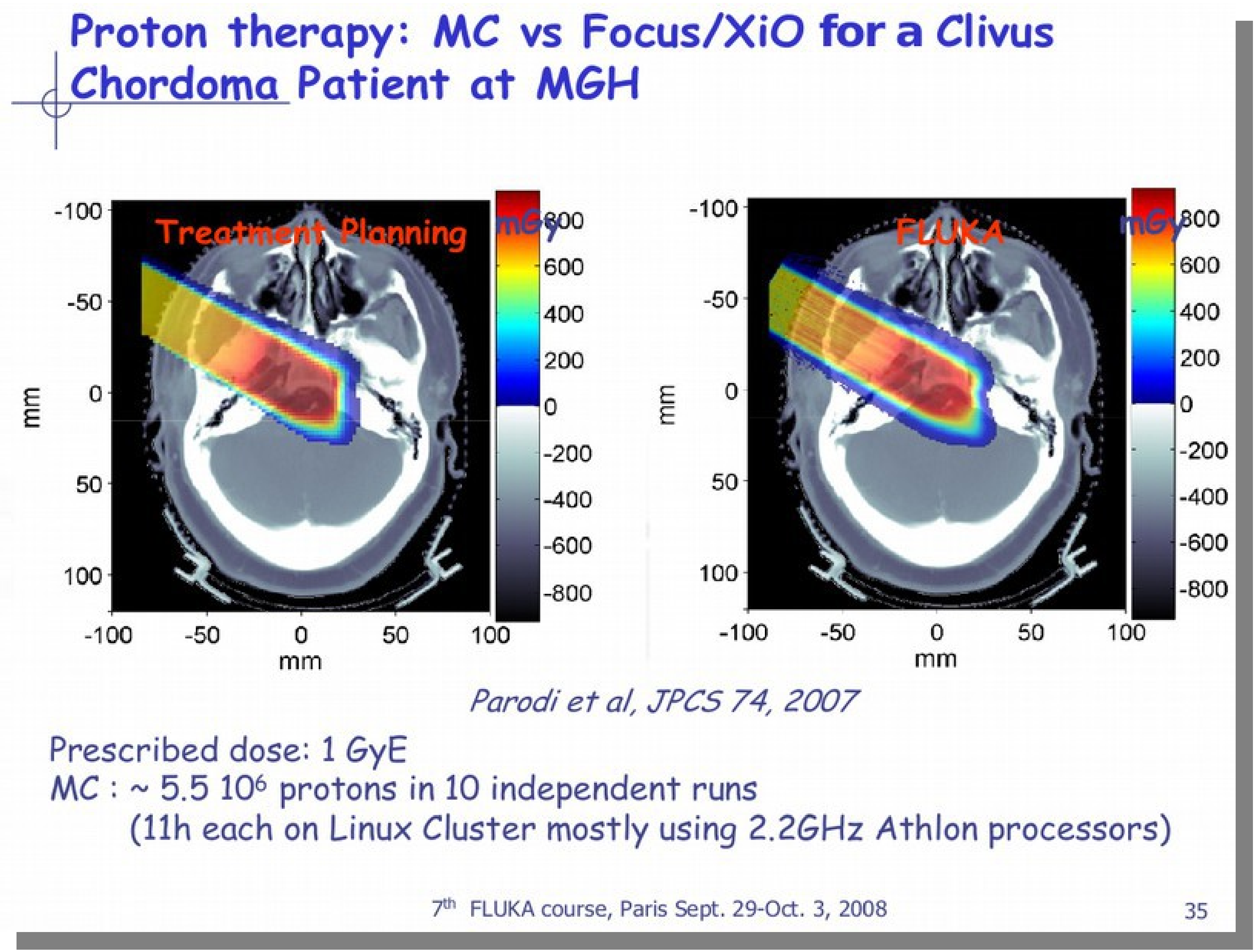
Rationale for MC treatment planning

- AAPM report #85 (Papanikolau et al 2004)
  - Due to steep slope of TCP and NTCP a 5% dose error can lead to a TCP change of 10-20% and worse for NTCP.
  - Prescribed → delivered dose, ~ 5% (1σ)
  - Improving dose engine, better than 3% (1σ)



- Tissue heterogeneities
  - Conventional superposition/convolution techniques give 5-10% deviations in heterogeneity (Mohan et al 1997) (e.g. lung), seen 15% for electrons (Ma et al 1999)

MC – Tissue Heterogeneity



Dosimetry

- Tools for determination of dose:

- **Experimental**
  - Ionisation chambers
  - Solid state detectors
  - Calorimetry
  - Chemical dosimeters
  - etc. etc

- **Calculation tools**
  - Paper and pencil (analytical)
  - Exact numerical solution
  - Pencil beam / collapsed cone
  - Monte-Carlo codes

Calculation tools are also needed to establish necessary correction factors for dosimetry, e.g.:

- stopping power ratios,
- fluence correction factors,
- relative effectiveness

are **dependent** on the charged particle **fluence** spectrum

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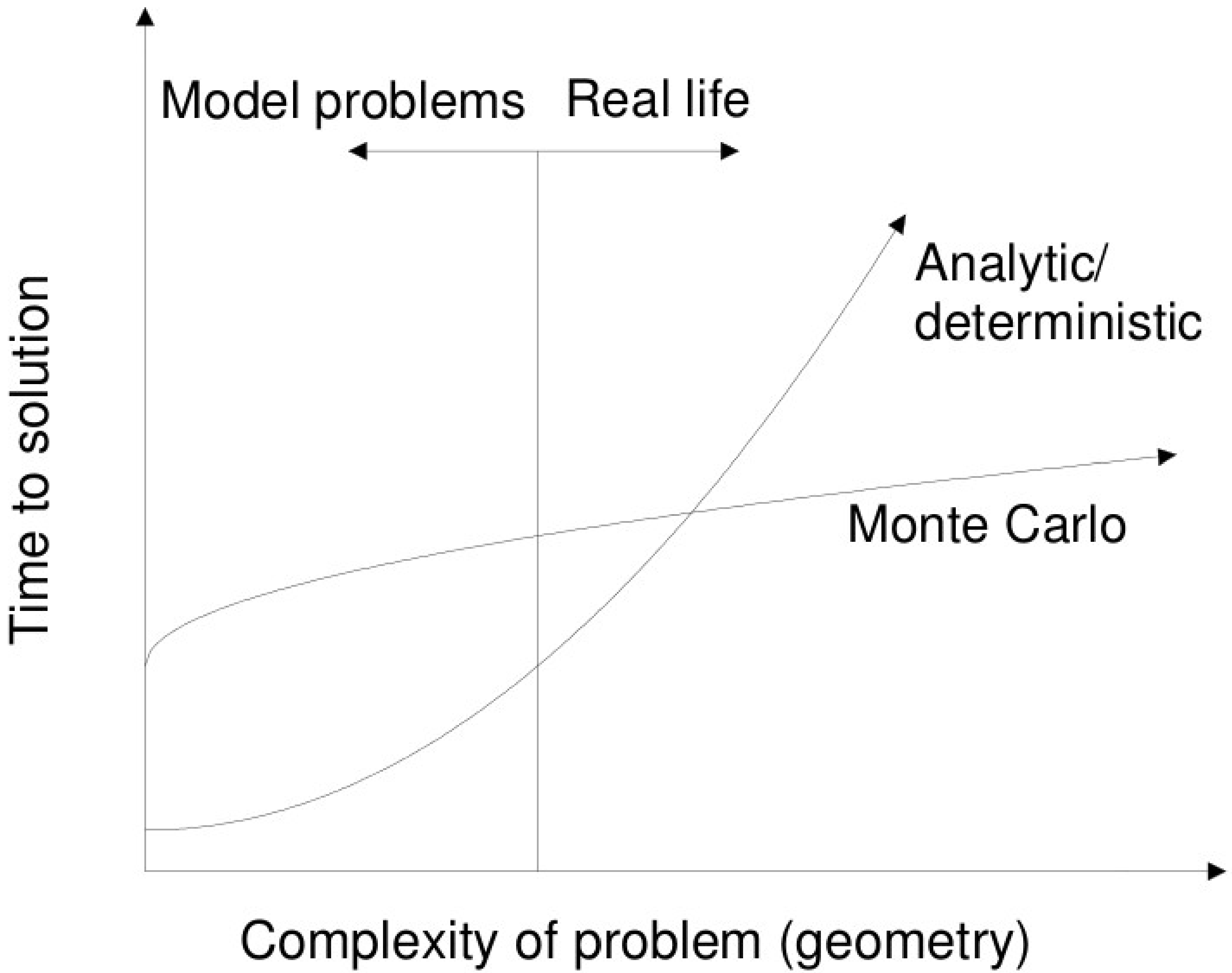
Monte Carlo Algortihms

- Often pencil+paper or **analytical** calculations are impossible, e.g.:
  - when CPE does not apply
  - when geometries are complicated
  - dealing with fluence spectra
- **Numerical** calculations becomes quickly be impossible due to *many degrees of freedom* in complex geometries and multitude of physics models
- **Monte Carlo** (MC) techniques can help
  - Idea by E. Fermi and S. Ulam while they worked with shielding (?) at Los Alamos
  - MC particle transport: follow particle and interaction histories, when plenty, it simulates real life
  - == solving the radiation transport equation with MC methods!
  - Widespread use limited by ***computing power***

Monte Carlo *vs* deterministic/analytic methods



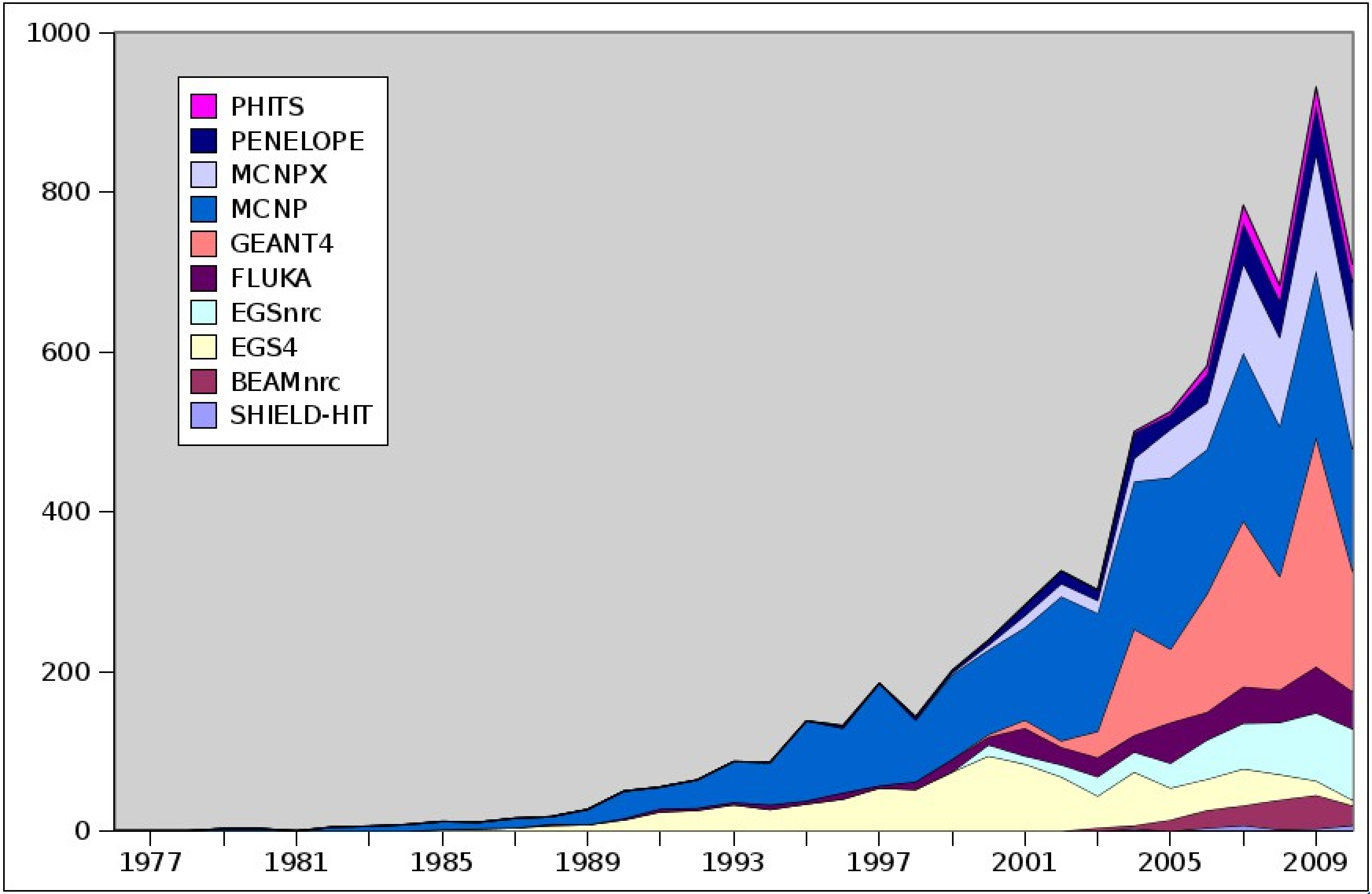
(Bielajew)

