Lecture 1

An Introduction to Particle Transport and the Geant4 Toolkit

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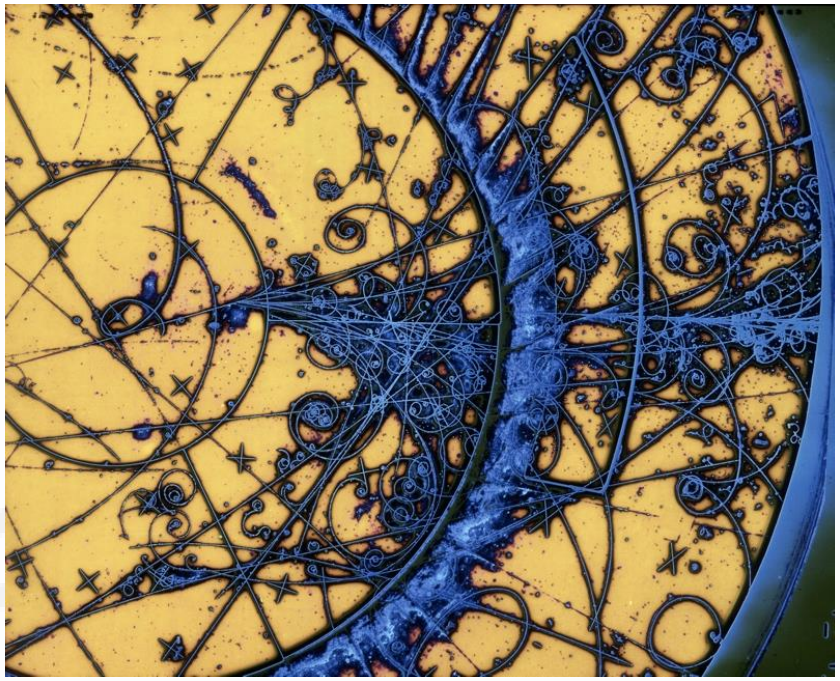
Adapted from talk by **Andrea Dotti** (SLAC- formely CERN)
at the Second African School of Physics, August 2012

Overview

- What is particle transport ?
- Geant4 and its components
  - Geometry & material
  - Recording information
  - Physics processes
  - Installing Geant4 on your machine
- Application Domains
- Future Challenges

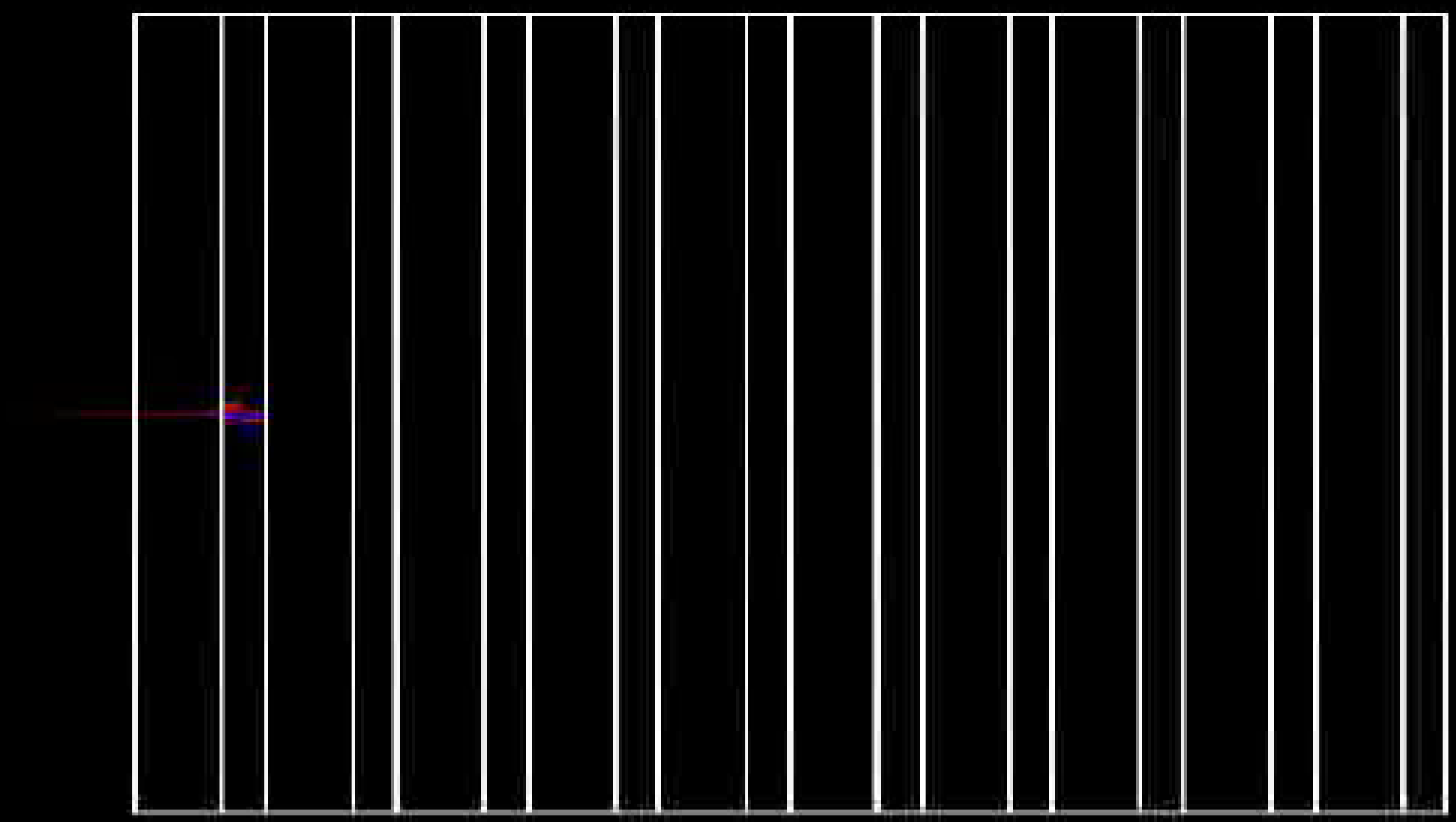
You can find these slides at http://bit.ly/g4asp2016n1 which links to https://dl.dropboxusercontent.com/u/540317/ASP2016/Snapshots/Geant4-ASP2016.pptx



What is Particle Transport Simulation?

- What does it involve ?
- What can we use it for ?

'Radiation' Transport



red: electrons
blue: gammas

Electromagnetic shower from a 100 MeV electron

What is Simulation?

- ‘Physical’ system
- Model = equations
- Evolve (usually in time)
- Extract results

What is particle transport?

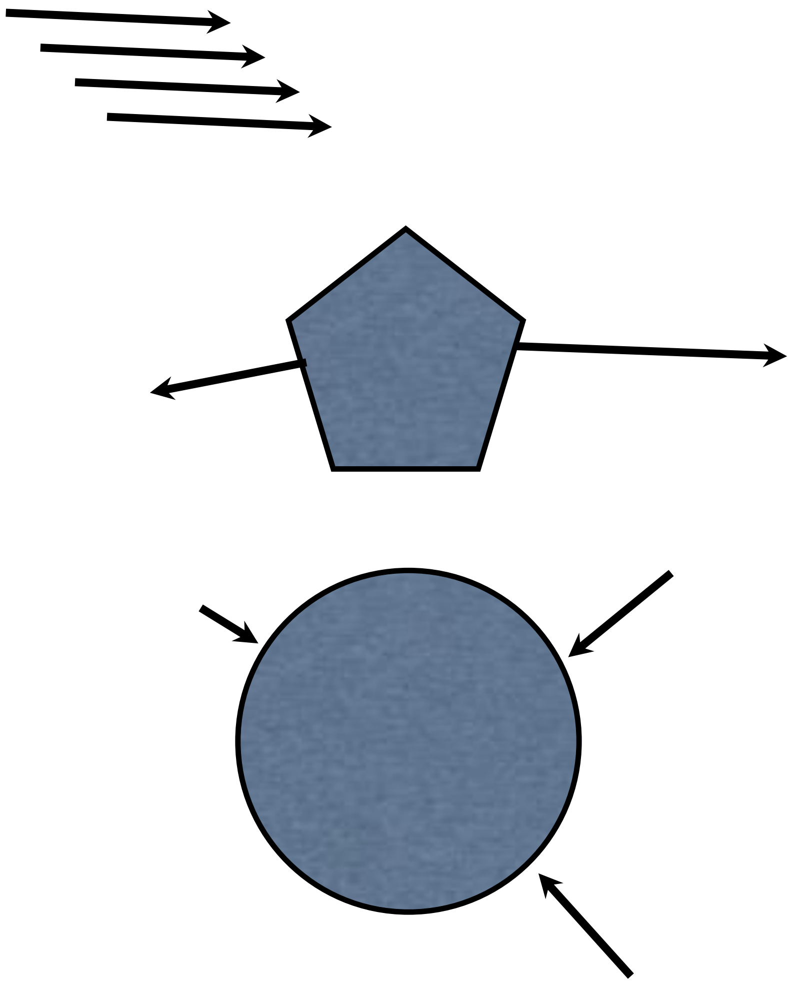
- It is a way to estimate the effects of radiation in a particular region
- We use it to ‘measure’ or better estimate
  - Energy deposition (e- displaced)
  - Dose - weighted by its biological effect
  - Fluxes, e.g. of neutrons (=> nuclear reactions) in a particular region
- It can also estimate complicated observables:
  - Width of distribution of energy deposition
  - correlations - e.g. coincidence of gammas (PET)

The parts

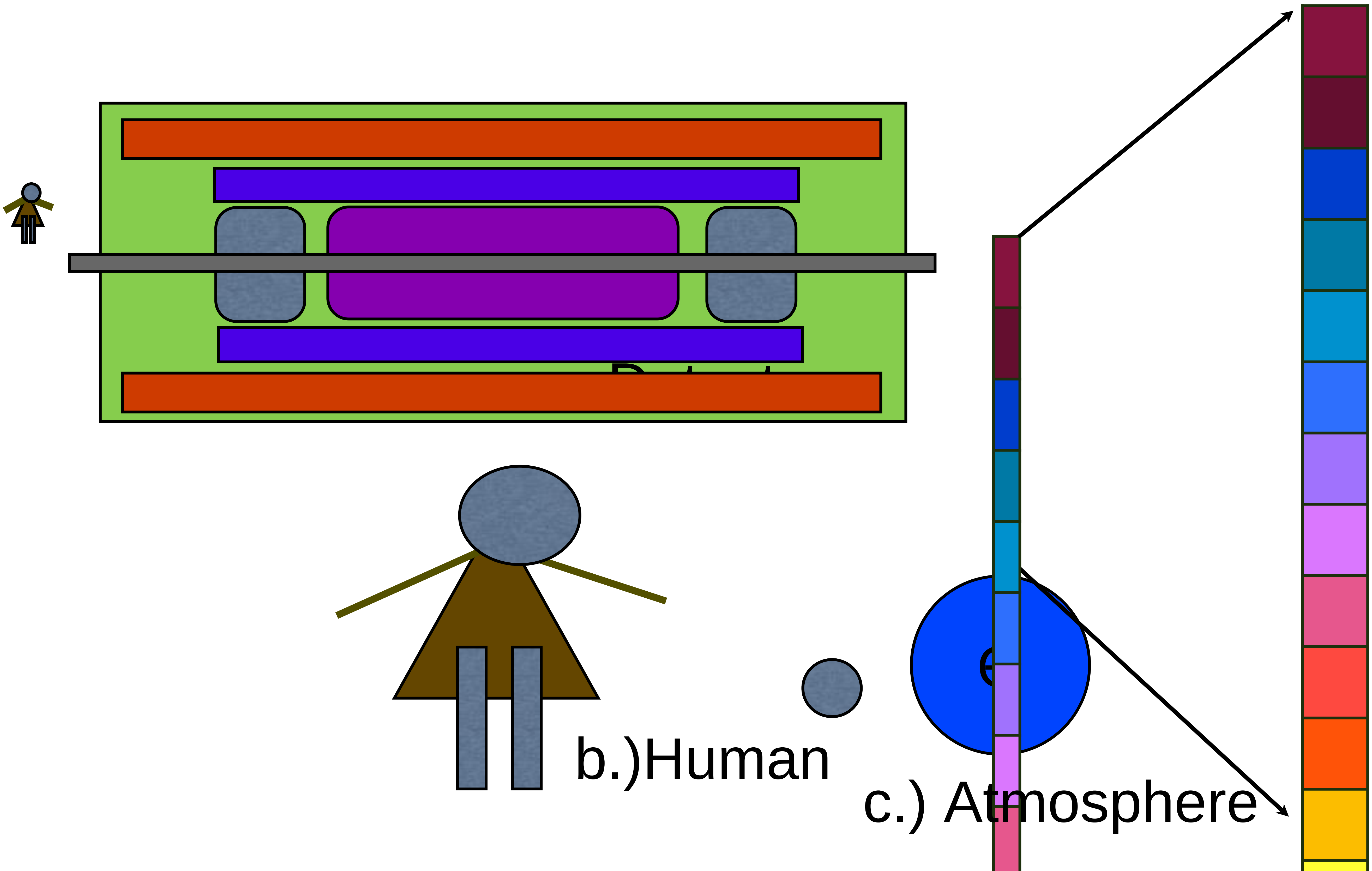
- Source or beam
- Geometry model (material, shape, location)
- ‘Sensitive’ regions - where to measure
- Transport (the ‘engine’ at the core)

1. The particle source

- Beam, 'source'
- Determines the initial particles
  - type (e.g. e-, proton)
  - momentum
- Distributions or unique

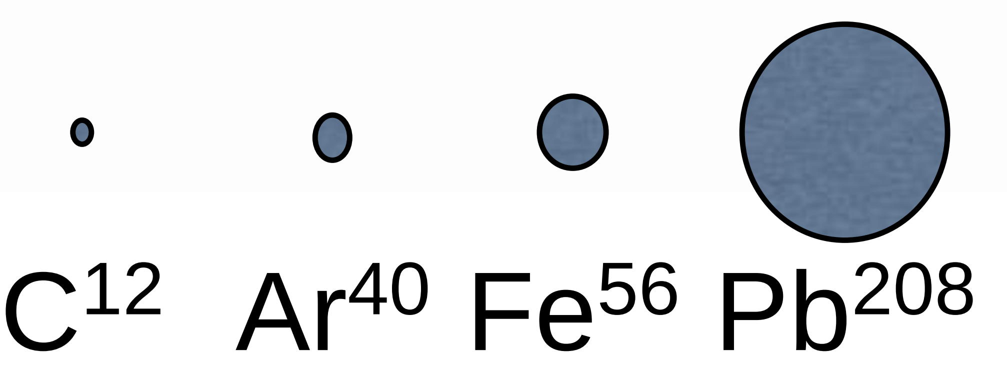


2. The geometry model



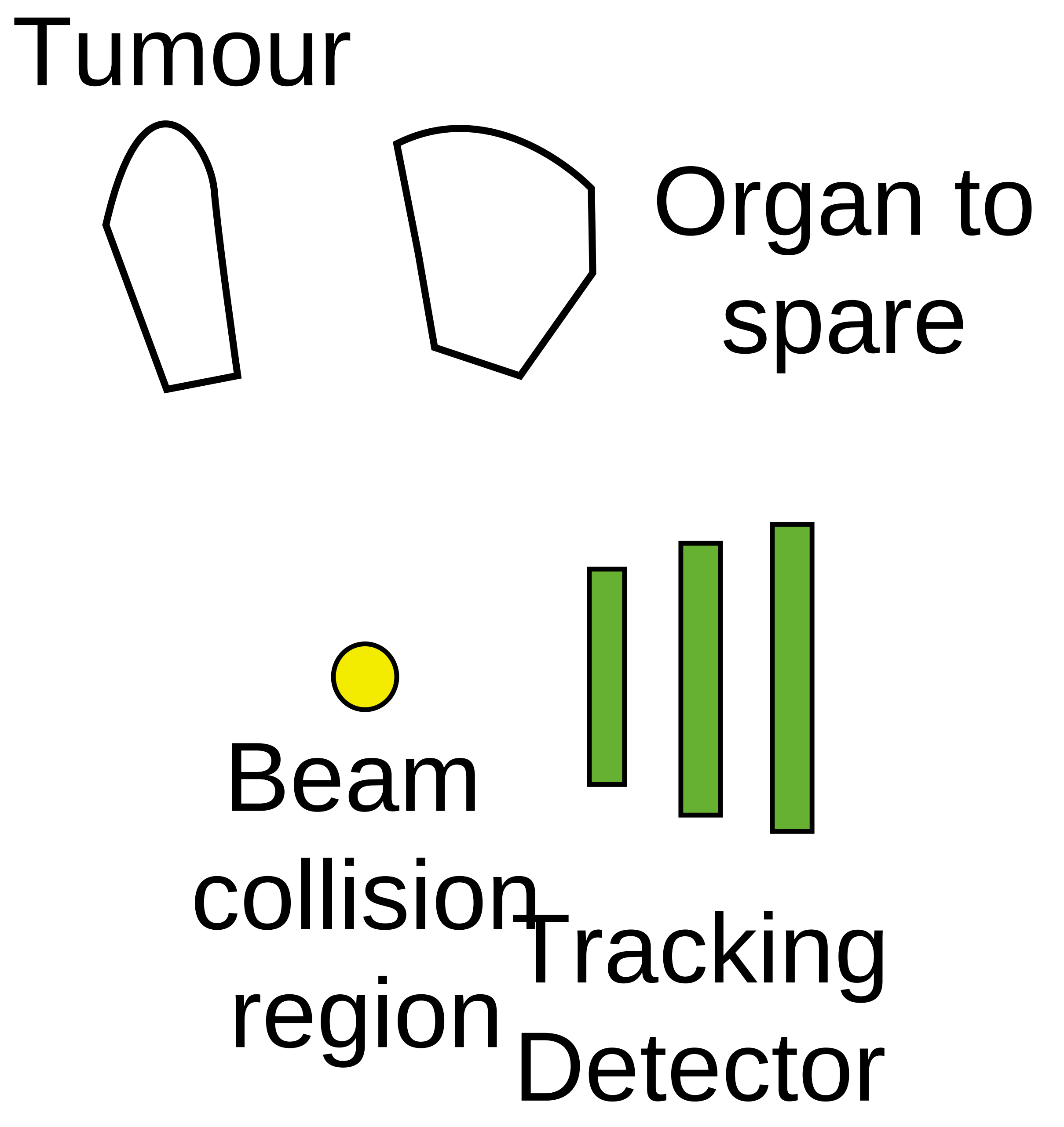
Geometry/material

- Volumes fill the simulation ‘world’
- Each Volume has
  - Shape, size, material
  - Location, orientation (rotation)
- Each Material fully defined - as ‘target’ atoms
  - Atomic composition, density



3. Sensitive Volume/Region

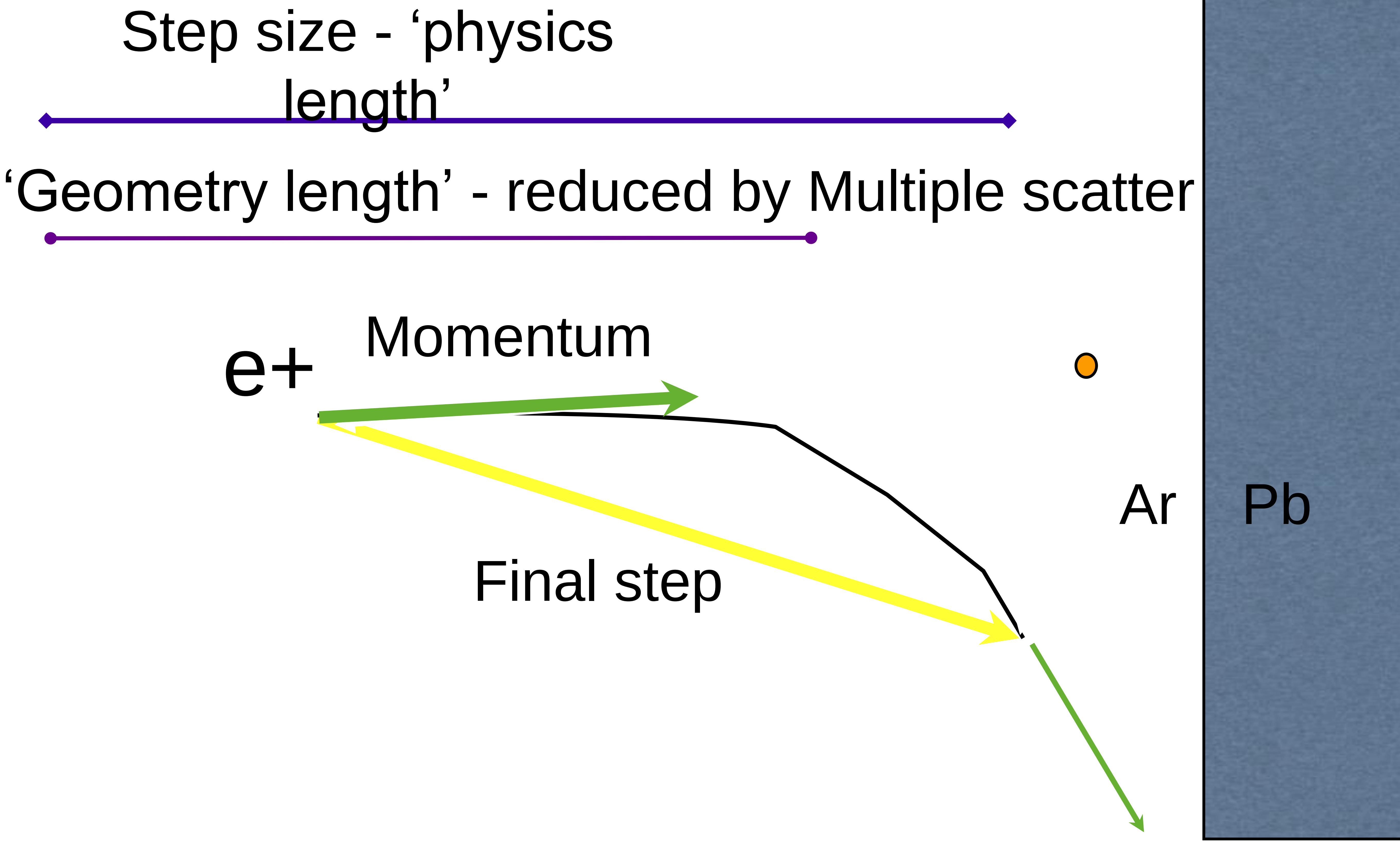
- It is a Geometry volume
- It records attribute(s) of each passing particles
  - E, p (momentum)
  - Particle type
  - ΔE, Energy deposition



