http://www.geant4.org

Detector Simulations

A brief introduction

Andrea Dotti (adotti@slac.stanford.edu) ; SD/EPP/AMS

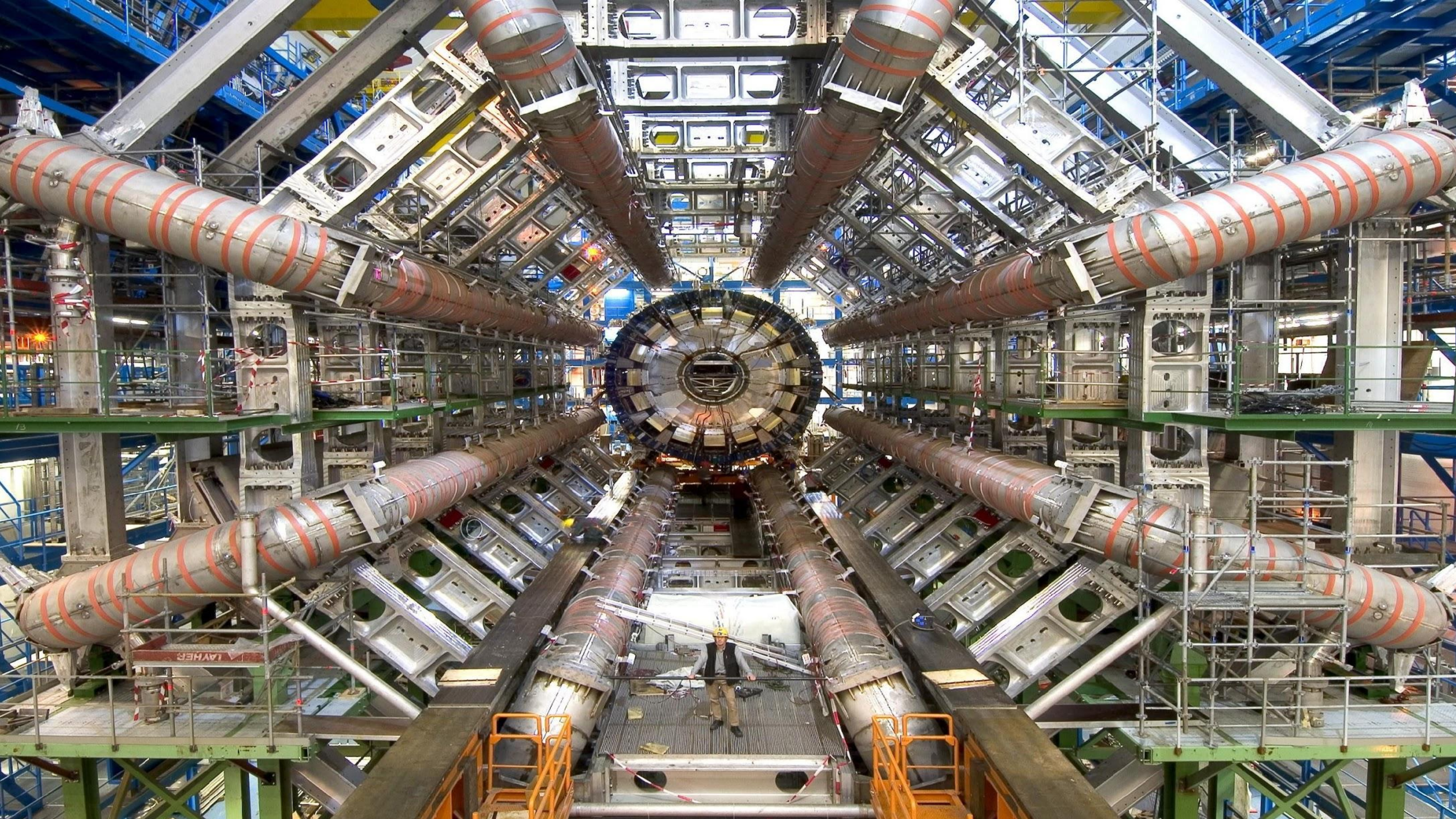
Short Detector Simulation Course @ Pisa School On Future Colliders 2018

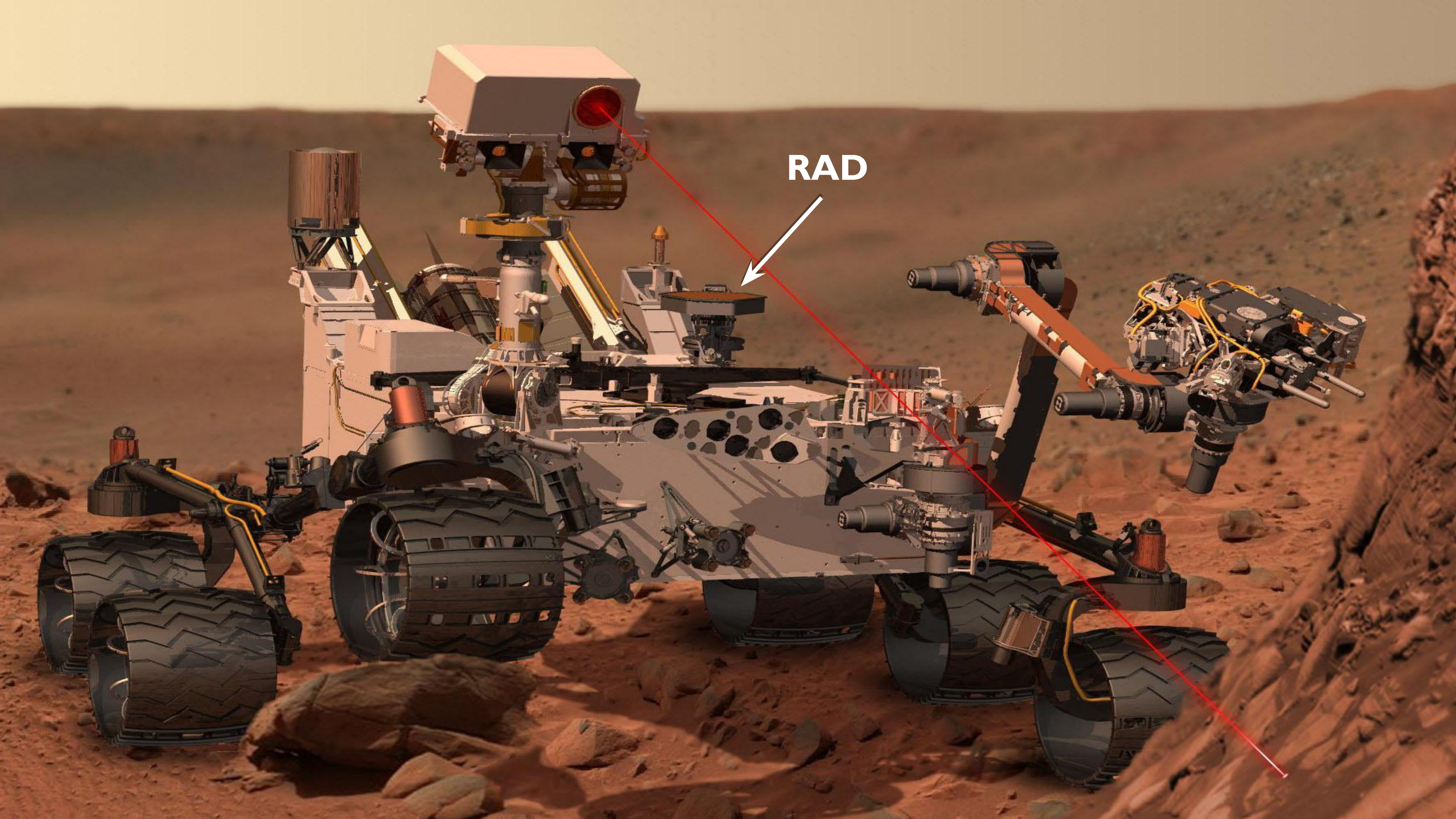
Important note

A “Geant4 course” is typically one week long, here we can only do a very short introduction to characterize what the tool can do.

Hands on exercises are provided with this course, today we can only start doing the exercises, but you can keep the Virtual Machine I have created and the code, so you can continue to test them out on your own if you are interested.

There are several full-week courses organized around the world, we are always happy to organize a course at your university, check Geant4 website for announcements (http://www.geant4.org)


LAYHER


RAD

What do these applications have in common?

The study of the interaction of radiation (e.g. particles, x-rays) with matter has applications in several scientific areas:

- Basic research (e.g. at accelerators to discover new phenomena)
- Medical imaging (e.g. x-rays)
- Medical treatment (e.g. radio-therapy)
- Industrial (e.g. energy production, shielding)

Essential tools in these fields are simulation programs. The most precise are based on Monte Carlo techniques

Several codes exists: Geant4 is one of them, the most widely adopted

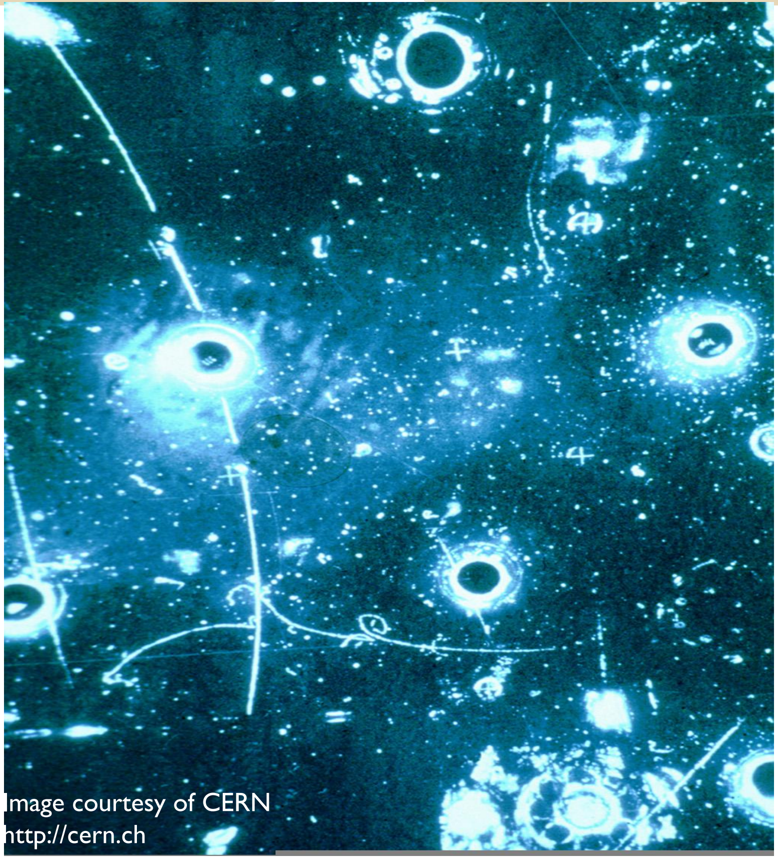
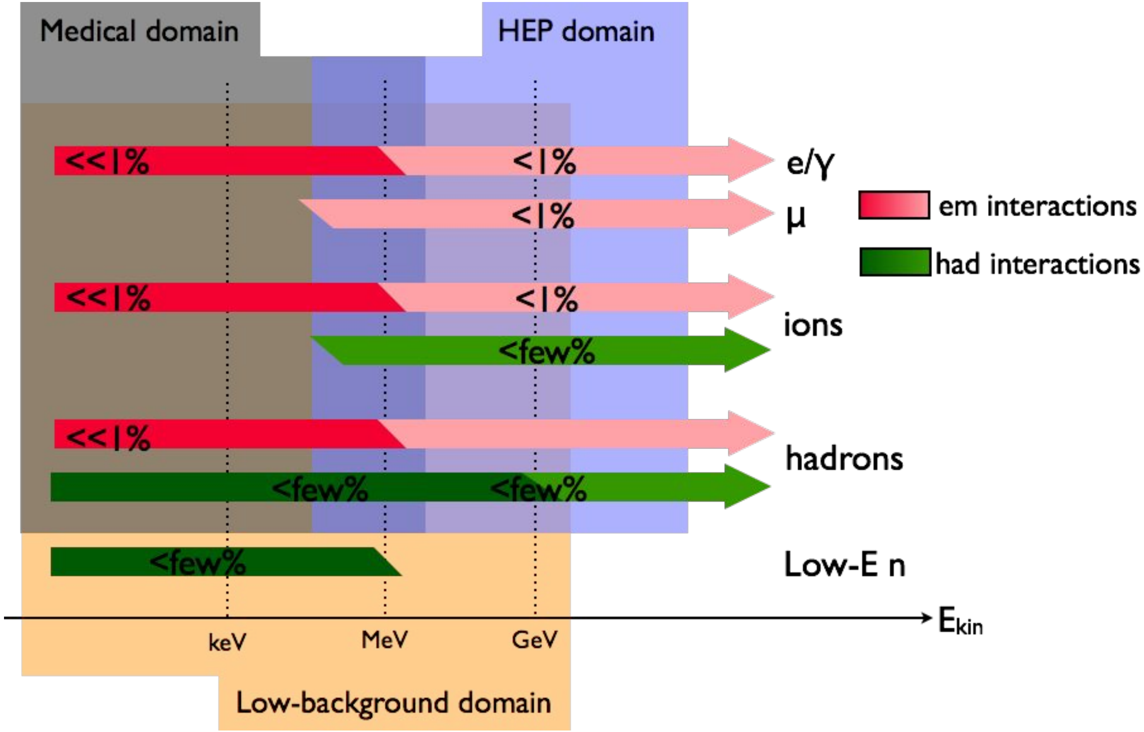
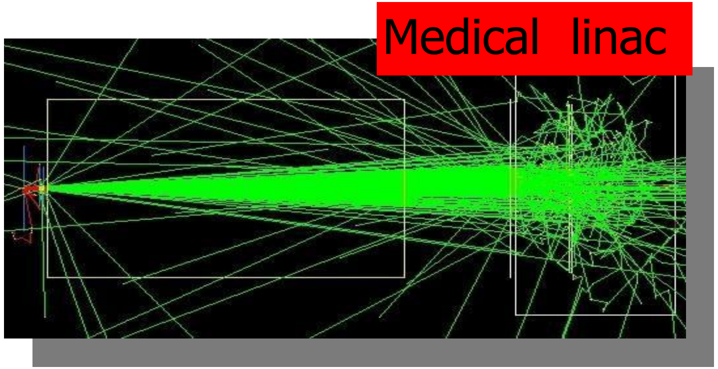
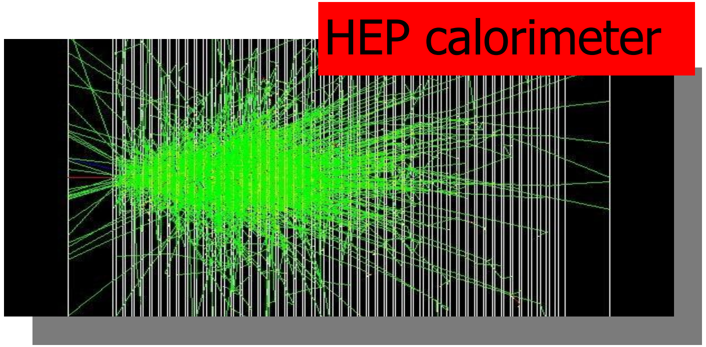