Common MC Codes

- Photons & Electrons only
  - EGS4, EGSnrc, BEAMnrc (National Research Council of Canada)
  - Penelope (Facultat de Fisica (ECM), Universitat de Barcelona)
  - MCNP (including neutrons)
- Photons & Electrons + Ions
  - FLUKA (CERN)
  - Geant4 (CERN)
  - PHITS (Japan Atomic Energy Agency)
  - MCNPX (Los Alamos National Laboratory)
- Ions only:
  - SHIELD(-HIT) (Institute for Nuclear Research RAS)

Common MC Codes in Use

Number of publications *ISI Web of Knowledge*



Year

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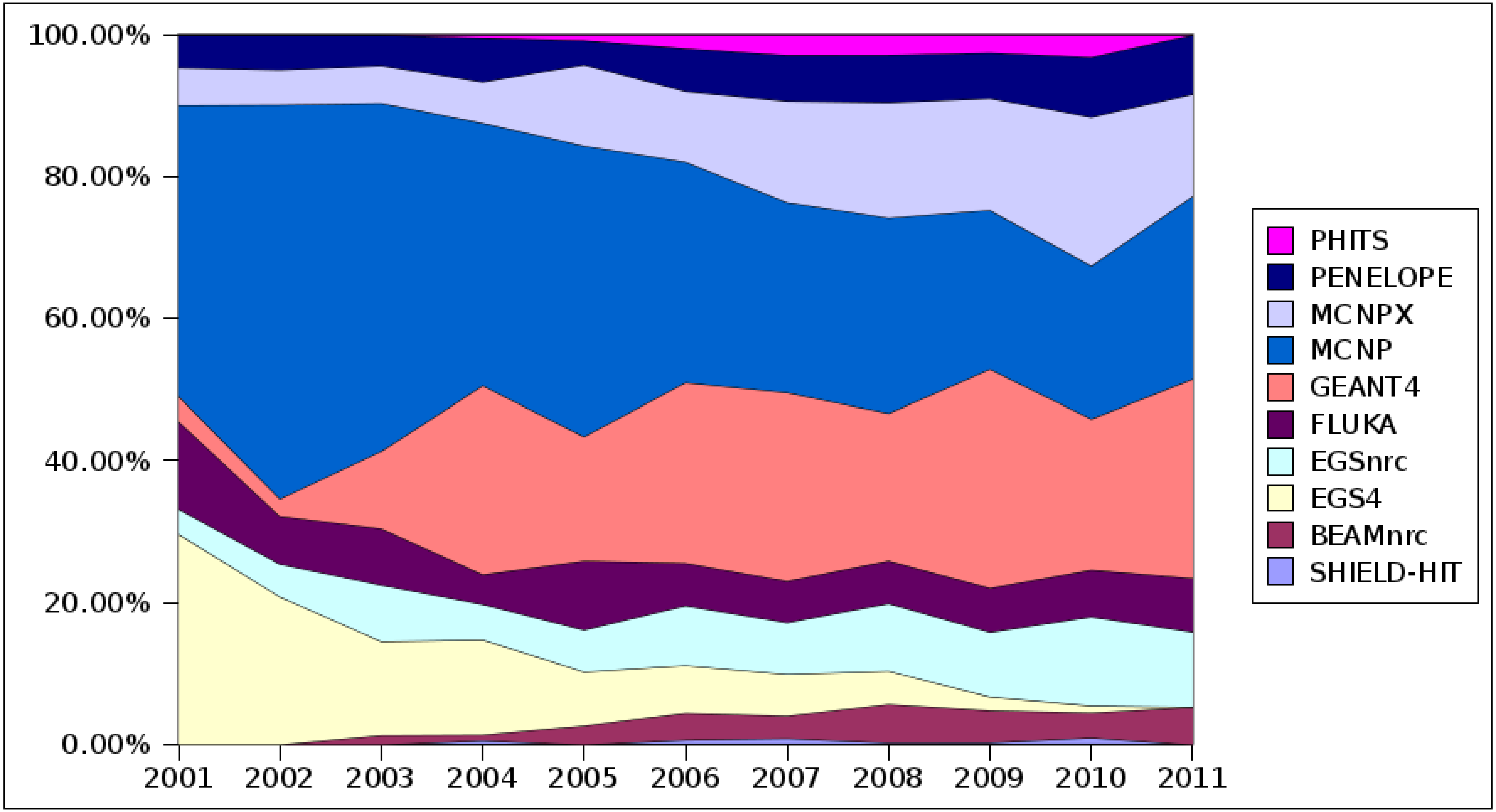
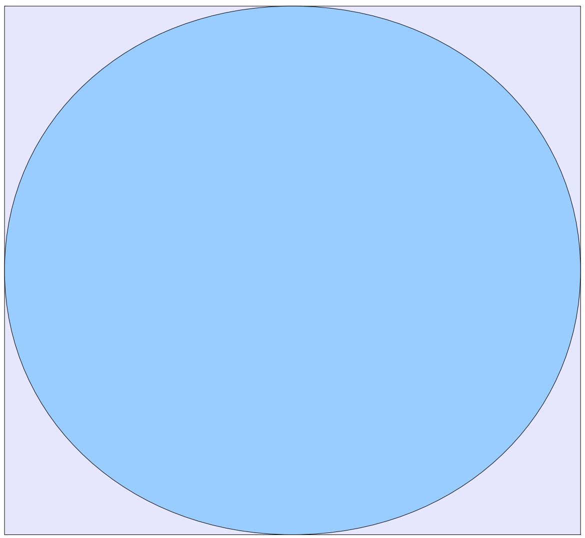
Common MC Codes in Use



Monte Carlo Techniques

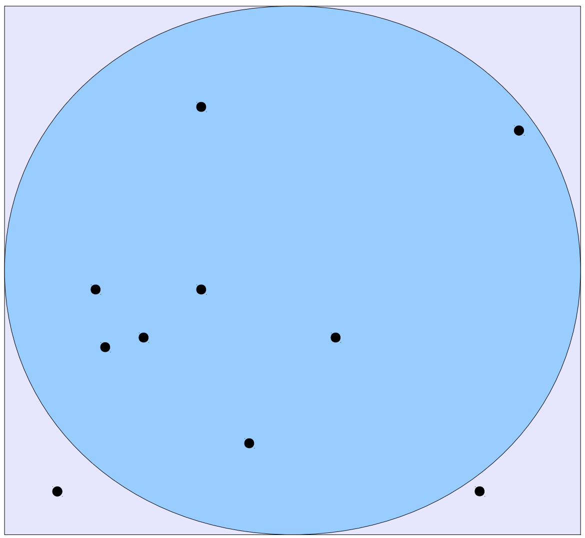
Throwing Darts



Area of square = $(2r)^2$
Area of circle = πr^2

Ratio of areas circle/square
= $\pi/4$ = 0.785398...

Throwing Darts



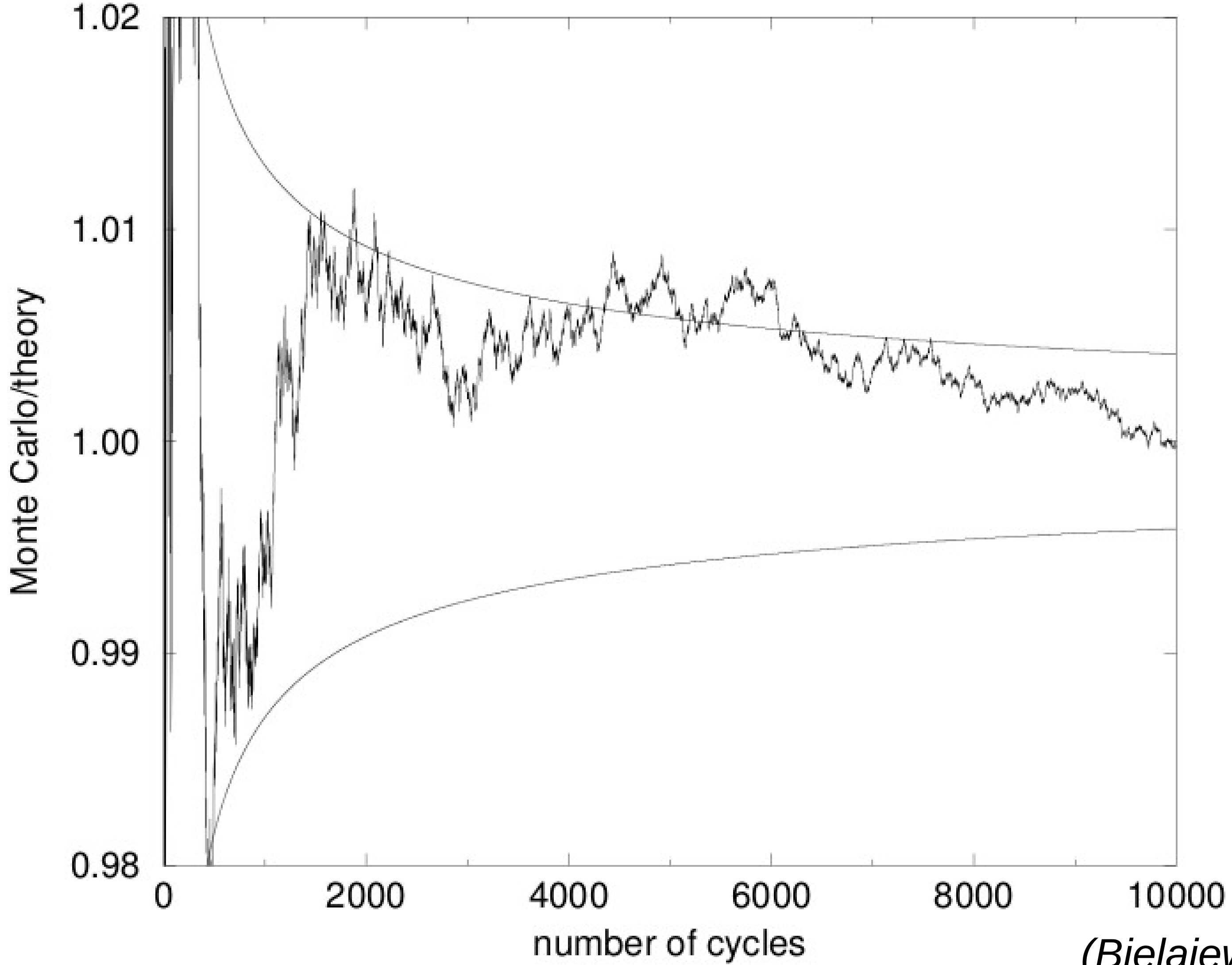
Area of square = $(2r)^2$
Area of circle = πr^2

Ratio of areas circle/square
= $\pi/4$ = 0.785398...

Throwing N = 10 darts
8 inside circle, 10 inside square → 8/10 = 0.800...

increase N for more precision

Monte Carlo determination of π



Error has slow convergence:

1/sqrt(N)

Need to quadruply N in order to reduce error by factor of 2.

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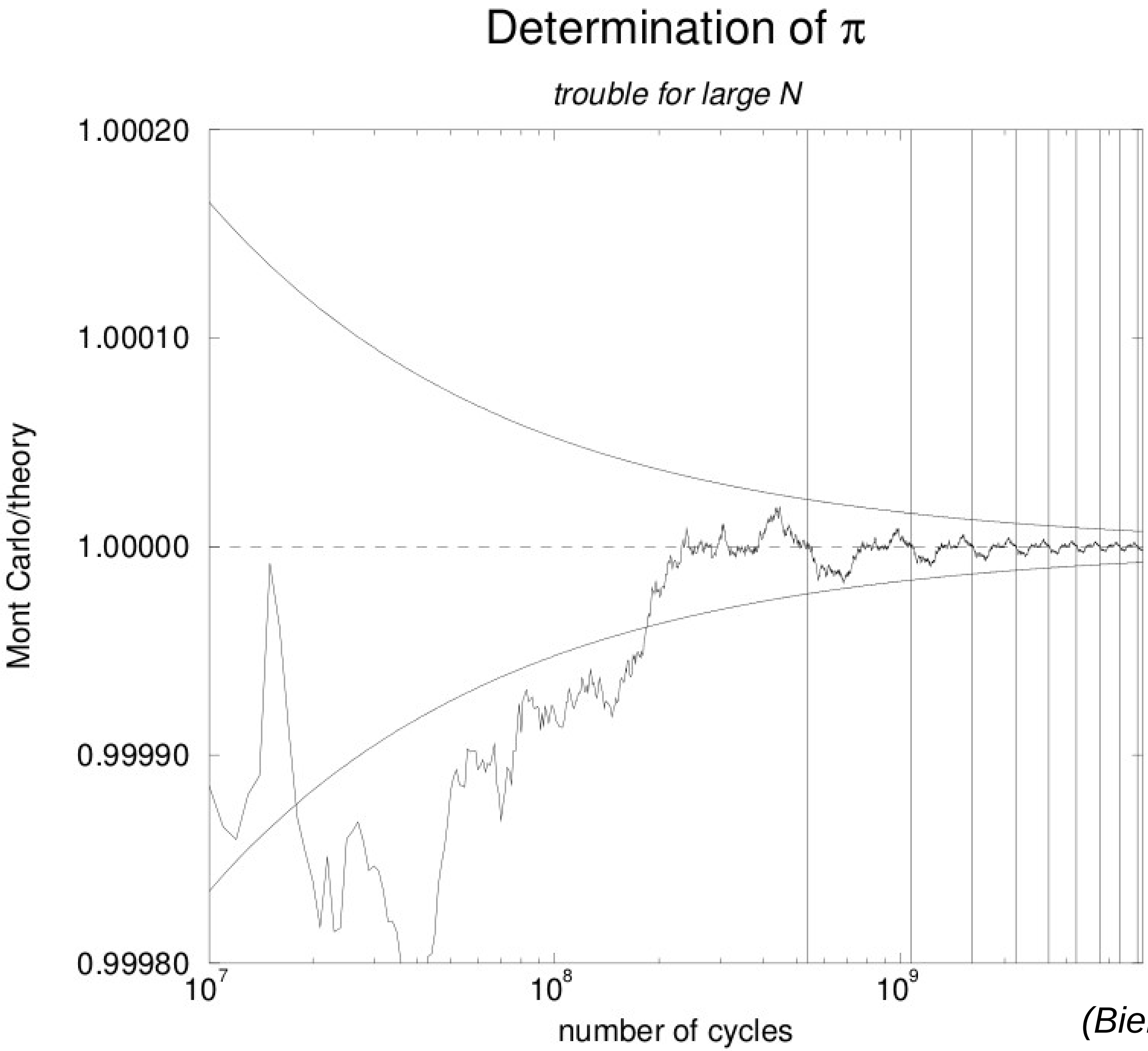


Example of false convergence due to insufficient random numbers.