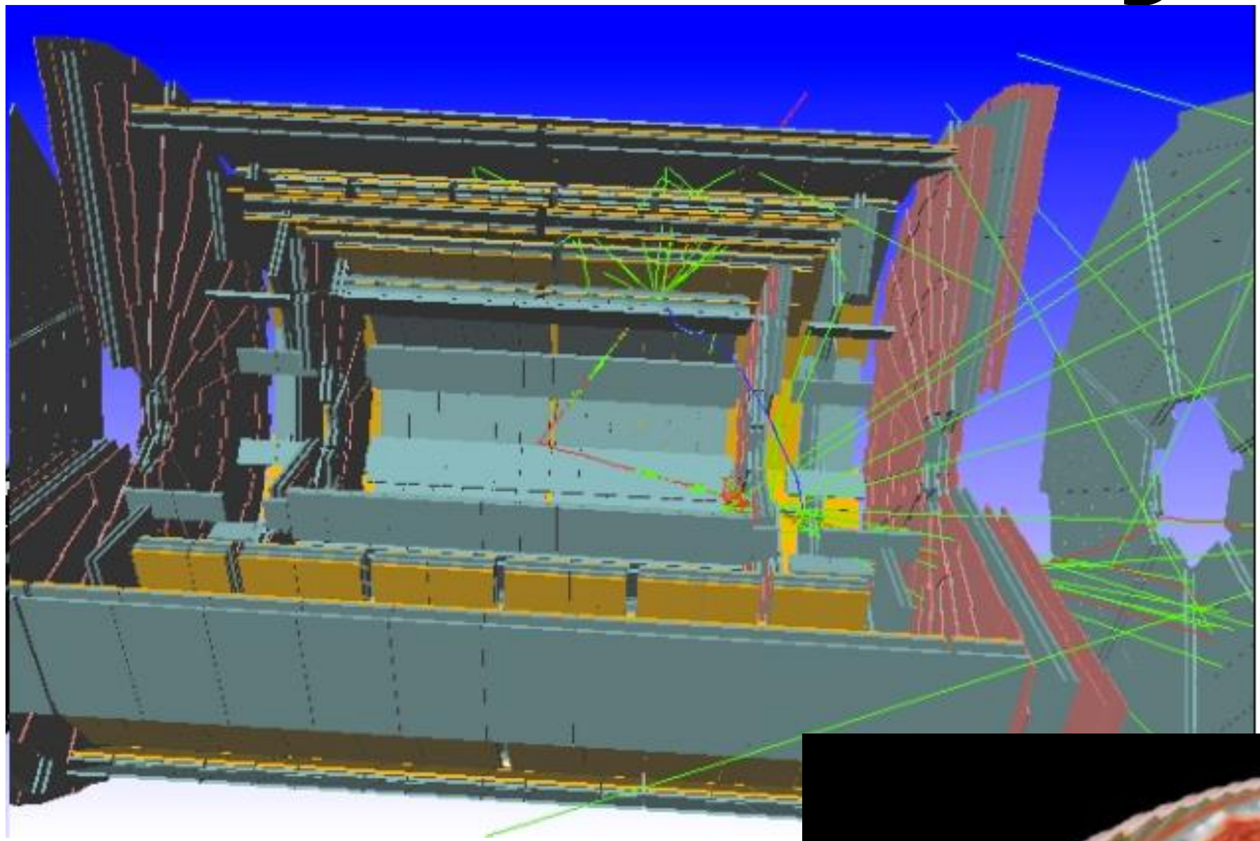
4. Transport ‘engine’

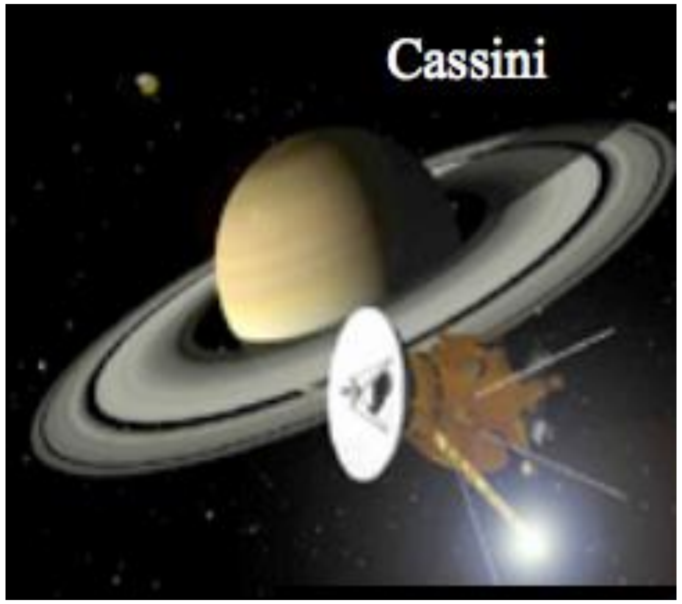
- It ‘transports’ the initial particles = tracks
- It ‘reacts’ each particle in turn with atoms, nuclei of material
  - producing new particles (secondaries)
- It moves particle tracks to new volumes
- Each track exits world, dies or is abandoned

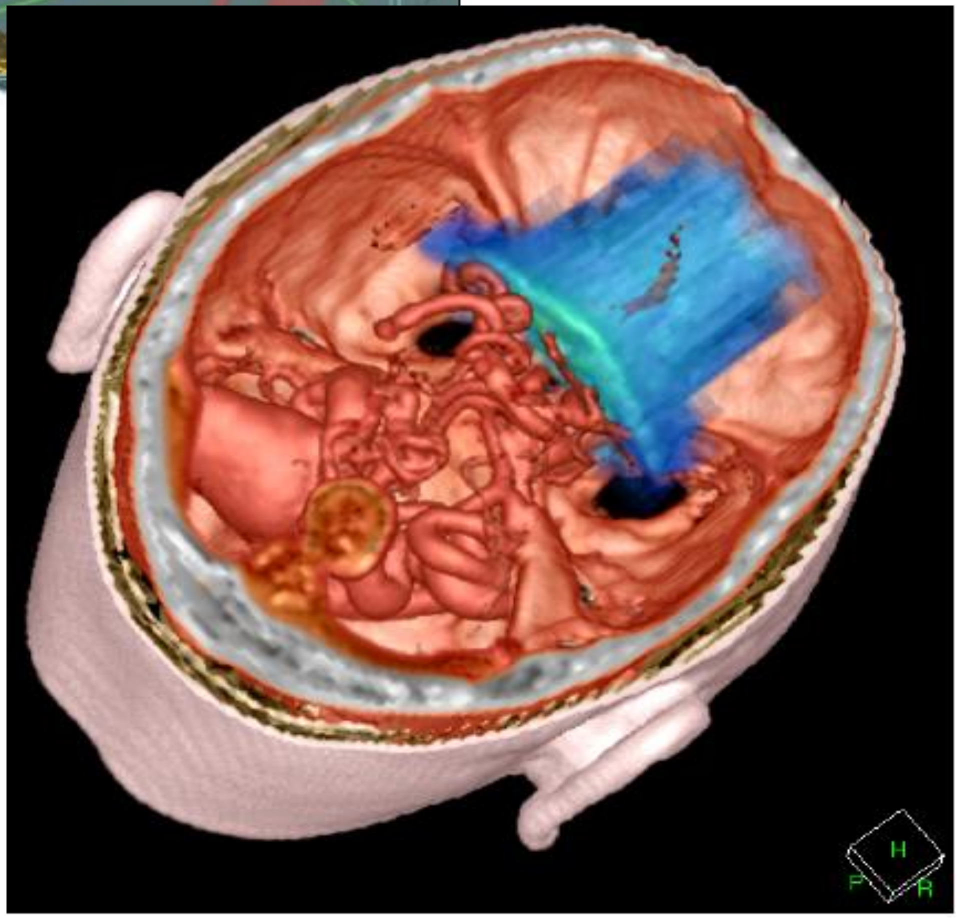
One step at a time



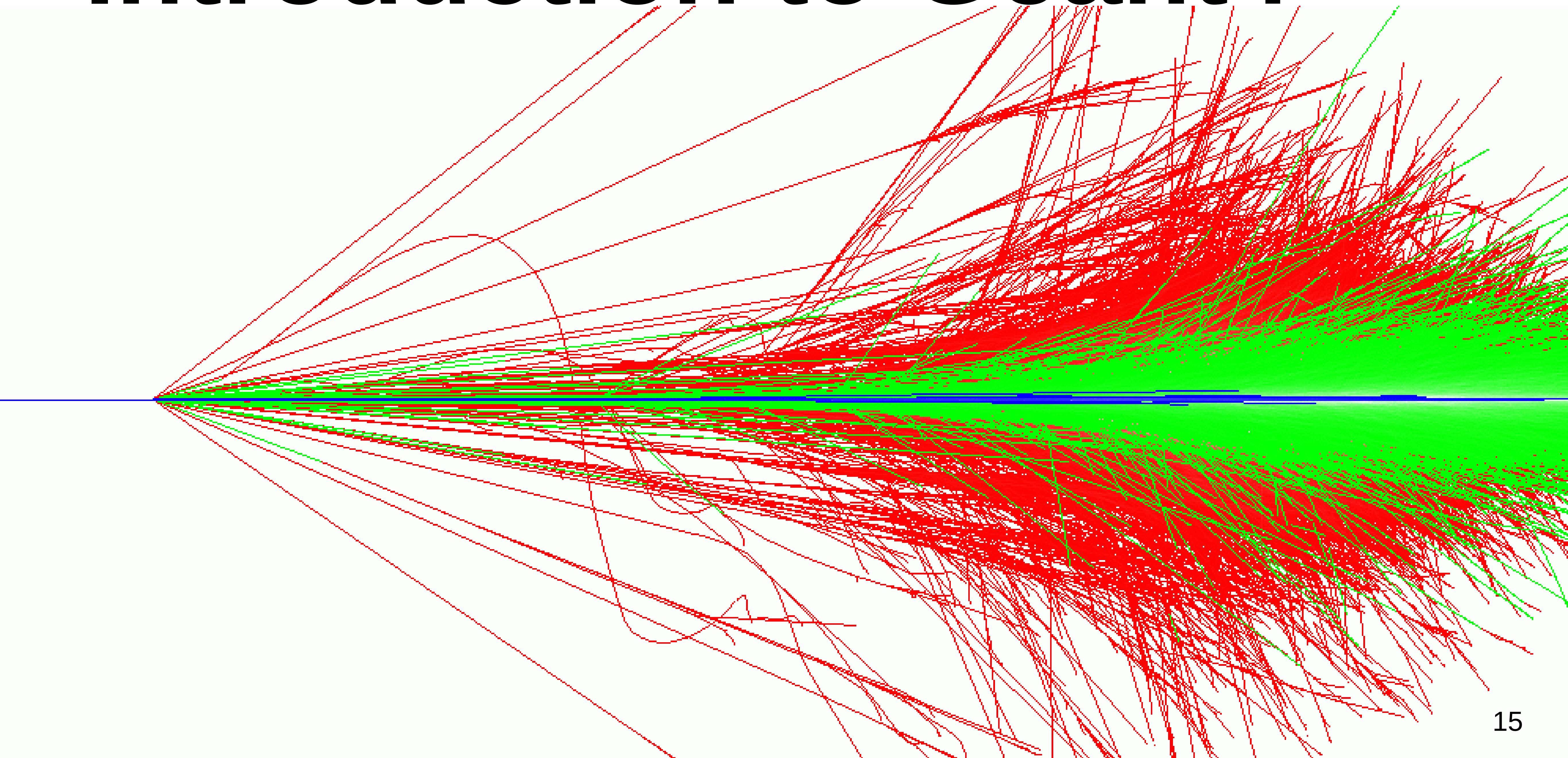
Where / why use it ?



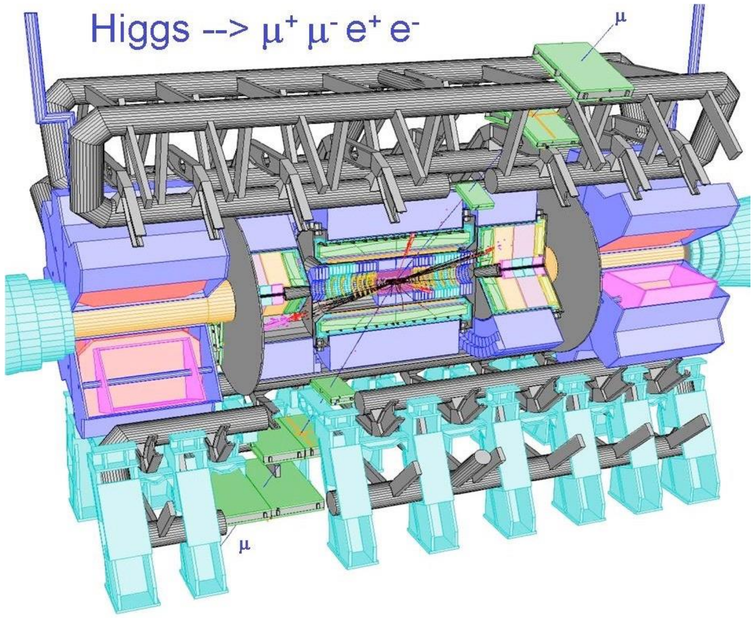




Introduction to Geant4



What is Geant4?



"Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science"

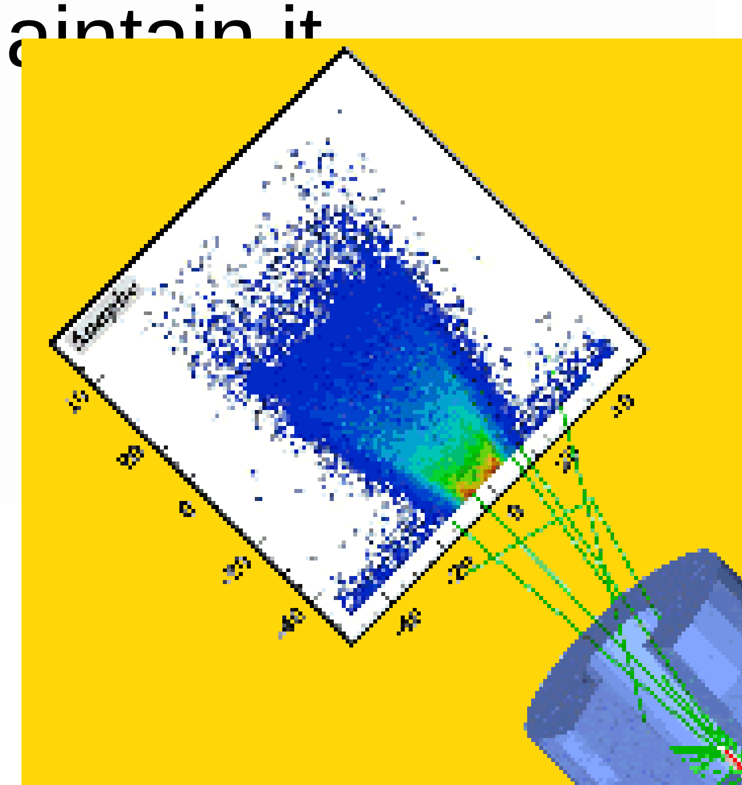
http://www.cern.ch/geant4

Geant4: GEometry ANd Tracking

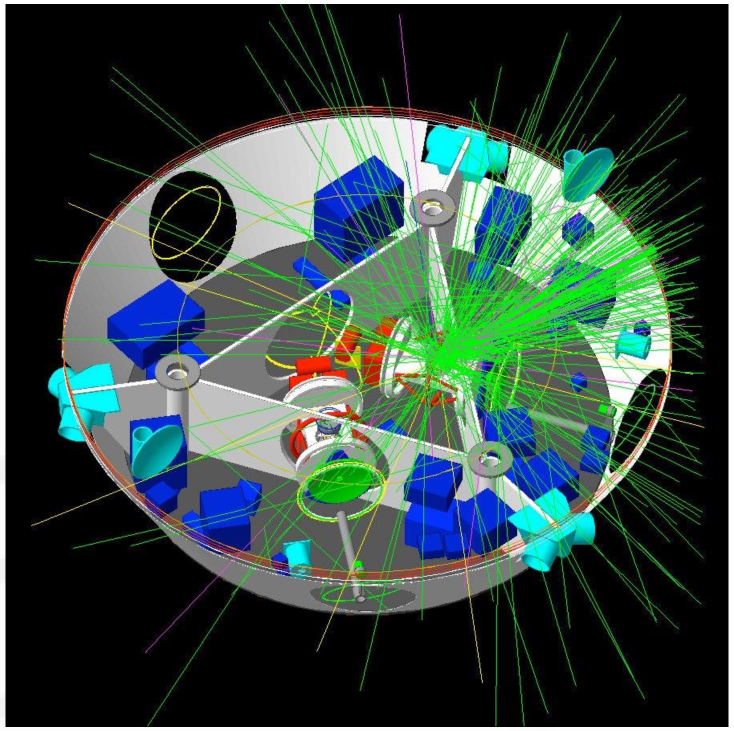
- A toolkit provides "general" tools to undertake (some or all) of the tasks:
  - tracking and geometrical propagation
  - modelling of physics interactions
  - visualization, persistency
- A toolkit enables you to describe your setup:
  - detector geometry
  - radiation source
  - details of sensitive regions

Geant4

- Detector simulation tool-kit from HEP
  - full functionality: geometry, tracking, physics, I/O
  - offers alternatives, allows for tailoring
- Software Engineering and OO technology (C++)
  - provide the architecture & methods to maintain it
- Requirements from:
  - current and future HEP experiments
  - medical and space science applications
- World-wide collaboration



Key capabilities



- ‘Kernel’: create, manage, move
  - tracking, stacks, geometry, hits, …
  - Extensible, flexible
- Physics Processes: cross-section, final-state
  - models for electromagnetic, hadronic, …
  - Can be ‘assembled’ for use in an application area
- Tools for faster simulation
  - ‘Cuts’, framework shower parametrisation
  - Event biasing, variance reduction.
- Open interfaces for input/output
  - User commands, visualization, persistency

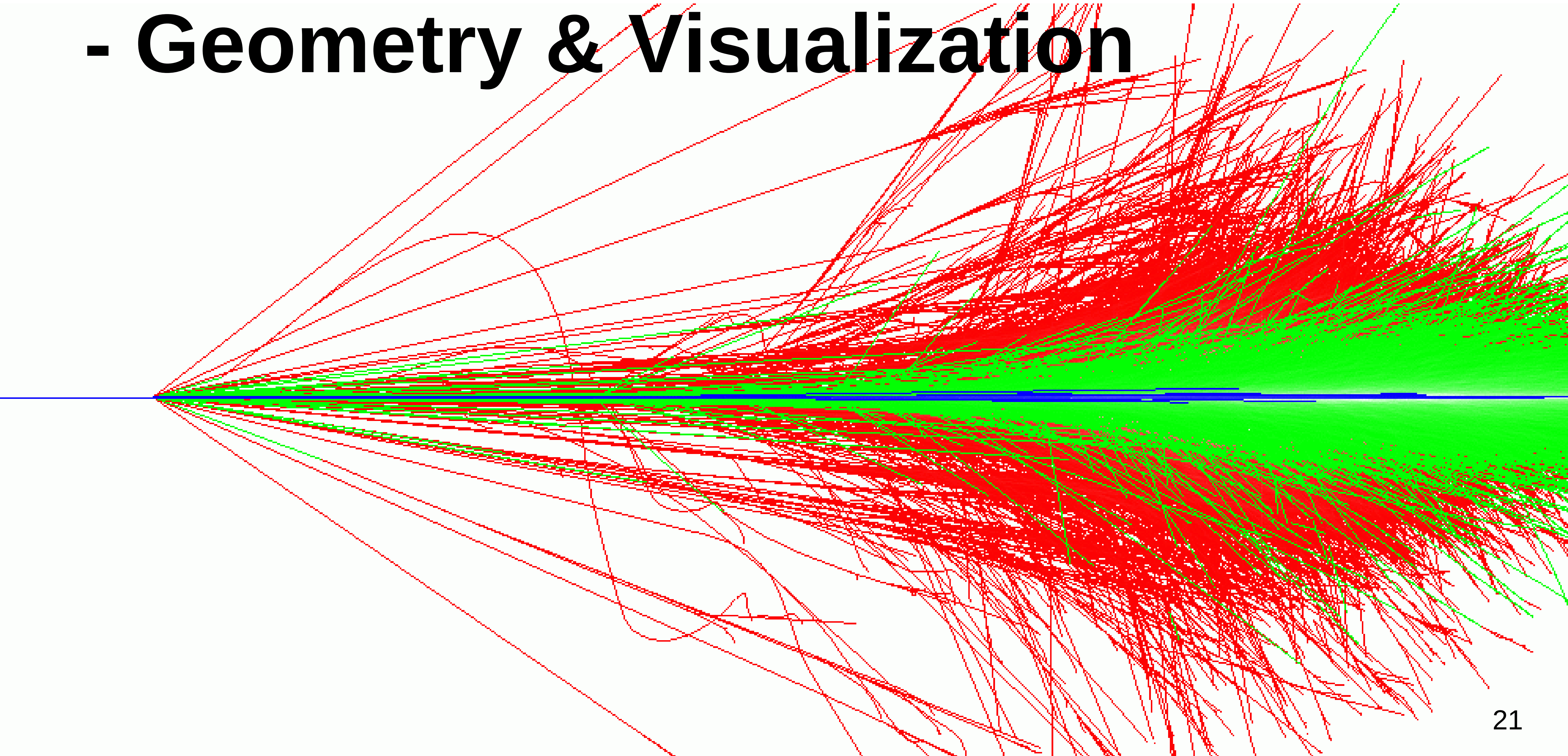
Practical Considerations

- Starting off: what you need
  - Compatible platform
  - One or more visualization libraries (possibly from system, e.g. OpenGL)
- CLHEP is used for key common classes
  - ThreeVector (G4ThreeVector is a name for CLHEP::HepThreeVector)
  - FourVector
  - Random Number Generators,
  - Starting from version 9.5 (Dec 2011) CLHEP included in G4

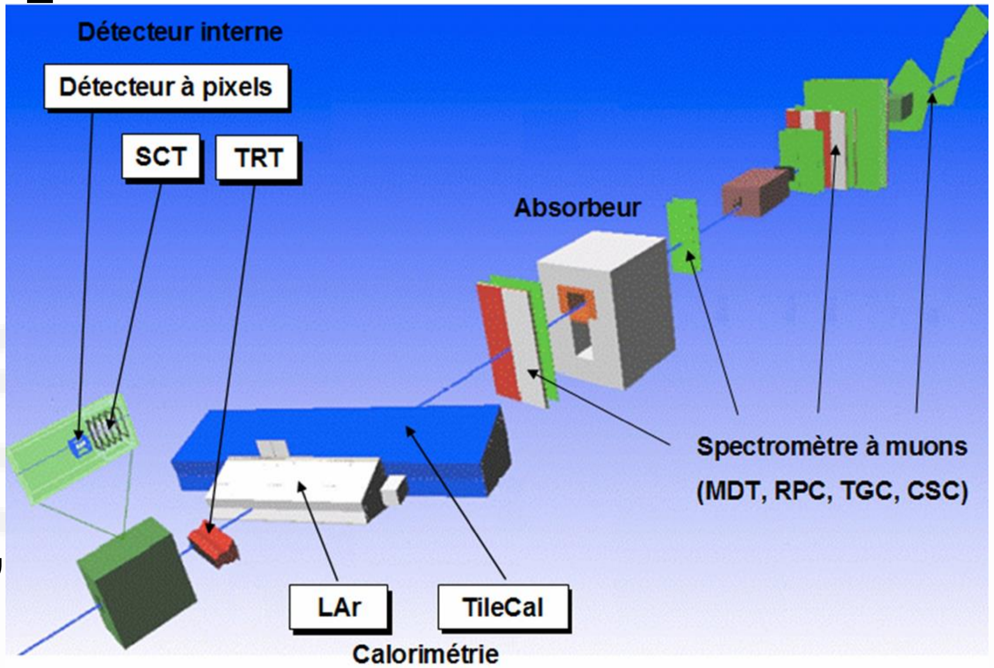
Platforms

- What works 'best' (used by developers, main testing)
  - Linux (Scientific Linux 6 or Centos7) gcc 4.8+ (HEP production)
  - MacOS 10.10 or 10.11 with Xcode/clang
  - Windows 7, 8 or 10 (w/ recent Visual C++)
- What is known and/or expected to work
  - Other Linux flavours with gcc 4.x (at least x>7); icc 15+
  - Possibly fewer options (visualization choices depend on libraries.)
- Likely to work
  - Other Unix/similar systems with gcc or other C++ compiler
  - Expect fewer visualisation options to work "out of the box".