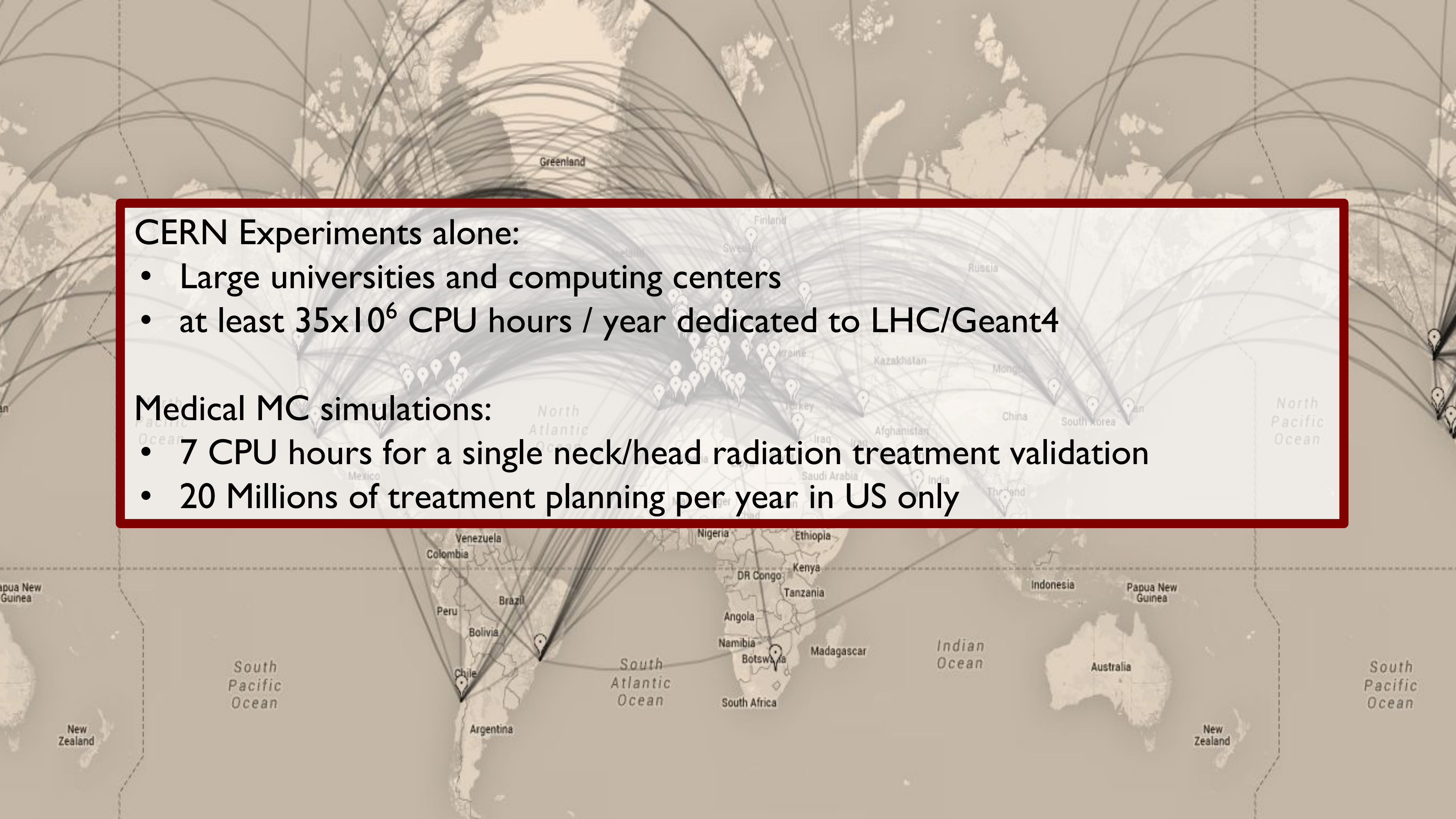
Image courtesy of CERN
http://cern.ch

Physics Requirements









CERN Experiments alone:

- Large universities and computing centers
- at least 35x10^6 CPU hours / year dedicated to LHC/Geant4

Medical MC simulations:

- 7 CPU hours for a single neck/head radiation treatment validation
- 20 Millions of treatment planning per year in US only

Overview

Part 1: Introduction

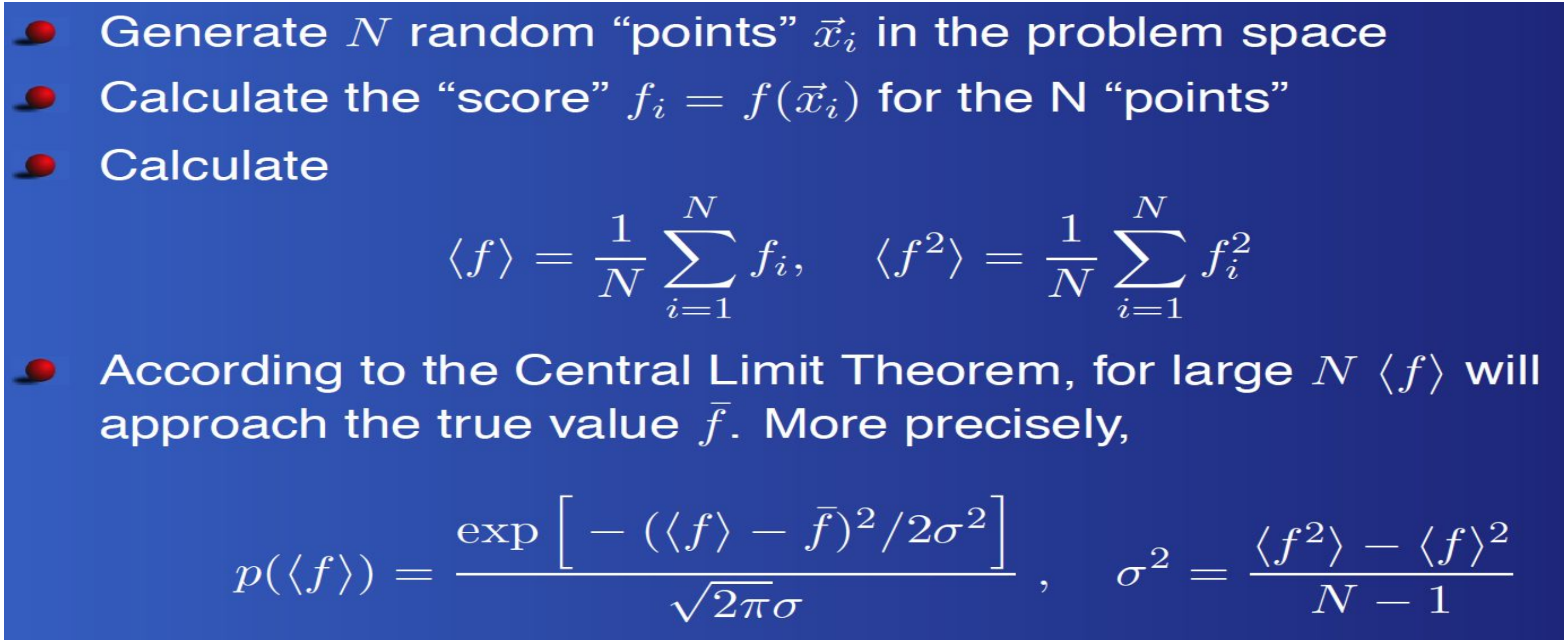
- Historical Notes
- Basics of Monte Carlo Method
- Basics of Monte Carlo for Radiation Transport

Part 1

Historical Notes: Monte Carlo Method

Monte Carlo method : definition

- The Monte Carlo method is a stochastic method for numerical integration.



- Generate N random "points" $\vec{x}_i$ in the problem space
- Calculate the "score" $f_i = f(\vec{x}_i)$ for the N "points"
- Calculate

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f_i, \qquad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} f_i^2$$

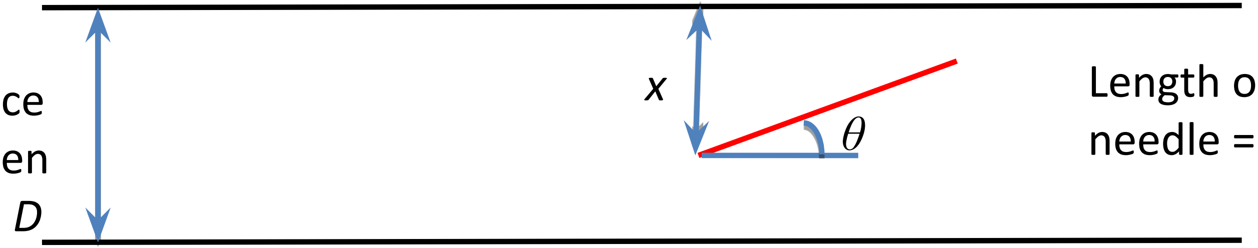
- According to the Central Limit Theorem, for large N $\langle f \rangle$ will approach the true value $\bar{f}$. More precisely,

$$p(\langle f \rangle) = \frac{\exp\left[-(\langle f \rangle - \bar{f})^2 / 2\sigma^2 \right]}{\sqrt{2\pi}\sigma}, \qquad \sigma^2 = \frac{\langle f^2 \rangle - \langle f \rangle^2}{N-1}$$

Buffon’s needle

- Buffon's Needle is one of the oldest problems in the field of geometrical probability. It was first stated in 1777. It involves dropping a needle on a lined sheet of paper and determining the probability of the needle crossing one of the lines on the sheet. The remarkable result is that the probability is directly related to the value of π.
- The needle in the picture misses the line. The needle will hit the line if $x \leq L\sin(\theta)$. Assuming $L \leq D$, how often will t

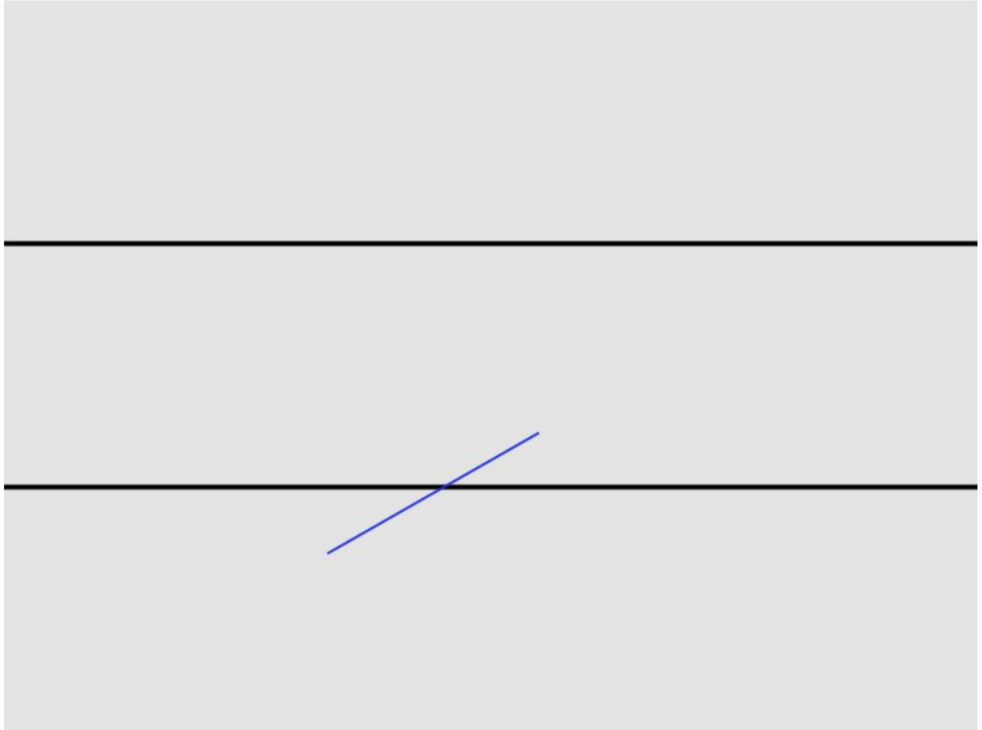
$$P_{cut} = \int_0^{\pi} P_{cut}(\theta)\frac{d\theta}{\pi} = \int_0^{\pi} \frac{L\sin\theta}{D}\frac{d\theta}{\pi} = \frac{L}{\pi D}\int_0^{\pi} \sin\theta\, d\theta = \frac{2L}{\pi D}$$