(Bielajew)

Random numbers in MC algorithms

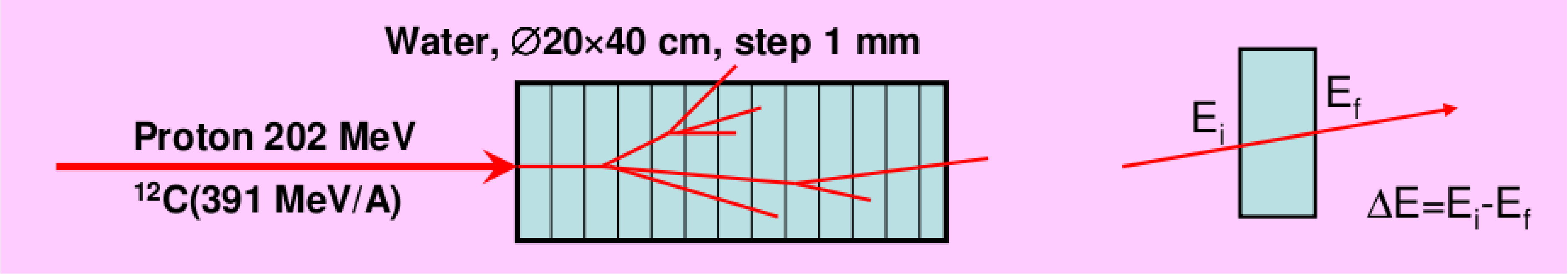
- Default random number generators (e.g. rand() of stdlib in c) are usually sh*t and not applicable for serious MC calculations.
- Plenty of different random number generators exist
  - MCRNG, LCRNG, RANLUX, RANSHI …
  - Sequence lengths of e.g. 10^19 random numbers

- Avoid experiments, use configurations and seeds which are well tested
- Several “random number” **hardness** testing packages exist (e.g. DIEHARD)
- Beware of **pitfalls** when parallelizing MC computations (e.g. accidentally running 100 parallel runs with same RND sequence)

MC Particle Transportation

MC Particle Transportation

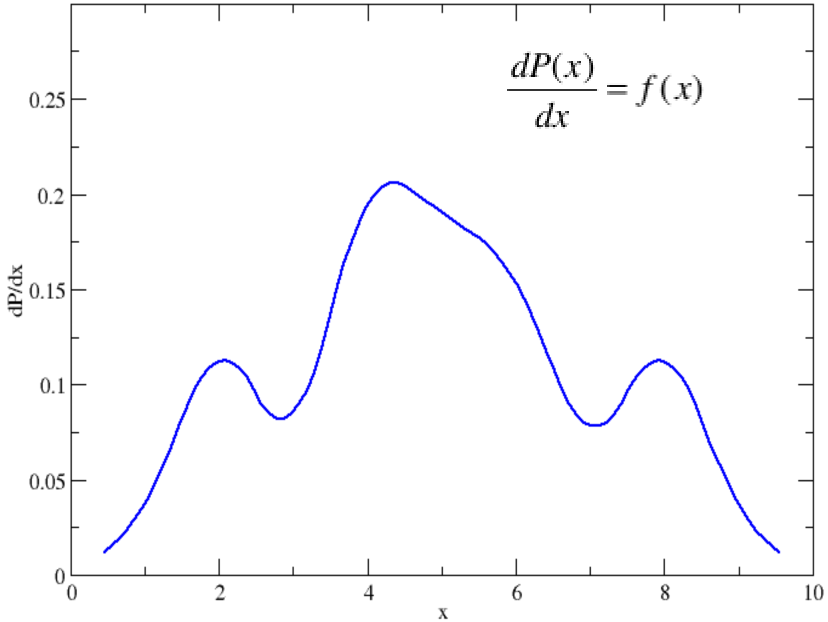
- MC particle transport:
  - Include probability distributions of all relevant physics
  - follow particle and interaction histories, when plenty, it simulates real life

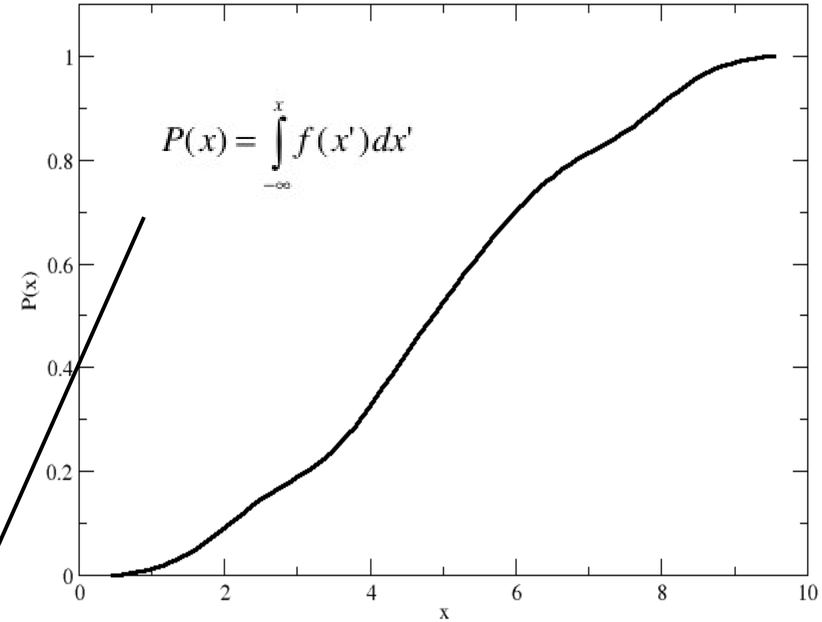


- Conservation of **energy** and **momentum** are always obeyed.
- Relies on good random number generator

Monte Carlo – Probability Distributions

$$1 = \int_{-\infty}^{\infty} f(x')dx'$$





Cumulative distribution function (CDF).
The probability to measure P(x) is
described by number between [0;1]

$$r = P(x)$$

The MC trick: *invert function, fill in a (flat distributed) random number r [0;1], and get x.*

$$x = P^{-1}(r)$$

Repeat a lot of times to get realistic simulation of f(x).

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Example: Compton Scattering

$\gamma + e^- \rightarrow \gamma + e^-$

The distance before next interaction, l, is a random variable.

We need to find its probability distribution, so we can convert a flat probability R [0:1] to the probability for next interaction.

cross section per atom : $\sigma(E,z)$

nb of atoms per volume : $n_{at} = \frac{\rho N}{A}$

cross section per volume : $\eta(E,\rho) = n_{at}\sigma$ (η is in 1/cm)

- $\eta(E,\rho)$ is the probability of Compton interaction per cm
- $\lambda(E,\rho) = \eta^{-1}$ is the mean free path associated to the process (Compton)

The probability distribution of l:
Invert it, and substitute f(l) with random number R:

$$f(l) = \eta \exp(-\eta l) = \frac{1}{\lambda} \exp(-\lambda^{-1} l)$$

$$\ln(R\lambda)\lambda = l$$

Similar calculation can be done for angles of scattering, for the photon and electron.
This is just one example, there is tons of physics implemented in similar ways

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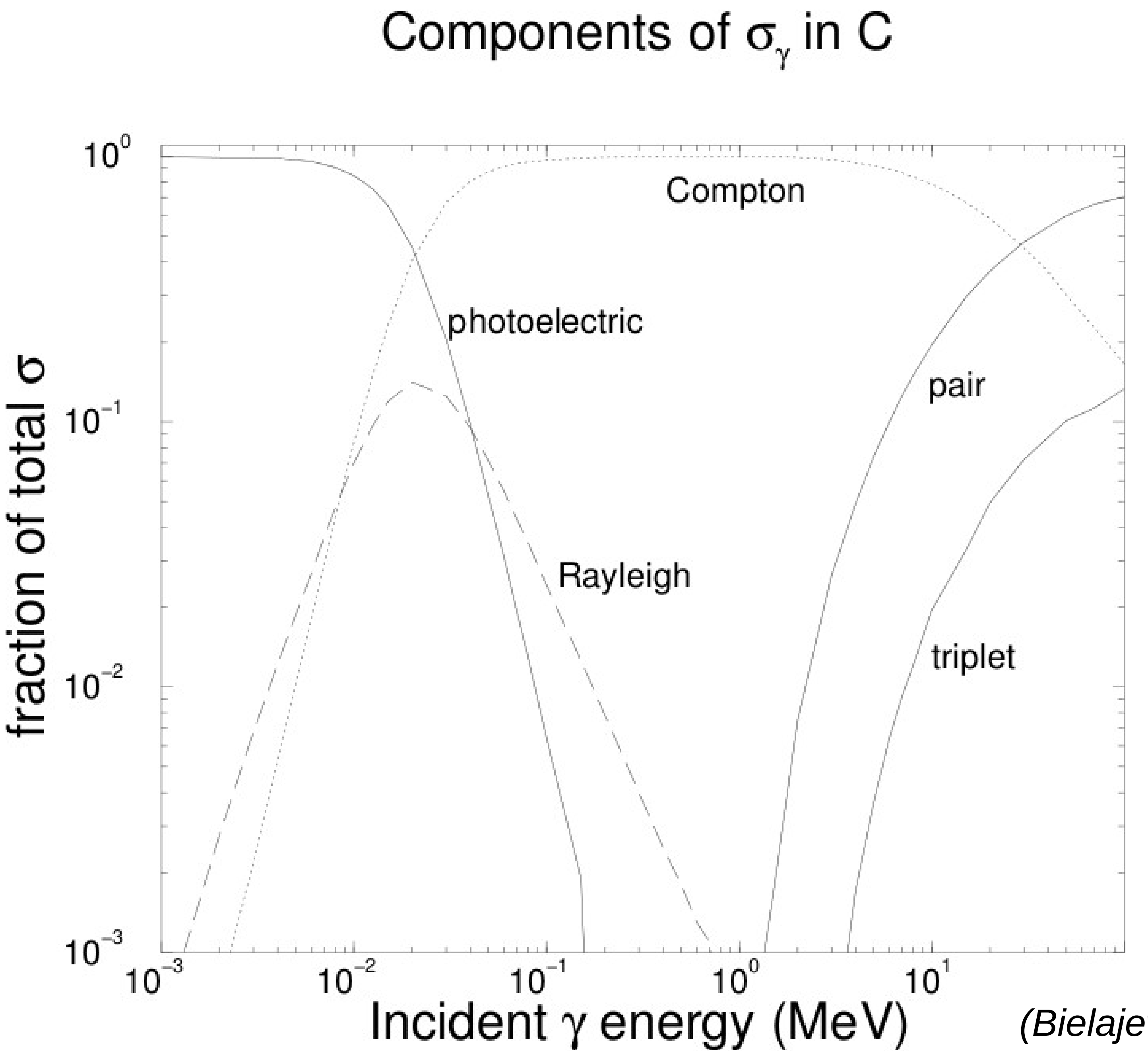
Photon Interactions – Reaction Channels