Creating a simulation:
- Geometry & Visualization



Building a G4 Application



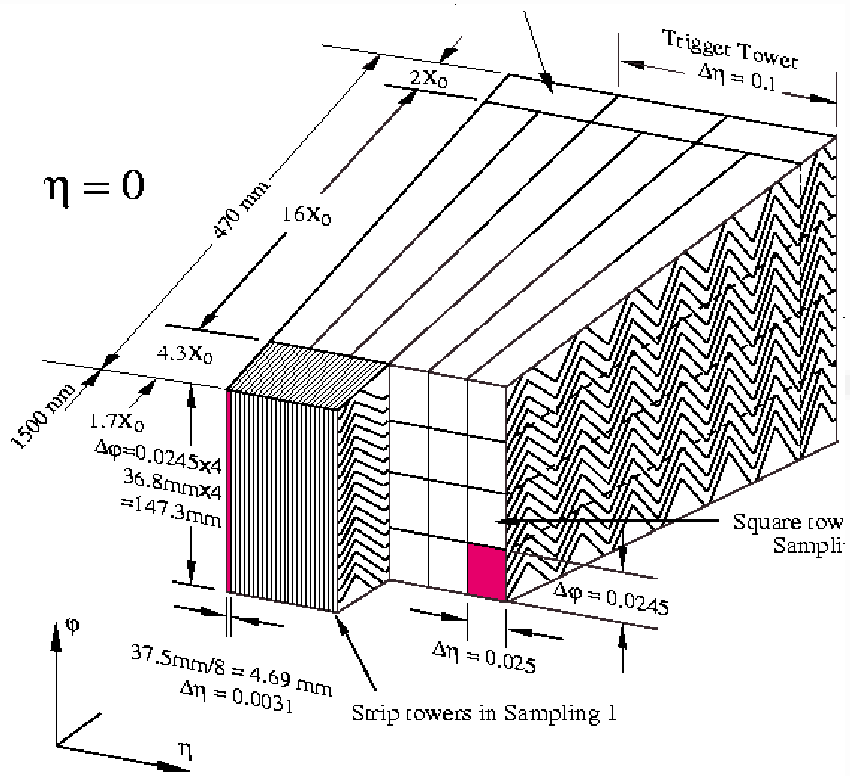
ATLAS Test-beam setup 2004

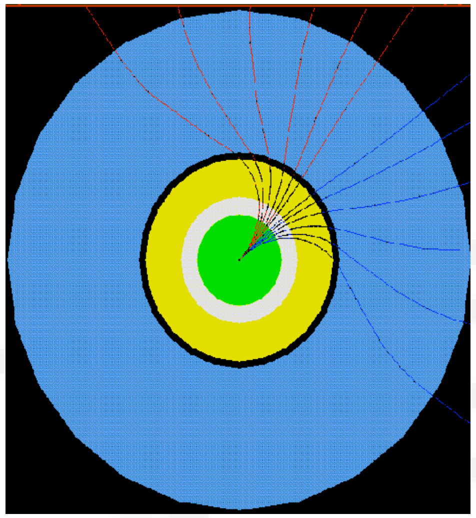
- How do you create a Geant4 simulation
  - Get a ready-made application, or
  - Modify a similar, existing, application,
  - Piece together a custom application

- What are the key steps for creating an application
  - Describing the setup: geometry, material, ..
  - Creating the primary tracks
  - Choosing the *physics* to use
  - Designating the "sensitive" volumes
  - And collecting physics observables.

Often the most
"coding" intensive steps:
build your own detector/device

geometry: what G4 does

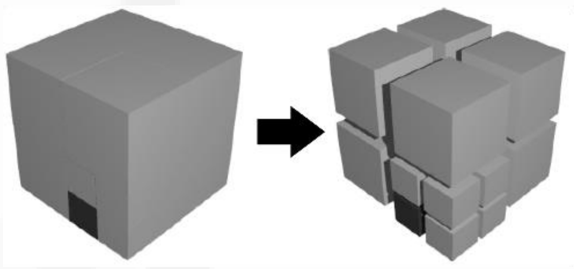




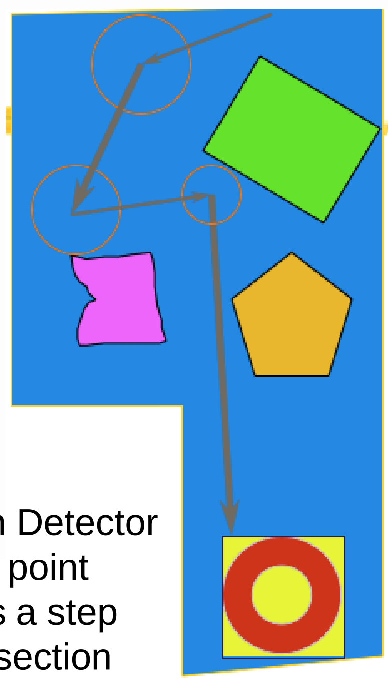
All charged particles ‘feel’ the effect of EM fields

Automatically following paths that approximate their curved trajectories

- User must describes a Setup
  - Hierarchy of volumes
  - Materials
- Up to hundreds of thousands of volumes
- Importing solids from CAD systems



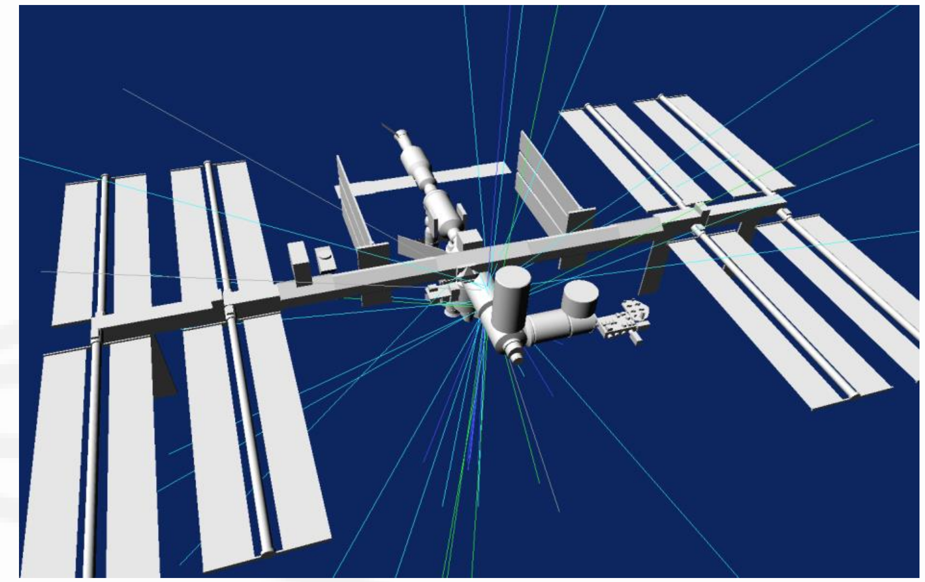
Automatic optimization of complex geometries (voxelization): efficient tracking



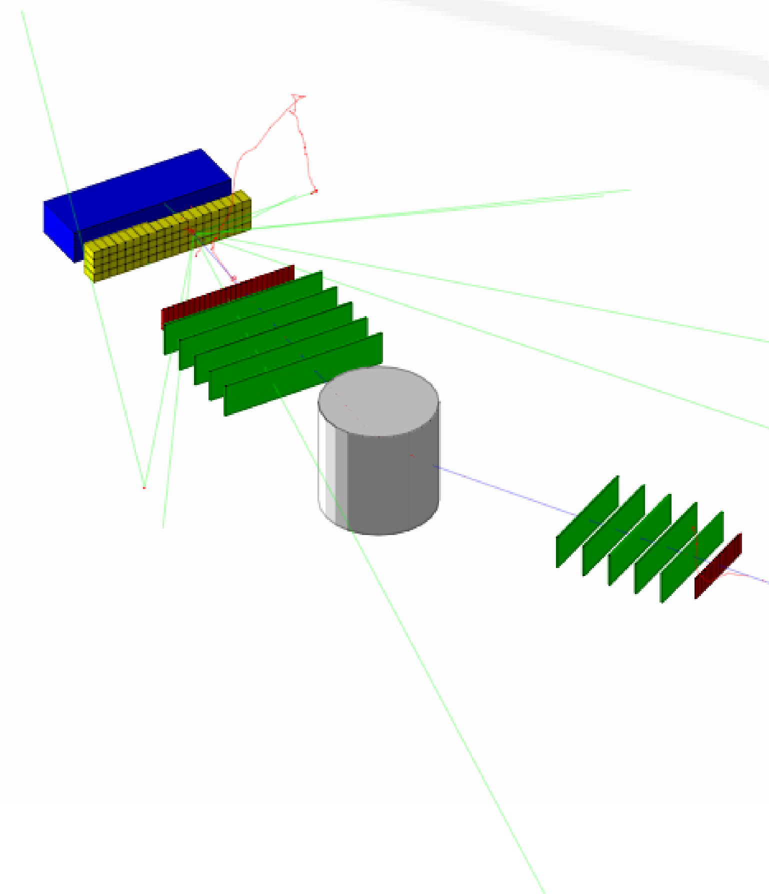
Navigates in Detector
☑Locates a point
☑Computes a step
Linear intersection

Visualization

- Much functionality is implemented
- Several drivers:
  - OpenGL, VRML, Open Inventor, DAWN renderer (G4),...
- Also choice of User Interfaces:
  - Terminal (text) or
  - GUI
- Editors for geometry
- Visualization of:
  - Volumes
  - Tracks
  - Energy deposits (“hits”, doses)



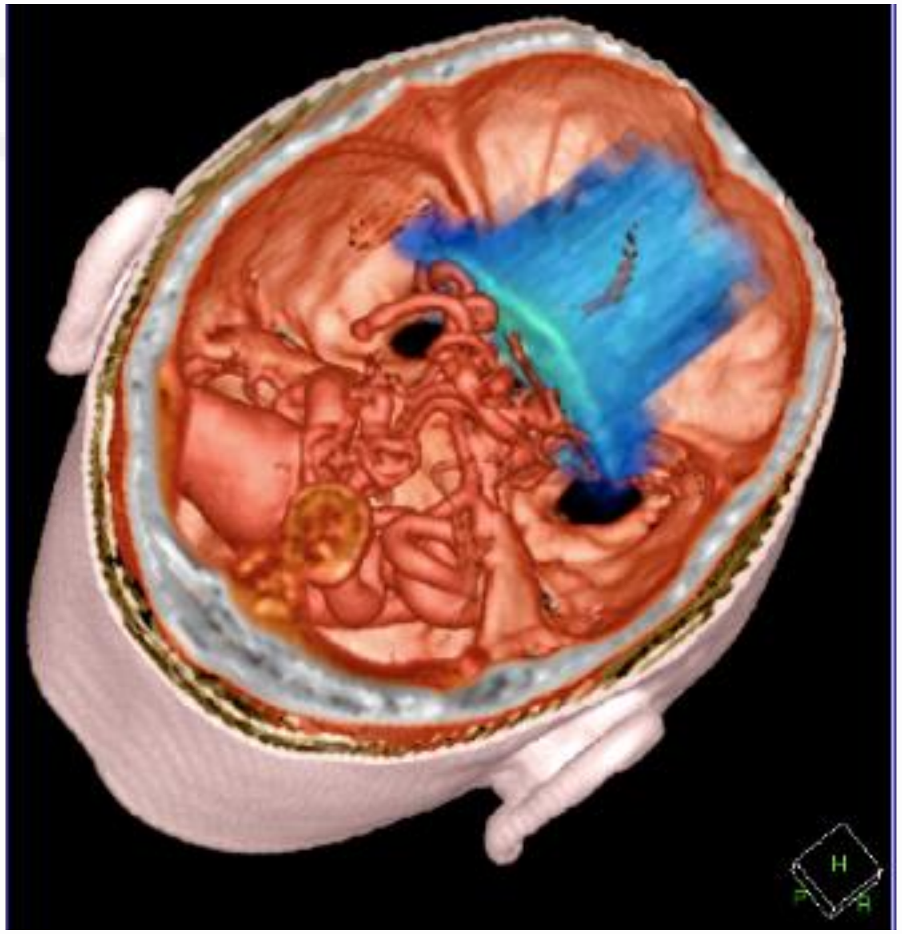
OpenGL driver



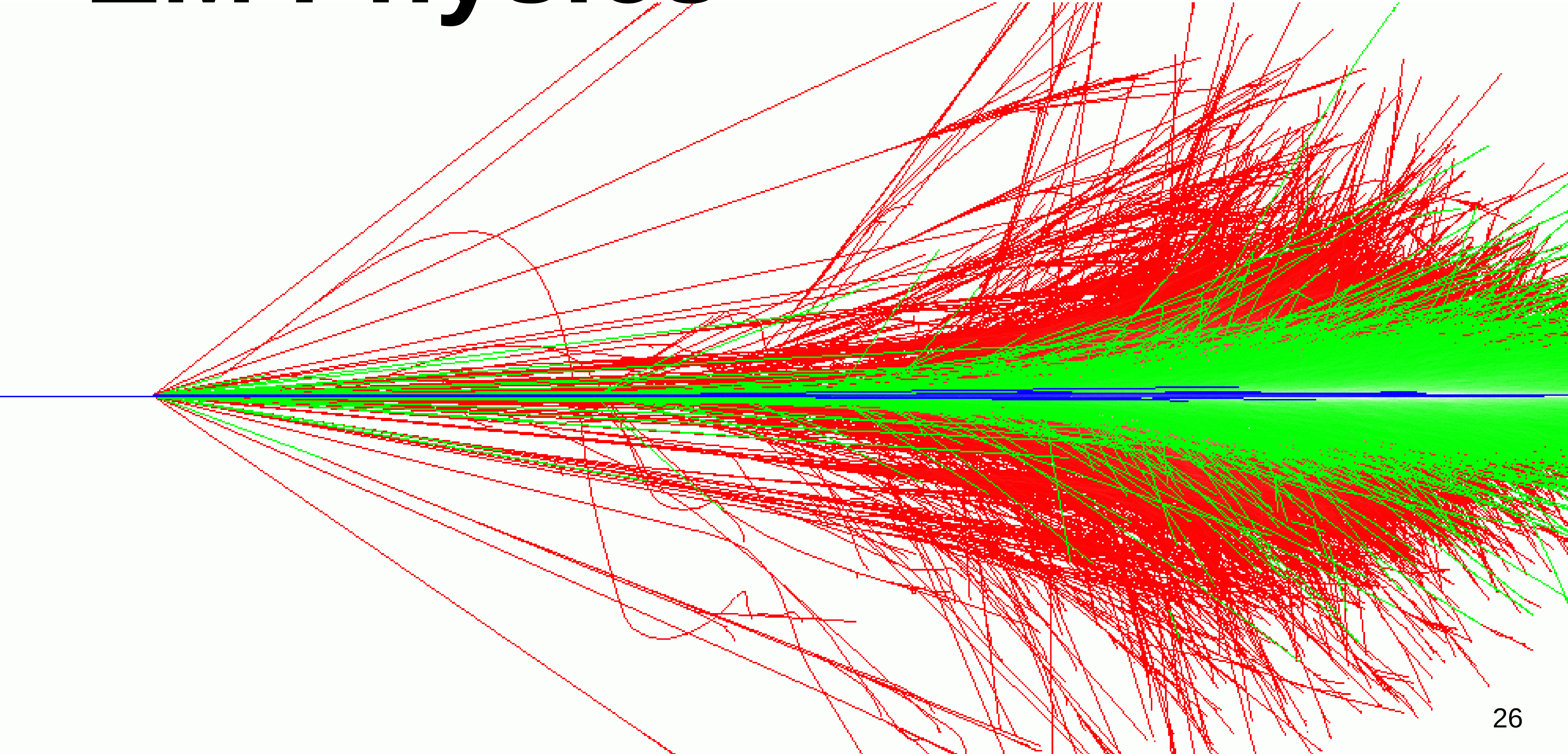
DAWN driver

An advanced Tool: gMocren

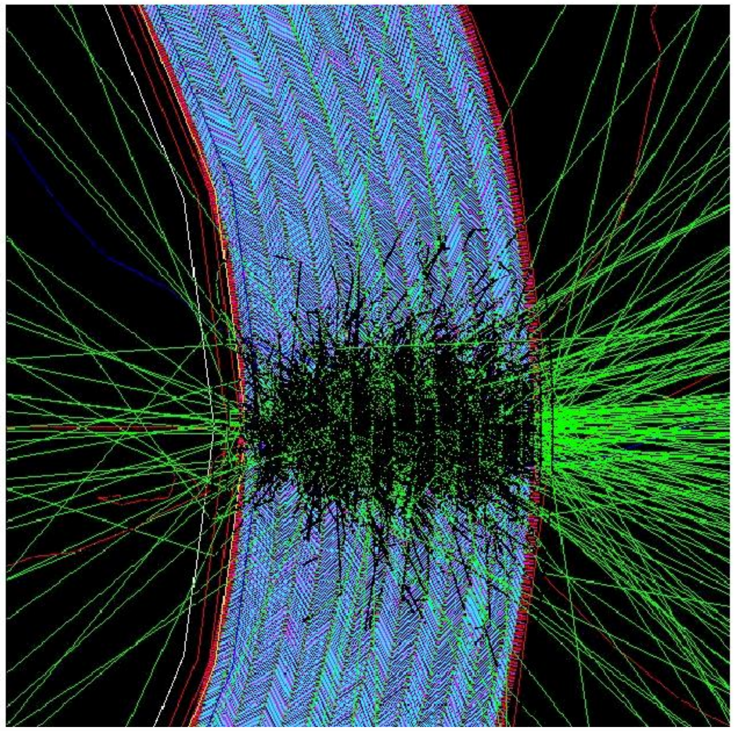
- Created by the JST/CREST project (Japan) to improve Geant4 for medical physics
- Able to visualize:
  - Volume data (including overlay of more than one set)
  - Trajectories
  - Geometry
- Runs on:
  - Windows and Linux
  - Mac - future ?
  - Based on a commercial package but offered freely to all Geant4 users
- http://geant4.kek.jp/gMocren



EM Physics



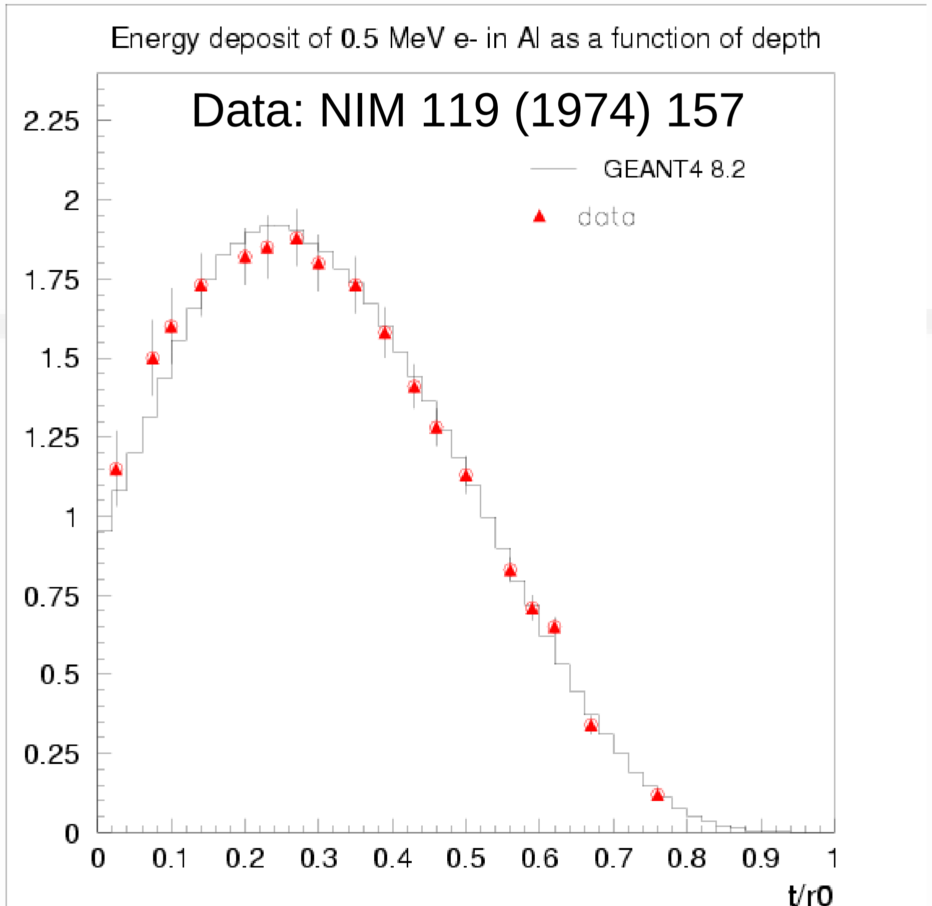
Processes



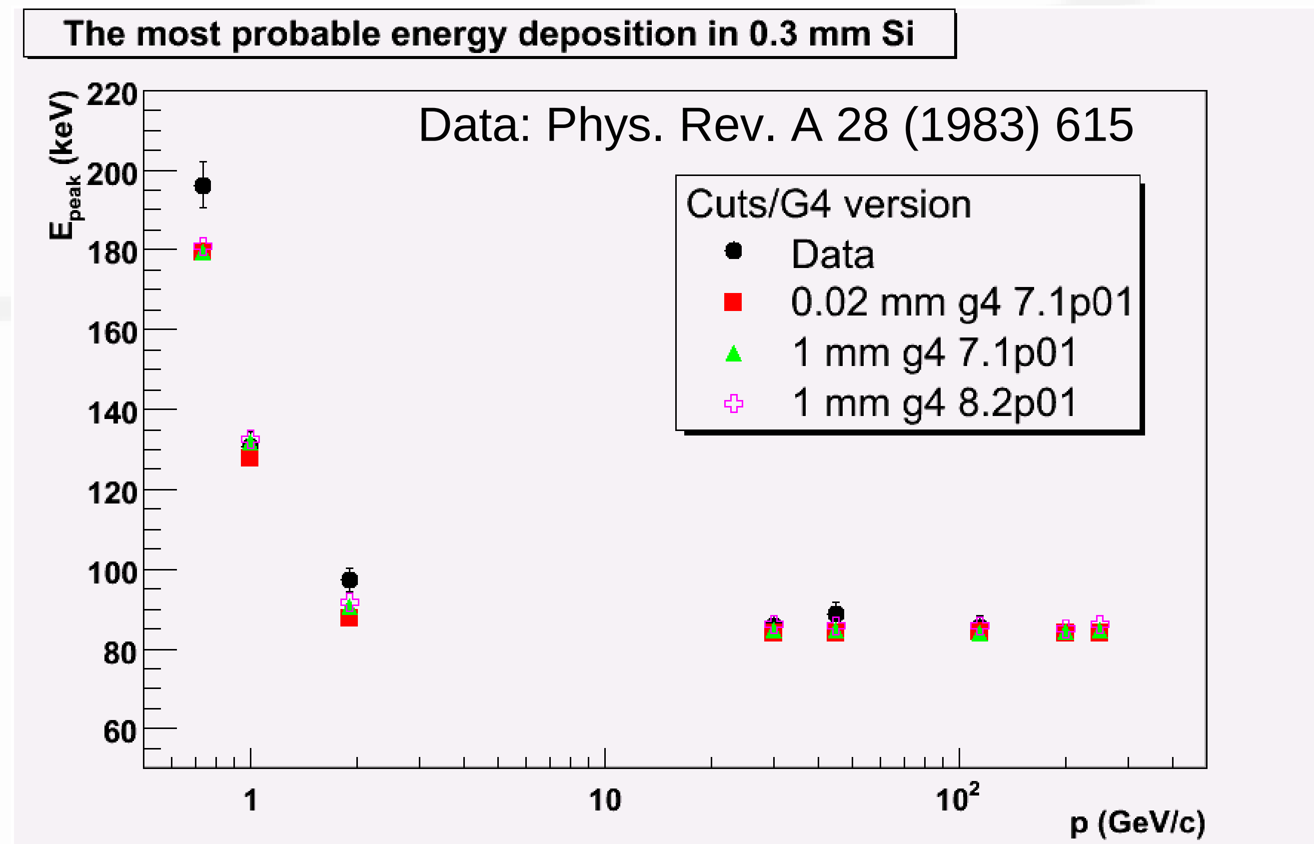
- Gammas:
  - Gamma-conversion, Compton scattering,

  Photo-electric effect
- Leptons(e, μ), charged hadrons, ions
  - Energy loss (Ionisation, Bremsstrahlung), Multiple scattering, Transition radiation, Synchrotron radiation, e+ annihilation.
- Photons:
  - Cherenkov, Rayleigh, Reflection, Refraction, Absorption, Scintillation
- High energy muons
- A choice of implementations for most processes
  - “Standard”: performant when relevant physics above 1 KeV
  - “Low Energy”: Extra accuracy for application delving below 1 KeV