Distance between lines = D

Length of the needle = L

Buffon’s needle



Number of drops (n) = 1

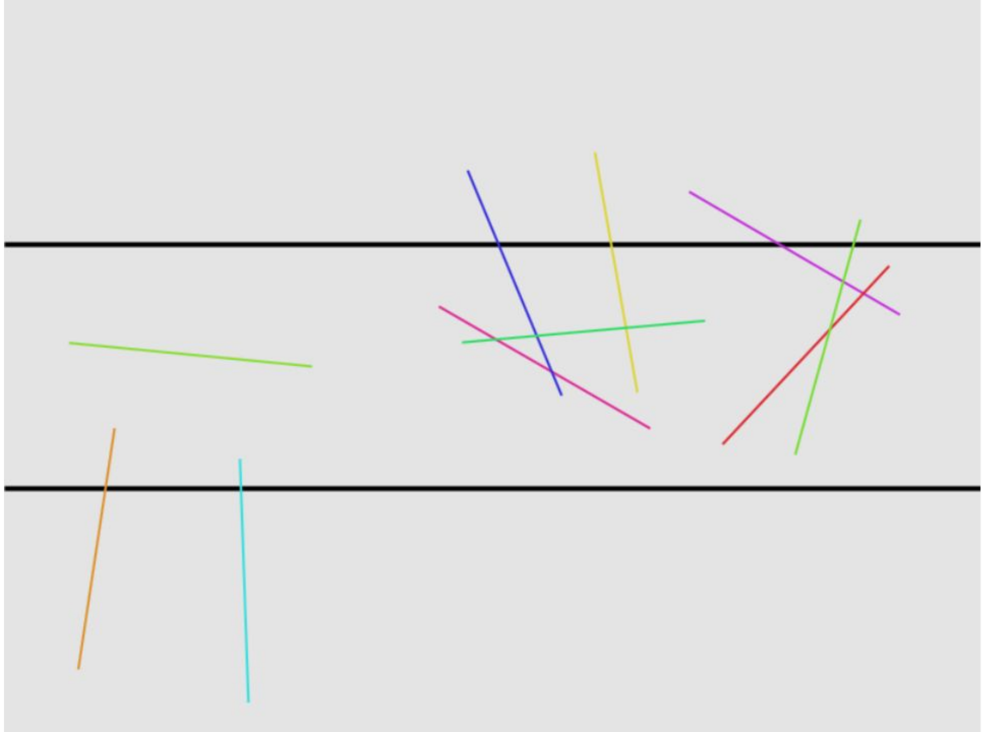
Number of hits (h) = 1

P_{cut} = h/n = 1

$\pi = (2\,L\,/\,D) * (\,n\,/\,h\,)$

$= 2\,/\,P_{cut} \sim 2$

Buffon's needle



Number of drops (n) = 10

Number of hits (h) = 6

$P_{cut} = h/n = 0.6$

$\pi = (2\,L\,/\,D) * (\,n\,/\,h\,)$

$\quad = 2\,/\,P_{cut} \sim 3.33333\ldots$

Buffon’s needle

Number of drops (n) = 100

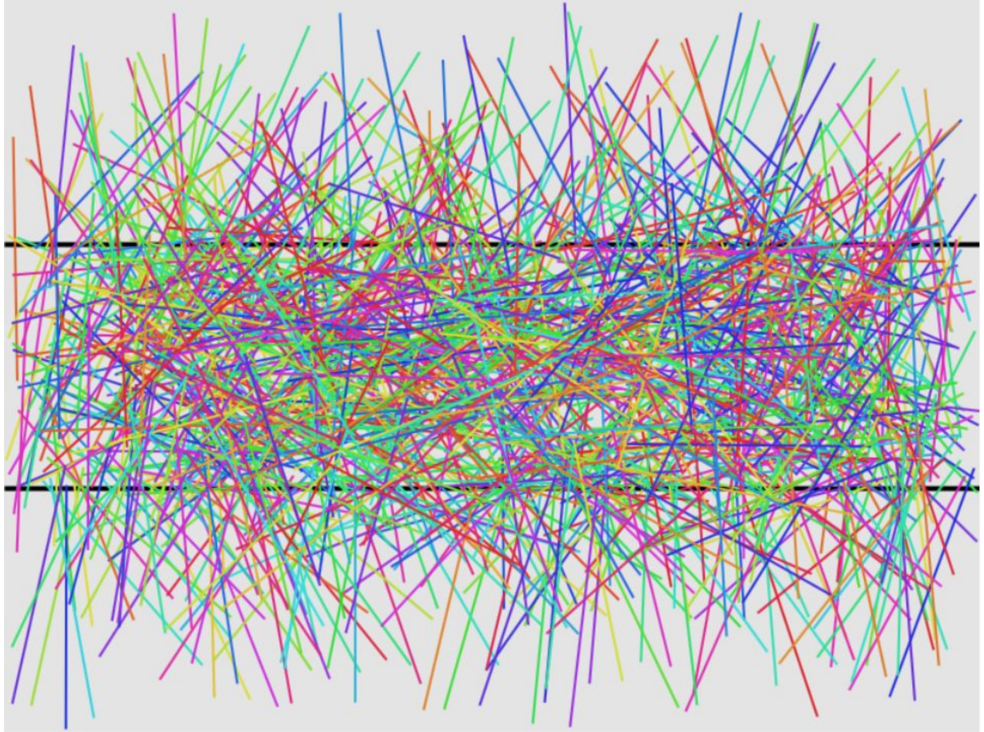
Number of hits (h) = 65

P_{cut} = h/n = 0.65

$\pi = (2\, L\, /\, D) * (\, n\, /\, h\,)$

$= 2\, /\, P_{cut} \sim 3.0769231$

Buffon’s needle



Number of drops (n) = 1000

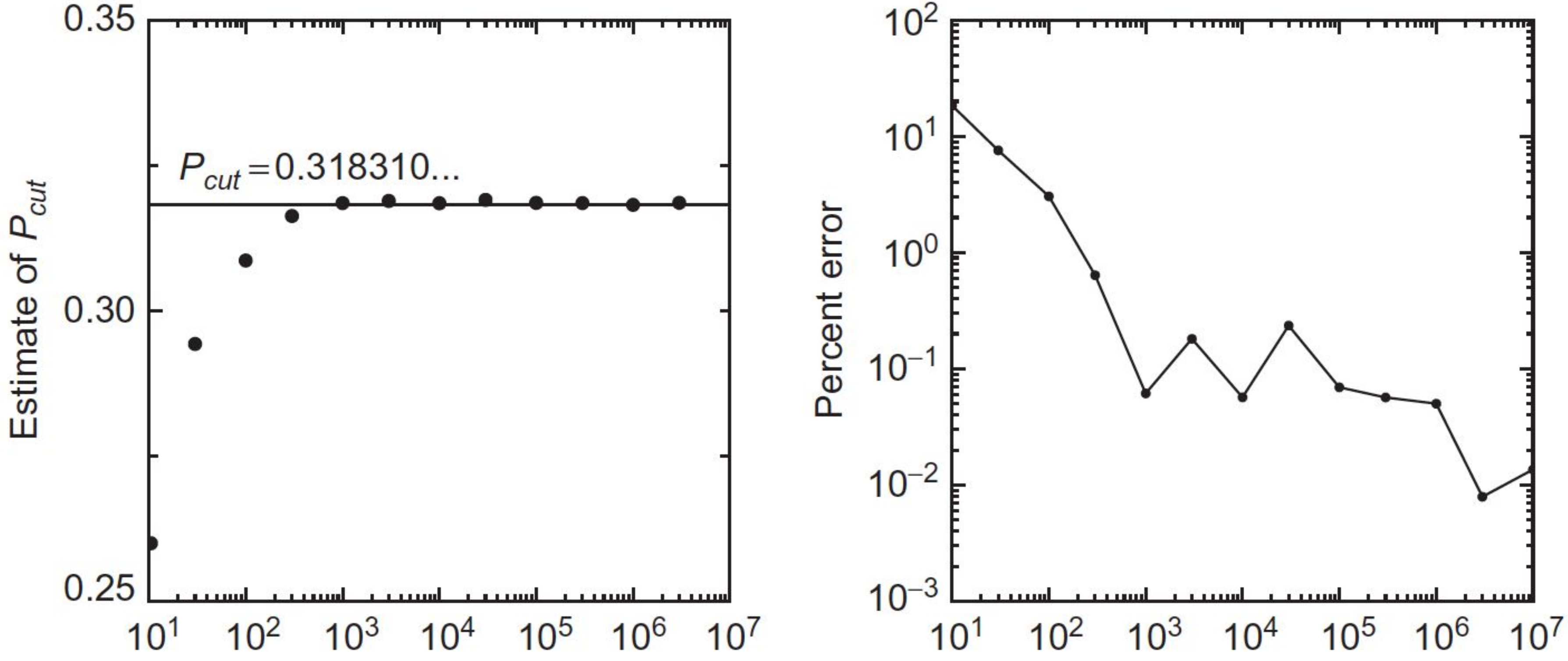
Number of hits (h) = 640

P_{cut} = h/n = 0.64

$\pi = (2\,L\,/\,D) * (\,n\,/\,h\,)$

$= 2\,/\,P_{cut} \sim 3.125$

Buffon’s needle



P_{cut} = h/n = 0.318310… ➡$\pi = (2\,L\,/\,D) * (\,n\,/\,h\,) = 2\,/\,P_{cut}$ ~

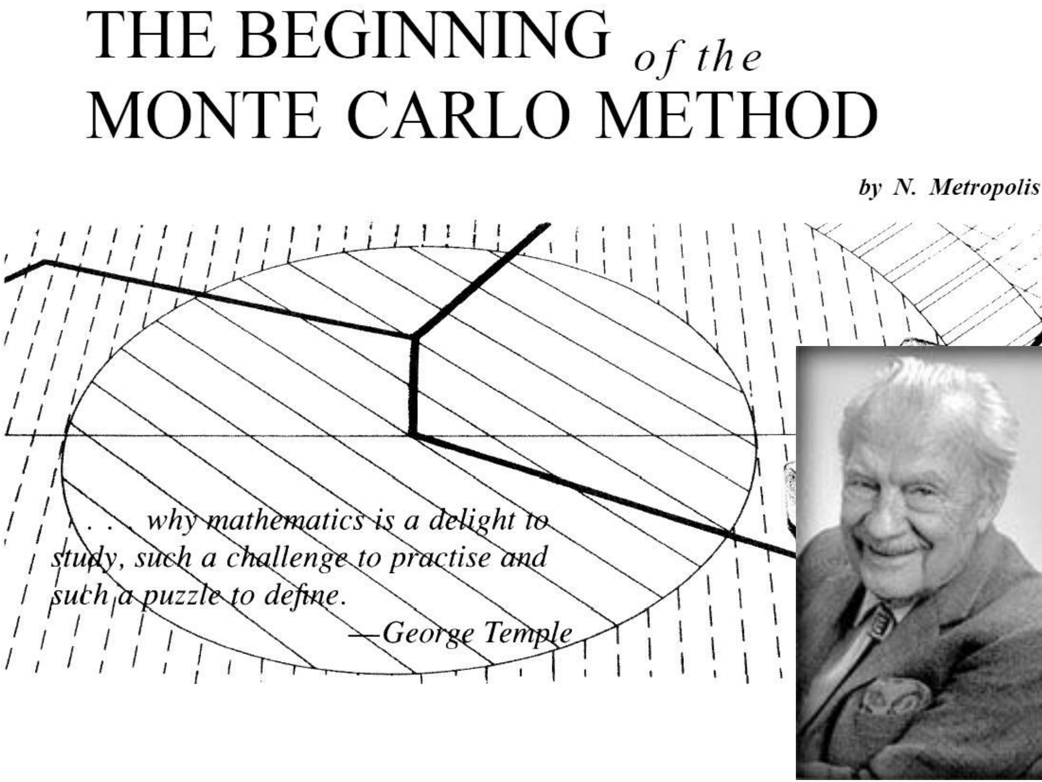
Monte Carlo methods for radiation transport

- Fermi (1930): random method to calculate the properties of the newly discovered neutron
- Manhattan project (40’s): simulations during the initial development of thermonuclear weapons. Von Neumann and Ulam coin the term “Monte Carlo”
- Field growth with the availability of digital computers
- Berger (1963): first complete coupled electron-photon transport code that became known as ETRAN
- Exponential growth since the 1980’s

Pioneers of the Monte Carlo simulation method

A team headed by Nicholas Metropolis (1915-1999) carried out the first actual Monte Carlo calculations on the ENIAC computer in 1948.

The Metropolis algorithm (1953 paper): cited in Computing in Science and Engineering as being among the top 10 algorithms having the "greatest influence on the development and practice of science and engineering in the 20th century."



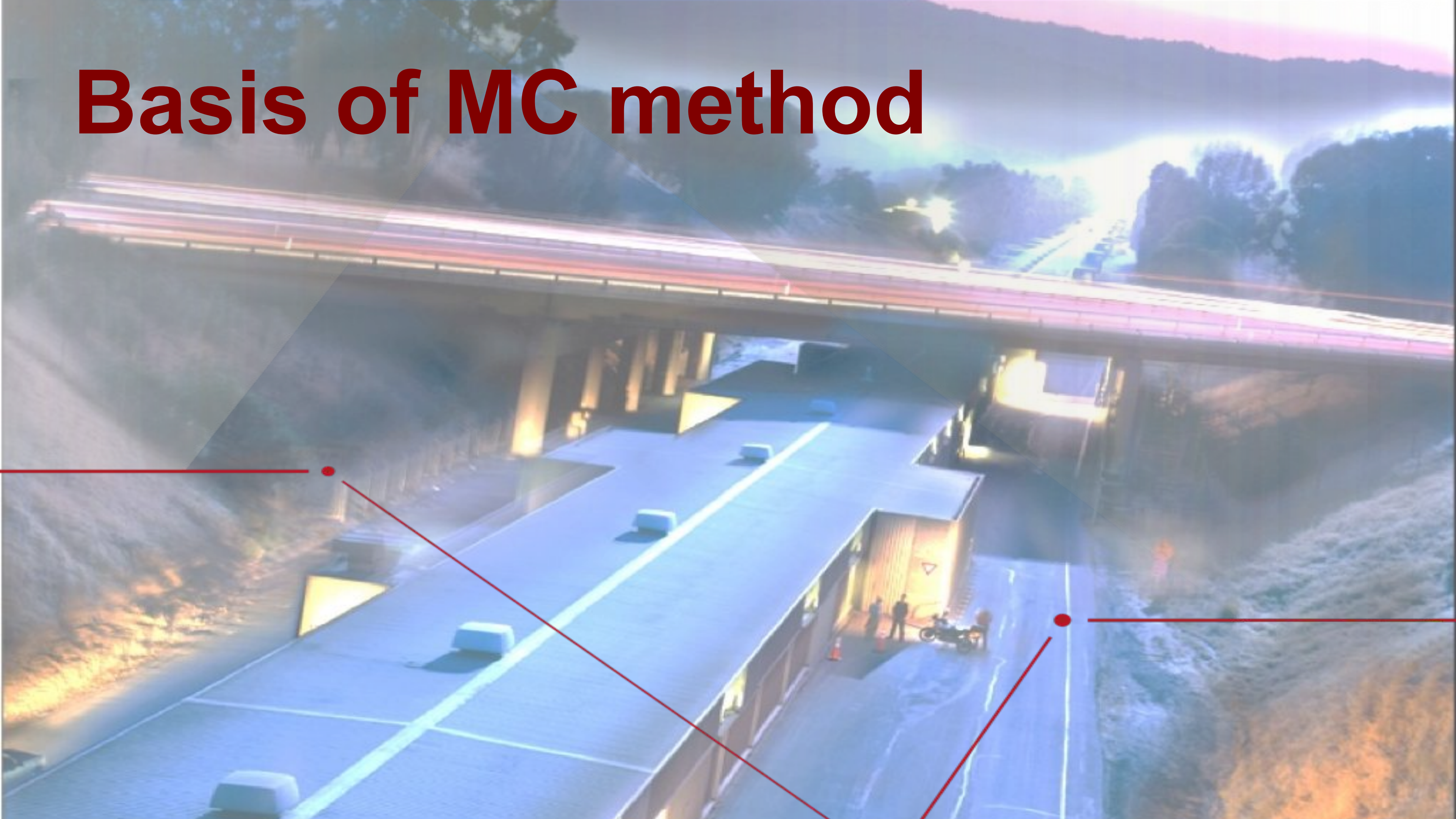
THE BEGINNING *of the*
MONTE CARLO METHOD

by N. Metropolis

. . . why mathematics is a delight to study, such a challenge to practise and such a puzzle to define.

—George Temple

Basis of MC method

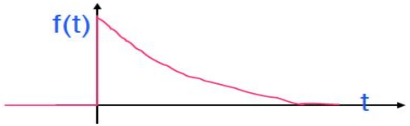


Simplest case – decay in flight (1)

- Suppose an unstable particle of life time *t* is flying with initial momentum *p*.
  - Distance to travel before decay : *d* = *t v*
- The life time t is a random value with probability density function

$$f(t) = \frac{1}{\tau}\exp\left(-\frac{t}{\tau}\right) \qquad t \geq 0$$

τ is the mean life of the particle



- *t* is determined from the cumulative distribution function. Generate a random number *r* with uniform probability on [0,1)

$$r = F(t) = \int_{-\infty}^{t} f(u)du$$

- From *r* on [0,1), one can sample the value *t* with:

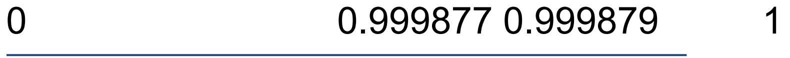
$$t = F^{-1}(\,r\,) = -\tau \ln(\,1 - r\,) \qquad 0 \leq r < 1$$

Simplest case – decay in flight (2)

- When the particle has traveled the *d* = *t v*, it decays.

- Decay of an unstable particle itself is a random process

$\pi^+ \rightarrow \mu^+ \nu_\mu$	(99.9877 %)
$\pi^+ \rightarrow \mu^+ \nu_\mu \gamma$	(2.00×10^{-4} %)
$\pi^+ \rightarrow e^+ \nu_e$	(1.23×10^{-4} %)
$\pi^+ \rightarrow e^+ \nu_e \gamma$	(7.39×10^{-7} %)
$\pi^+ \rightarrow e^+ \nu_e \pi^0$	(1.036×10^{-8} %)
$\pi^+ \rightarrow e^+ \nu_e e^+ e^-$	(3.2×10^{-9} %)

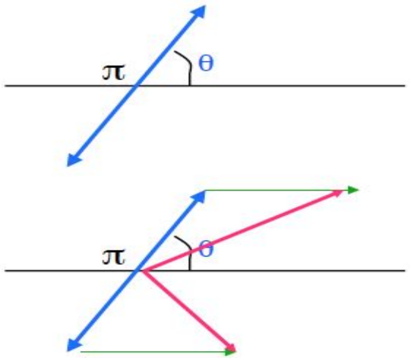


- Select a decay channel by shooting a random number

- In the rest frame of the parent particle, rotate decay products in θ $[0,\pi)$ and φ $[0,2\pi)$ by shooting two random numbers

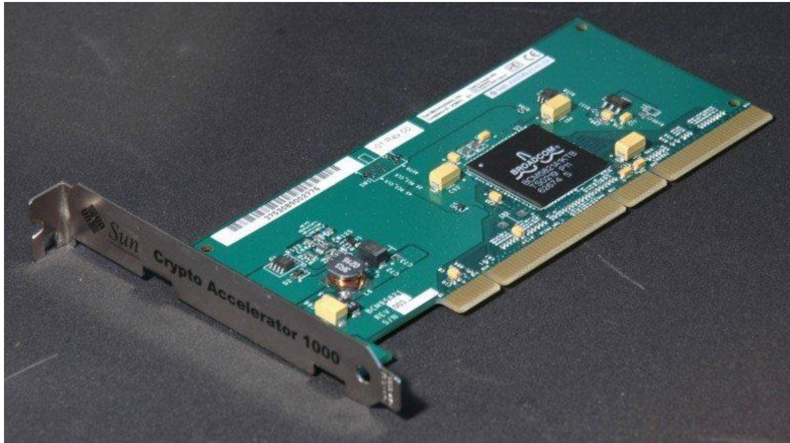
- Finally, Lorentz-boost the decay products

- You need 4 random numbers to simulate one decay in flight



Random number generators (RNG)

- At the core of all Monte Carlo calculations is some mechanism to produce a long sequence of random numbers r_i that are uniformly distributed over the open interval [0,1)
- A true random sequence could, in principle, be obtained by coupling to our computer some external device that would produce a truly random signal.
- Would be impossible to debug a Monte Carlo code if, on every run, a different sequence of random numbers were used: reproducibility



pRNG: properties

A pRNG needs a seed to start a sequence. It will always produce the same sequence when initialized with that state.