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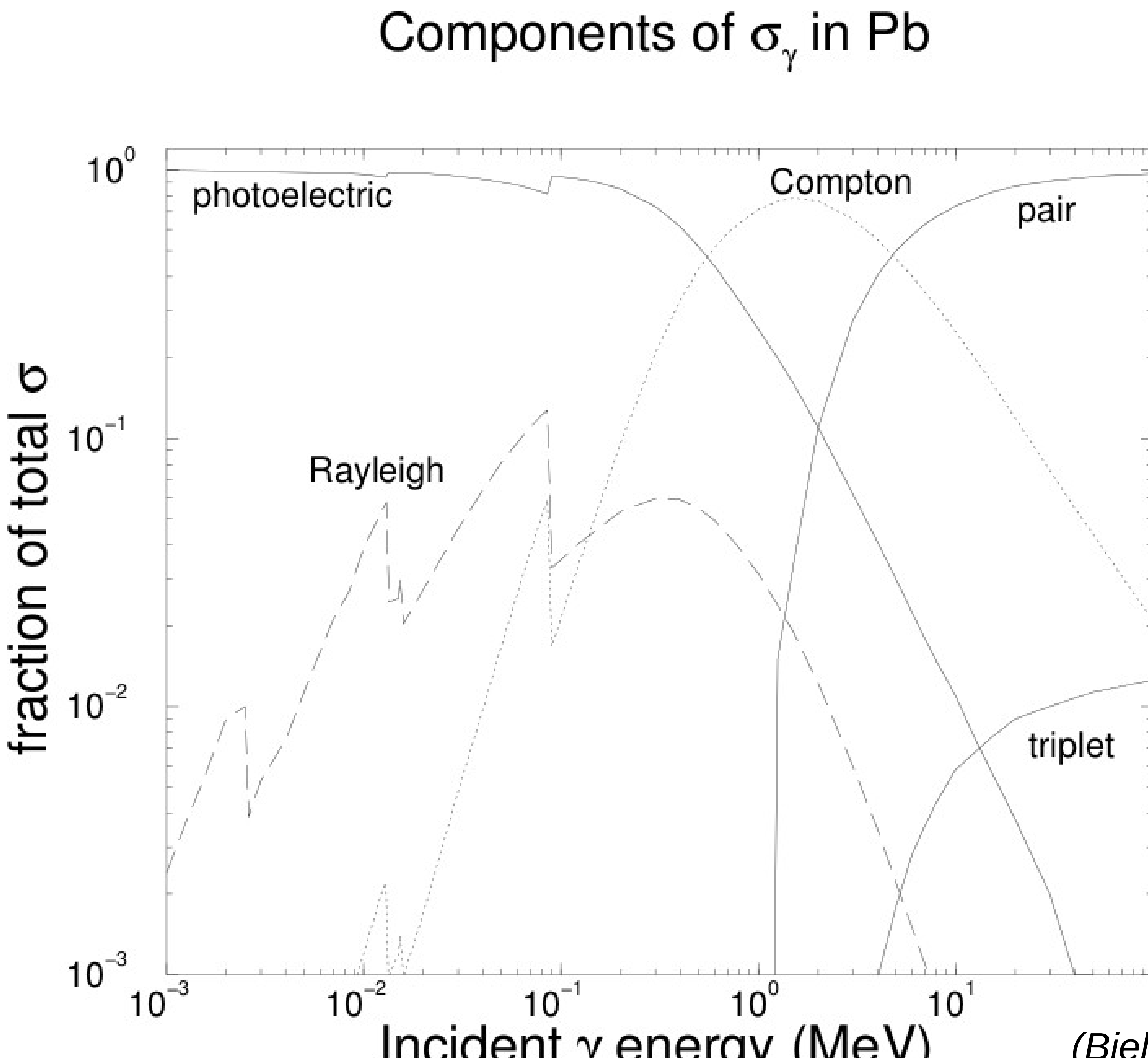
Photon Interactions



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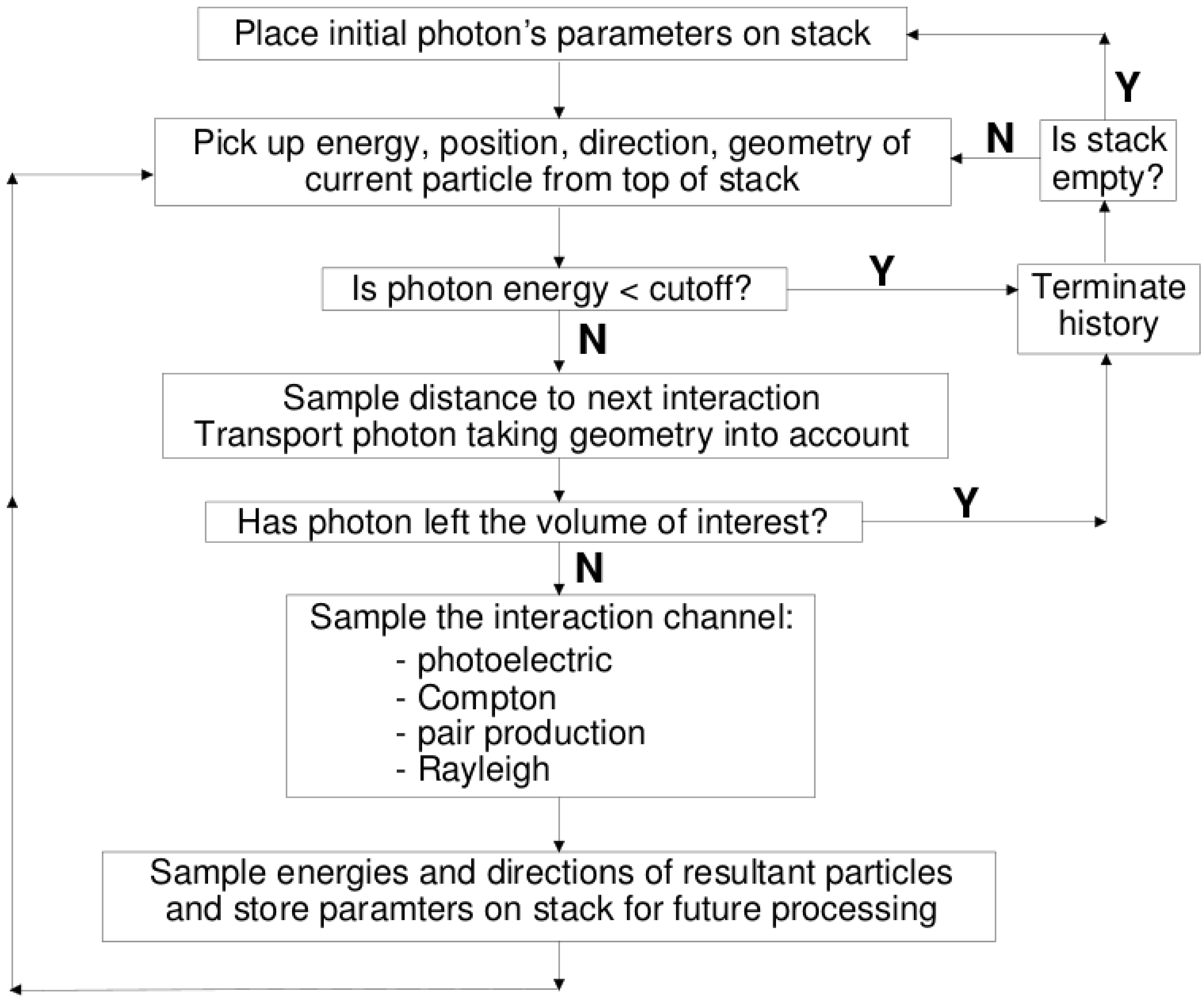
Photon Transport



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Charged Particle Interactions

- A single 1 MeV ***photon***:
  - Number of interactions app. 10, i.e. ~ 10 ions created by photon.

- A single 1 MeV ***charged particle***:
  - Large number of interactions, ~ 10^4 ions created

Not feasible in MC (depending on the task to be solved),
very CPU intensive for necessary precision.

Q: in what disciplines would you want a full *ab-initio* simulation?

Groups of Charged Particle Interactions

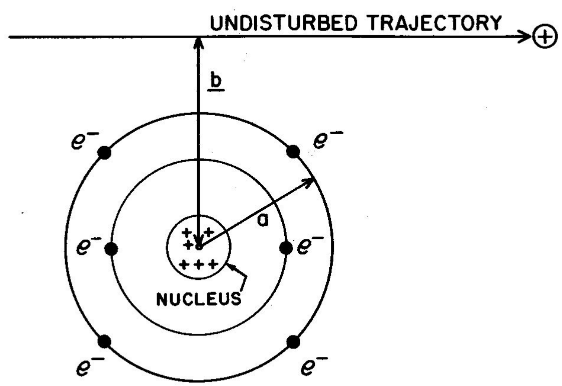

FIGURE 8.1. Important parameters in charged-particle collisions with atoms: *a* is the classical atomic radius; *b* is the classical impact parameter.

(b>>a): ***Soft collisions*** Coulomb interaction with the whole atom. Large number of interactions. Small energy transfers.

(b≈a): ***Hard collisions*** Coulomb interaction with a single atomic electron. Large energy transfers. Creation of δ-particles (high energy e-)

(b<<a): ***Interactions with the nuclear field***
For incident electrons:
Eleastic scattering (resulting in multiple scattering).

Occasionally: Inelastic scattering. Creation of bremsstrahlung.

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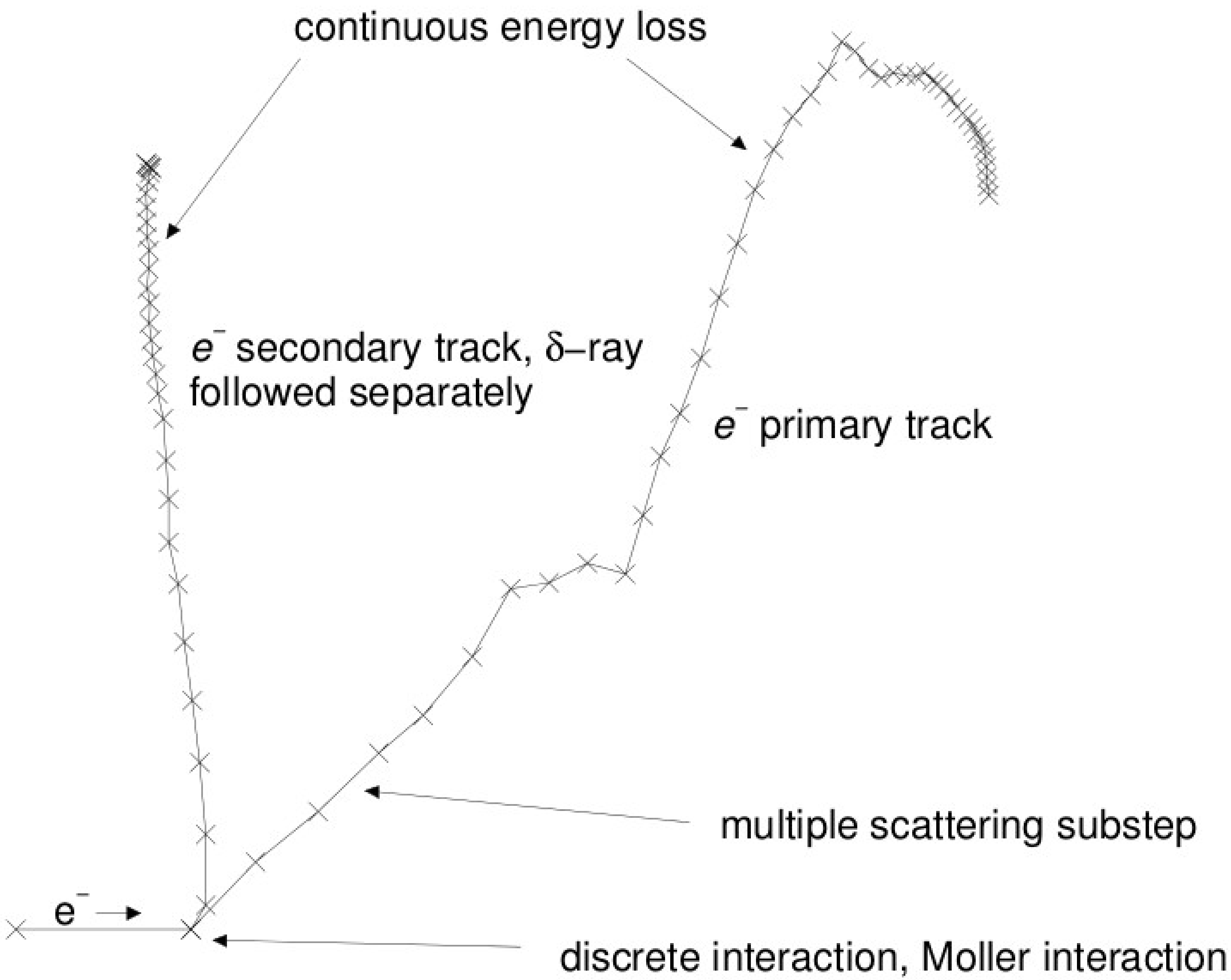
Simulation of a single electron track



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Electron MC Transportation

- "Catastrophic"
  - large energy-loss Møller scattering ($e^-e^- \longrightarrow e^-e^-$),
  - large energy-loss Bhabha scattering ($e^+e^- \longrightarrow e^+e^-$),
  - hard bremsstrahlung emission ($e^\pm\mathrm{N} \longrightarrow e^\pm\gamma\mathrm{N}$), and
  - positron annihilation "in-flight" and at rest ($e^+e^- \longrightarrow \gamma\gamma$).
- "Soft"
  - low-energy Møller (Bhabha) scattering (modeled as part of the collision stopping power),
  - atomic excitation ($e^\pm\mathrm{N} \longrightarrow e^\pm\mathrm{N}^*$) (modeled as another part of the collision stopping power),
  - soft bremsstrahlung (modeled as radiative stopping power), and
  - elastic electron (positron) multiple scattering from atoms, ($e^\pm\mathrm{N} \longrightarrow e^\pm\mathrm{N}$).