Validation: examples



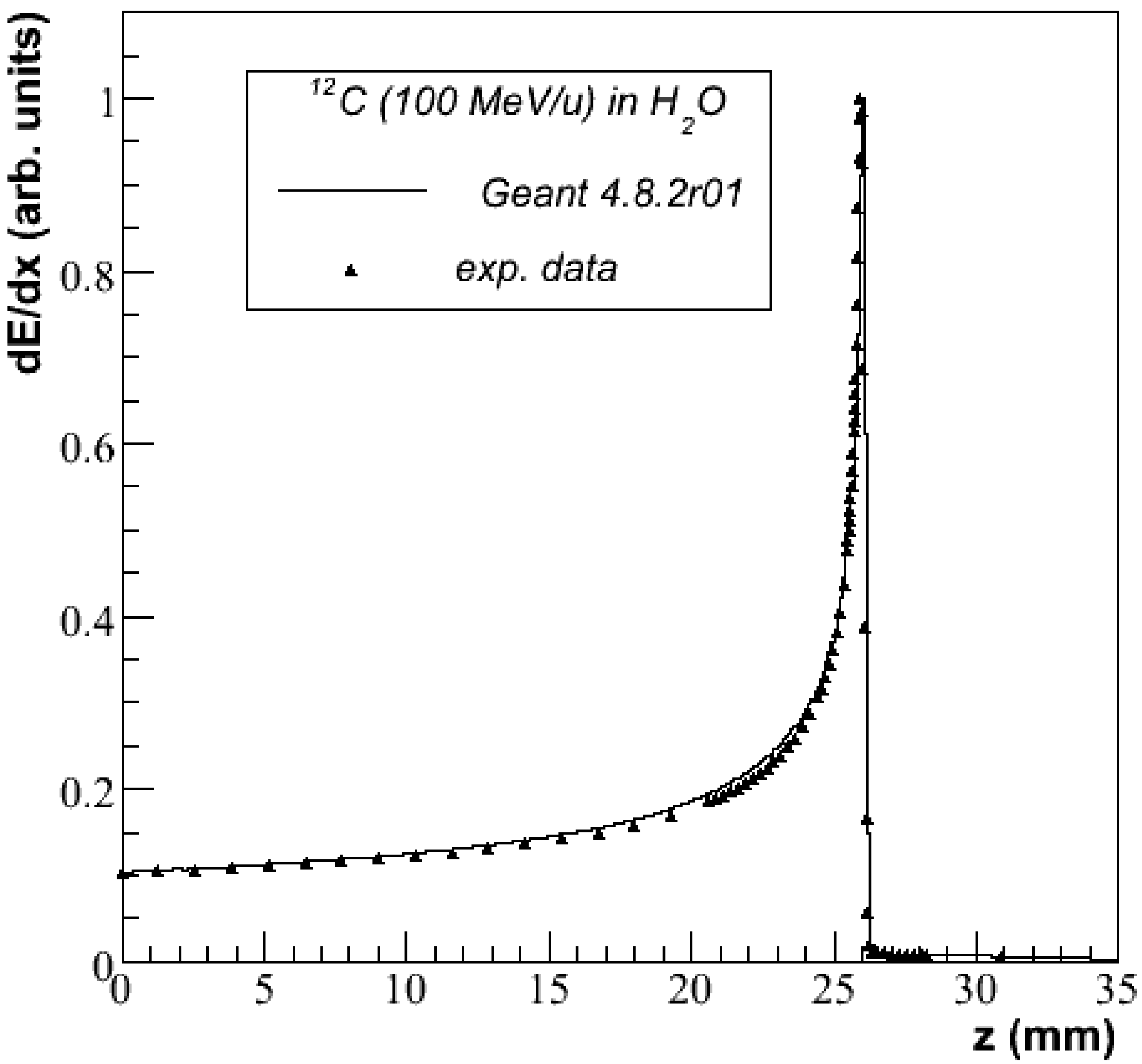
Dose calculation



Ionisation in thin layers

- Very good level of agreement reached from keV to TeV of kinetic energy range
- Results available at: http://geant4.web.cern.ch/geant4/collaboration/working_groups/electromagnetic/tests.shtml

Validation: Medical physics



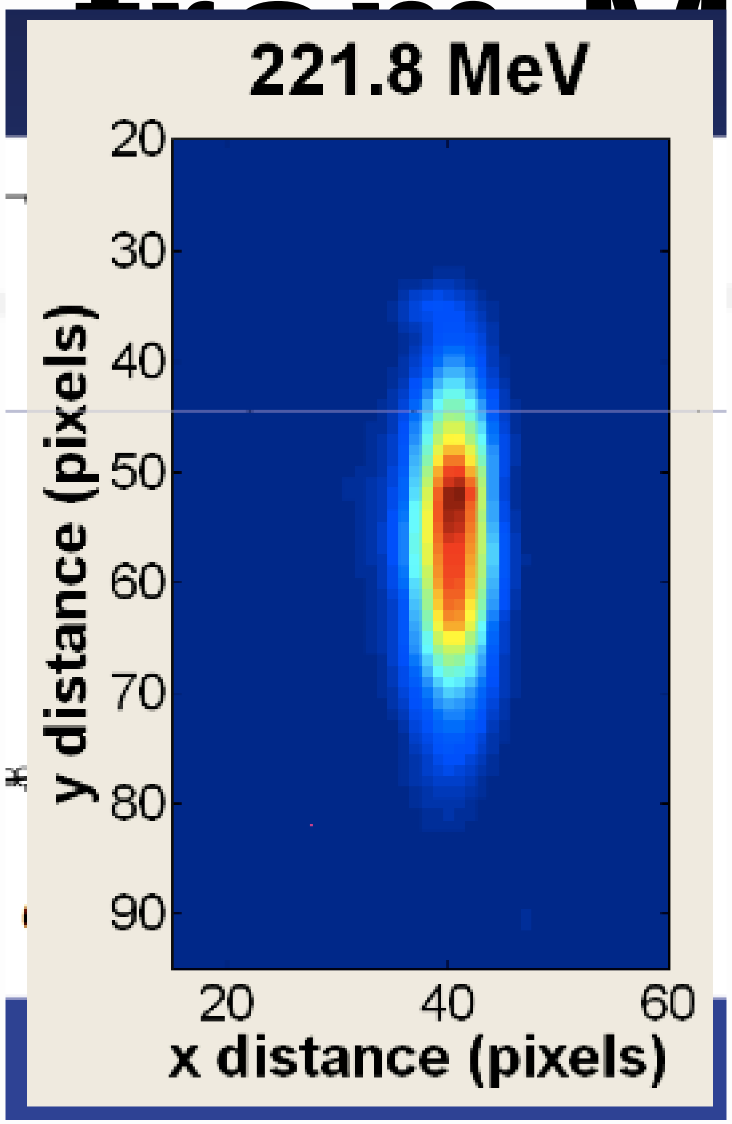
- Bragg Peak in water

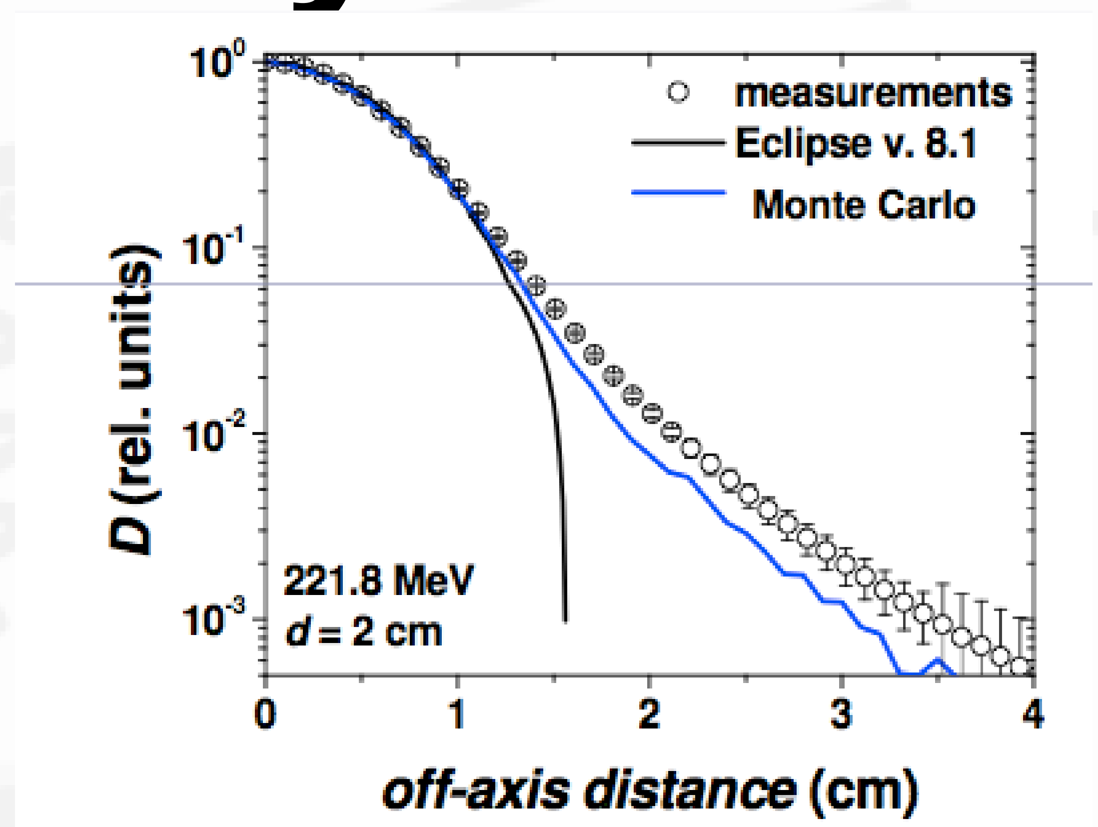
for a 100MeV/u ^{12}C beam

Precision of the position of the peak is the key observable to judge simulation quality

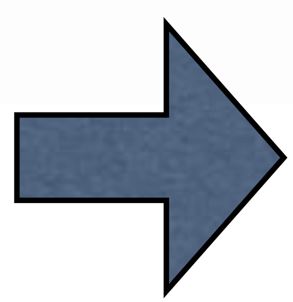
But...

Challenges: An example from Medical Physics



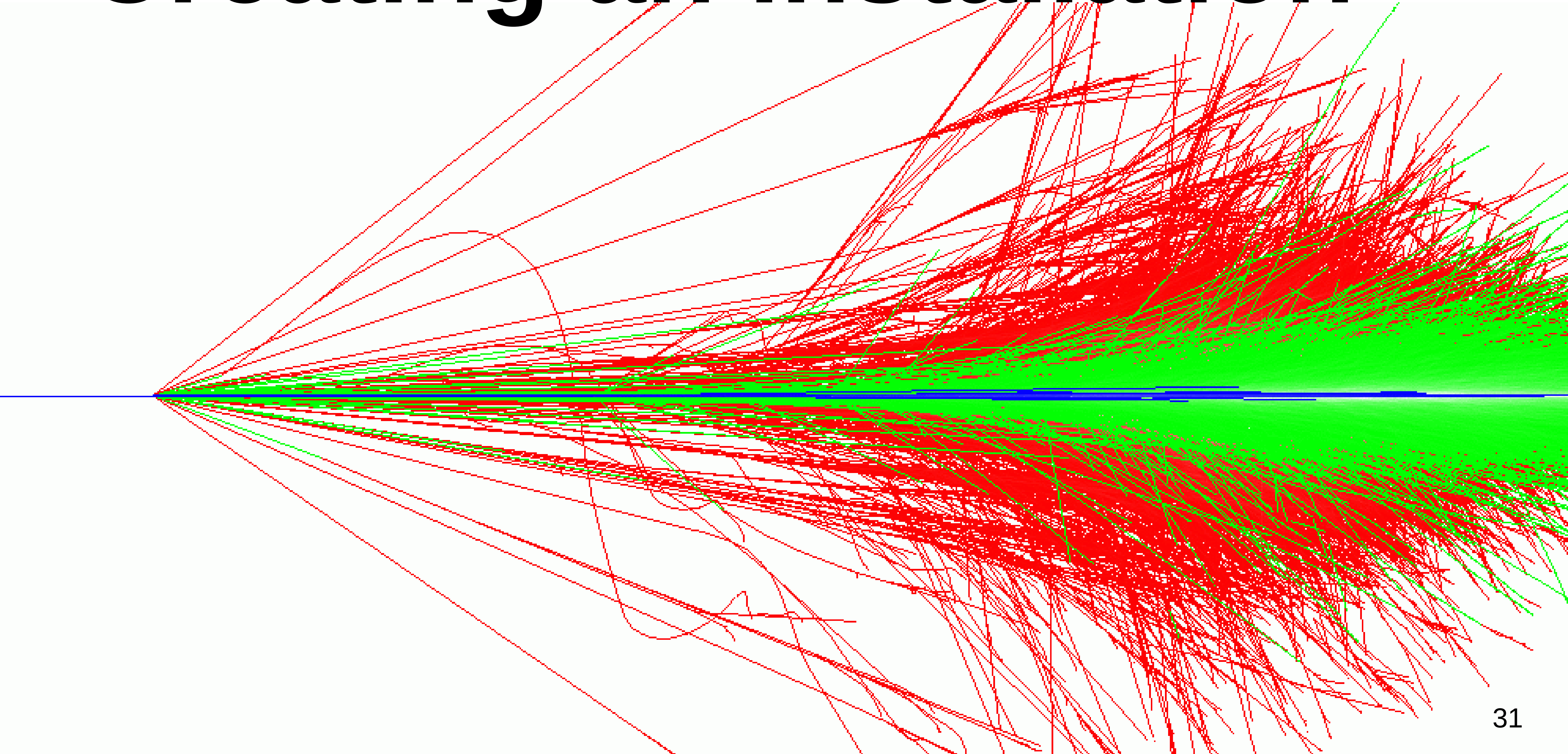


Use a beam for patient treatment:
send thousands/millions of particles (protons, C)



Tails become important:
1 spot, difference <0.1% (perfectly ok for ATLAS, CMS, ...)
10000 spots, difference > 5%

Creating an installation



Installing Geant4

- We will create a Geant4 installation on your local machine
  - it will be a copy of an installation I created on the local server
  - I created it by downloading Geant4 & following the installation instructions

- Later this week, I offer to help you create or upgrade your own installation
  - on your laptop (Linux or Windows)
  - on a machine at your institute - if you can connect

Geant4 installation

- We will now create a Geant4 installation
  - copying the files from another machine
  - deploying them in your machine / account
  - running the setup script
  - building your first Geant4 executable

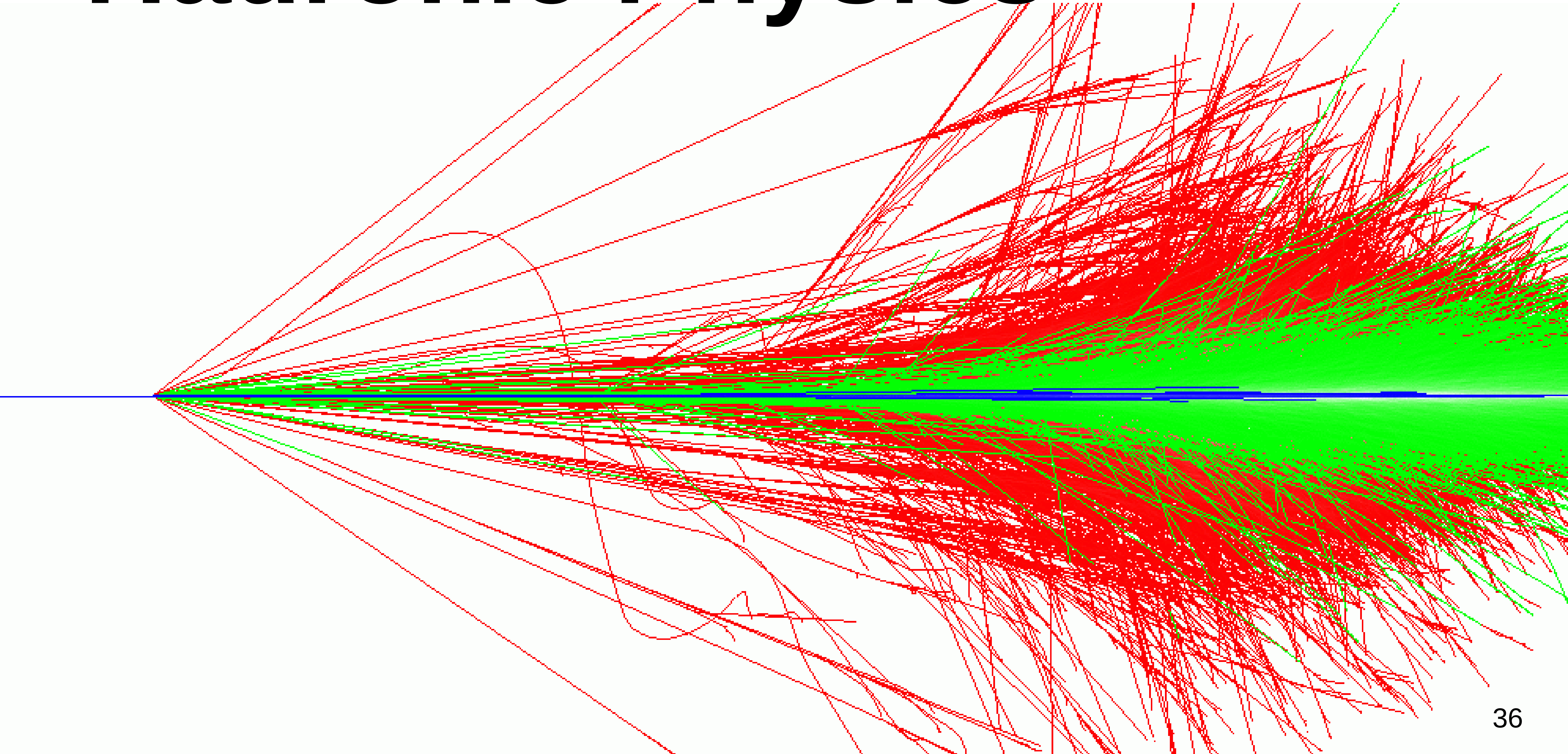
- You can follow all the steps at
  - http://bit.ly/2b7zVwW
  - or, if you prefer, its full address
  - https://dl.dropboxusercontent.com/u/540317/ASP2016/DownloadG4.txt

Getting Geant4 machine

- cd
- *# Download a 'tarball' of Geant4 & cmake*
- scp student12@172.17.33.213:Geant4.gtz .
- *# Check its size & date stamp*
- ls -l Geant4.gtz
- *# Expect it to be: 527518149 Aug 8 10:59*
- *# Check contents*
- tar tvf Geant4.gtz | head
- *# 'Un-tar' to get the contents into your directory*
- tar xf Geant4.gtz
- ls -lt   *# Let’s see if ‘geant4’ and ‘bin’ appear*

- cd geant4
- *# Run the commands to setup Geant4 installation*
- source setupGeant4.sh
- setupG4
- env | grep G4INS   # Check it
- *# Copy the examples to your working area*
- sh ./copy-examples.sh
- cd examples/basic/B1 # *First, basic example*
- mkdir build
- cd build
- buildG4 # Build it
- ls -lt exampleB1 # *last character is a ‘one’*
- ./exampleB1   # *Run it !*

Hadronic Physics



Processes

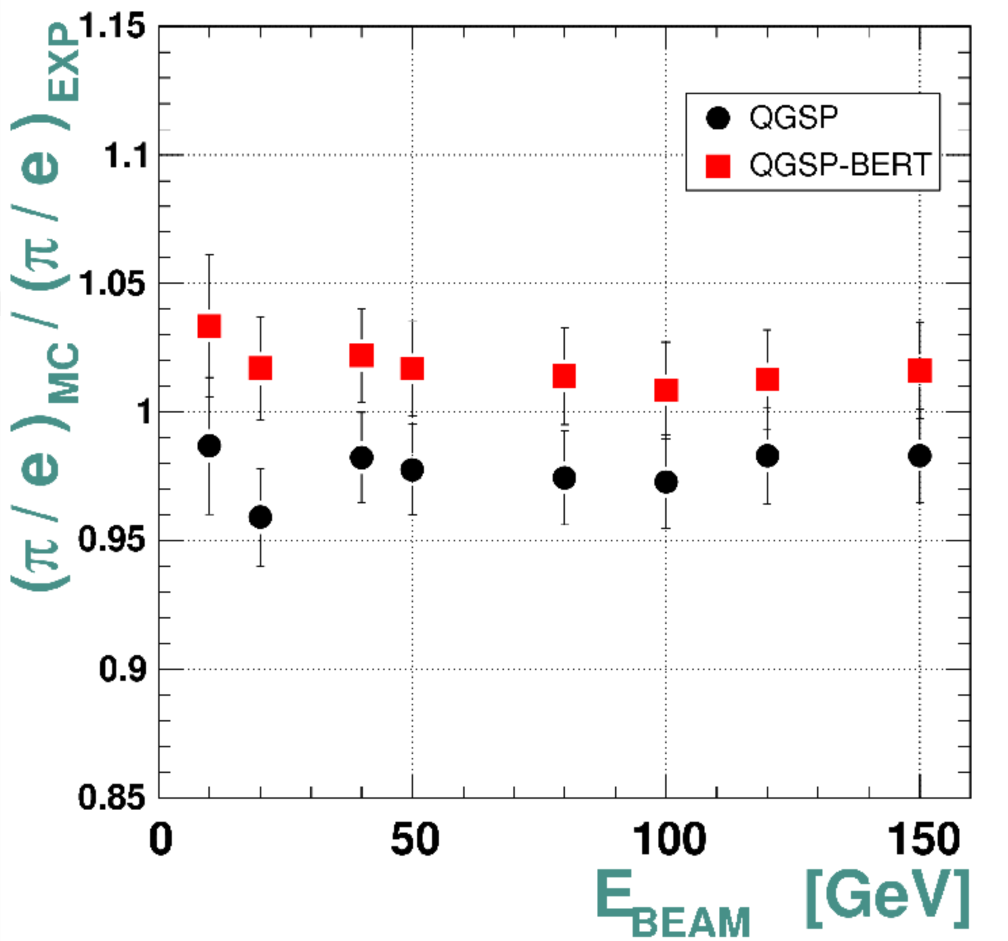
- Hadronic physics is included in Geant4
  - a powerful and flexible framework and
  - implementations of cross-sections & models.
- A variety of models and cross-sections
  - for each energy regime, particle type, material
  - alternatives with different strengths and computing resource requirements
- Components can be assembled in an optimised way for each use case.