The period of a pRNG is defined as the maximum, over all starting seeds, of the length of the repetition-free of the sequence. We want a large period

Most pRNG algorithms produce sequences which are uniformly distributed. We want an algorithm that does not show correlations on its output.

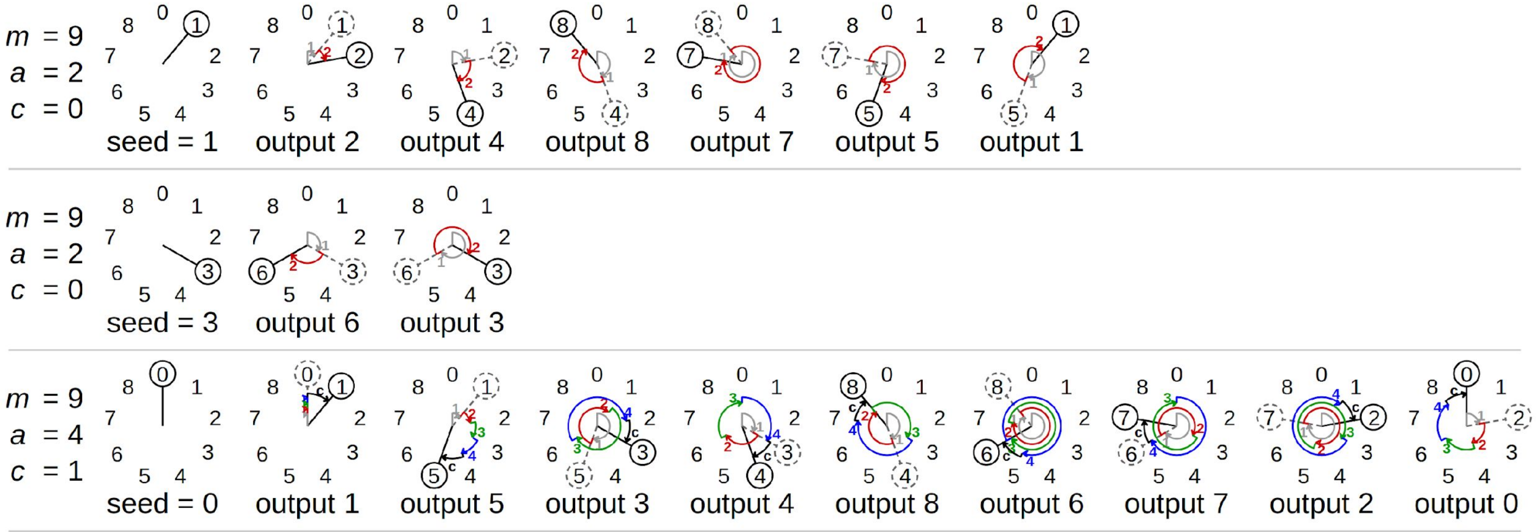
pRNG example: LCG

Linear Congruential Generator:

```
function lcg( $X_n$ , a , c, m ):
    return (a*$X_n$+c) % m
```

The “art” is to find a good set of parameters: a,c,m

For example for GCC implementation (`rand()` in `stdlib.h`): $m=2^{31}$, a=1103515245 , c = 12345



Part 2

Overview

Part 2: Geant4 Toolkit
- General architecture
- Geometry
- Physics
- Geant4 extensions

Basic components

A detector simulation program requires at least the following three components:

- Geometry description module: to describe the experimental setup in terms of shapes, materials, relative positioning
- Physics modules: to cover all particles, energies and interaction types of interest
- Primary definition/generation: to describe what are the properties (species, 4-momenta) of the first particles that “appear” in the setup (can be provided by an external tool, e.g. a *generator* -PYTHIA, HERWIG,...- for HEP)

A system (user-hooks) to interact with the simulation and extract the physics quantities must be provided (e.g. scorers that record energy deposits in specified regions)

Alternative, useful components:

- Analysis tools to create histograms and store data in files
- Visualization drivers (to display geometry and possibly tracks and doses)
- System integration tools: MPI interfaces to submit jobs on clusters, scripting/macro systems

The following is based on Geant4 internals, but many concepts are common to all MC detector simulation tools

Semi-classical Approach

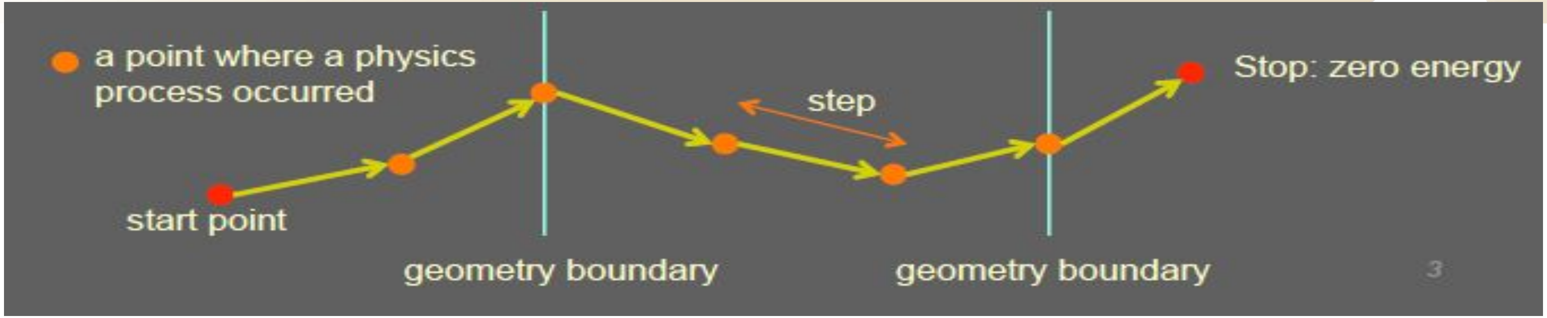
In Geant4, a particle that flies through a detector is **treated as a classical particle**, as a point-like object which has a well-defined momentum at each instant:

- Space-time position (t, x, y, z)
- Energy-momentum (E, px, py, pz)

This is a reasonable approximation, given that in most practical situations particles are seen as "tracks" in macroscopic detectors

Geant4 is based on a semi-classical approach, because the particles are treated classically, but **their interactions** - cross sections and final states - **often take into account the results of quantum-mechanical effects**

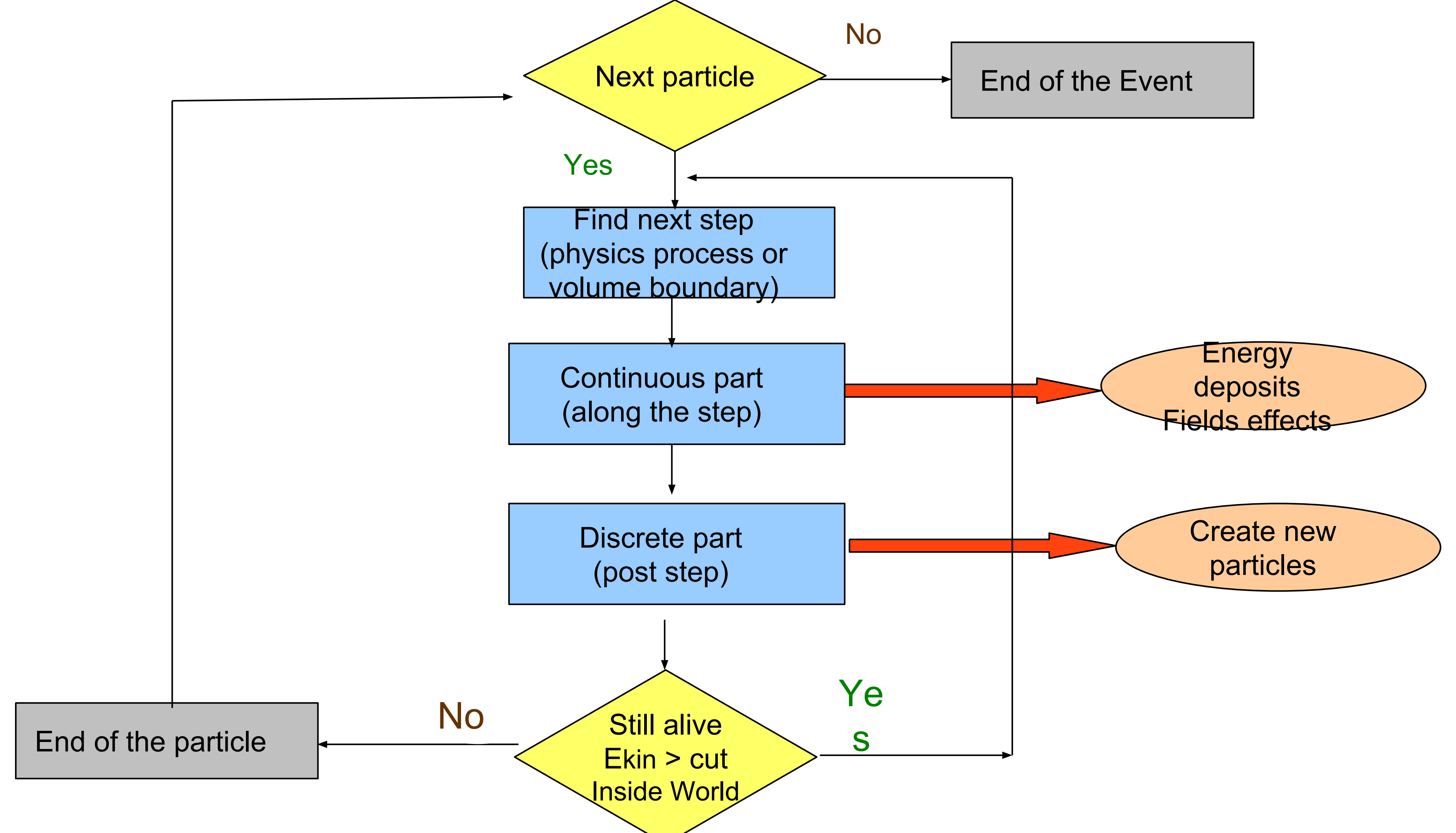
Simulation in Steps



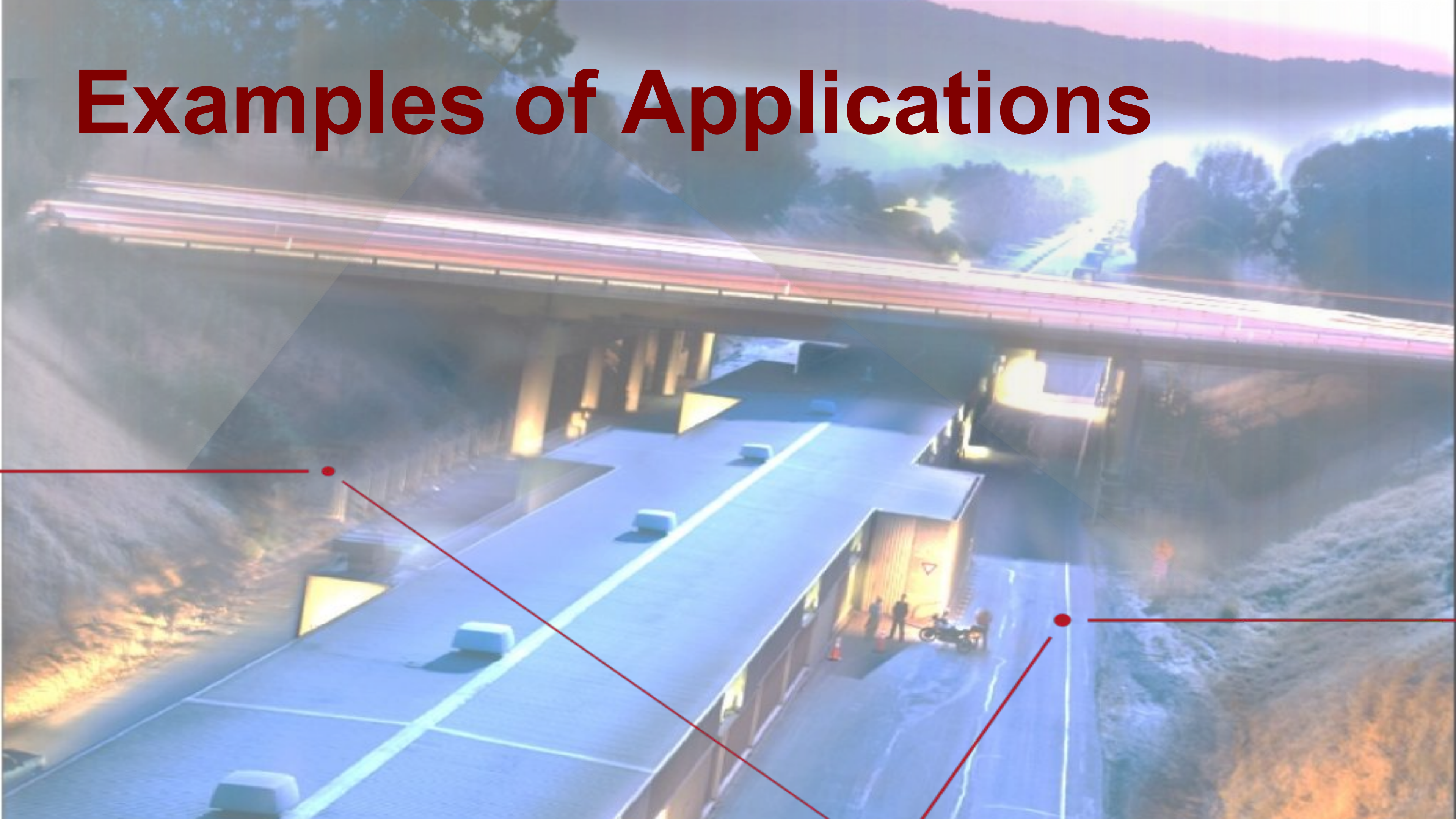
Treat **one particle at the time** and treat a particle **in steps**