"Soft" interactions are small and numerous -> ***condensed*** simulation.

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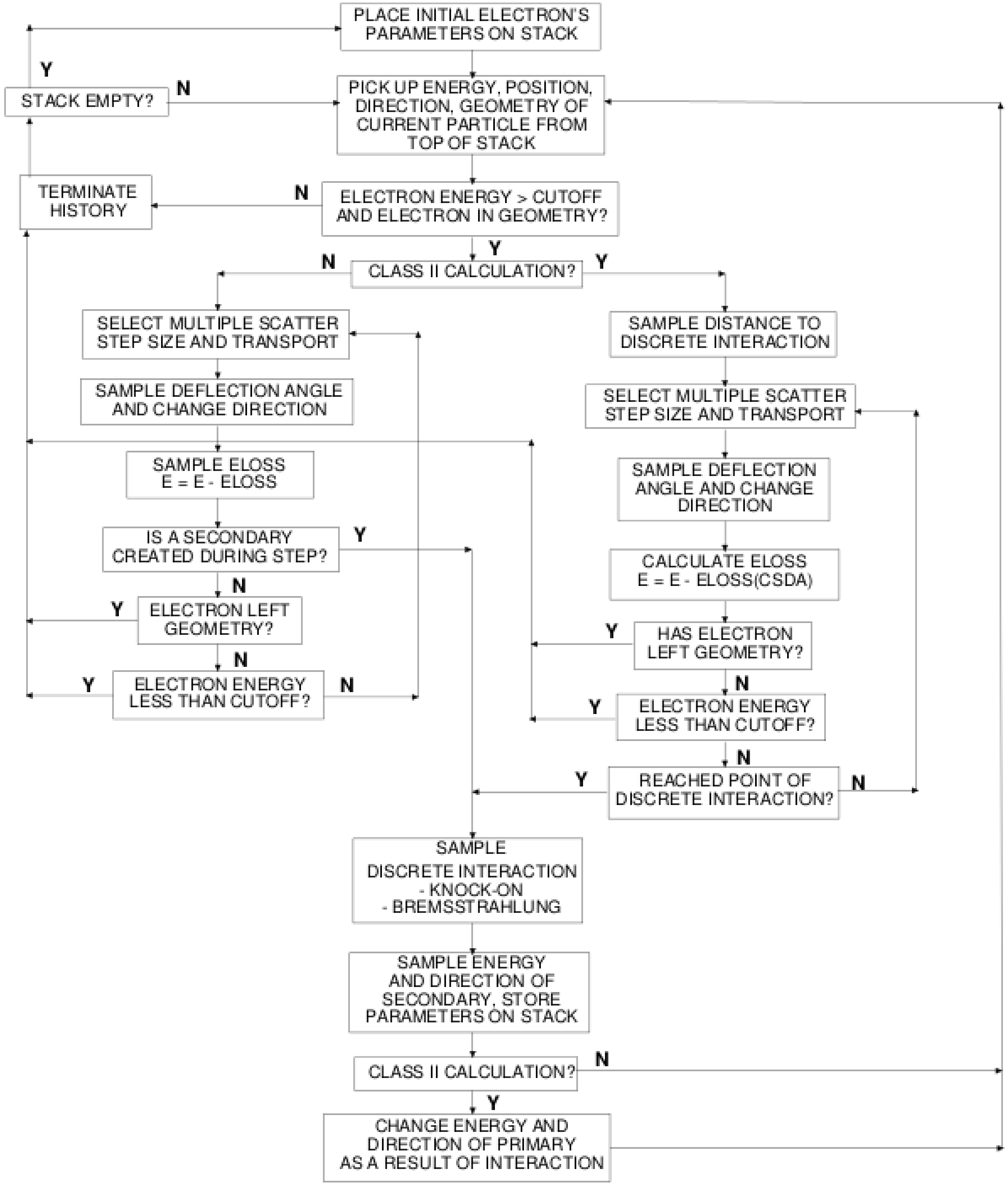
Electron transport



(Bielajew)

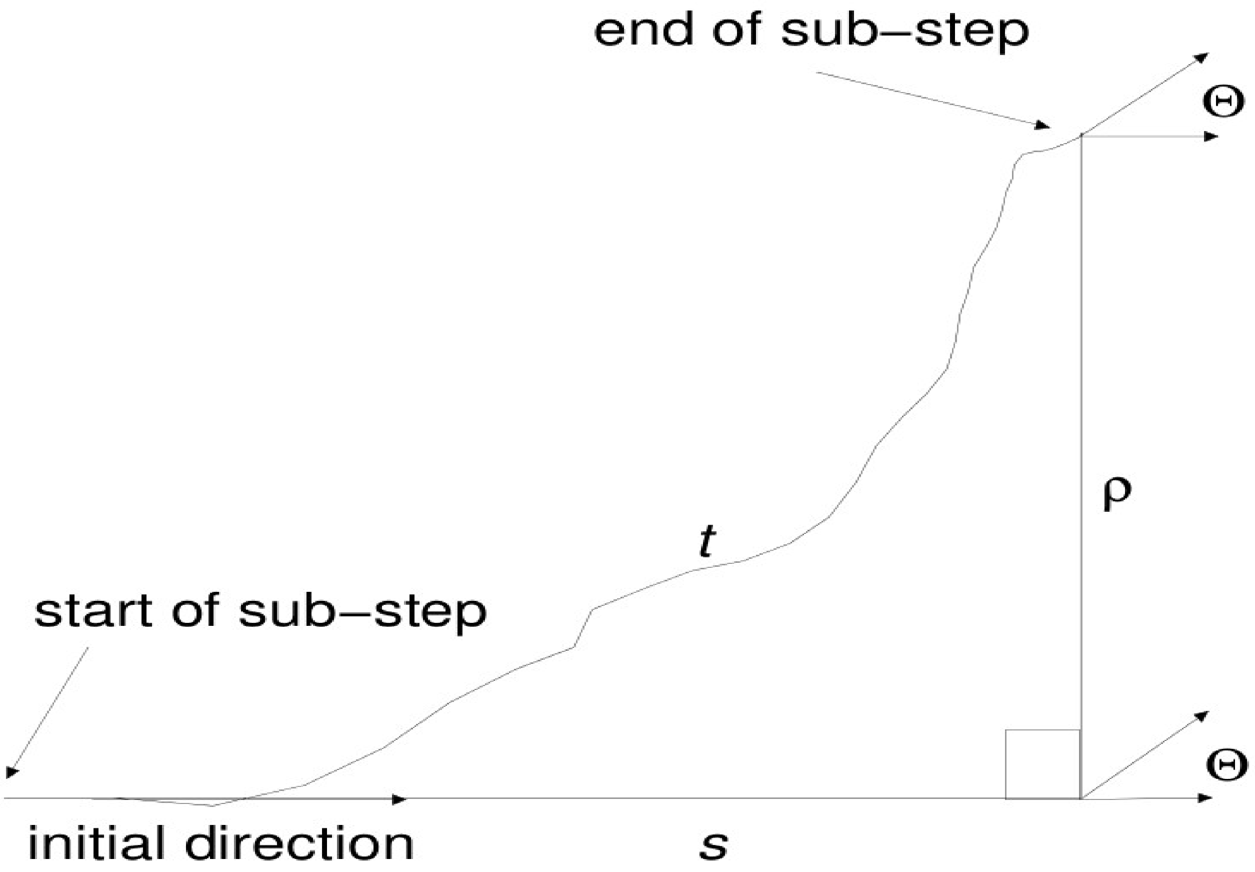
Condensed MC

- charged particle interactions are not described individually (contrary to photon interactions)
- **Average effects** are described and put into groups

Examples of macroscopic (averaged) treatment of quantities in MC particle transport:

- **Scattering** is described as “multiple scattering” (Moliere scattering, thin targets)
- **Stopping power dE/dx** is macroscopic
  - **Ions** are typically treated classically
  - **Electrons and positrons** are “always” relativistic
- **Energy fluctuations** “energy straggling” are described by Gaussian, Vavilov or Landau distributions.

A single charged particle sub-step



- ***No simple relationship between t and s***
- ρ is often not calculated (ignored)
- Scattering is still happening due to Θ (Moliere scattering)

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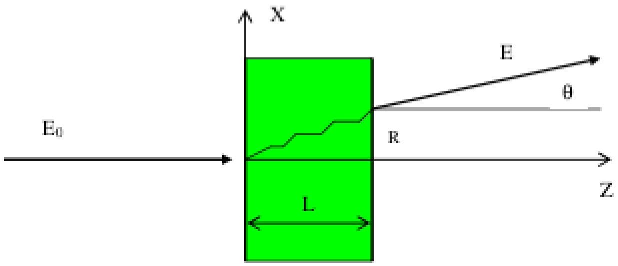
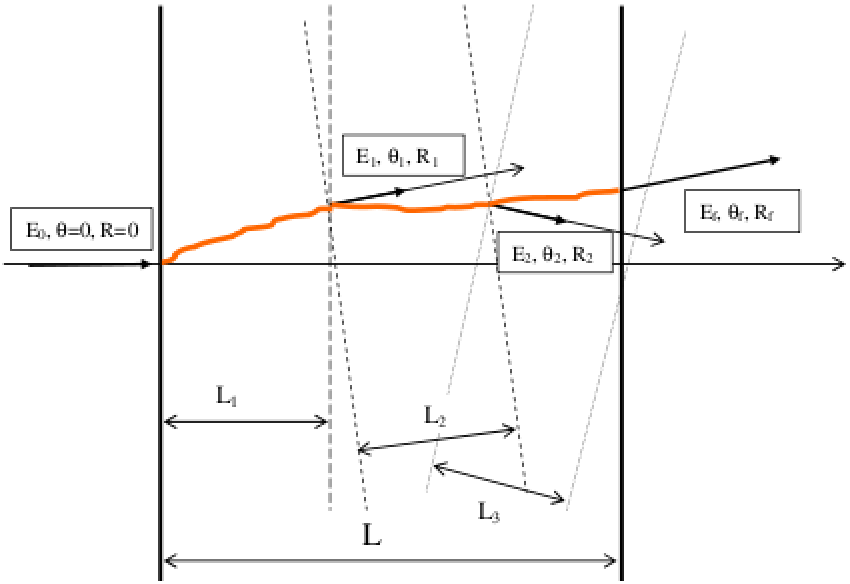


Прохождение тяжелой заряженной частицы с энергией E_0 через слой вещества толщины L.

(Heavy ion transportation code SHIELD-HIT does take new position into account)



Слой толщины L как набор тонких слоев L_i.

L is defined by user as a ***minimum step length***, within this condensed physics is applied instead of discrete sampling

Typical ion step lengths: 5% energy loss (HADRONthe default FLUKA and SH12A)..

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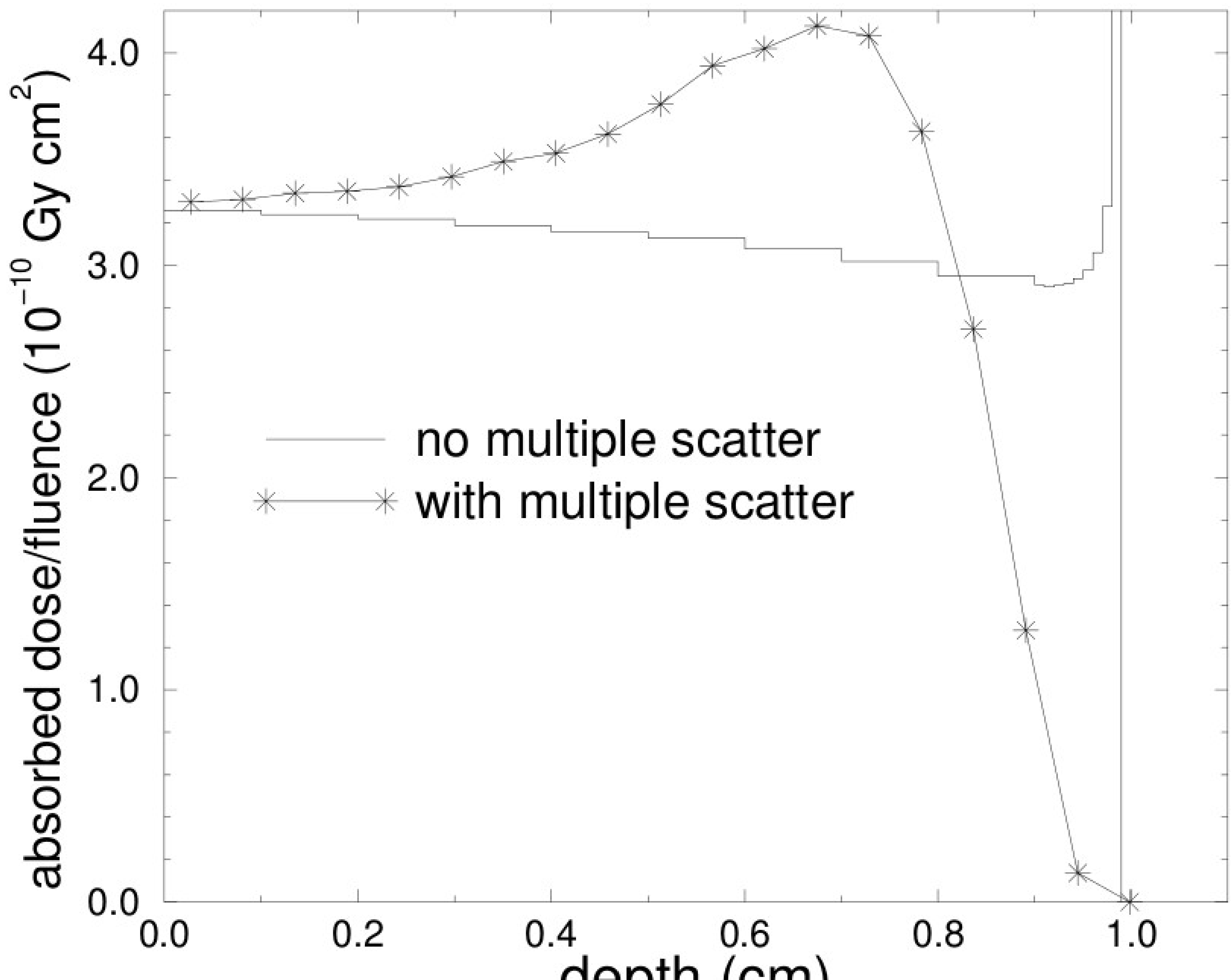
20 MeV e^- on water