Models Summary

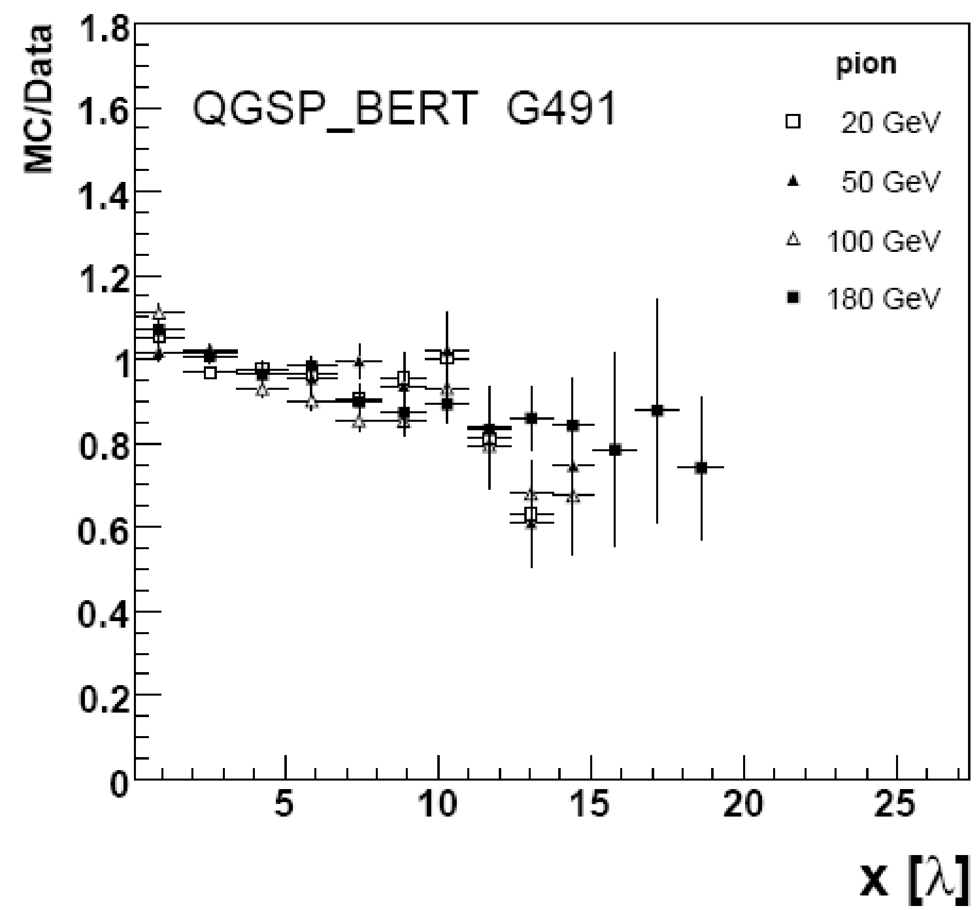
- Parameterized models (1997): all E and particles - data driven
- Fritjof, “FTF” (new developments): p,n,k,π of high energy (E_{kin}>10 GeV) Nucl. Phys. 281 289 (1987)
- Quark-Gluon-String, “QGS”: p,n,k,π of high energy (E_{kin}>20 GeV) See Sec. IV, Chap. 22 of Geant4 Physics Reference Manual and bibliography within
- Bertini cascade: low energy intra-nuclear cascade (E_{kin} < 5 GEV) Nucl. Instr. Meth, 66, 1968, 29 ; Physical Review Letters 17, (1966), 478-481
- Binary cascade: low energy intra-nuclear cascade (E_{kin} < 5 GEV) See Sec. IV, Chap. 25 of Geant4 Physics Reference Manual and bibliography within

Validation: examples

Response to pions: ATLAS HEC



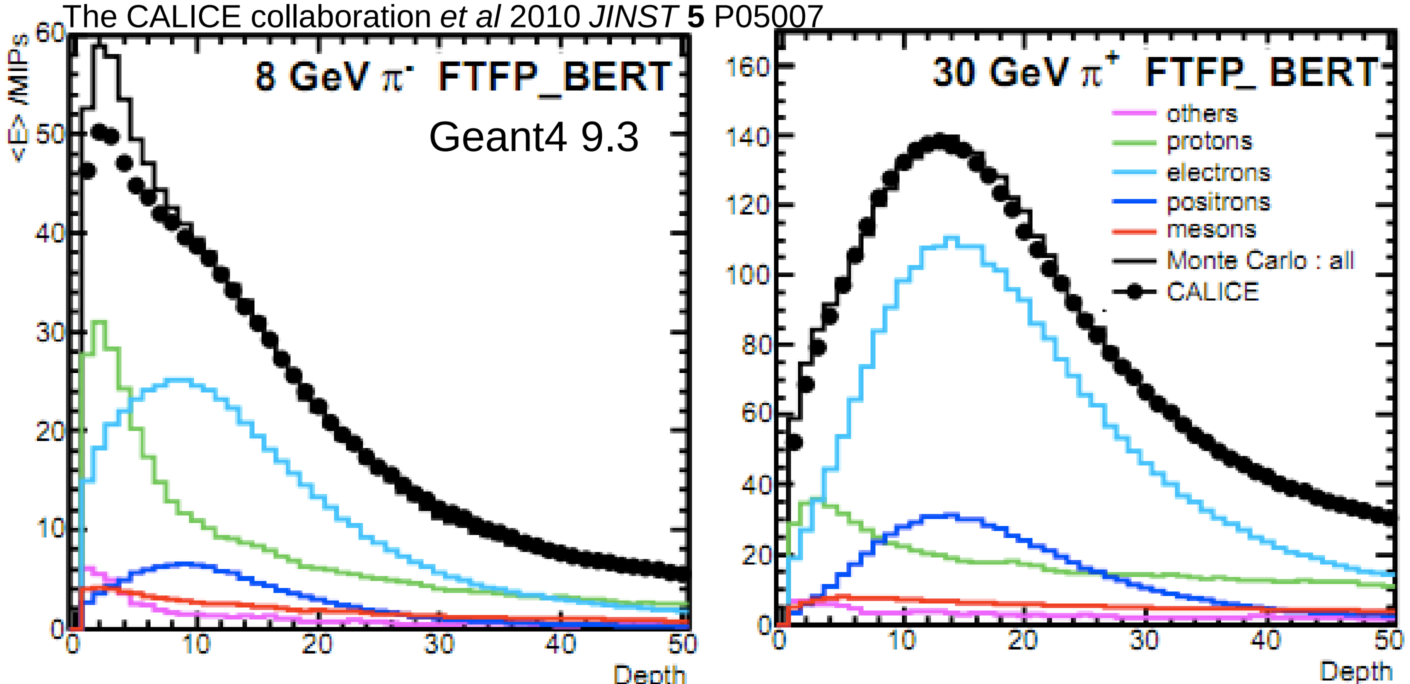
Longitudinal Shower shape: ATLAT TileCal



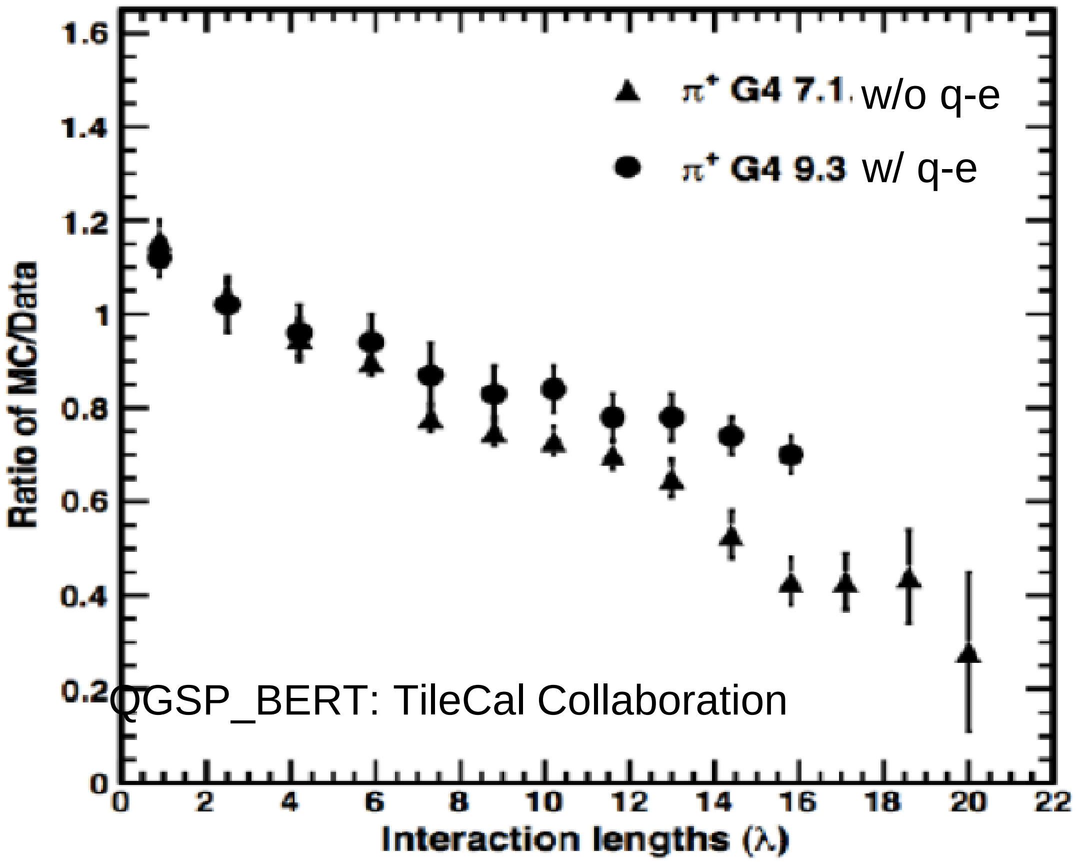
- Hadronic models are of primary interest for LHC experiments: close collaboration
  - Example: ATLAS plans to use extensively G4 to extract “corrections” and “calibration constants” for jet calibration
- Comparison with thin target experiments and LHC test-beams data
- More details: http://geant4.fnal.gov/hadronic_validation/validation_plots.htm

Longitudinal Shower Shape

The CALICE collaboration *et al* 2010 *JINST* **5** P05007



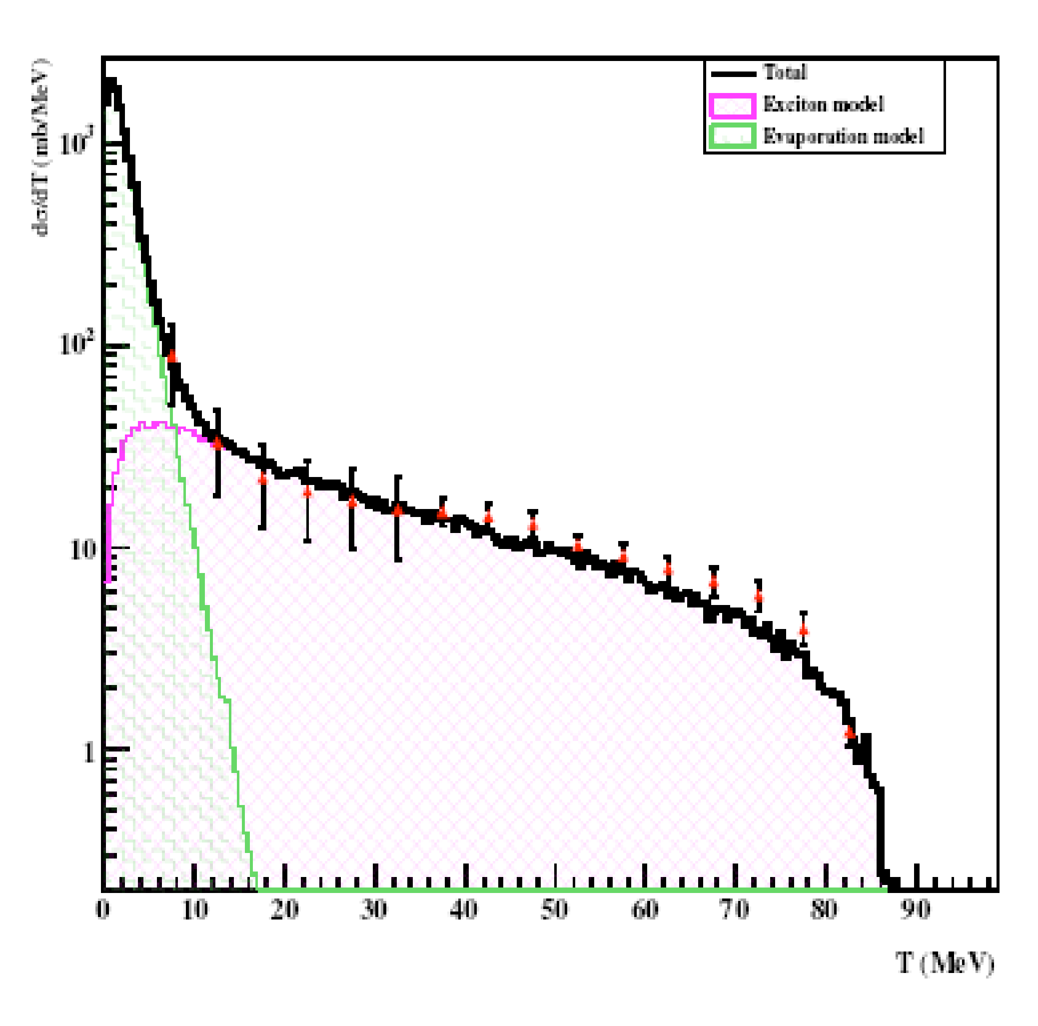
Shower profile: comparison with test-beam (SiW) data and MC break-down



- CALICE: unprecedented details in shower development
  - High energy: data better described
  - Low energy: too many protons (role of precompound: under investigation)
- LHC experiments showed “forward physics” processes (quasi-elastic, diffraction) are needed to describe longitudinal evolution of showers

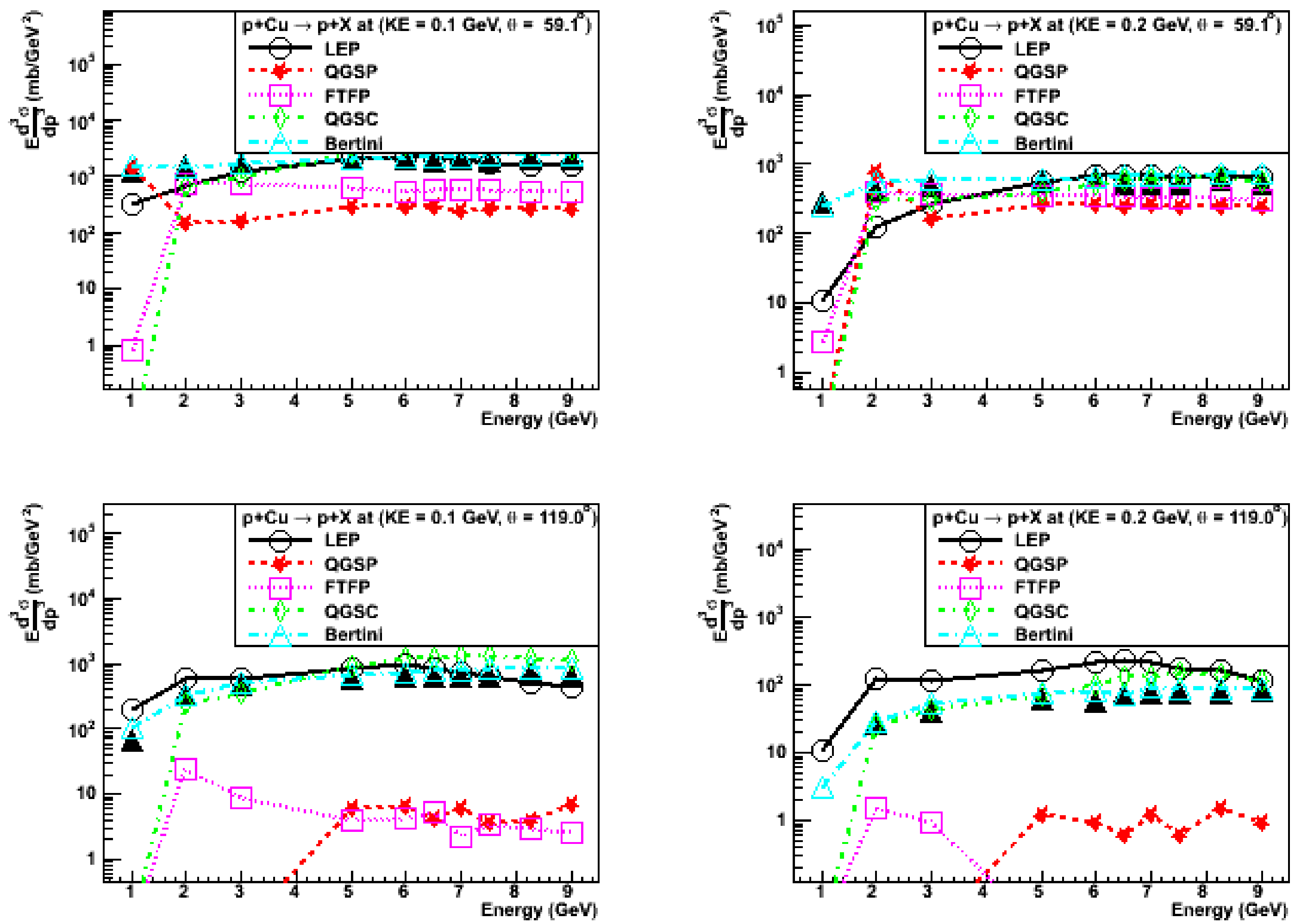
More Validation Examples

Neutron cross section



Protons of 90 MeV Bi(p,n) reaction:
Precompound model

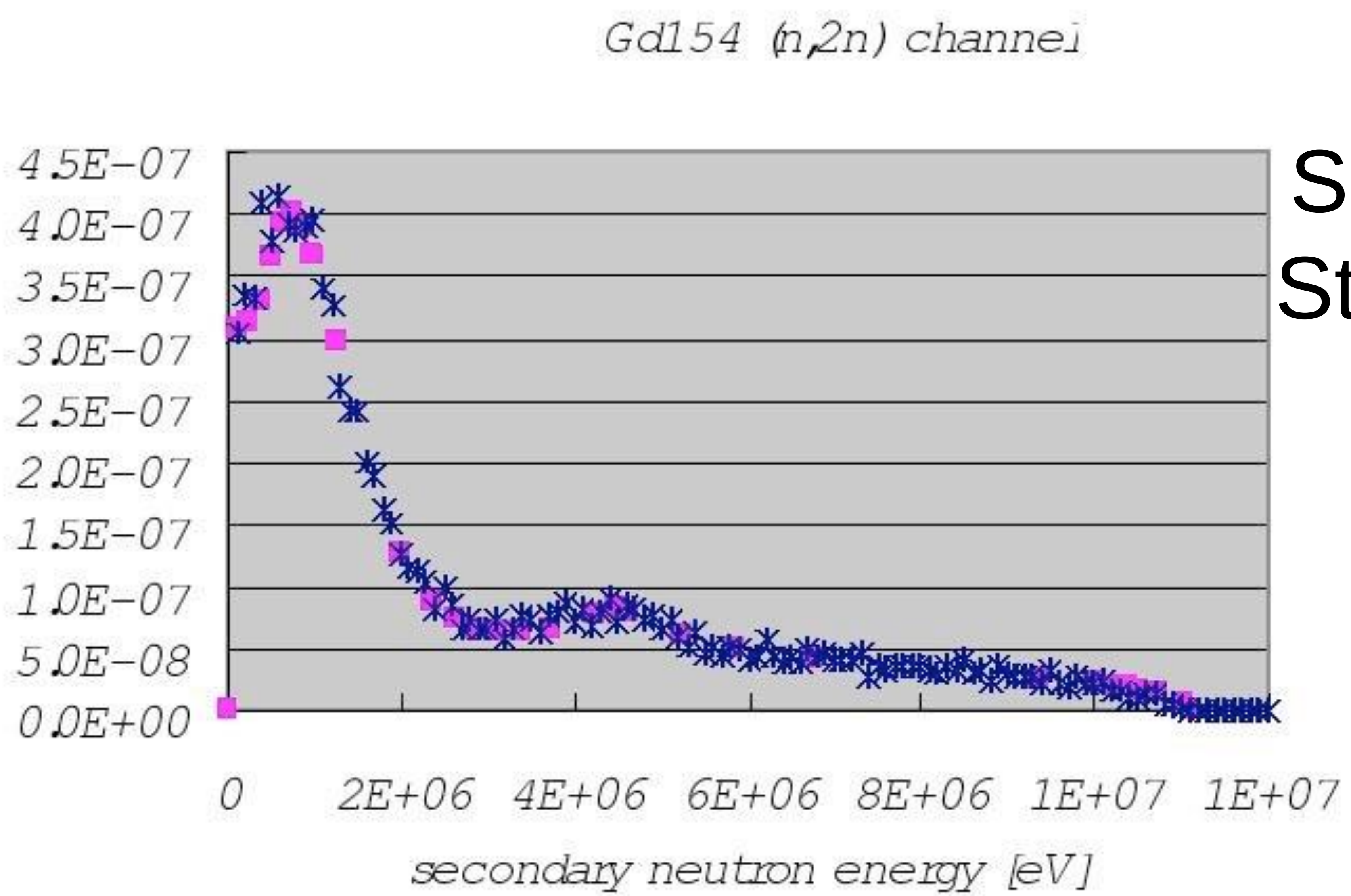
p cross-sections for various models at different angles



p on Cu with kinetic energy of 0.1/0.2 GeV

Another example: Thermal neutrons

HP (High Precision) extension is needed when interested in thermal neutrons. Expect up to x10 slower simulation!

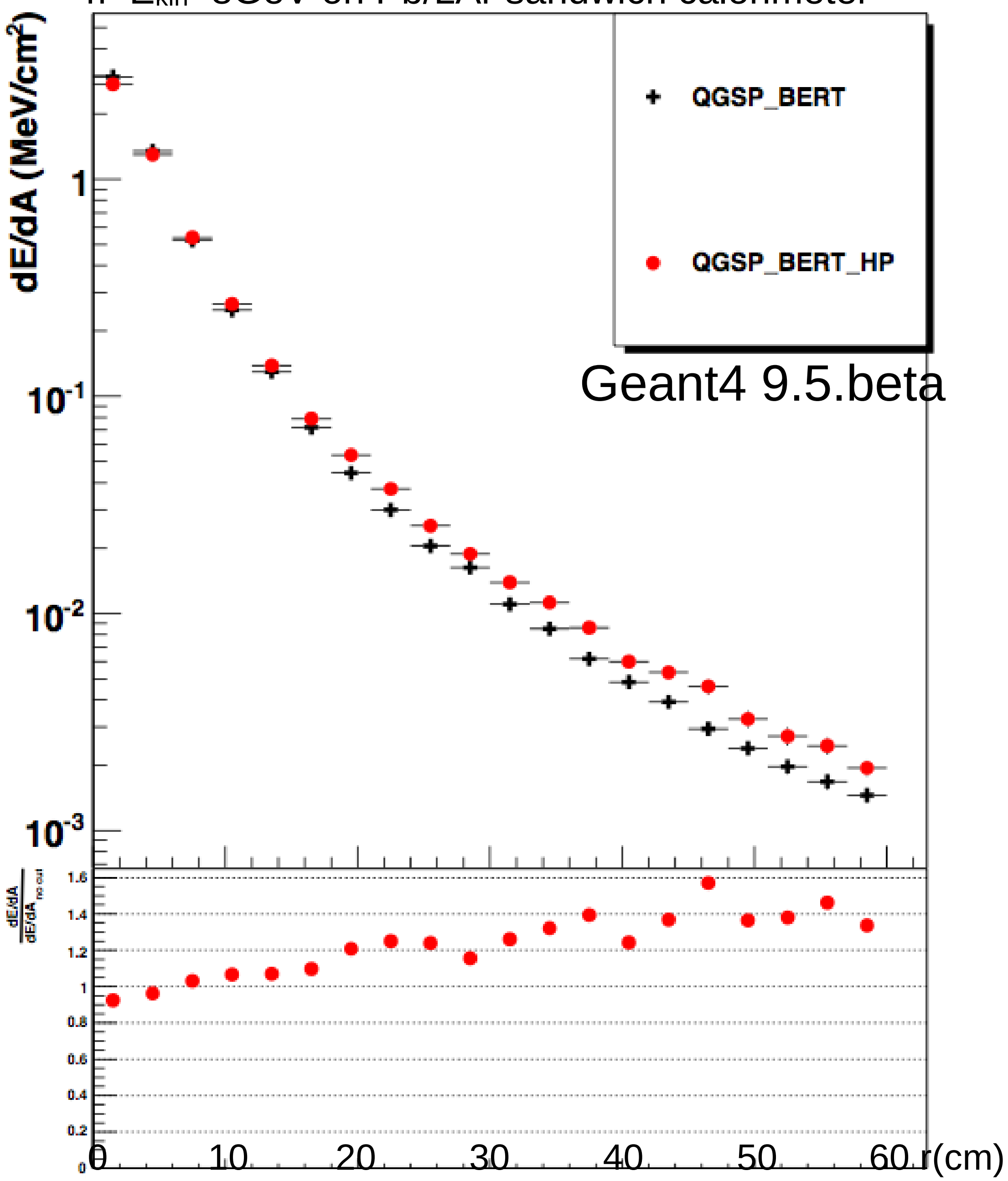


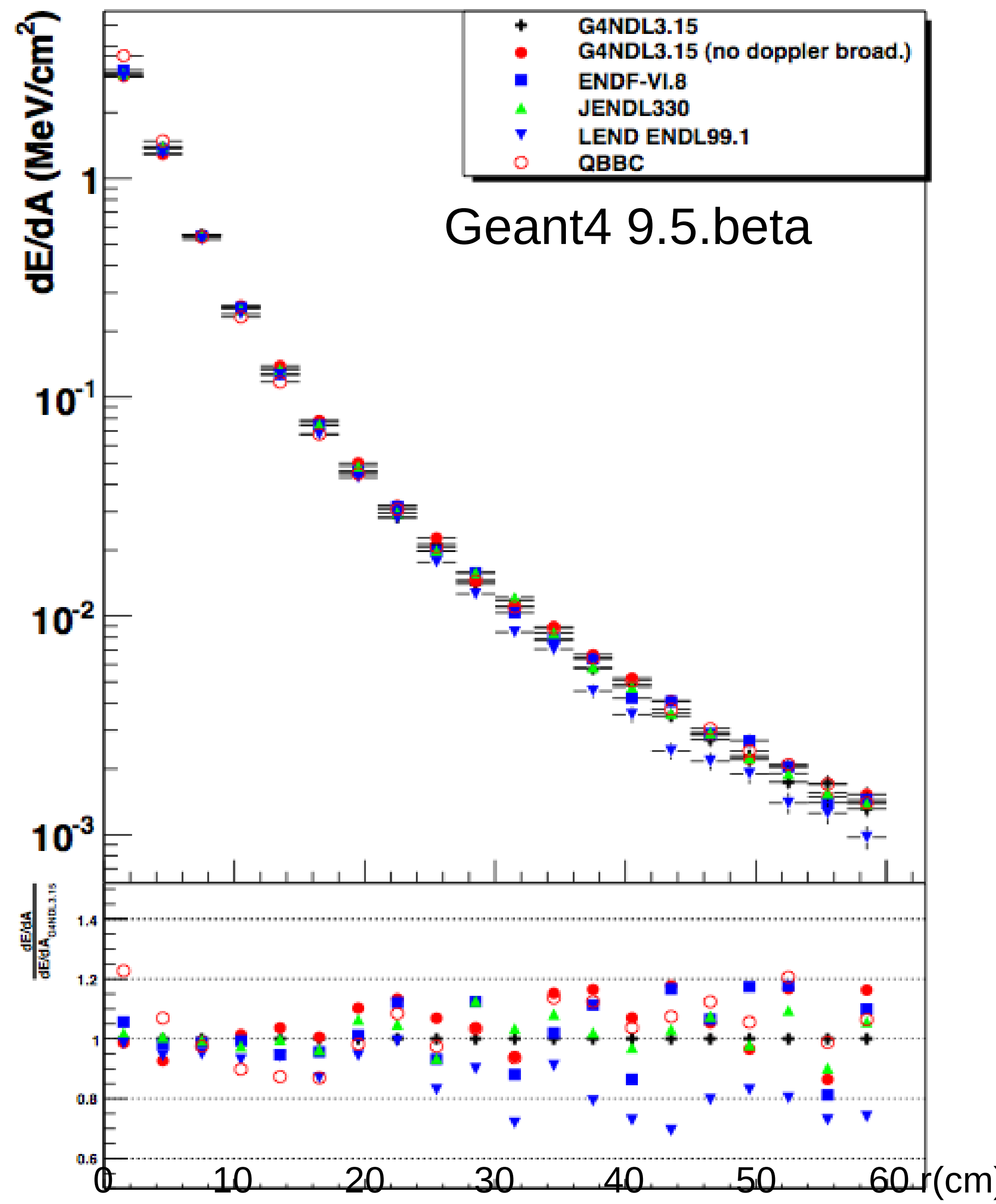
Squares: NDF data
Stars: G4 HP Model

Warning: this is a little bit a tautology, since HP is based on NDF data....