For each step

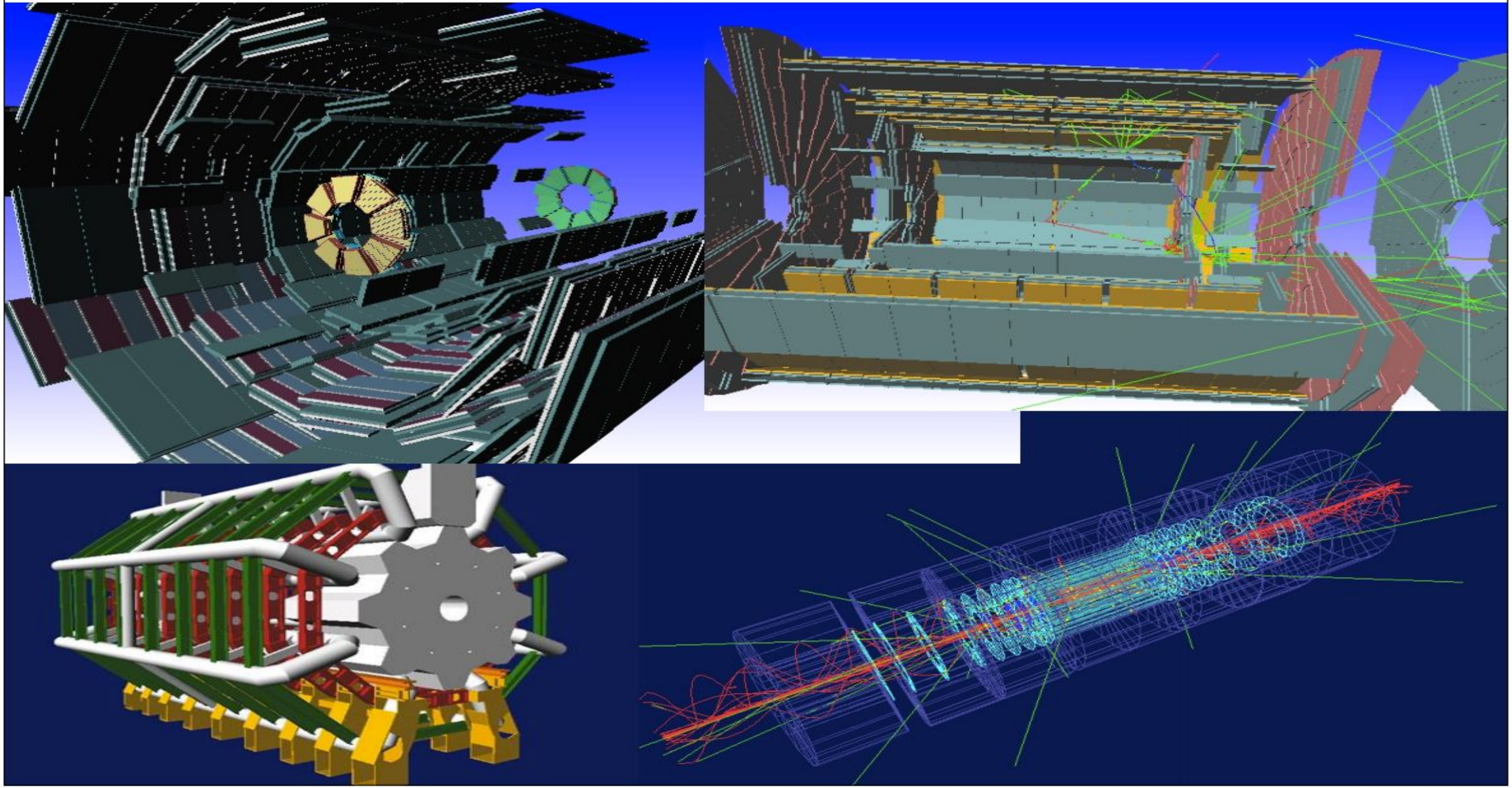
1. the step length is determined by the cross sections of the physics processes and the geometrical boundaries
2. if new particles are created, add them to the list of particles to be transported
3. local energy deposit; effect of magnetic and electric fields;
4. if the particle is destroyed by the interaction, or it reaches the end of the apparatus, then the simulation of this particle is done

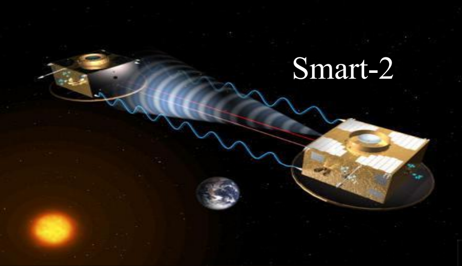

Next particle
No
End of the Event
Yes
Find next step (physics process or volume boundary)
Continuous part (along the step)
Energy deposits Fields effects
Discrete part (post step)
Create new particles
No
End of the particle
Still alive Ekin > cut Inside World
Yes

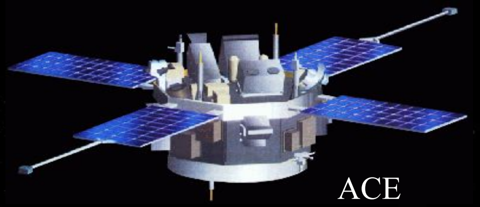
Examples of Applications

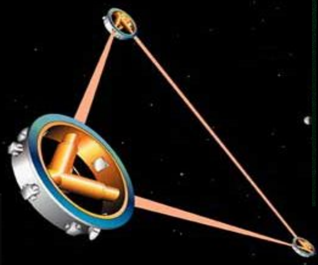


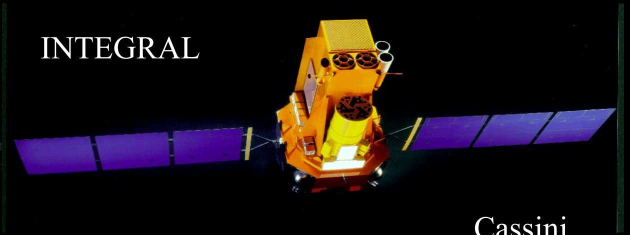
Geant4 in High Energy Physics (ATLAS at LHC)

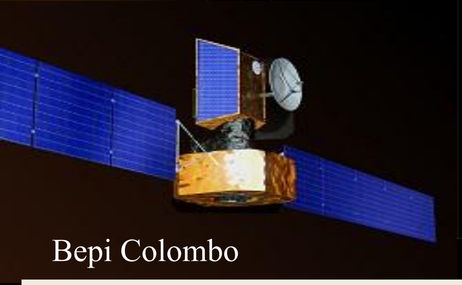


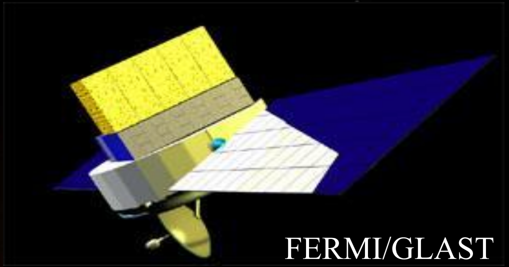

Smart-2


ACE

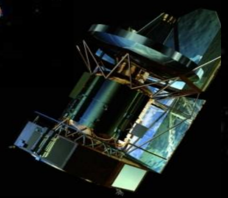

LISA


INTEGRAL


Bepi Colombo


FERMI/GLAST

Herschel

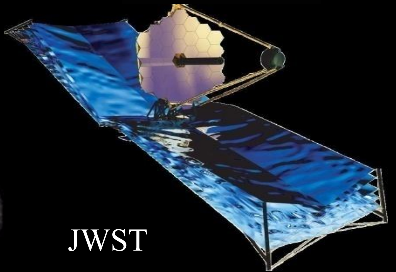


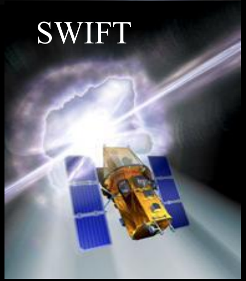
Cassini


Astro-E2


XMM-Newton

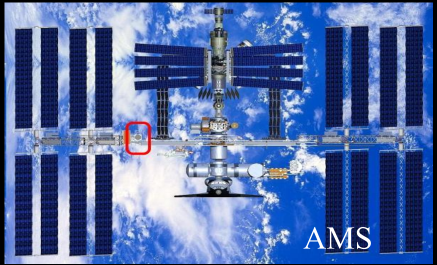

GAIA

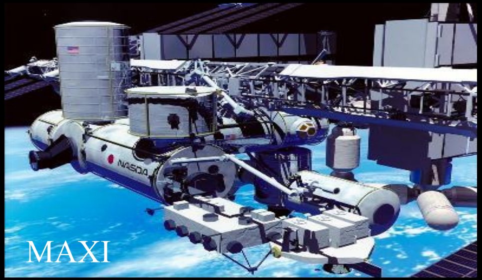

JWST


SWIFT

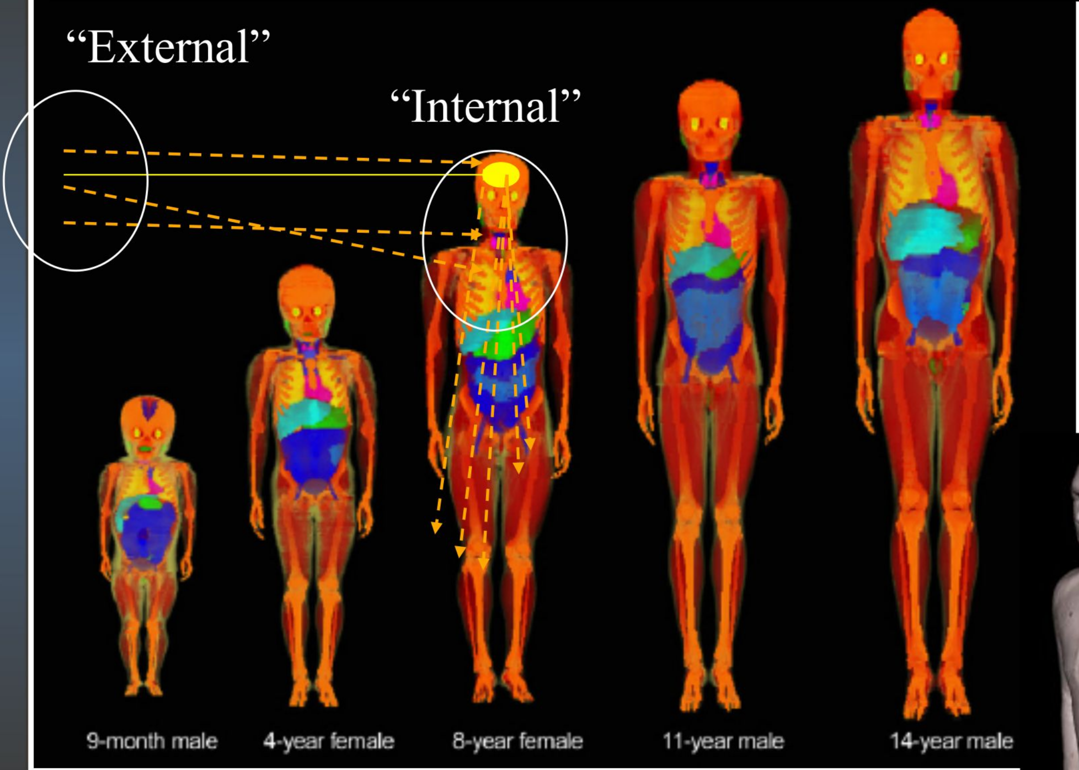

ISS Columbus


EUSO


AMS

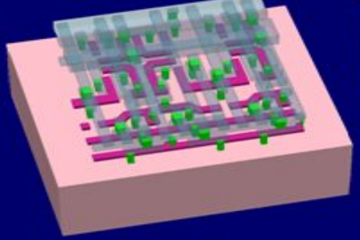

MAXI

The risk associated with neutron radiation in proton therapy

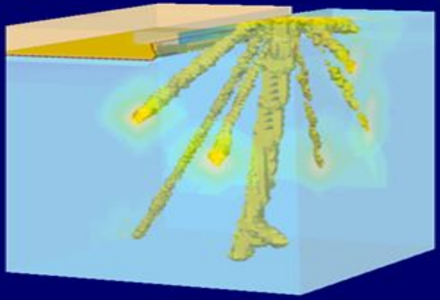


Phantoms implemented into the Geant4 Monte Carlo dose calculation environment at Mass. Gen. Hosp.

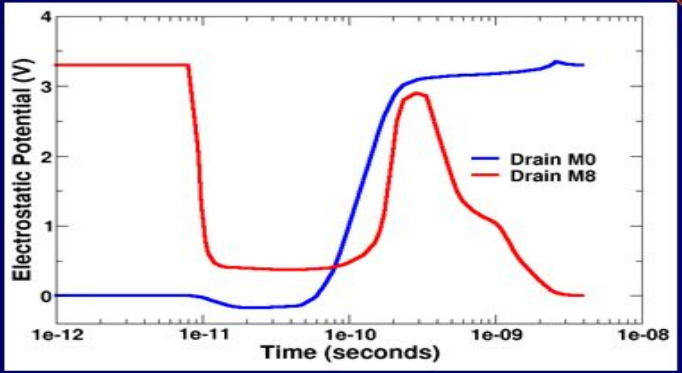
RADSAFE on SEE in SRAMs



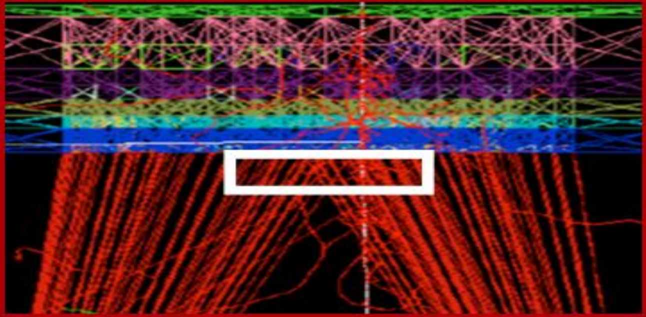
TCAD Cell Structure: SRAM Cell



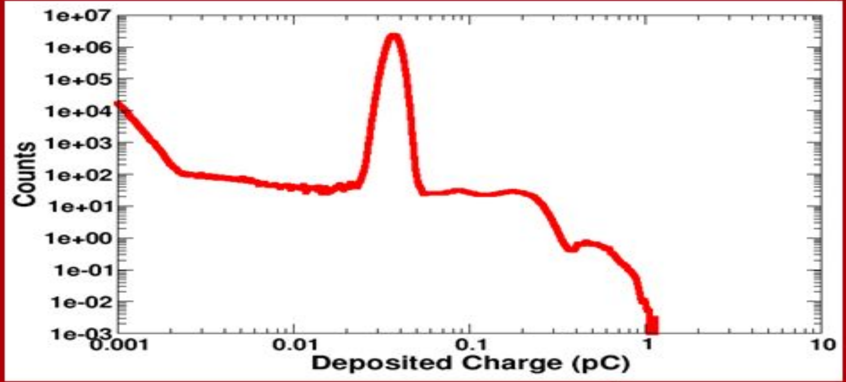
Single Charge Deposition in TCAD: Ne+W Event



SRAM Cell Upset



Geant4 Geometry and 523 MeV Neon Event

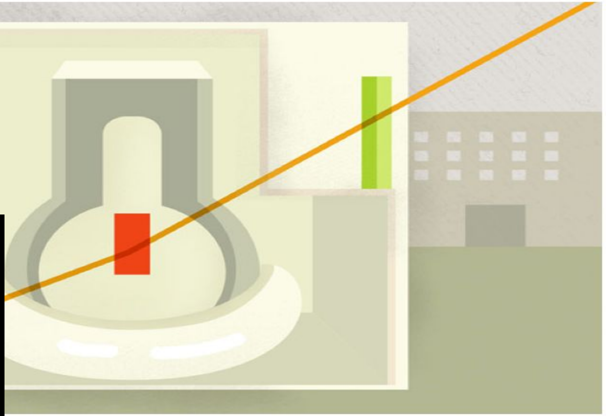


MRED Energy Deposition for 10^8 Events

symmetry of particle physics

Those exterior walls, made of concrete 10 feet thick, offer their own challenge. Based on computer simulations run with the particle physics software GEANT4, the walls are expected to reduce the resolution to about 30 centimeters.

In addition, the team must also prepare for the high radiation levels present just outside of the reactor units.



ors (shown here in green) on either side of
record the path of muons (represented by the
hrough the reactor. By determining how the
ectors, scientists will compile the first picture of

with Shawna X.

age

As time ticks down to the restart of the Large Hadron Collider, scientists are making sure their detectors run like clockwork.