broad parallel beam, CSDA calculation



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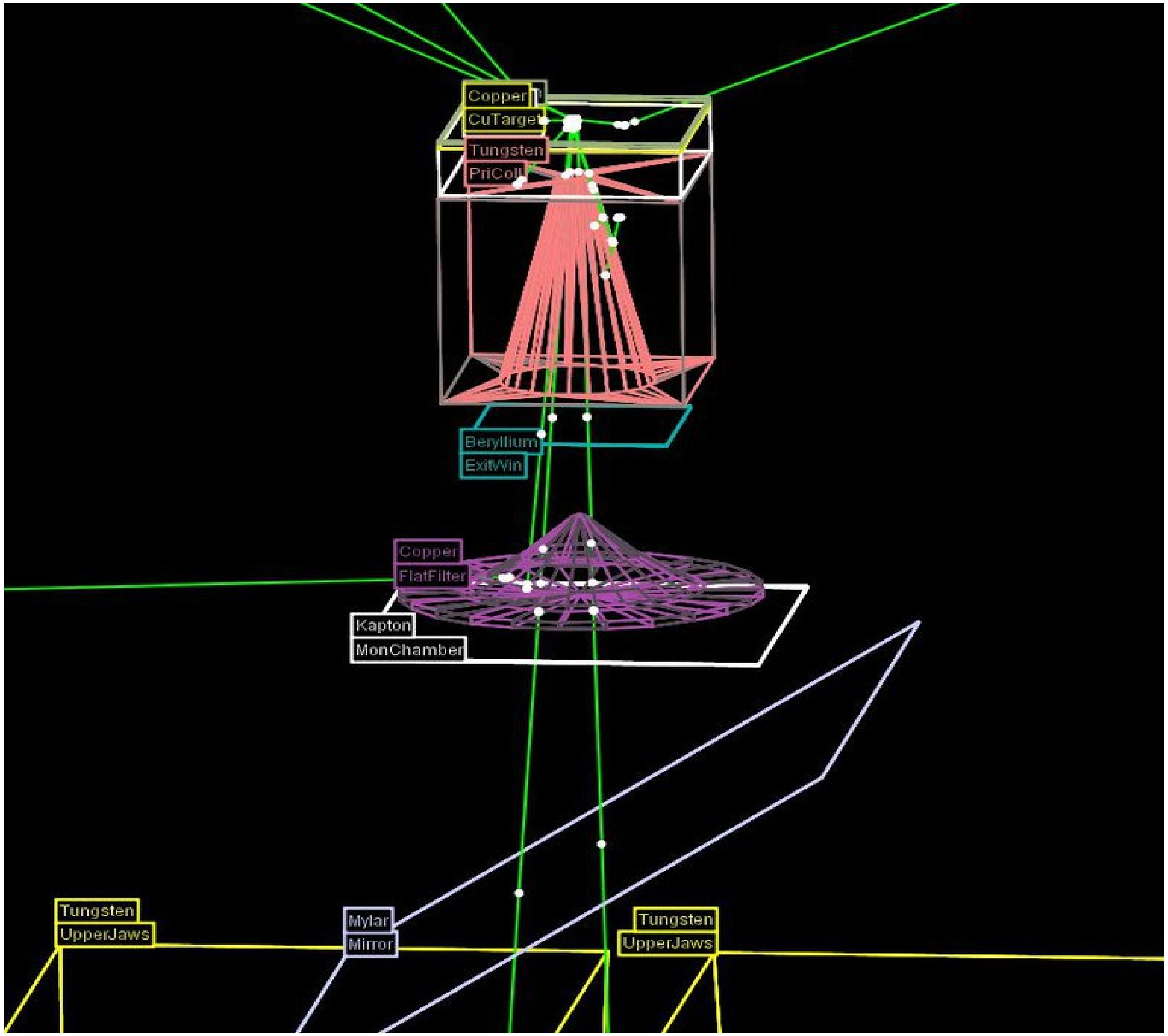
Geometry Considerations



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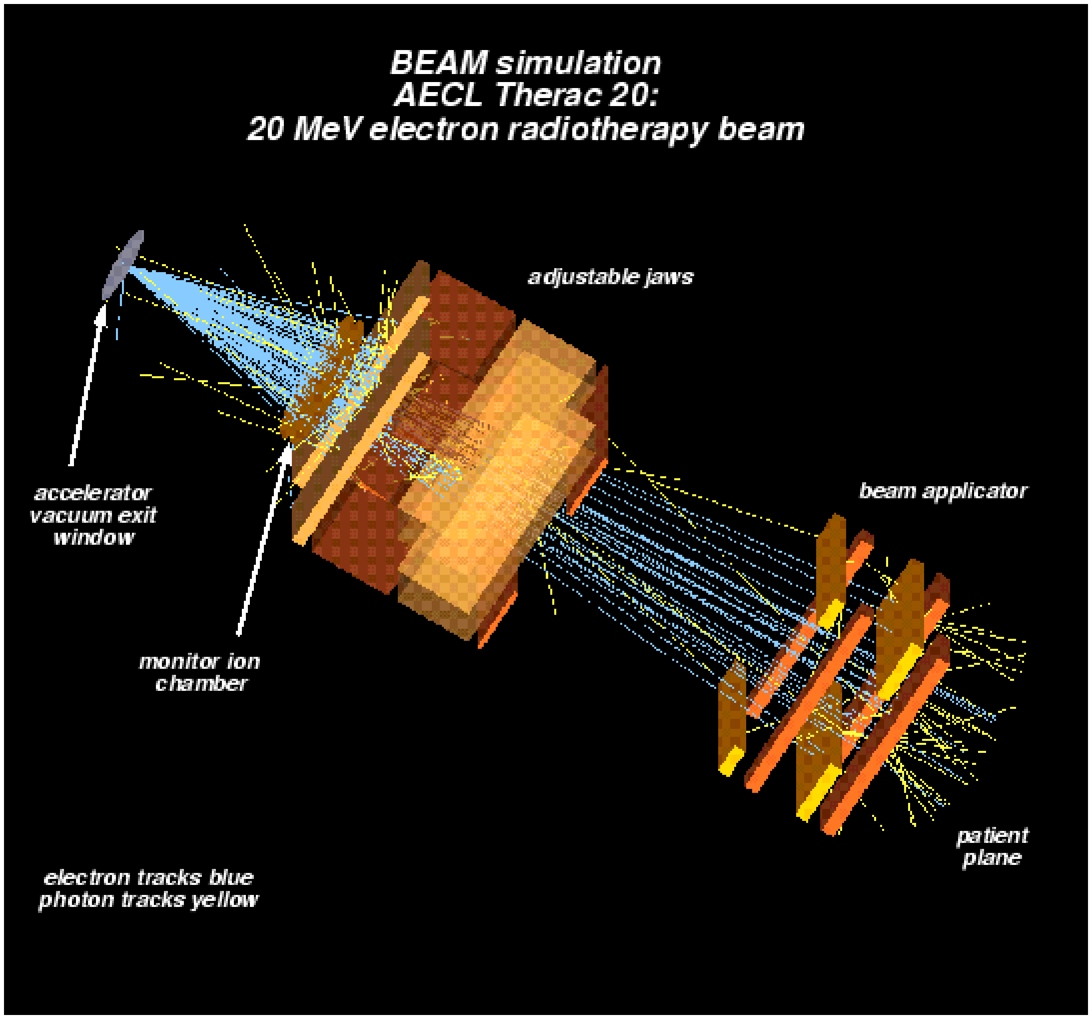
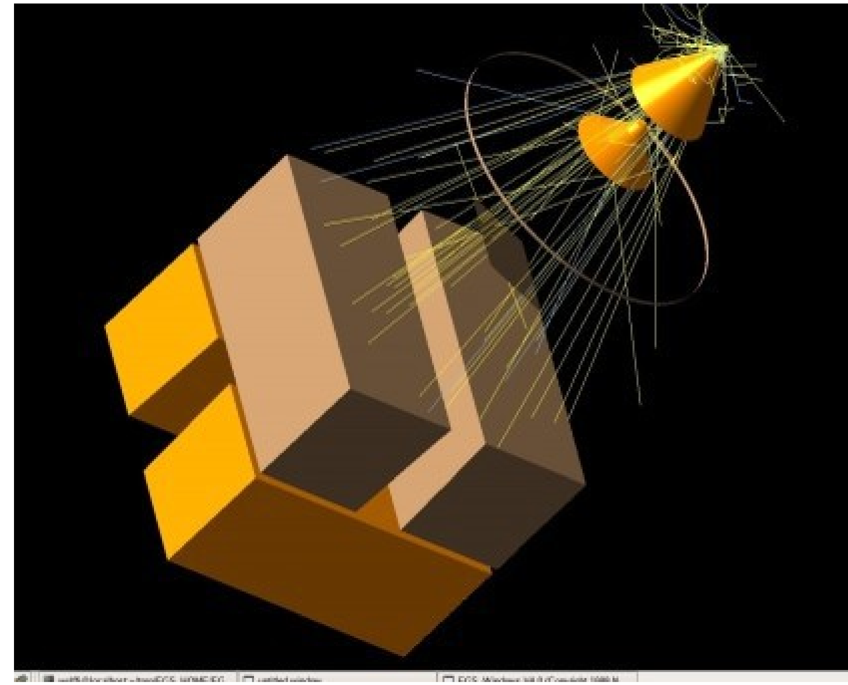
Beam Sources

1) Full simulation of treatment head
2) Virtual treatment head
3) Phase space file of pre-calculated values

1) Full simulation



Electron beam application (BEAMnrc)



Photon therapy w. flattening filters

2) Virtual Source

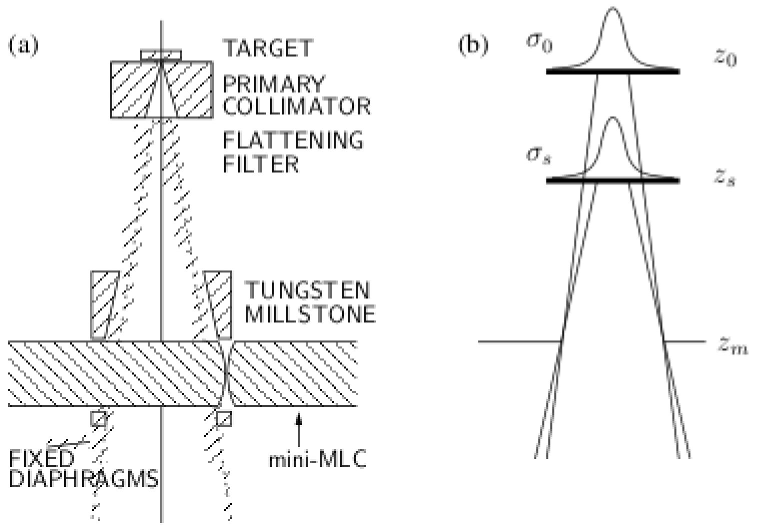


Figure 1. (a) The collimation system of the EBM with marked positions of a target and a flattening filter. (b) Scheme of the VEF of the EBM, where σ_0 and σ_s are standard deviations of the Gaussian intensity distribution of the primary and secondary photon sources respectively, z_0 the position of the primary photon source, z_s the position of the secondary photon source and the electron contamination source, z_m the position of the upper edge of the mini MLC.

A Virtual Source Model (VSM) described the beam above the MLC.