Role of neutrons: example

π^- E_{kin}=8GeV on Pb/LAr sandwich calorimeter

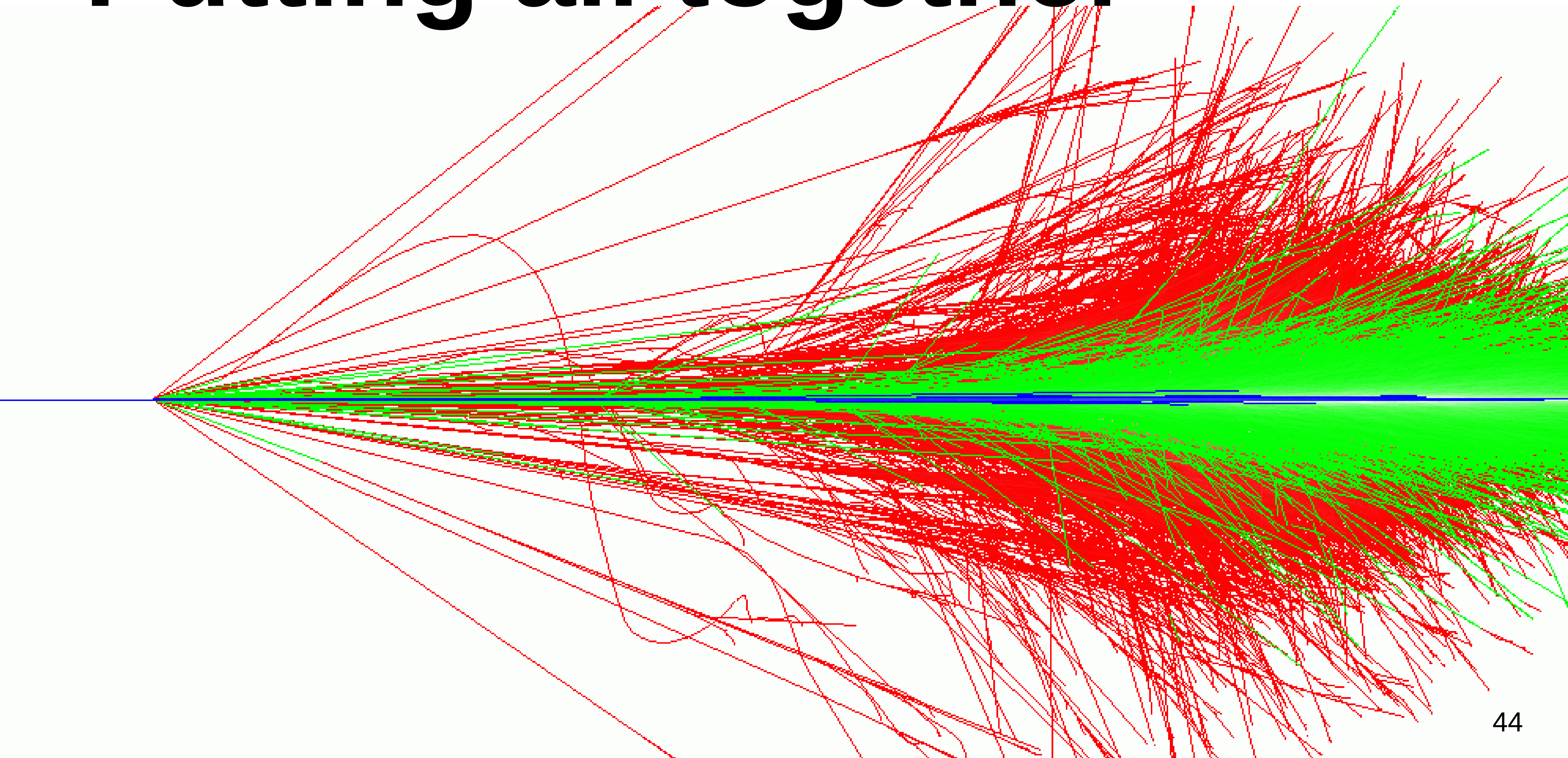




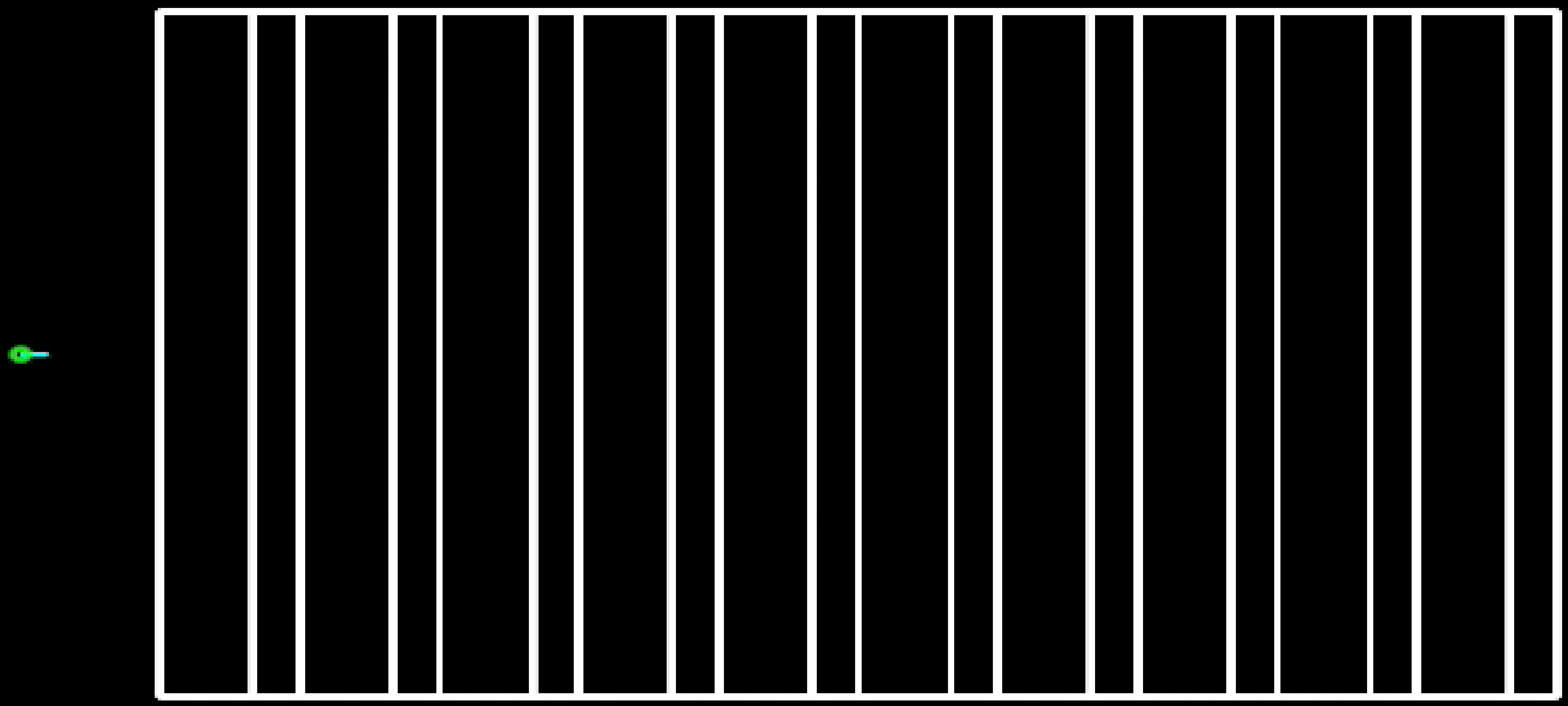
Low-E neutrons play important role for lateral profile

Need high granularity calorimeter for better understanding (CALICE)

Putting all together



Hadronic Shower



More examples at: http://www.hep.man.ac.uk/u/johna/pub/Geant4/Movies

A concrete Example: what you have seen

- 10 GeV/c pi- on lead (in a lead-liquid-argon calorimeter, exampleN03 with QGSP physics)
- A plethora of slow pions, protons and neutrons
  - Three fast pi- and one fast pi+ that subsequently interacts again
  - Neutrons (yellow) hang around for several ns
- Green circle is expanding at the speed of light

Physics Lists

- Since different (hadronic) models exists with different performances (quality of results and computing requirements) at different energy ranges, multiple choices are available:
  - Models are assembled in “physics lists”
- Can be built from scratch or use one of the provided “educated” physics lists, for applications in:
  - HEP calorimetry, tracking, low-E dosimeter with neutrons, shielding, medical applications, air shower applications, low background experiments, space applications

Currently suggested physics lists:

- FTFP_BERT : recommended for HEP
  - High Energy: Fritiof model
  - Intermediate Energy: Bertini style cascading
  - Low Energy: Pre-compound and evaporation
- QGSP_BERT_HP or Shielding: recommended for shielding, nuclear studies
  - Add High Precision extension for low-energy neutrons (<20MeV)
- EM low-energy variants: recommended for medical applications
  - Livermore, Penelope treatment of low-energy gammas and electrons
  - Under-development: G4-DNA, simulate also physio-chemical step of DNA damage

Test-beam summary (G4 9.4.p01)

Status Sept-Oct 2011

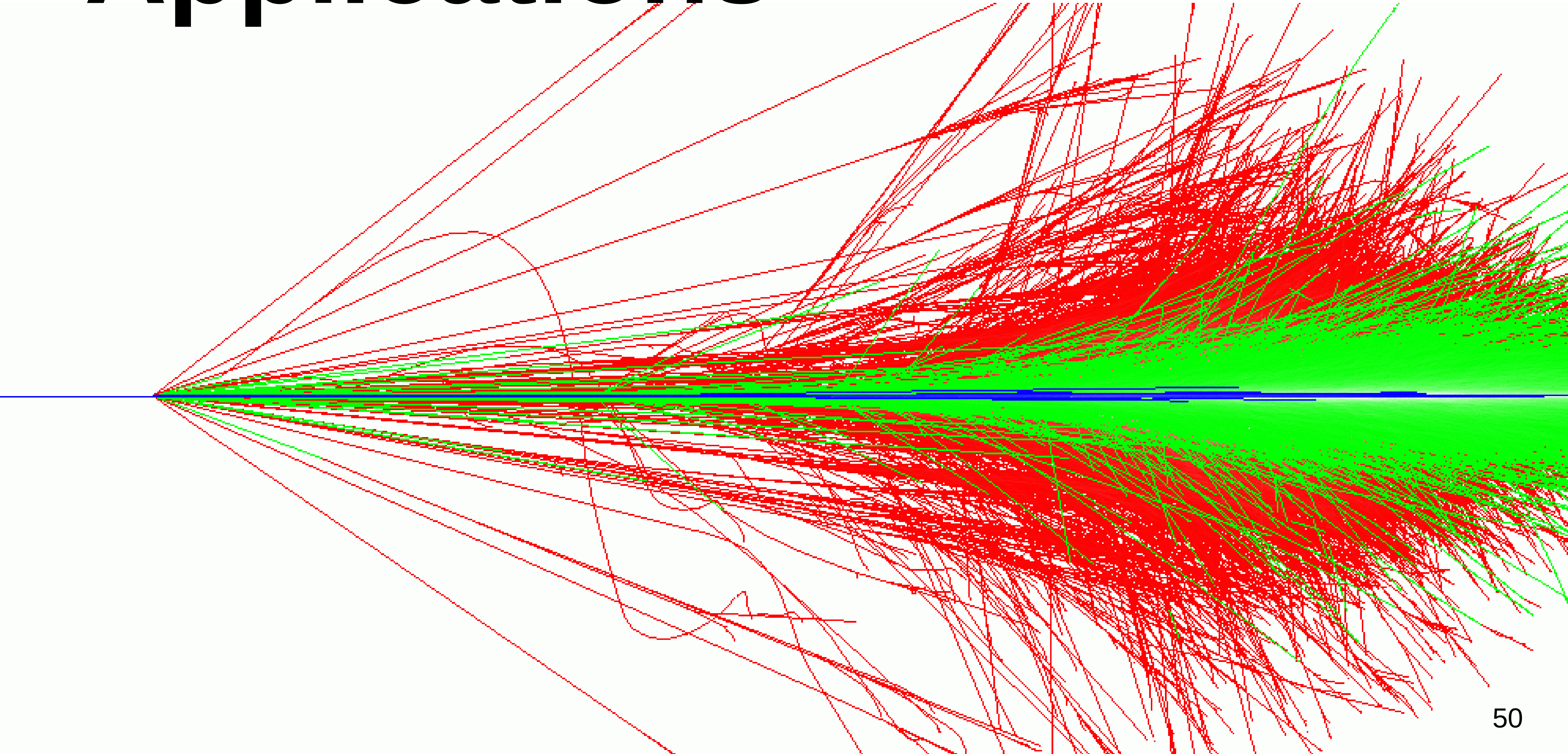
	Response	Resolution	Smoothness	Lateral Shape	Longitudinal Shape @10λ	Peculiarities, comments
QGSP_BERT	+(1-3)%	-(5-10)%	Δ~5%@10GeV	π,p: -(10-20)%	π: -10% p: -20%	Extensive use of LHEP
FTFP_BERT QGSP_FTFP_BERT	+(0-5)% (***)	-(3-7)%	Δ~0	π: -(10-20)% p: -(3-10)%	π: +10% p: +(10-20)%	anti-nucleons, hyperons via CHIPS(*), no LHEP
CHIPS	+(5-10)%	-(10-20)%	Δ~0	π: -(3-10)% p: -(10-20)%	π: -10% p: -20%	anti-nucleons, hyperons, single model
FTF_BIC(**)	+(3-5)%	-(2-6)%	Several irregularities	-	π: +10%	Implements re-scattering at high E, Extensive use of LHEP

(*): Native FTF model under testing

(**): Much less tested at LHC

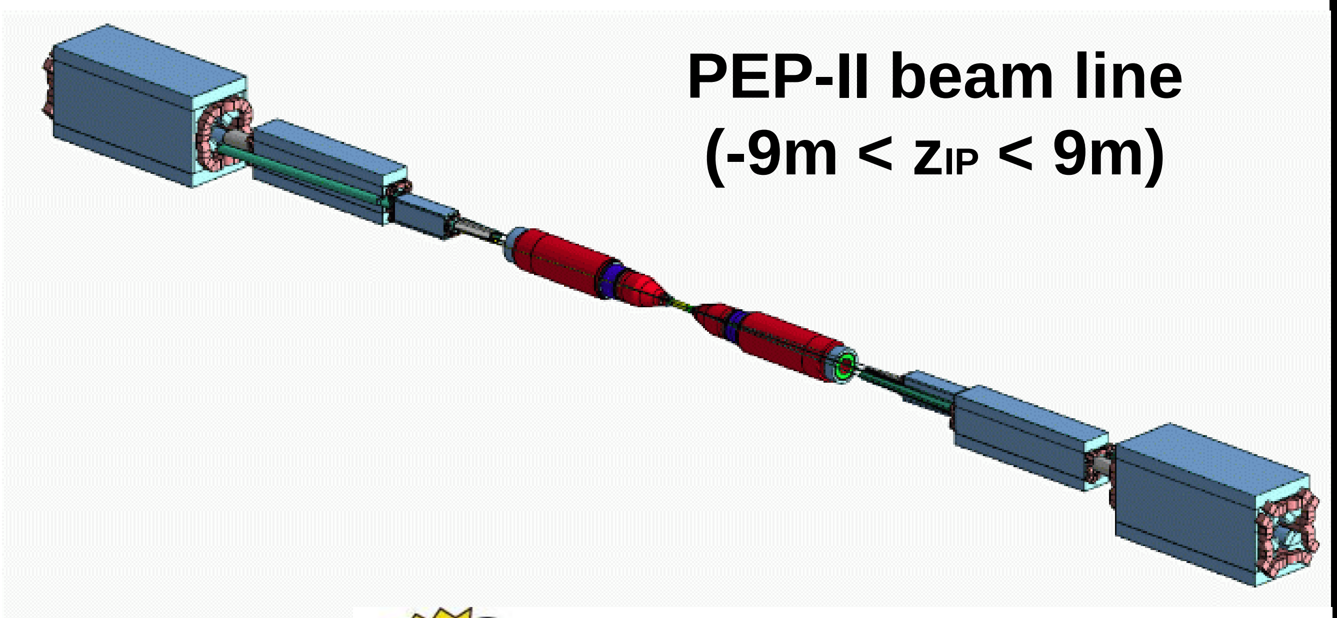
(***): Lower limit: CMS; Upper limit ATLAS

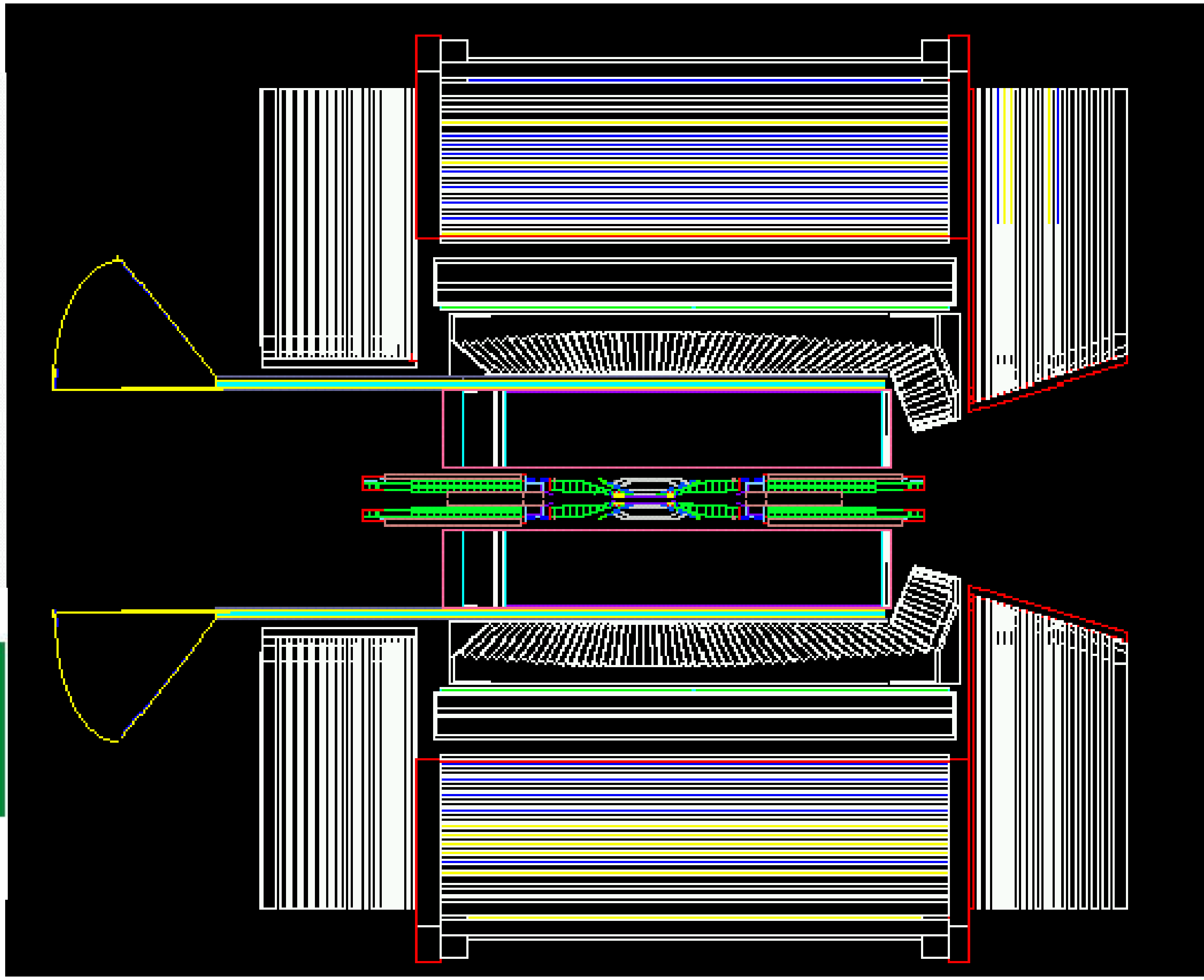
Applications



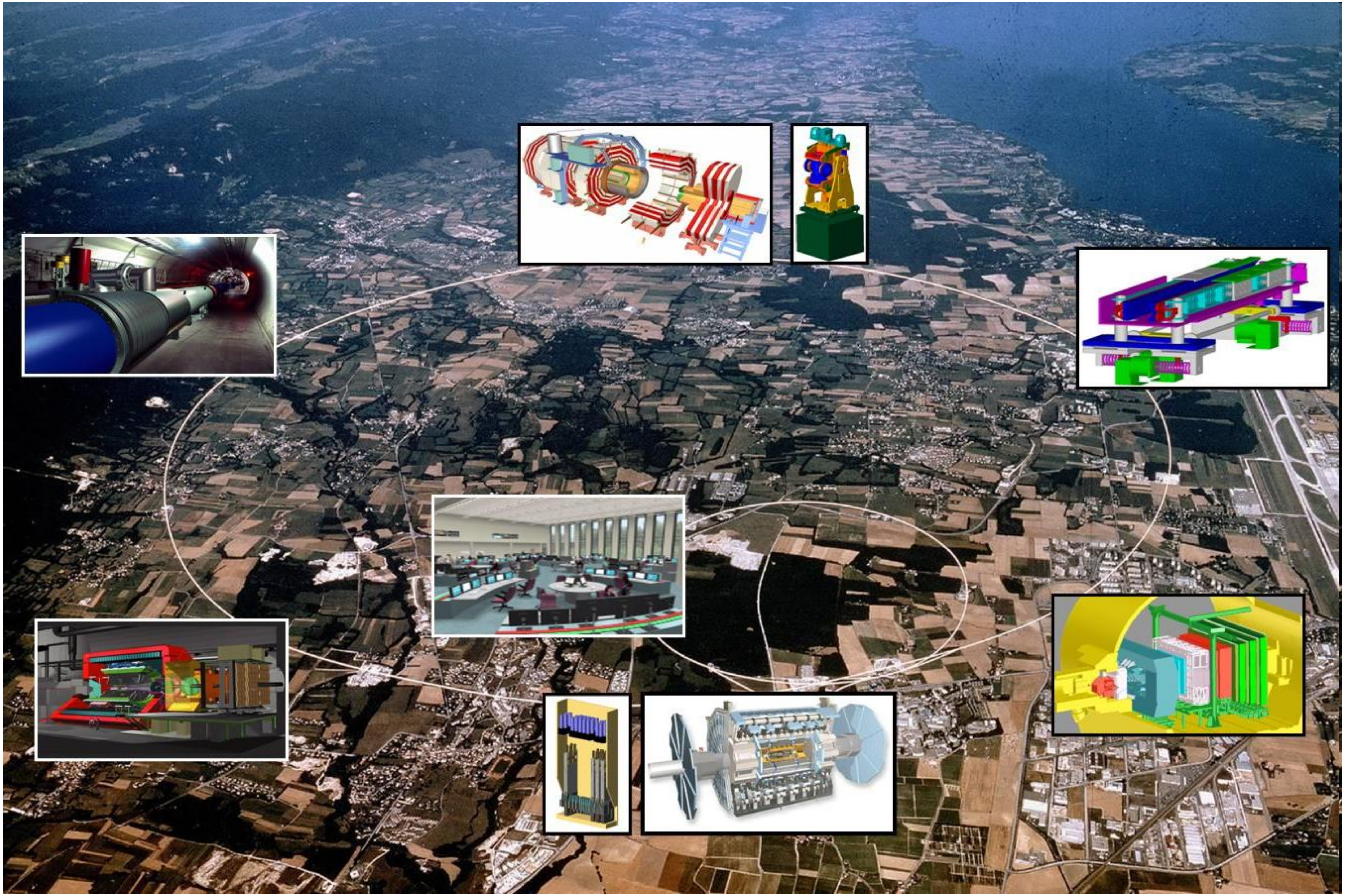
BaBar and Geant4

- BaBar is the pioneer HEP experiment in use of OO technology, and the first customer of Geant4.
  - During the R&D phase of Geant4, we acknowledge lots of valuable feedbacks were provided by BaBar.
- BaBar started its simulation production in 2000 and had produced more than 10 billion events at more than 20 sites in Europe and North America.