Geometry

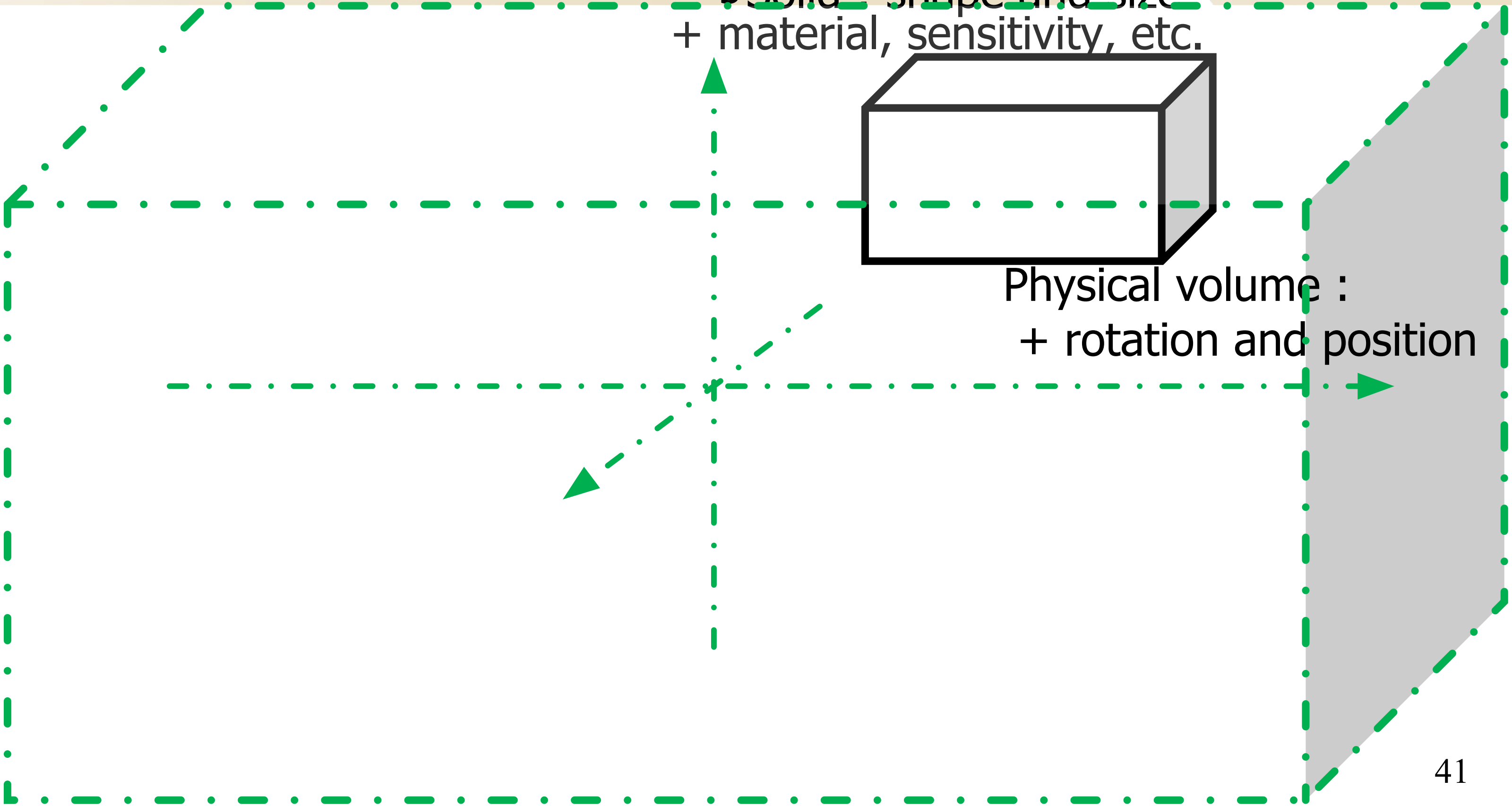
Creating a detector in Geant4

Three steps procedure:

1) G4Shape: Create a Volume (e.g. shape), with the correct dimension
2) G4LogicalVolume: Assign one (and only one) material to the shape, optionally assign a magnetic field and “sensitivity”
3) G4VPhysicalVolume: Place one (or more) logical volumes inside another logical volume, specifying the position and rotation w.r.t. the mother

Repeat for all volumes of the detector

Define detector geometry

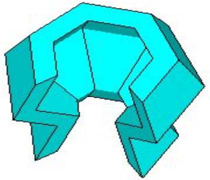


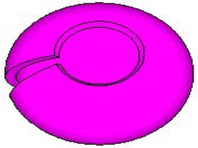
Solid : shape and size

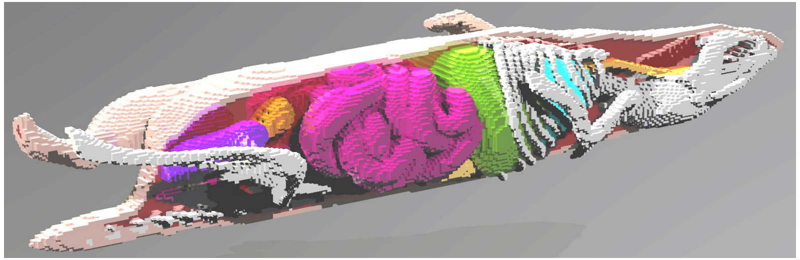
Logical volume :
+ material, sensitivity, etc.

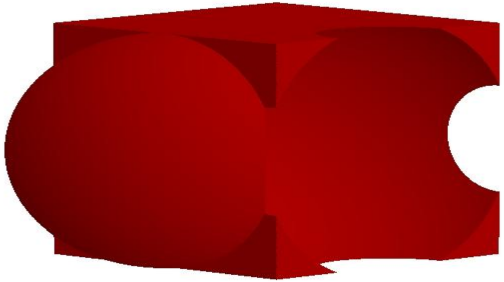
Physical volume :
+ rotation and position

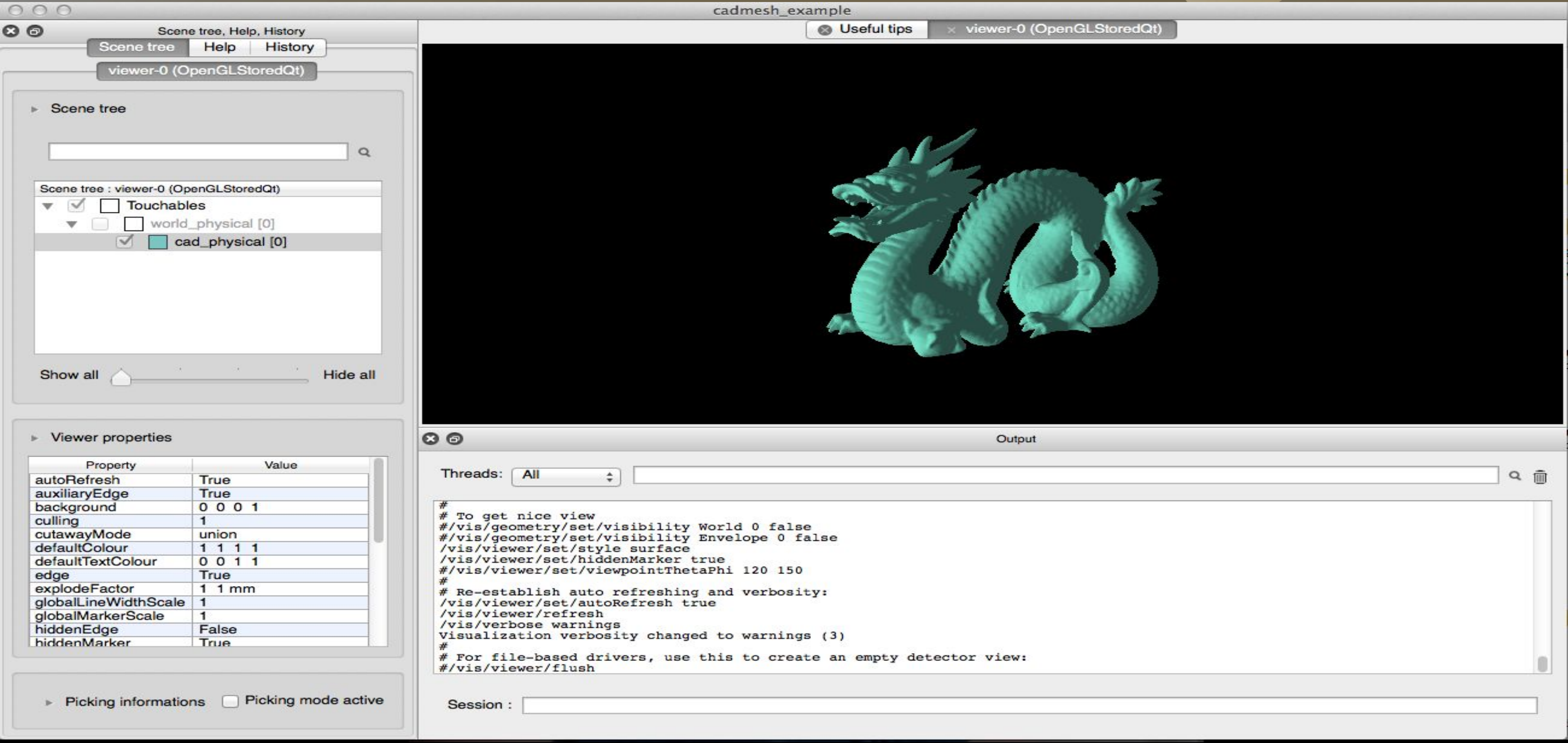
Key geometry capabilities











Property	Value
autoRefresh	True
auxiliaryEdge	True
background	0 0 0 1
culling	1
cutawayMode	union
defaultColour	1 1 1 1
defaultTextColour	0 0 1 1
edge	True
explodeFactor	1 1 mm
globalLineWidthScale	1
globalMarkerScale	1
hiddenEdge	False
hiddenMarker	True

```
#
# To get nice view
#/vis/geometry/set/visibility World 0 false
#/vis/geometry/set/visibility Envelope 0 false
/vis/viewer/set/style surface
/vis/viewer/set/hiddenMarker true
#/vis/viewer/set/viewpointThetaPhi 120 150
#
# Re-establish auto refreshing and verbosity:
/vis/viewer/set/autoRefresh true
/vis/viewer/refresh
/vis/verbose warnings
Visualization verbosity changed to warnings (3)
#
# For file-based drivers, use this to create an empty detector view:
#/vis/viewer/flush
```

Physics

Geant4 Physics

Geant4 provides a wide variety of physics components

Physics components are coded as processes

- a process is a class which tells a particle how to interact
- Geant4 provides many of these

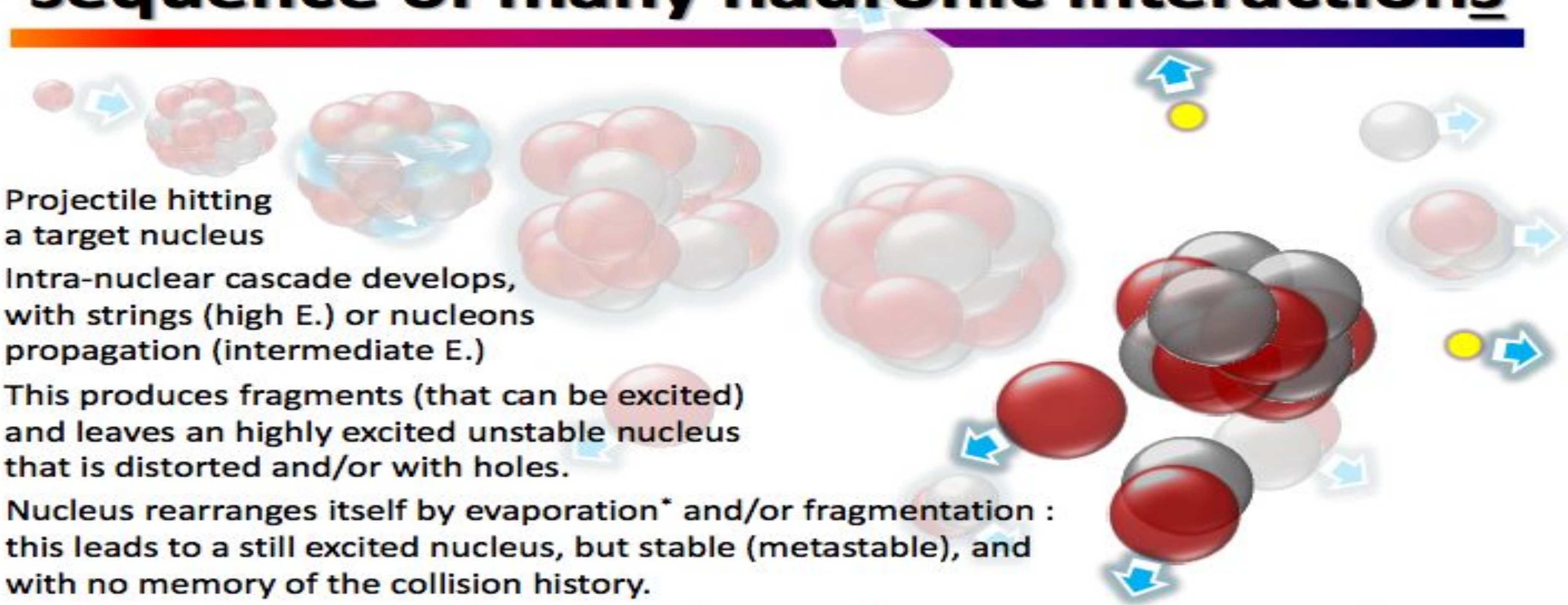
Processes are classified as

- electromagnetic, hadronic, decay, or transportation

Geant4 Electromagnetic Packages

- Standard
  - γ, e± up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV
- Muons
  - up to 1 PeV
  - energy loss propagator
- X-rays
  - X-ray and optical photon production proc.
- High-energy
  - processes at high energy (E>10GeV)
  - physics for exotic particles
- Polarisation
  - simulation of polarized beams
- Optical
  - optical photon interactions
- Low-energy
  - Livermore library γ, e- from 10 eV up to 1 GeV
  - Livermore library based polarized processes
  - PENELOPE code rewrite , γ, e- , e+ from 100 eV up to 1 GeV (2008 version)
  - hadrons and ions up to 1 GeV
  - atomic de-excitation (fluorescence + Auger)
- Geant4-DNA
  - microdosimetry models for radiobiology (Geant4-DNA project) from 0.025 eV to 10 MeV
- Adjoint
  - New sub-library for reverse Monte Carlo simulation from the detector of interest back to source of radiation
- Utils
  - general EM interfaces

One hadronic collision = sequence of many hadronic interactions



Projectile hitting a target nucleus

Intra-nuclear cascade develops, with strings (high E.) or nucleons propagation (intermediate E.)

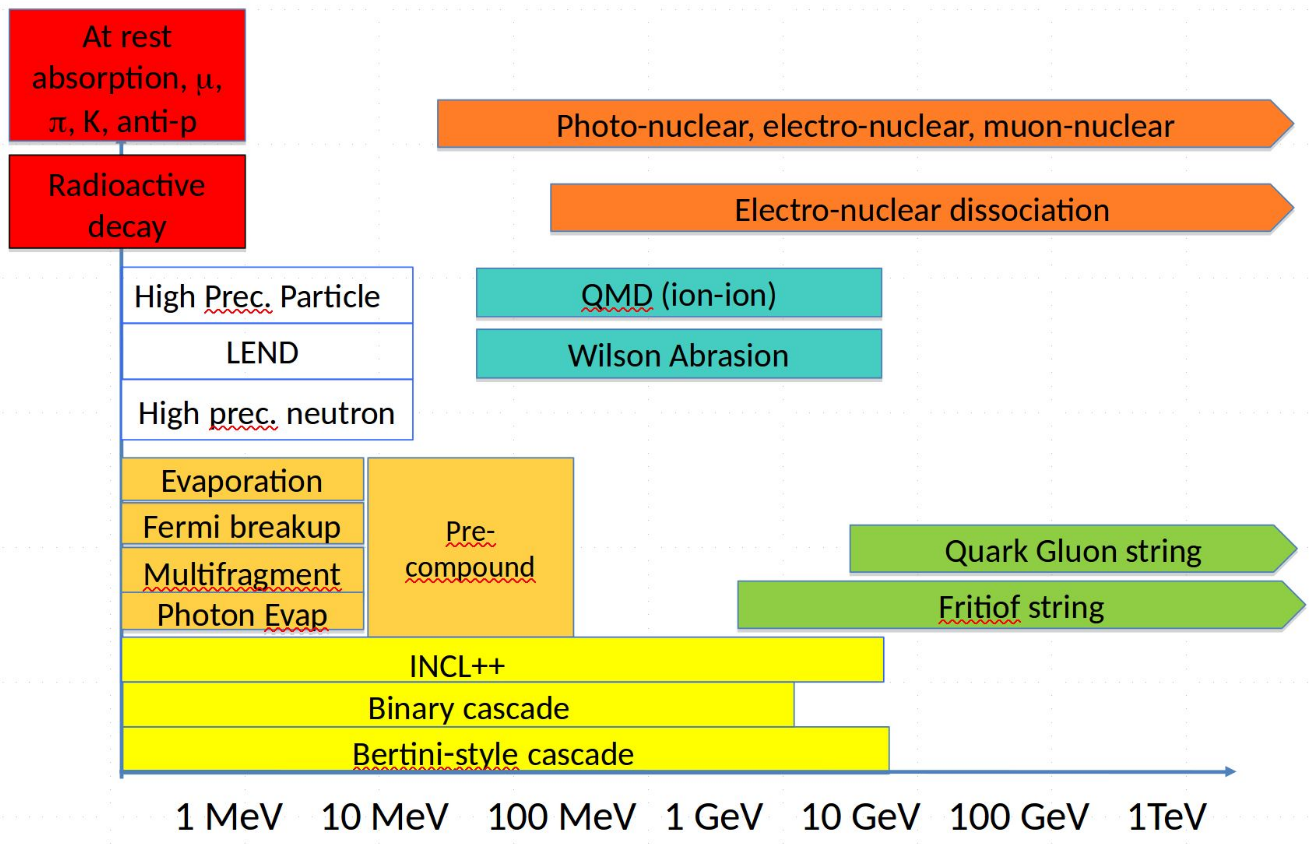
This produces fragments (that can be excited) and leaves an highly excited unstable nucleus that is distorted and/or with holes.