(Sikora et al, PMB 2007)

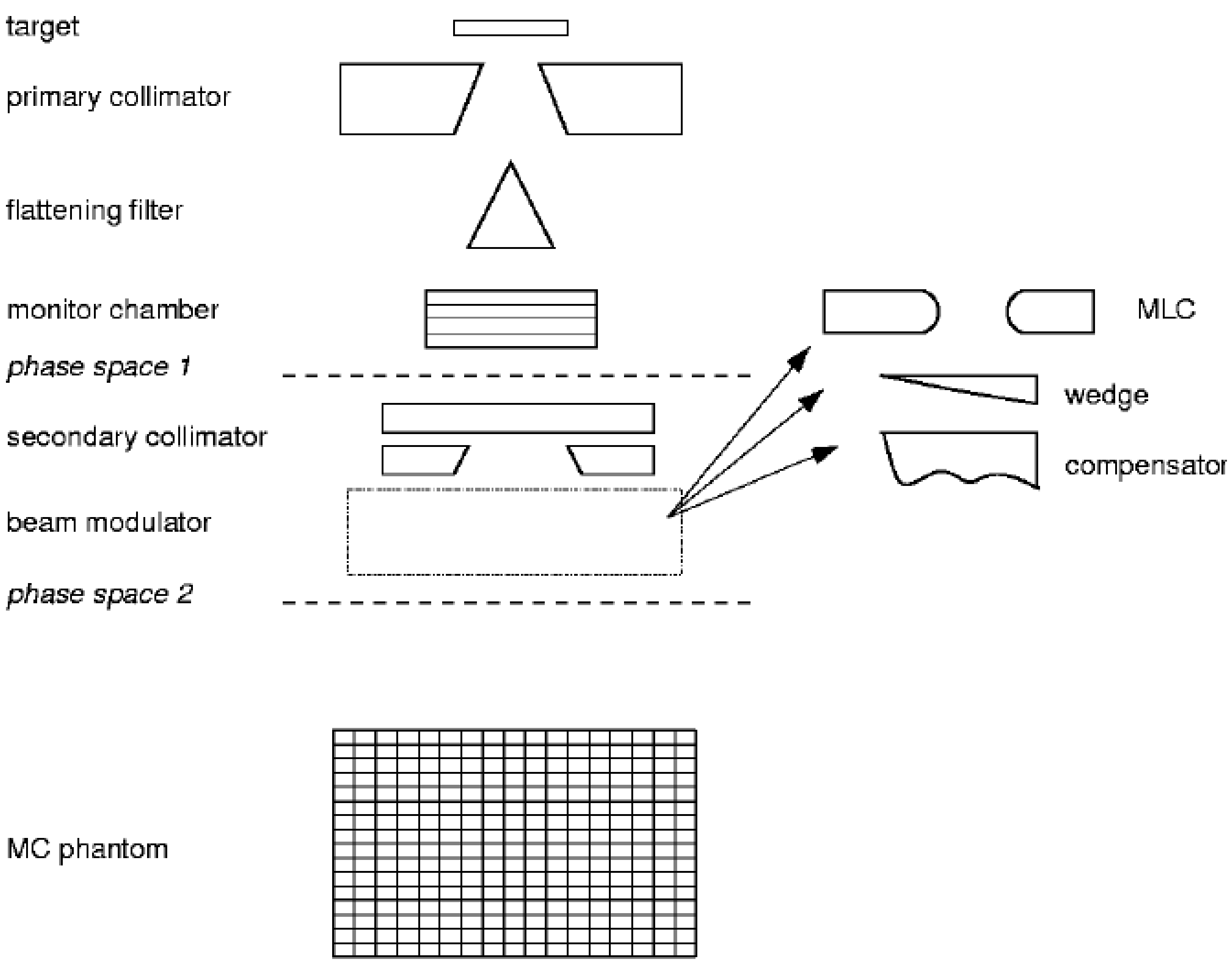
3) Using Phase Space Files

- Phase space file: list of particles, direction vector and energy
  - n(x,y,z,v1,v2,E)
- IAEA .phsp definition: http://www-nds.iaea.org/phsp/phsp.htmlx

IAEA provide a database with linacs and Co-60 phase-space files

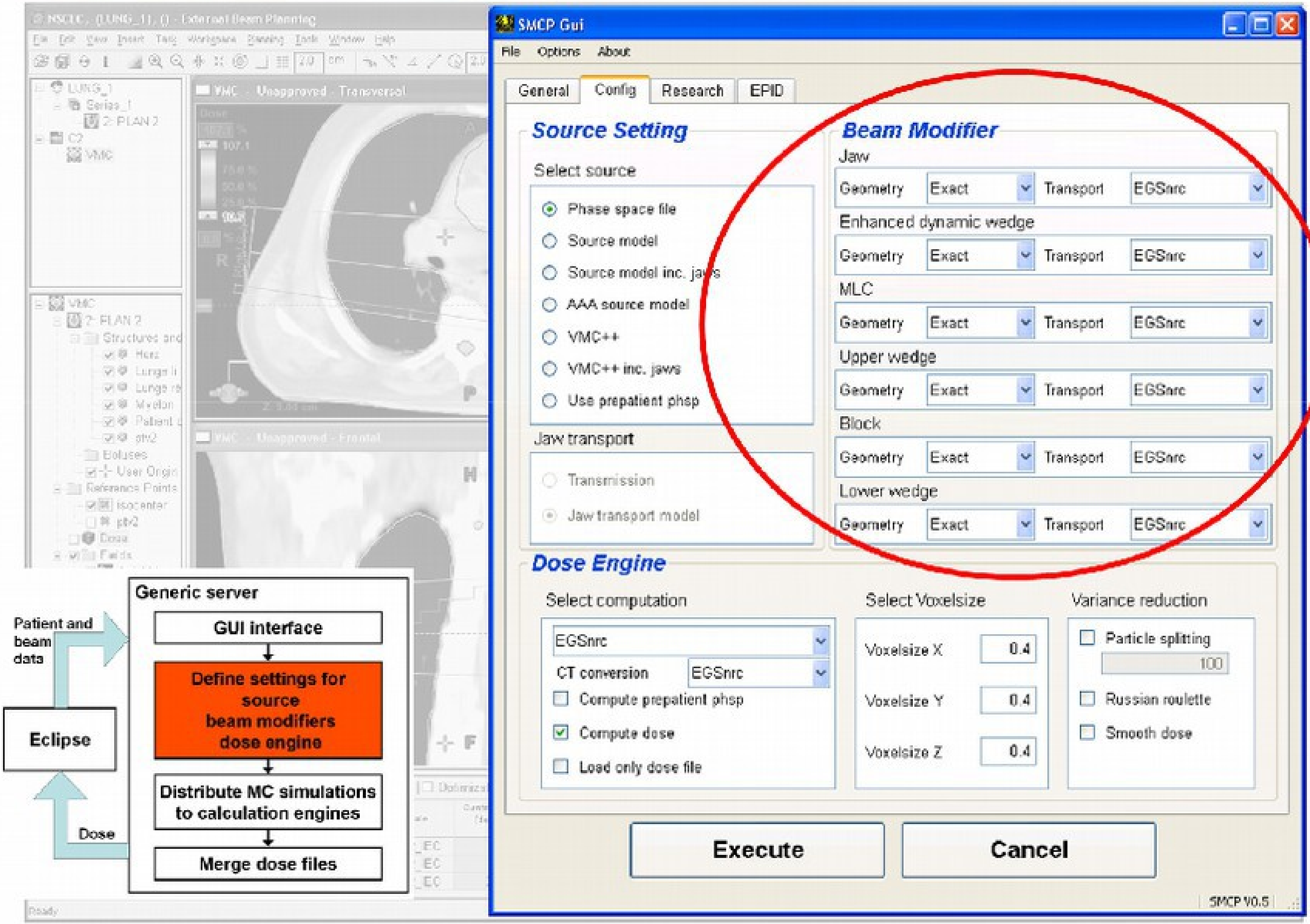
Variable	Meaning	Type of variable
X	First coordinate (usually X position in cm)	Real*4
Y	Second coordinate (usually Y position in cm)	Real*4
Z	Third coordinate (usually Z position in cm)	Real*4
U	First direction cosine	Real*4
V	Second direction cosine	Real*4
E	Kinetic energy in MeV	Real*4
Statistical_Weight	Particle statistical weight	Real*4
Particle_type	Type of the particle *Current list:* photons, electrons, positrons, protons and neutrons	Integer*2
Sign_of_W	Sign of W (Third direction cosine)	Logical*1
Is_new_history	Signifies if particle belongs to new history	Logical*1
Integer_extra	Extra storage space for integer variables *Currently defined variables:* Incremental history number EGS LATCH PENELOPE ILB	n*(Integer*4) (n ⩾ 0)
Float_extra	Extra storage space for real variables *Currently defined variables* XLAST YLAST ZLAST	m*(Real*4) (m ⩾ 0)

3) Using Phase Space Files (cont.)



a representative recording of particles in a plane, typically (but not necessarily) before any modifies which are specific to the treatment.

SMCP-Interface with Eclipse



Courtesy of M. Fix

Calculation Speed

TABLE I. Summary of timing and accuracy results from the ICCR benchmark. Timing comparisons were performed using 6 MV photons, 10×10 cm^2 field size, and those for the accuracy test, using 18 MV photons and a 1.5×1.5 cm^2 field size, as detailed in the ICCR benchmark (Ref. 99). All times have been scaled to the time it would take running on a single, Pentium IV, 3 GHz processor. Readers should be aware that the timing results, as well as the method used to scale the times, are subject to large uncertainties due to differences in compilers, memory size, cache size, etc.

Monte Carlo code	Time estimate (min)	% mean difference relative to ESG4/PRESTA/DOSXYZ
ESG4/PRESTA/DOSXYZ	43	0, benchmark calculation
VMC++	0.9	±1
XVMC	1.1[a]	±1
MCDOSE (modified ESG4/PRESTA)	1.6	±1
MCV (modified ESG4/PRESTA)	22	±1
DPM (modified DPM)	7.3[b]	±1
MCNPX	60[c]	Maximum difference of 8% at Al/lung interface (on average ±1% agreement)
PEREGRINE	43[d]	±1
GEANT4 (4.6.1)	193[e]	±1 for homogeneous water and water/air interfaces

Chetty et al. PMB 2007

Computer Clusters

← cluster maintained by APTG in Heidelberg

Future is cloud computing! See e.g. Amazon Web Services.

Dose to Water vs Dose to Medium

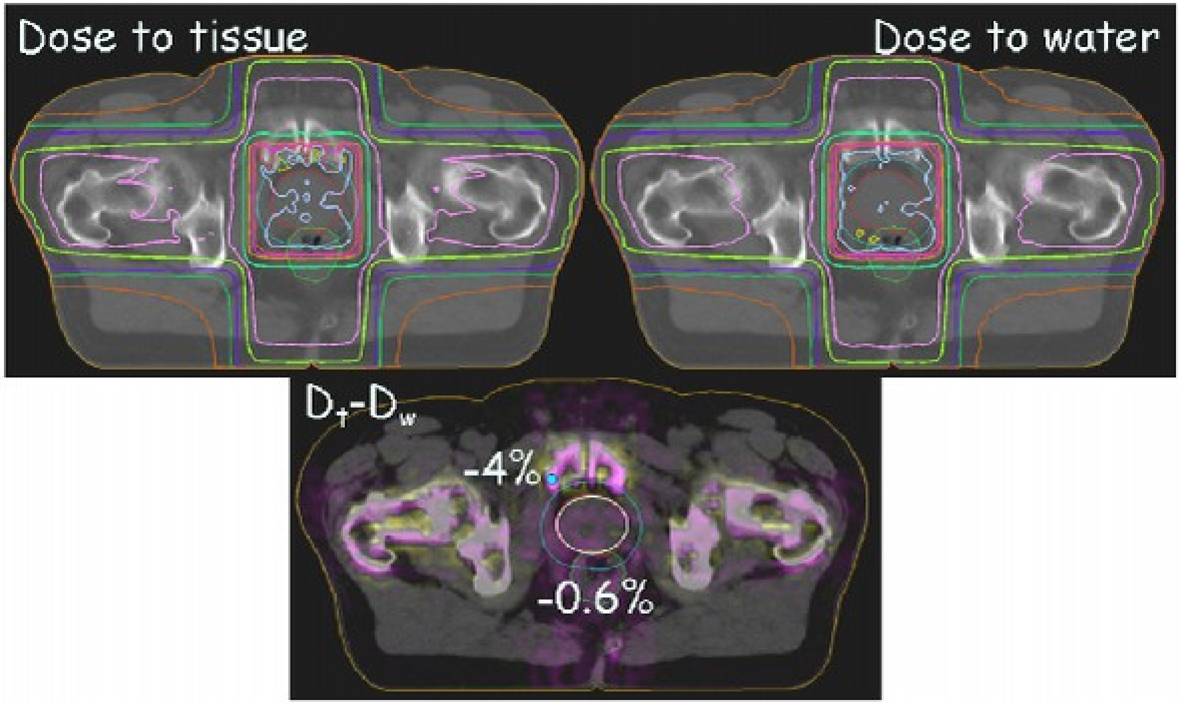


Figure 3. The four-field box technique for the prostate case with MC calculations for all tissues mapped as tissues (upper left) and mapped as water (upper right). The difference is shown in the lower panel. The isodoses shown are 115, 112.5, 110, 107.5, 105, 102.5, 100, 97.5, 95, 90, 70, 50, 30, 10, 5 and 2%. The dose in cortical bone at the blue dot is −4% and the average dose in the PTV is −0.6% compared to the dose to water plan.