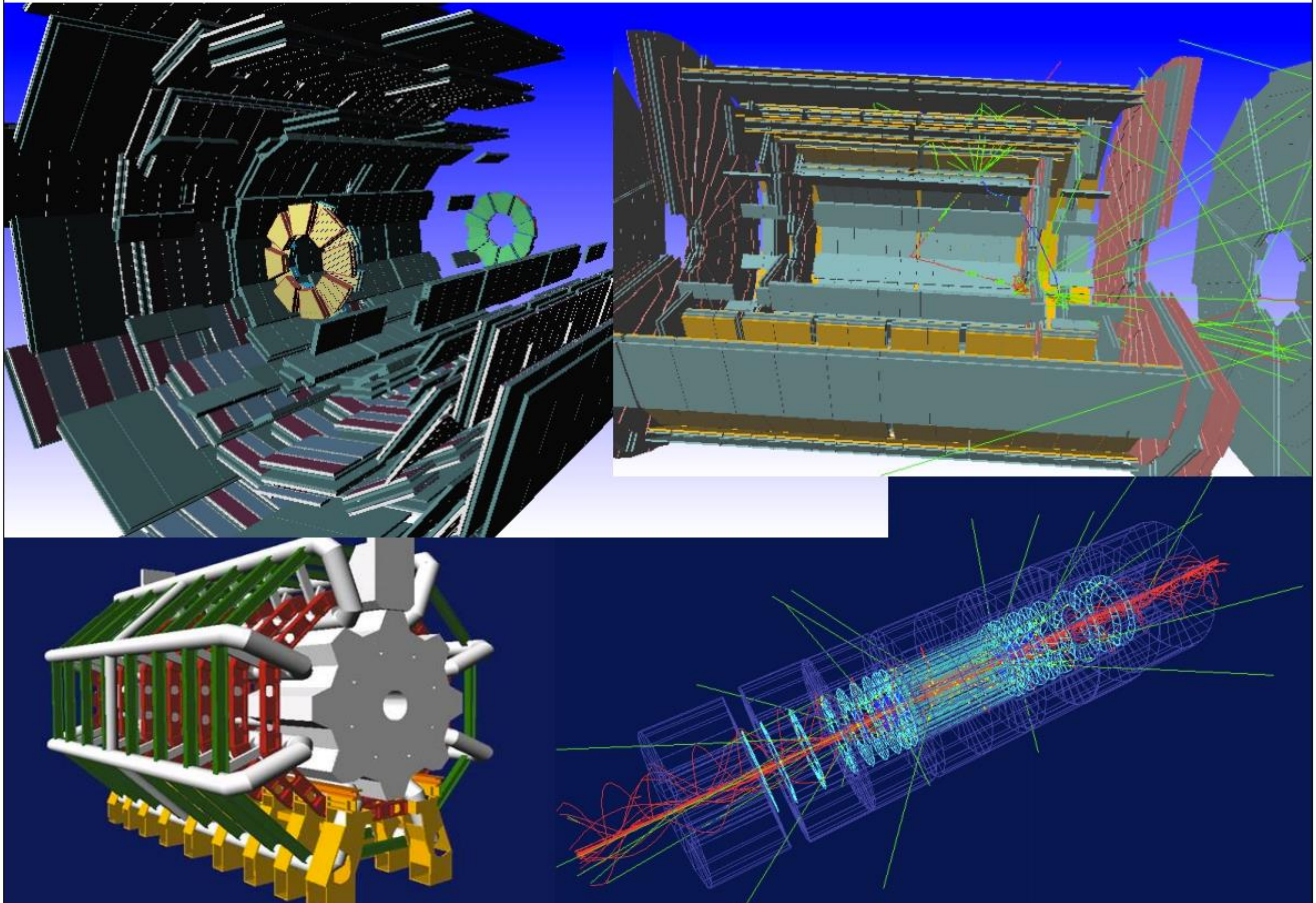




Large Hadron Collider (LHC) @ CERN



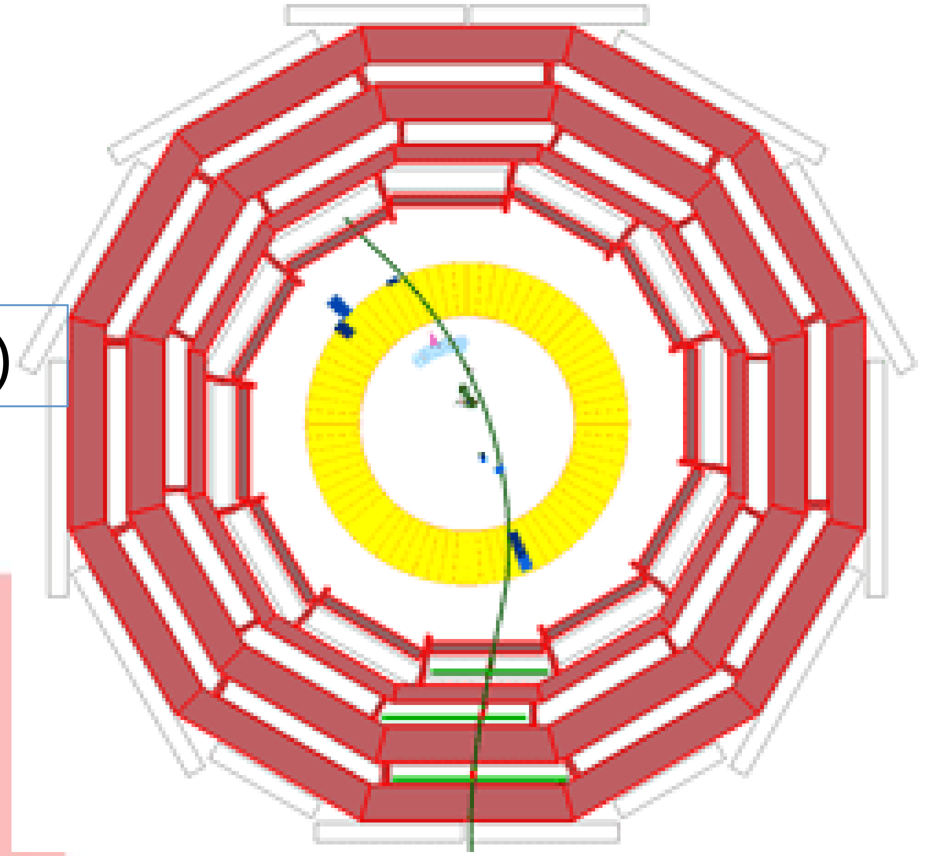
Geant4 in High Energy Physics (ATLAS at LHC)



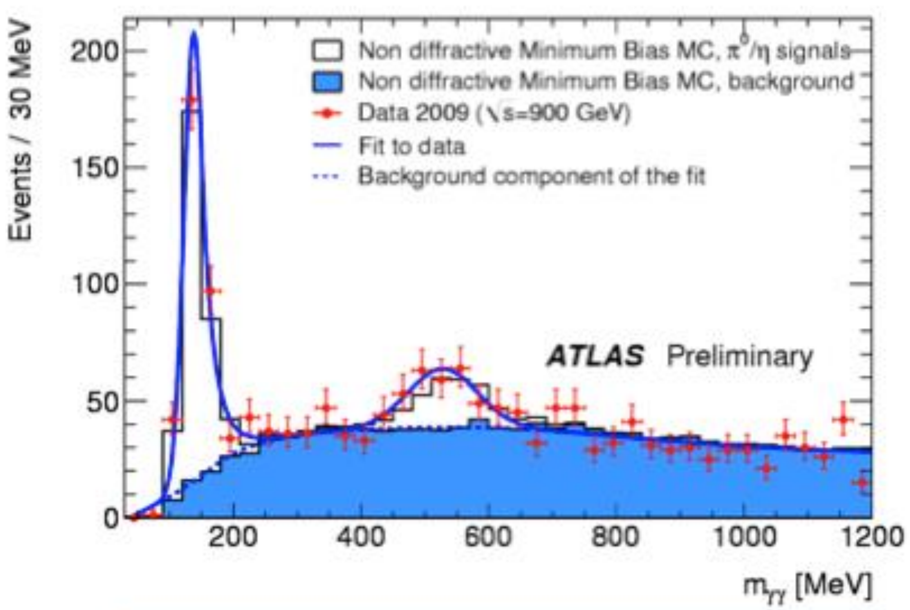
Geant4 has been successfully employed in many HEP experiments

- Detector design
- Calibration / alignment
- First analyses

T. LeCompte (ANL)



GEANT4 Comparisons with the Calorimeters



Invariant mass of pairs of well-isolated electromagnetic clusters.

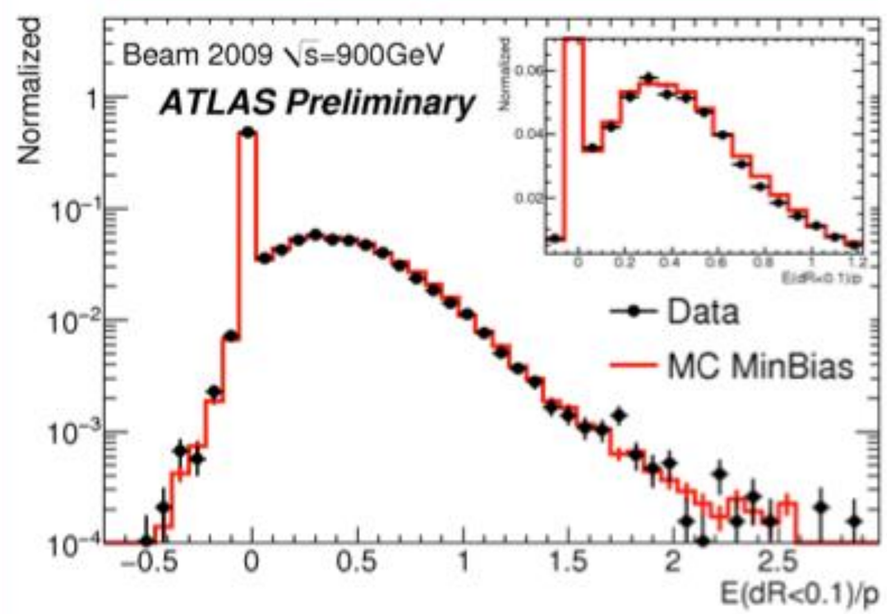
The π^0 mass is within 0.8 ± 0.6% of expectations.

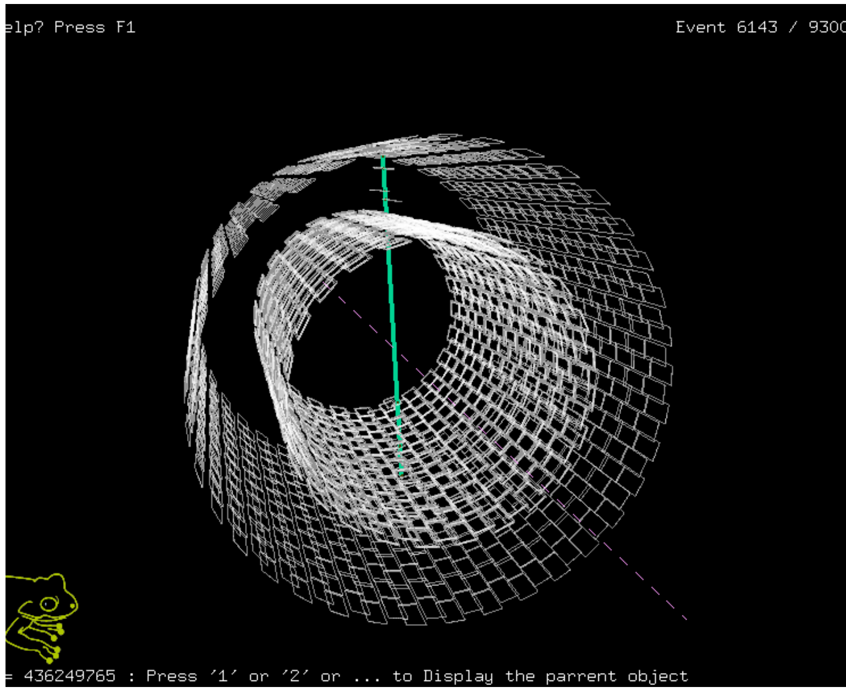
The η^0 mass is within 3 ± 2% of expectations.

The detector uniformity is better than 2%.

Response of the calorimeter to single isolated tracks. To reduce the effect of noise, topological clusters are used in summing the energy.

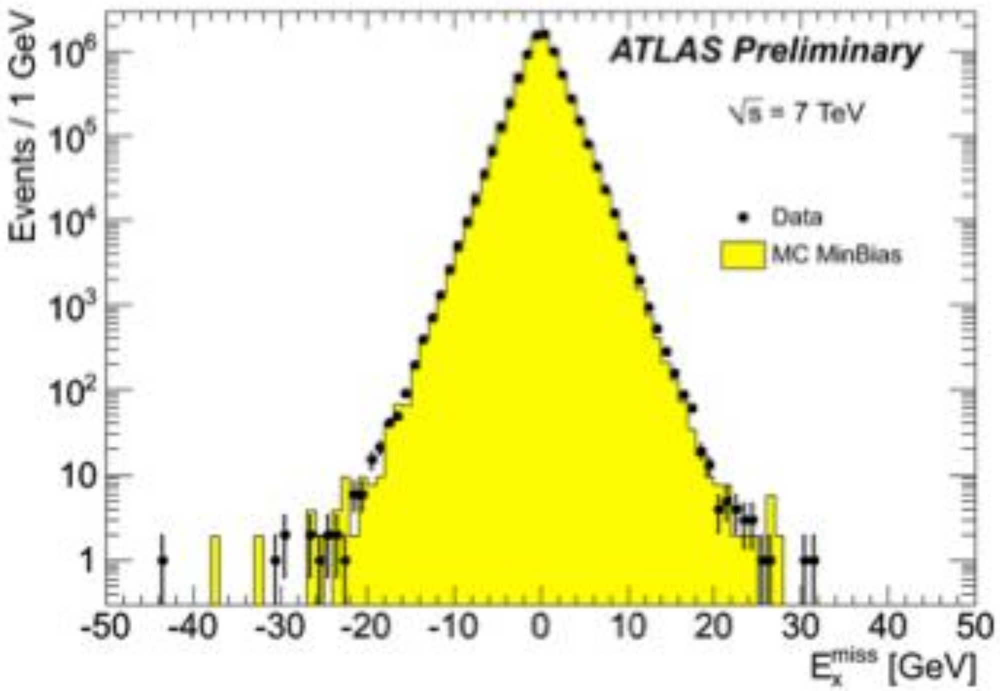
This plot agreed better than we ever expected. (I sent the student who made it back to make sure that they didn't accidentally compare G4 with G4.

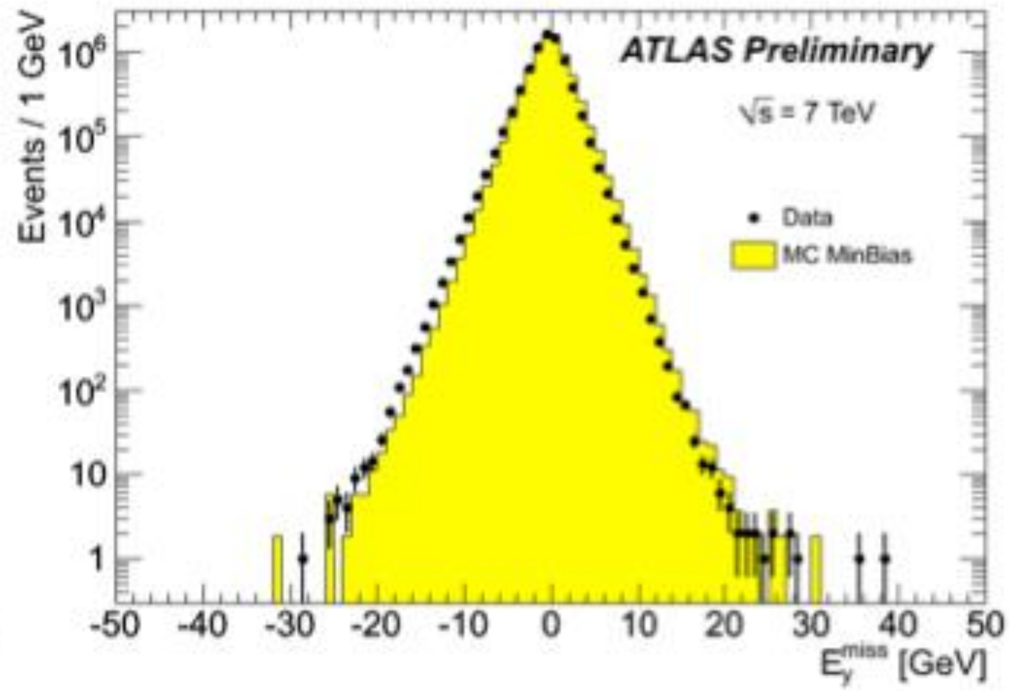




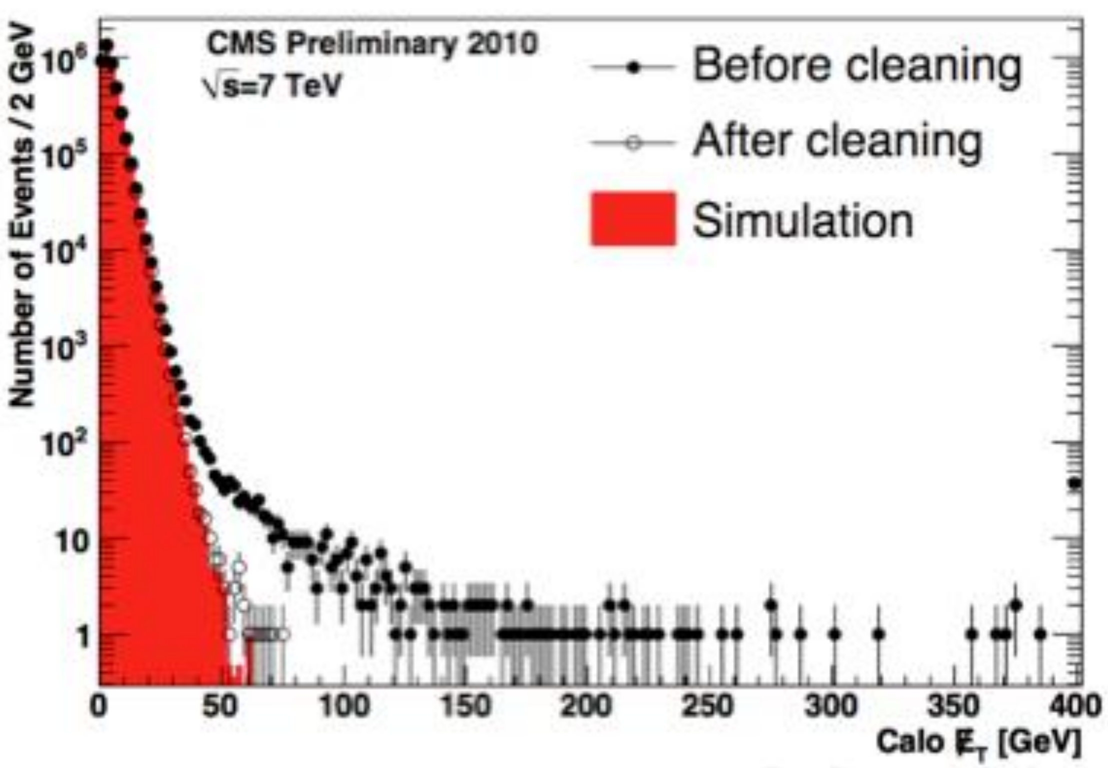
Figures from CMS

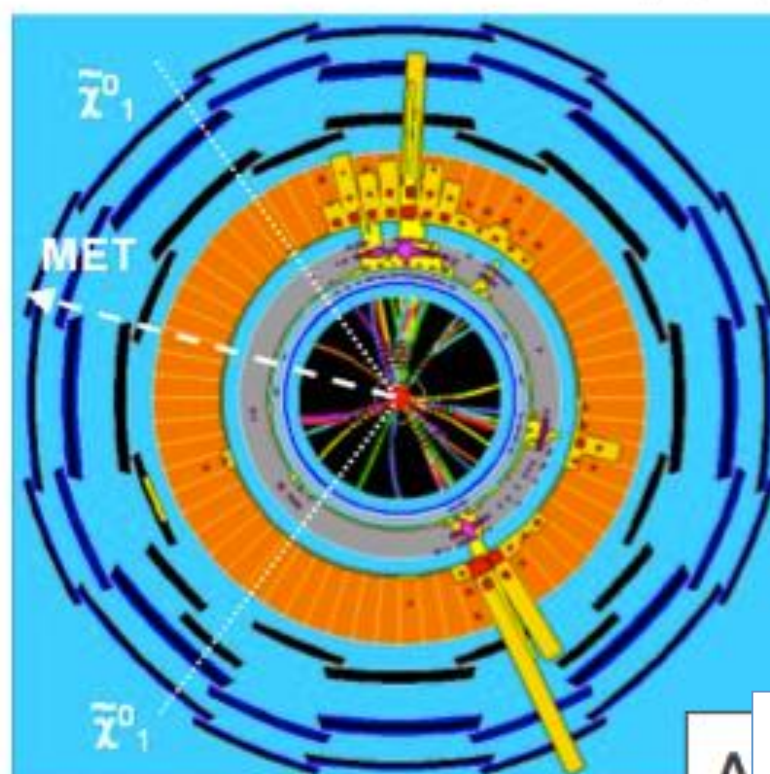
Missing E_T





This is one of the hardest things to get right. MET incorporates everything measured in the detector and attempts to identify non-interacting particles, such as neutrinos or dark matter.