Nucleus rearranges itself by evaporation* and/or fragmentation : this leads to a still excited nucleus, but stable (metastable), and with no memory of the collision history.

The nucleus undergoes final de-excitation by evaporation* or fission and ends-up in its ground state. In case of fission, further de-excitation of fragments may occur.

(*) **Evaporation** = de-excitation by emission of light nuclei $\in$ {n, p, d, t, 3He, α} or photon

Partial Hadronic Catalog



What is a Physics List?

A software artifact that collects all the particles, physics processes and production thresholds needed for your application

It is a very flexible way to build a physics environment

- user can pick the particles he wants
- user can pick the physics to assign to each particle

Geant4 provides several “production physics lists” which are routinely validated and updated with each release

Production Physics Lists

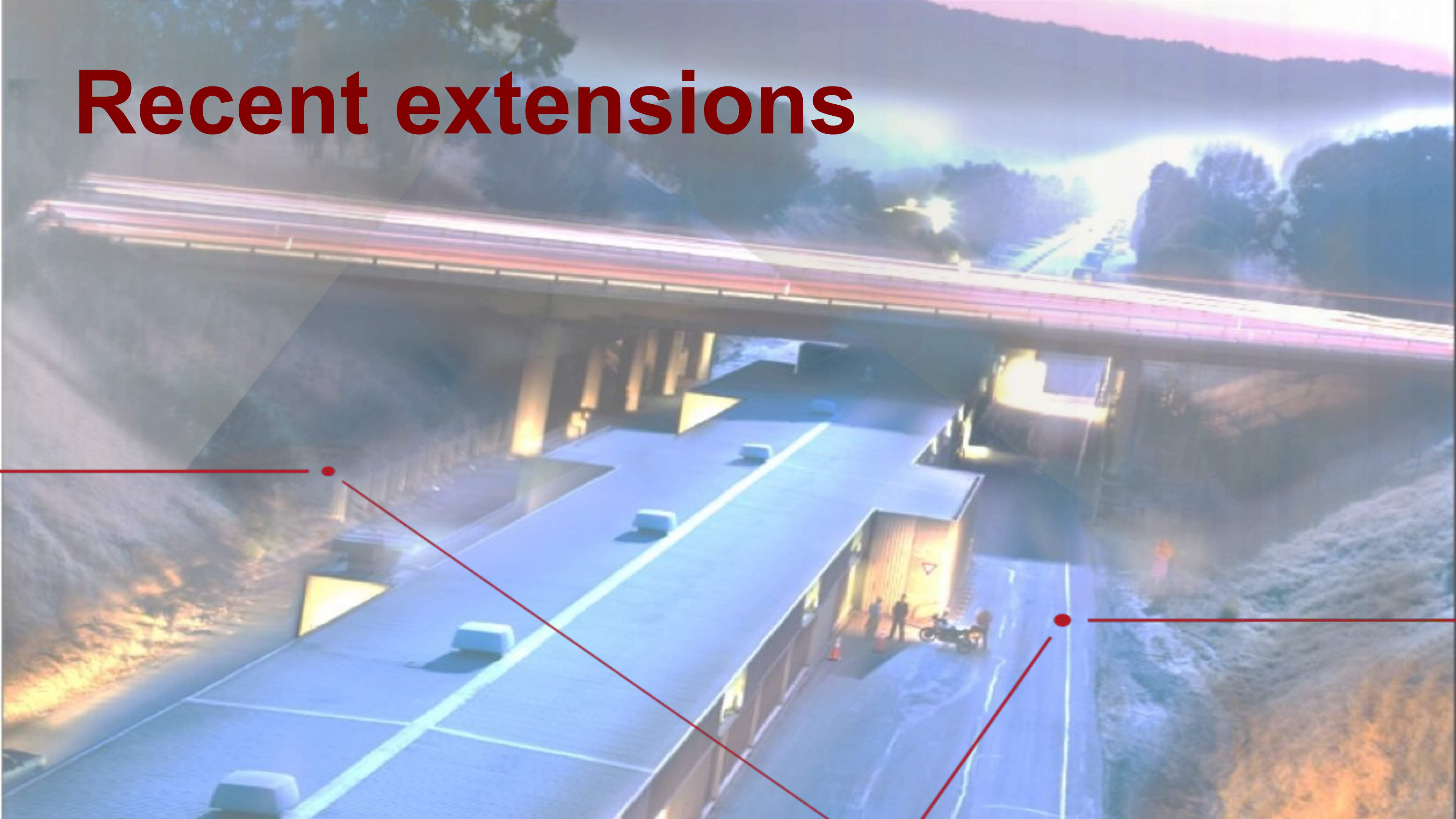
FTFP_BERT

- recommended by Geant4 for HEP
- contains all standard EM processes
- uses Bertini-style cascade for hadrons < 5 GeV
- uses FTF (Fritiof) model for high energies (> 4 GeV)

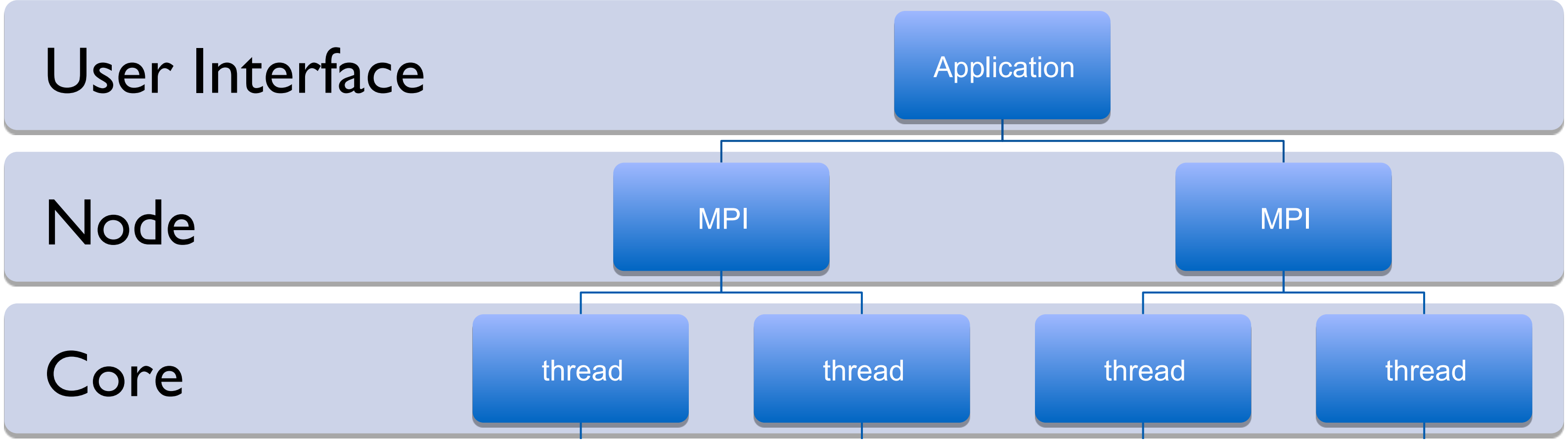
QGSP_BERT

- all standard EM processes
- Bertini-style cascade up to 9.9 GeV
- QGS model for high energies (> ~18 GeV)
- FTF in between

Recent extensions



Geant4 Strategy for parallelism



We provide defaults for all level of parallelism, users can overwrite with experiment framework specific technologies

E.g. LHC experiments: GRID instead of MPI, TBB instead of pthread

What to do when this is not enough or you cannot compromise on physics precision?

An example outside of Geant4 collaboration

N. Henderson http://goo.gl/dPhI9i

Monte Carlo for e/γ radiotherapy simulation

radiotherapy simulation

Analytic methods

- Time: minutes to seconds
- accurate to 3-5%
- used in treatment planning

Monte Carlo methods

- Time: several hours to days of CPU time
- accurate within 1-2%
- used to verify treatment plans

Good candidate for GPU implementation

- 3 particle kinds {ɣ,e-,e+}
- Low energy electromagnetic physics
- 1 material (H_2O)
- Uniformly discretized geometry

N. Henderson http://goo.gl/dPhI9i

MPEXS: a GPU–Accelerated MC for radiation therapy

Goal: at least x100 speedup to make real-time medical MC calculations possible

- enabling scientific breakthrough

How?

Reduce complexity and specialize:

choose correct tool for your problem

Geant4 @ SLAC

Geant4 @

ICME
INSTITUTE for COMPUTATIONAL & MATHEMATICAL ENGINEERING
at STANFORD UNIVERSITY

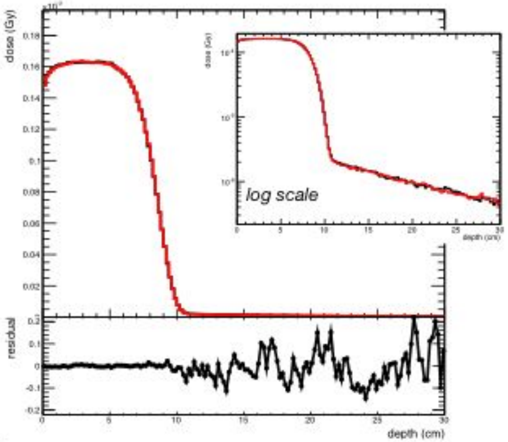
NVIDIA CUDA

Special thanks to the CUDA Center of Excellence Program

N. Henderson http://goo.gl/dPhI9i

Comparison of depth dose for e- 20MeV

(1) water



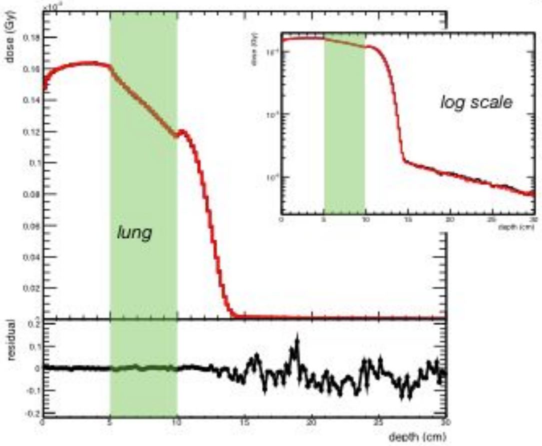
– G4 v9.6.3

– MPEXS

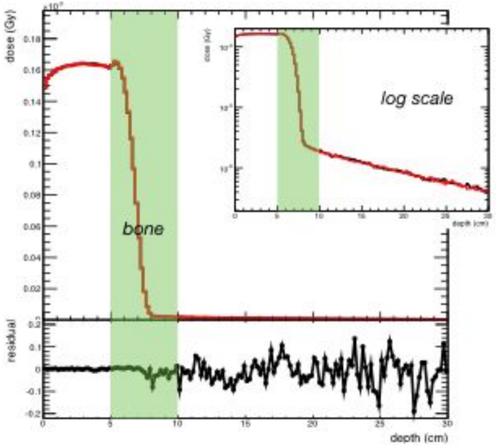
Physics Results compatible with Geant4 (host) application

- x-axis: z-direction (cm)
- y-axis: dose (Gy)
- residual = **(MPEXS-G4)/G4**

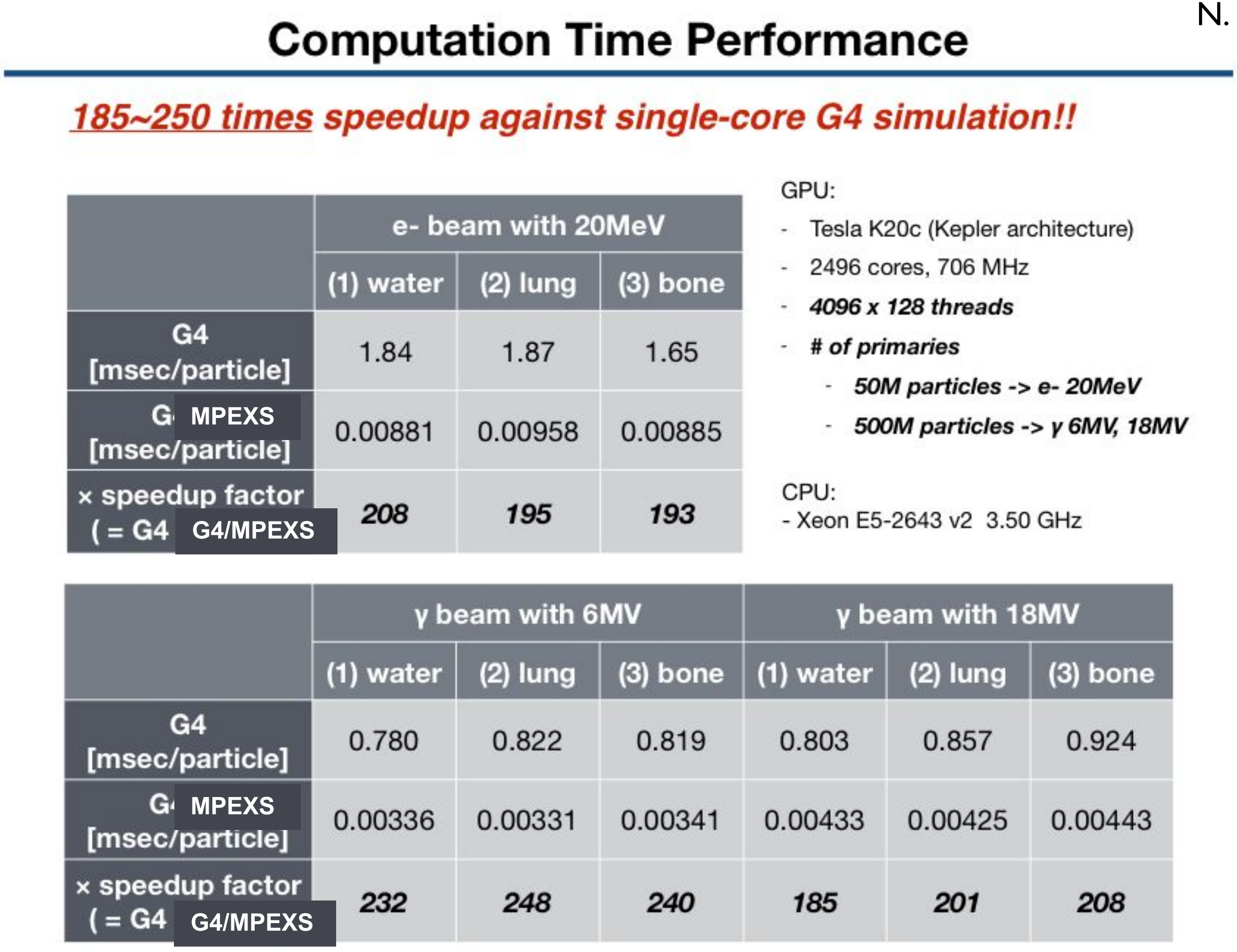
(2) lung



(3) bone



N. Henderson http://goo.gl/dPhI9i



Computation Time Performance

185~250 times speedup against single-core G4 simulation!!