(Knöös et al, 2006, PMB)

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Dose to Water vs Dose to Medium

IOP PUBLISHING PHYSICS IN MEDICINE AND BIOLOGY

Phys. Med. Biol. **56** (2011) 3073–3089 doi:10.1088/0031-9155/56/10/012

Dose specification for radiation therapy: dose to water or dose to medium?

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Online at stacks.iop.org/PMB/56/3073

MC codes calculated Dose to Medium. Should they be translated to dose to water?

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Dose to Water vs Dose to Medium

(1) Conventional photon dose calculation algorithms, either correction based or model based, compute doses using water with different electron densities, which are close (<4% differences) to doses to media, as computed by Monte Carlo, but significantly different (up to 11%) from doses to water converted from doses to media following AAPM TG105 recommendations.

(2) Our results suggest that for consistency with previous radiation therapy experience, Monte Carlo photon algorithms report dose to medium for radiotherapy dose prescription, treatment plan evaluation and treatment outcome analysis.

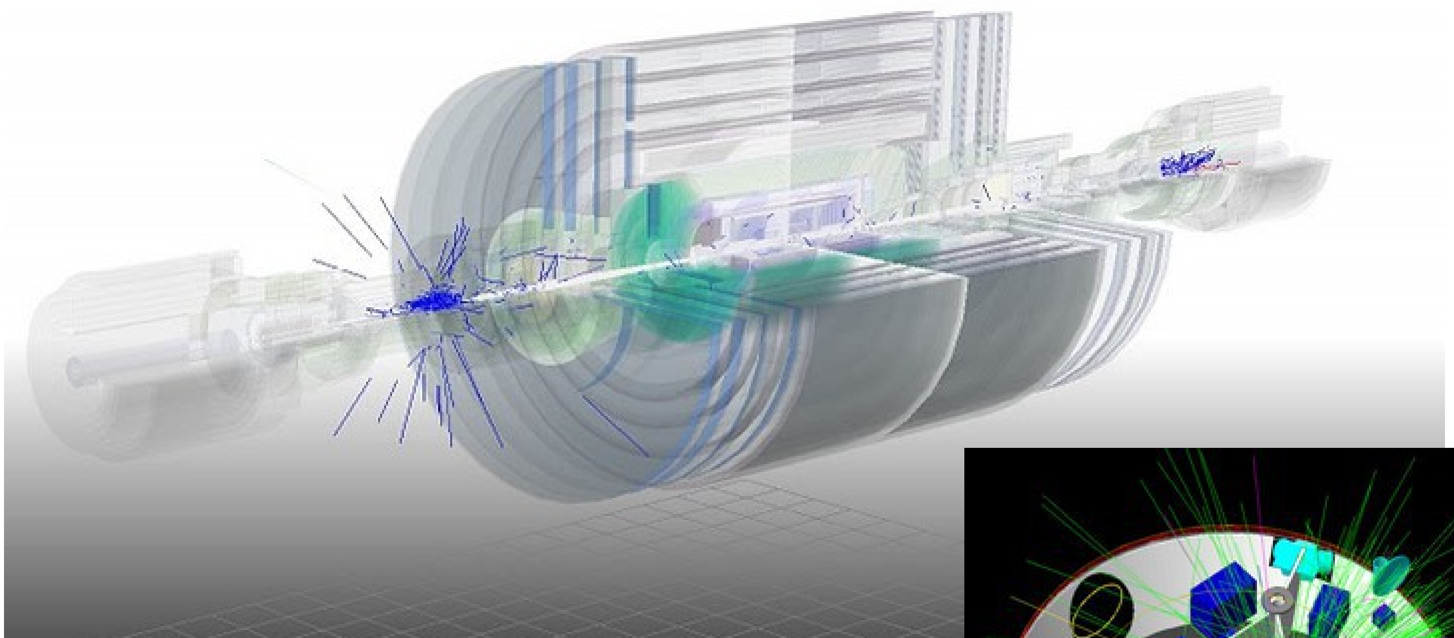
(… except.)
They also comment for electron plans:
use water with varying electron density.

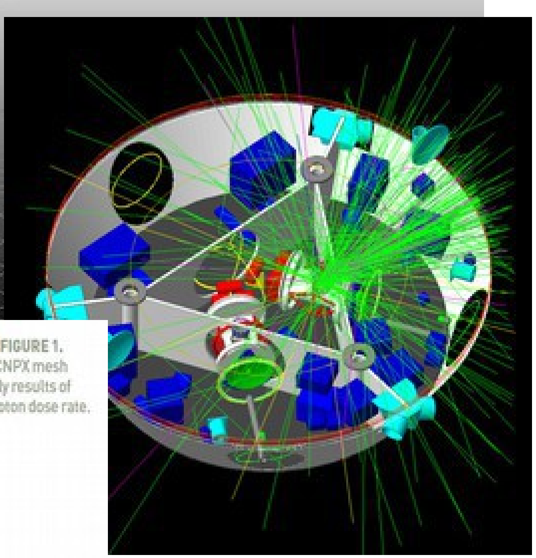
(Ma et al. 2011 PMB)

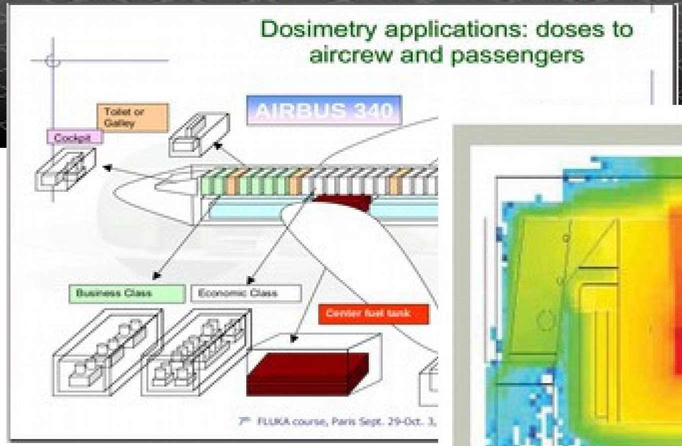
Monte Carlo – Usage Examples

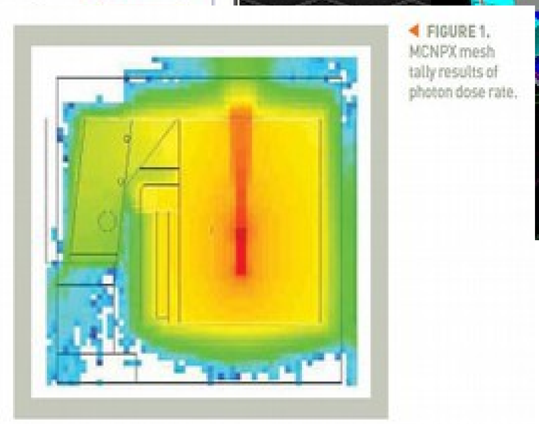
- CMS and ATLAS detector at CERN
- Shielding in space, airplanes, accelerator vaults
- Nuclear fission and fusion reactors, -bombs
- ...

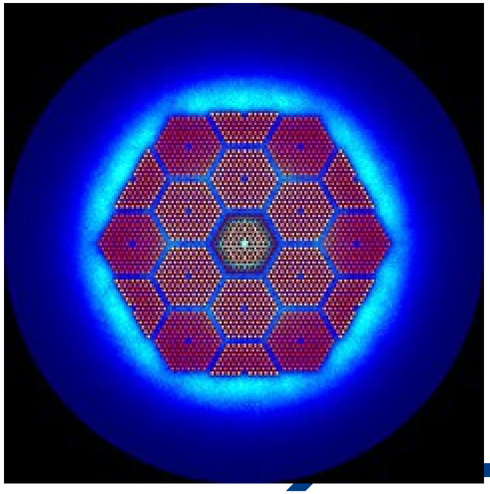
(FLUKA, Geant4)



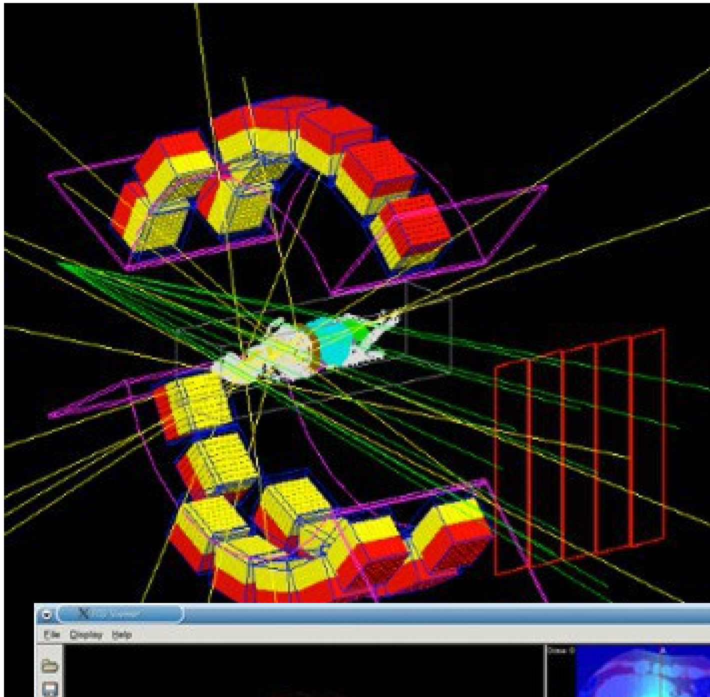


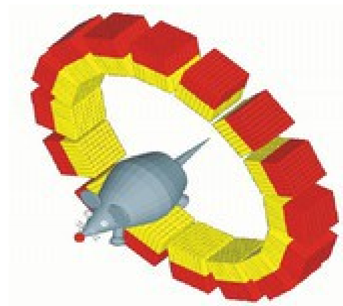






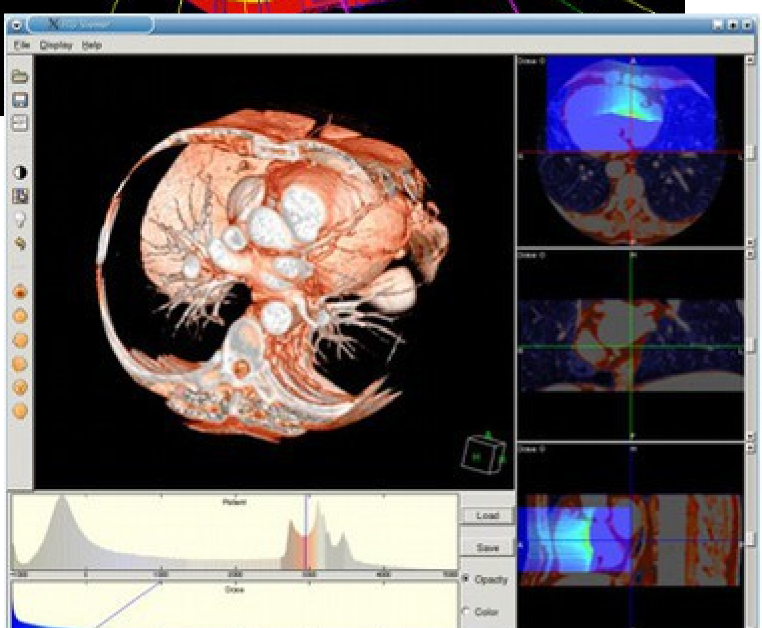
Monte Carlo – Usage Examples

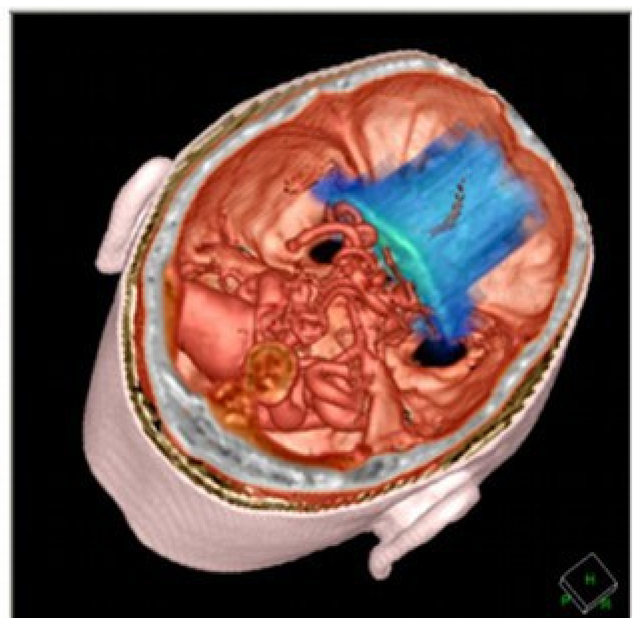




MEDICAL:
PET/CT, Photons, electrons, ions therapy.

Dose/fluence spectra calculations





Recommended Literature

Bielajews unfinished book on MC calculations:

http://www-personal.umich.edu/~bielajew/DosimetryBook/book.pdf

C-M Ma and Jinsheng Li 2011 Phys. Med. Biol. 56 3073
doi: 10.1088/0031-9155/56/10/012

Monte Carlo Treatment Planning An Introduction
Report 16 of the Netherlands Commission on Radiation Dosimetry

go to http://radiationdosimetry.org/ncs/documents/ncs-16-