	e- beam with 20MeV		
	(1) water	(2) lung	(3) bone
G4 [msec/particle]	1.84	1.87	1.65
MPEXS [msec/particle]	0.00881	0.00958	0.00885
× speedup factor (= G4/MPEXS	*208*	*195*	*193*

GPU:
- Tesla K20c (Kepler architecture)
- 2496 cores, 706 MHz
- ***4096 x 128 threads***
- ***# of primaries***
  - ***50M particles -> e- 20MeV***
  - ***500M particles -> γ 6MV, 18MV***

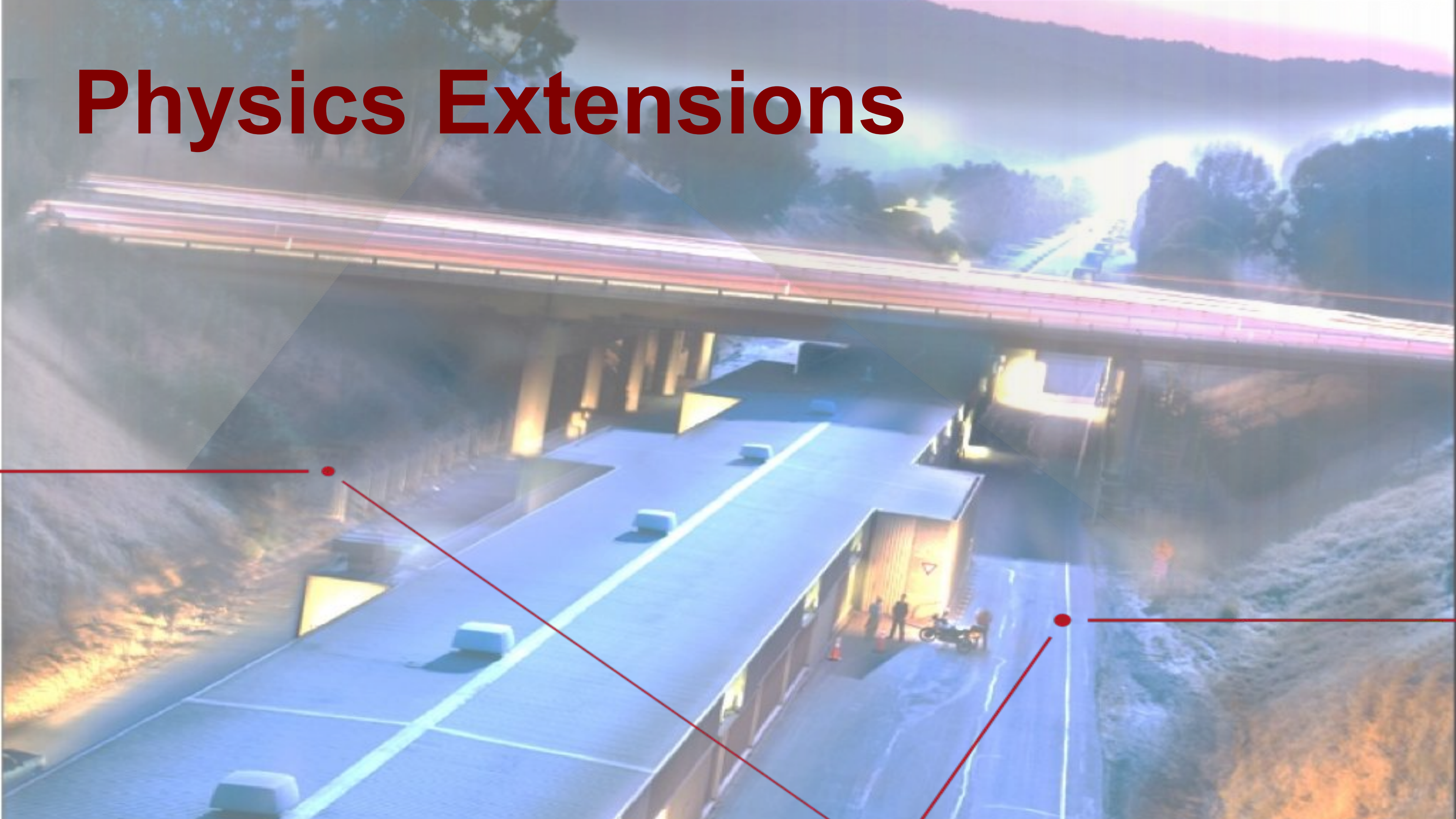
CPU:
- Xeon E5-2643 v2 3.50 GHz

	γ beam with 6MV			γ beam with 18MV		
	(1) water	(2) lung	(3) bone	(1) water	(2) lung	(3) bone
G4 [msec/particle]	0.780	0.822	0.819	0.803	0.857	0.924
MPEXS [msec/particle]	0.00336	0.00331	0.00341	0.00433	0.00425	0.00443
× speedup factor (= G4/MPEXS	*232*	*248*	*240*	*185*	*201*	*208*

Geant4-DNA already
Ported to CUDA

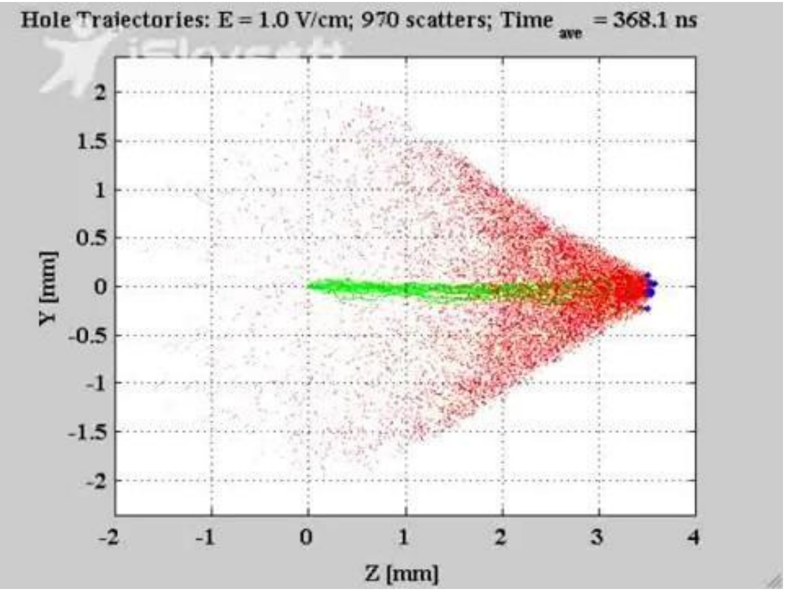
Working on Binary Cascade
(for proton therapy)

Physics Extensions



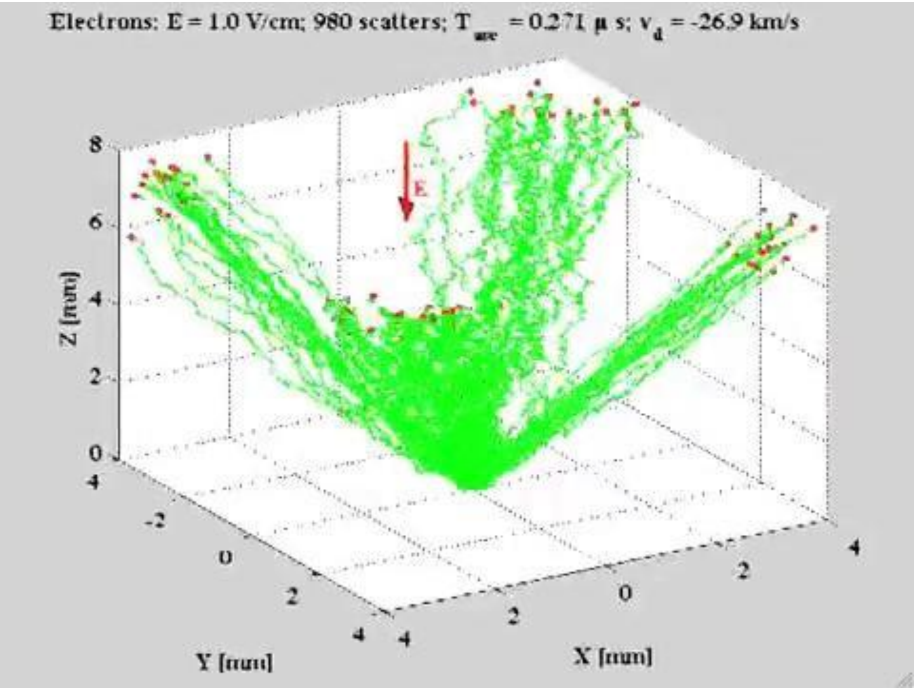
Holes / Phonons simulation

Simulation of **phonons** in ultra-cold crystals: isotope scattering and mode mixing ; anharmonic down conversion ; reflection processes implemented



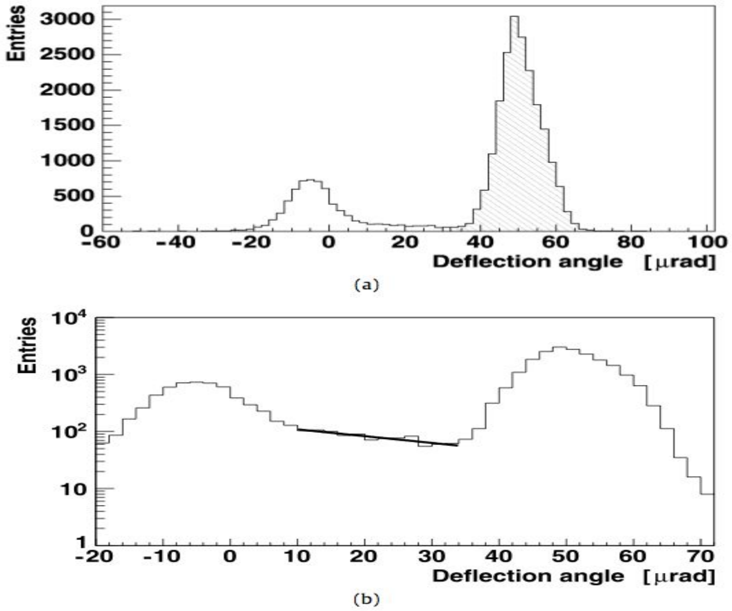
Electrons in crystals

Simulation of **drifting carriers in conduction bands**



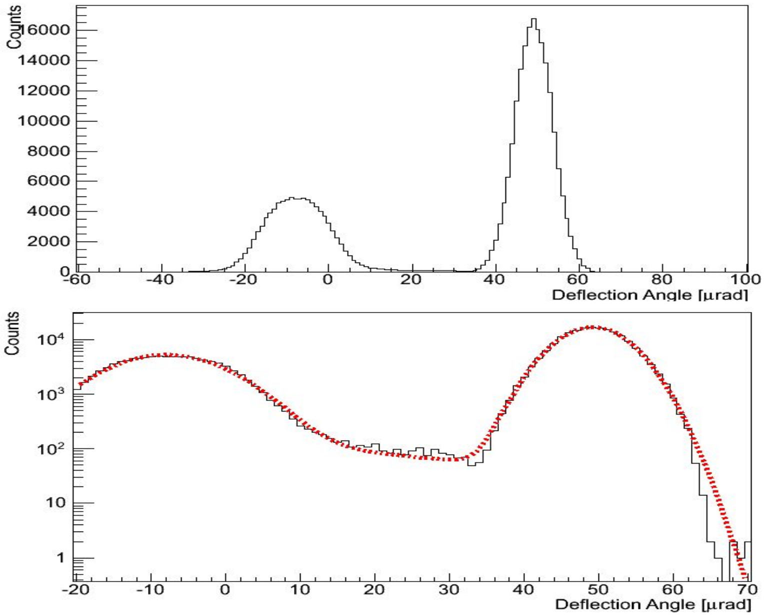
Nuclear dechanneling length

W. Scandale et al., Phys. Lett. B 680 (2009) 129



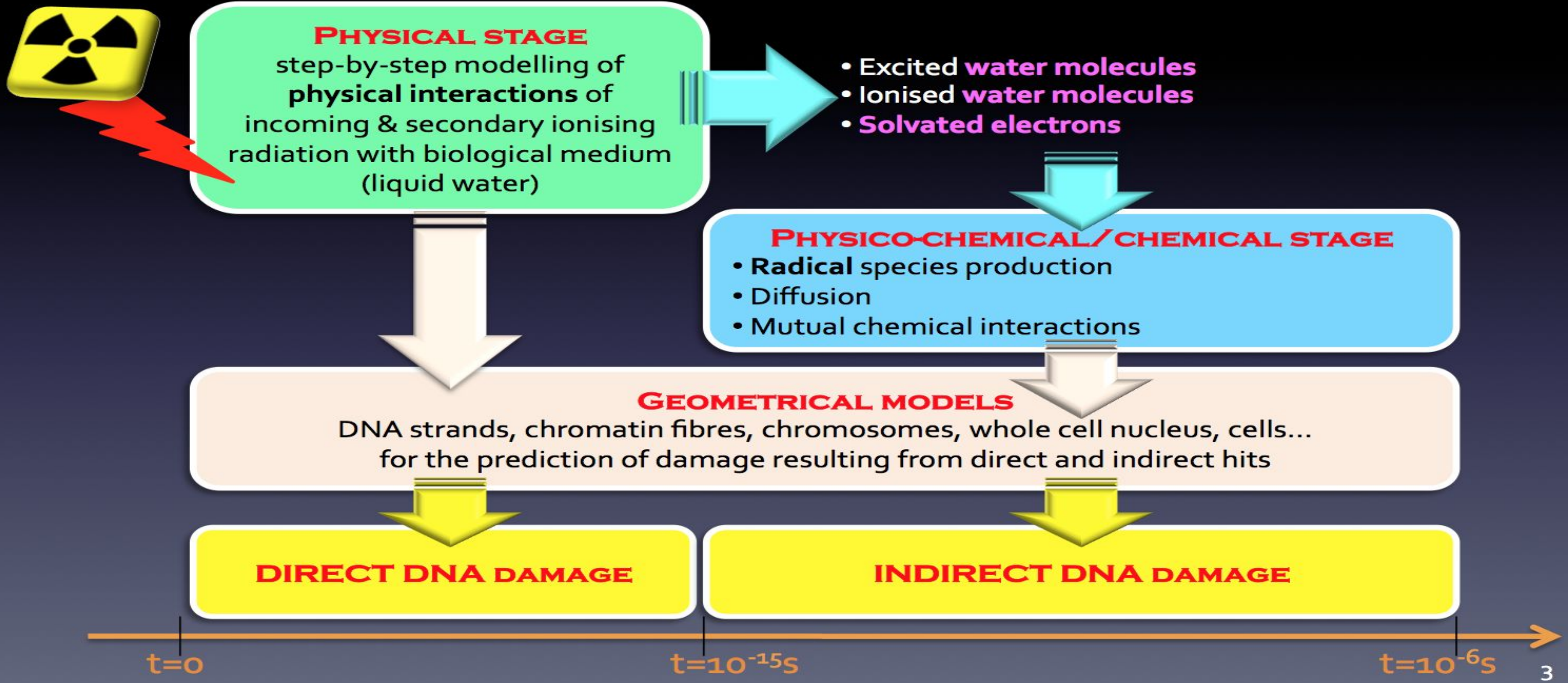
$L_n = (1.53 \pm 0.35 \pm 0.20)$ mm

Geant4 Channeling



$L_n = (1.31 \pm 0.05)$ mm

How can Geant4-DNA model early DNA damage ?



Physical stage
step-by-step modelling of **physical interactions** of incoming & secondary ionising radiation with biological medium (liquid water)

- Excited water molecules
- Ionised water molecules
- Solvated electrons

Physico-chemical/chemical stage

- **Radical** species production
- Diffusion
- Mutual chemical interactions

Geometrical models
DNA strands, chromatin fibres, chromosomes, whole cell nucleus, cells…
for the prediction of damage resulting from direct and indirect hits

Direct DNA damage

Indirect DNA damage

So Long, and Thanks for All the Fish