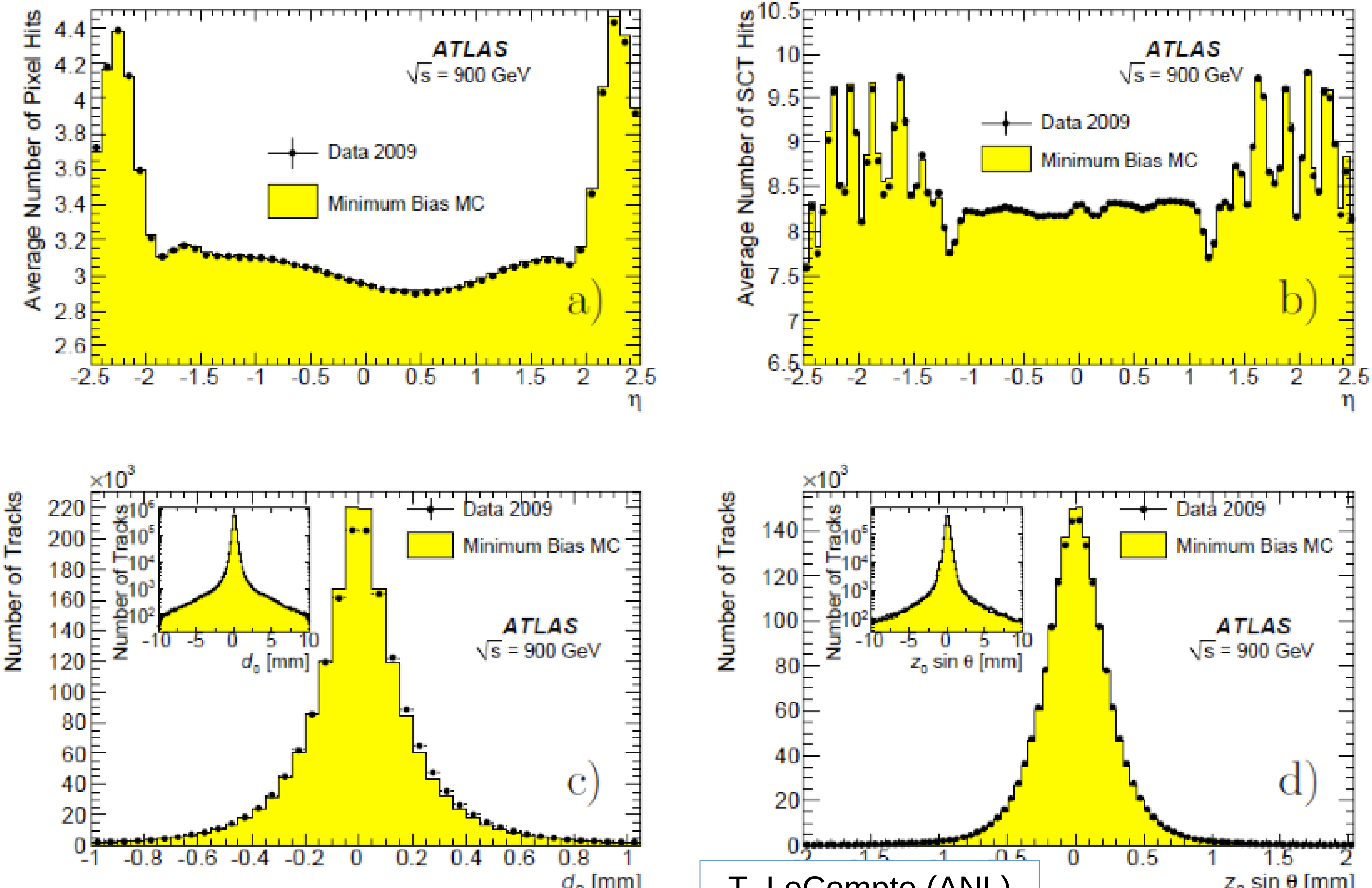
Agreement is astounding.

You can even see that the ATLAS detector is not quite centered – in both data and MC.

T. LeCompte (ANL)

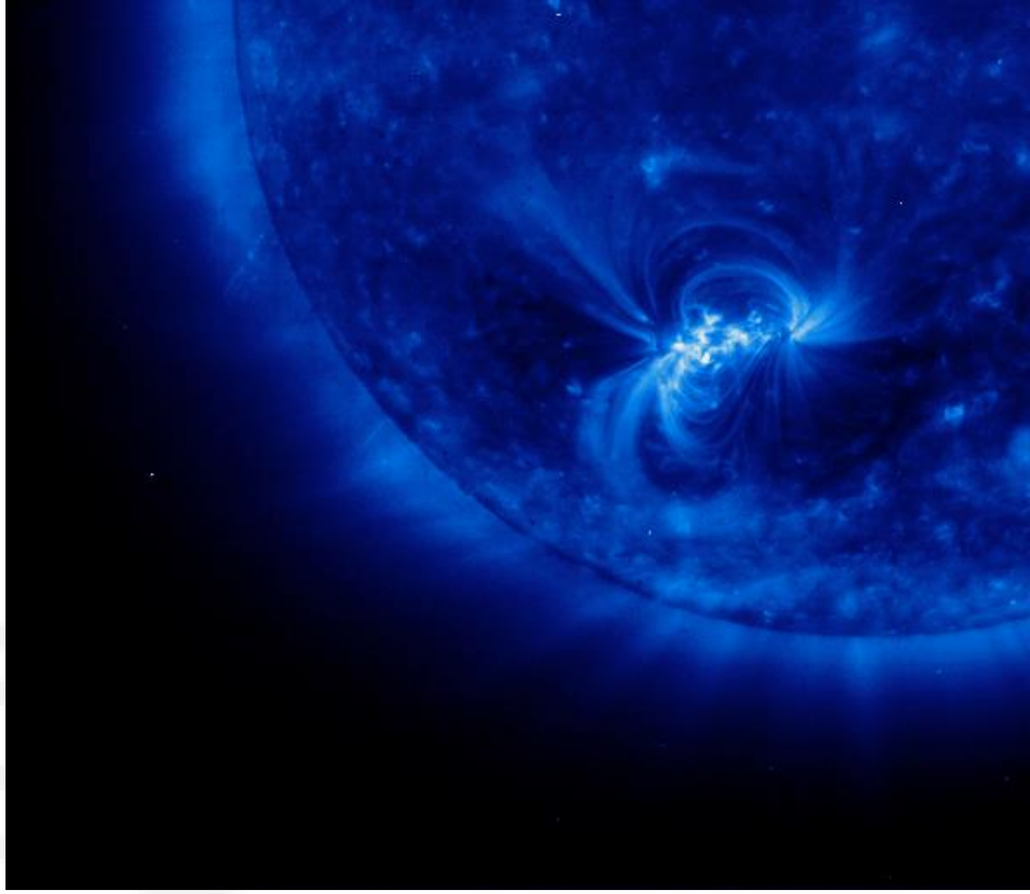
Both ATLAS and CMS plots are made from a tiny piece of the very earliest data.

Data and simulation agreements



T. LeCompte (ANL)

Solar event gamma-rays

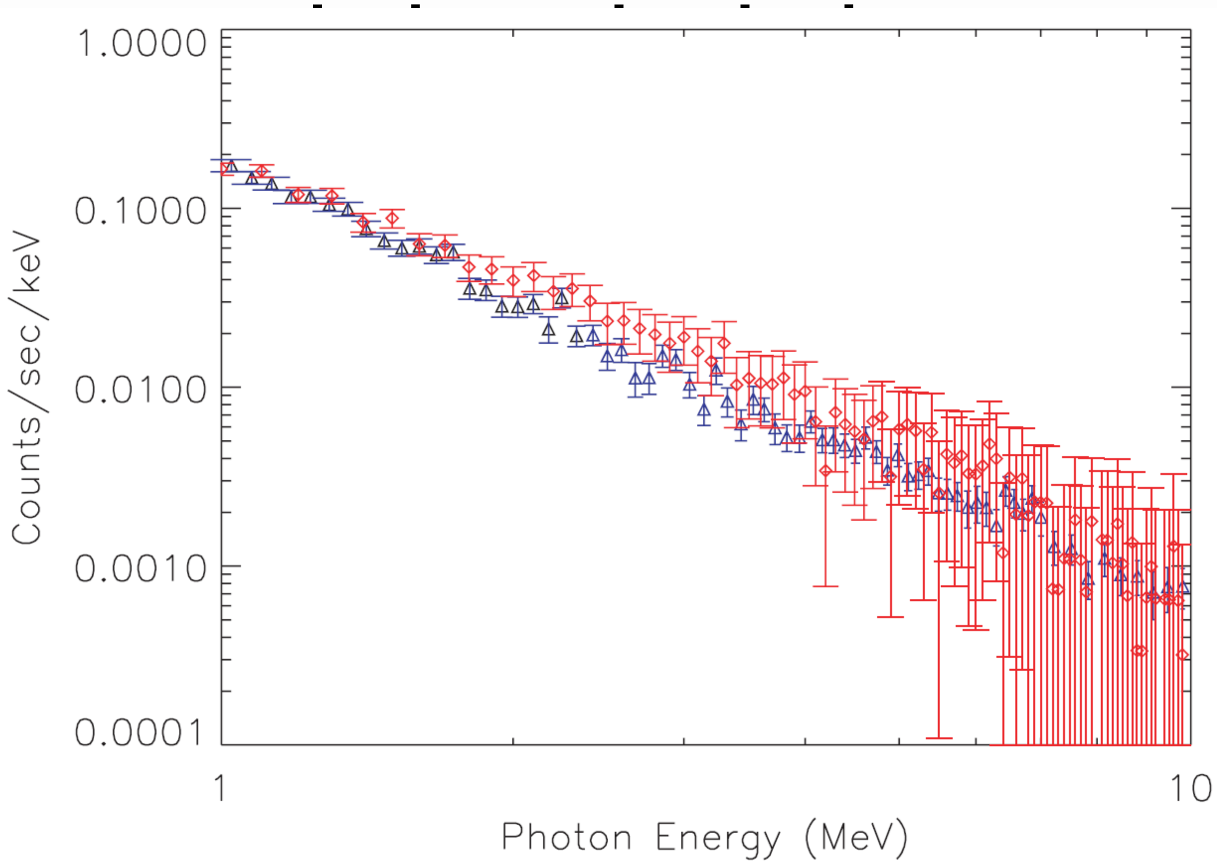


- Electron Bremsstrahlung – induced gammas in solar flares
- Compton back-scattering

  → observable gamma-ray spectrum

  much softer than predicte

  simple



Effects of Compton scattering on the Gamma Ray Spectra of Solar flares

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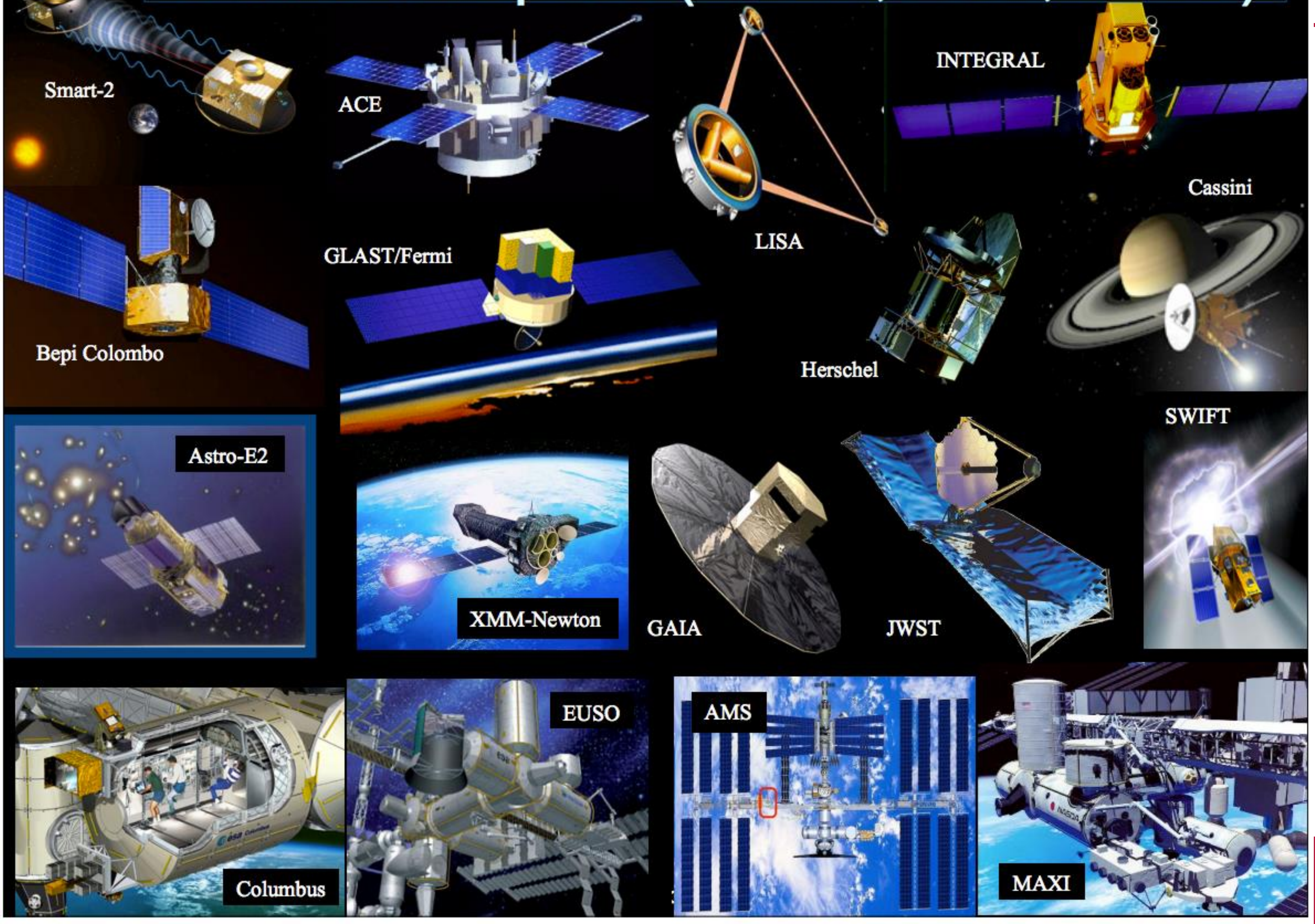
(Received ; accepted)

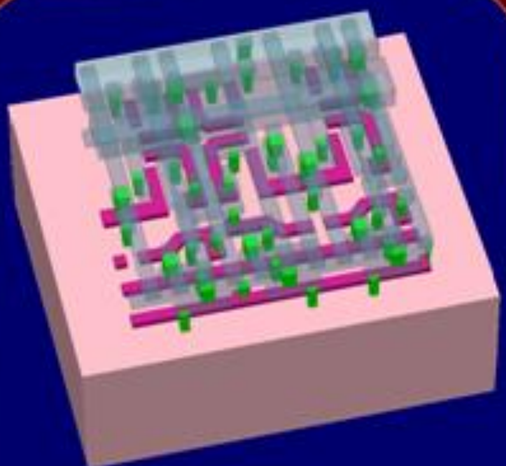
Abstract

Using fully relativistic GEANT4 simulation tool kit, the transport of energetic electrons generated in solar flares was Monte-Carlo simulated, and resultant bremsstrahlung gamma-ray spectra were calculated. The solar atmosphere was ap-

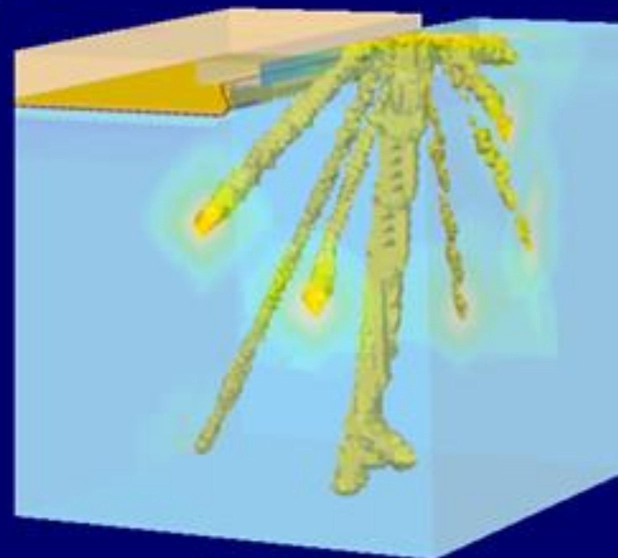
Geant4 in Space (NASA, ESA, JAXA)



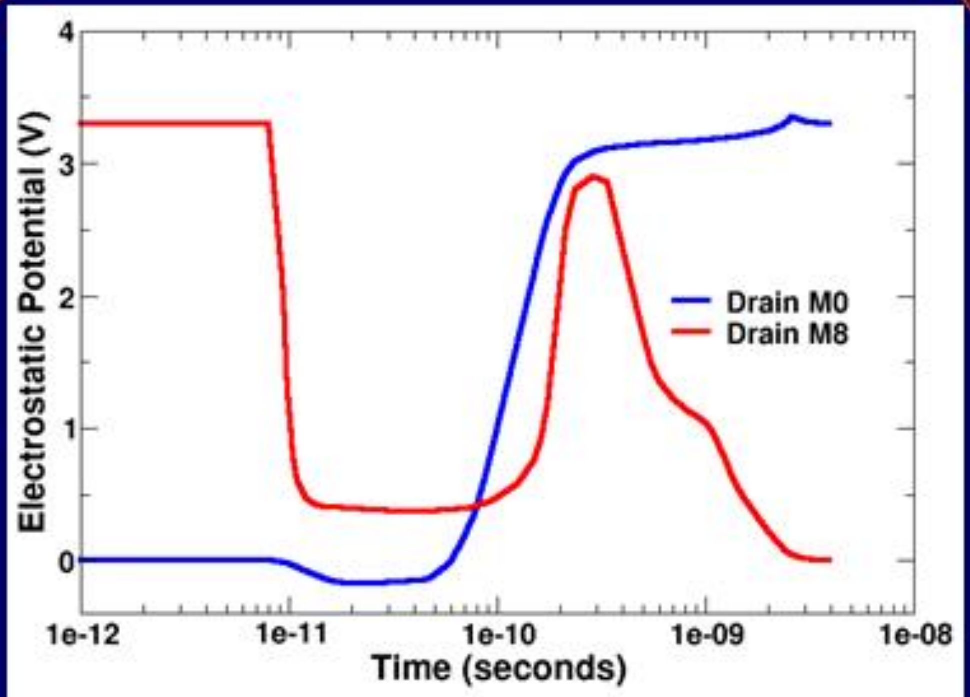
RADSAFE on SEE in SRAMs



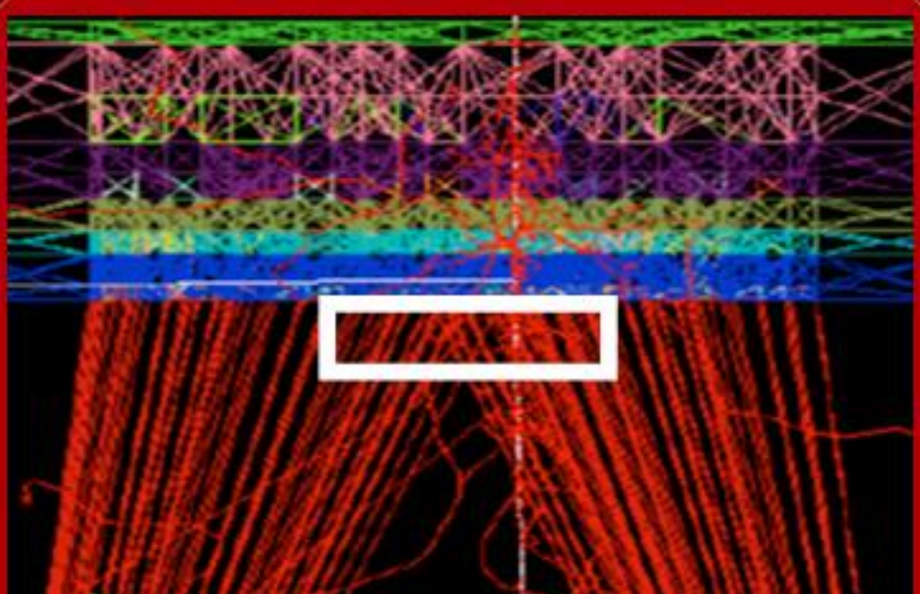
TCAD Cell Structure: SRAM Cell



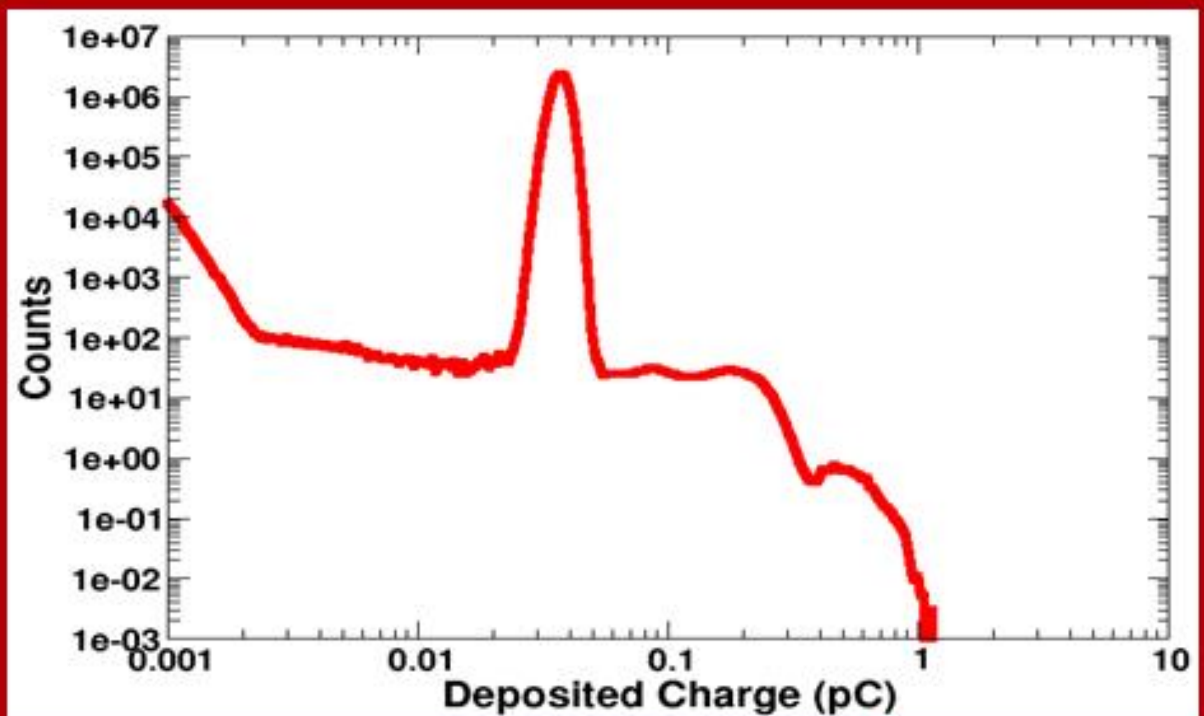
Single Charge Deposition in TCAD: Ne+W Event



SRAM Cell Upset



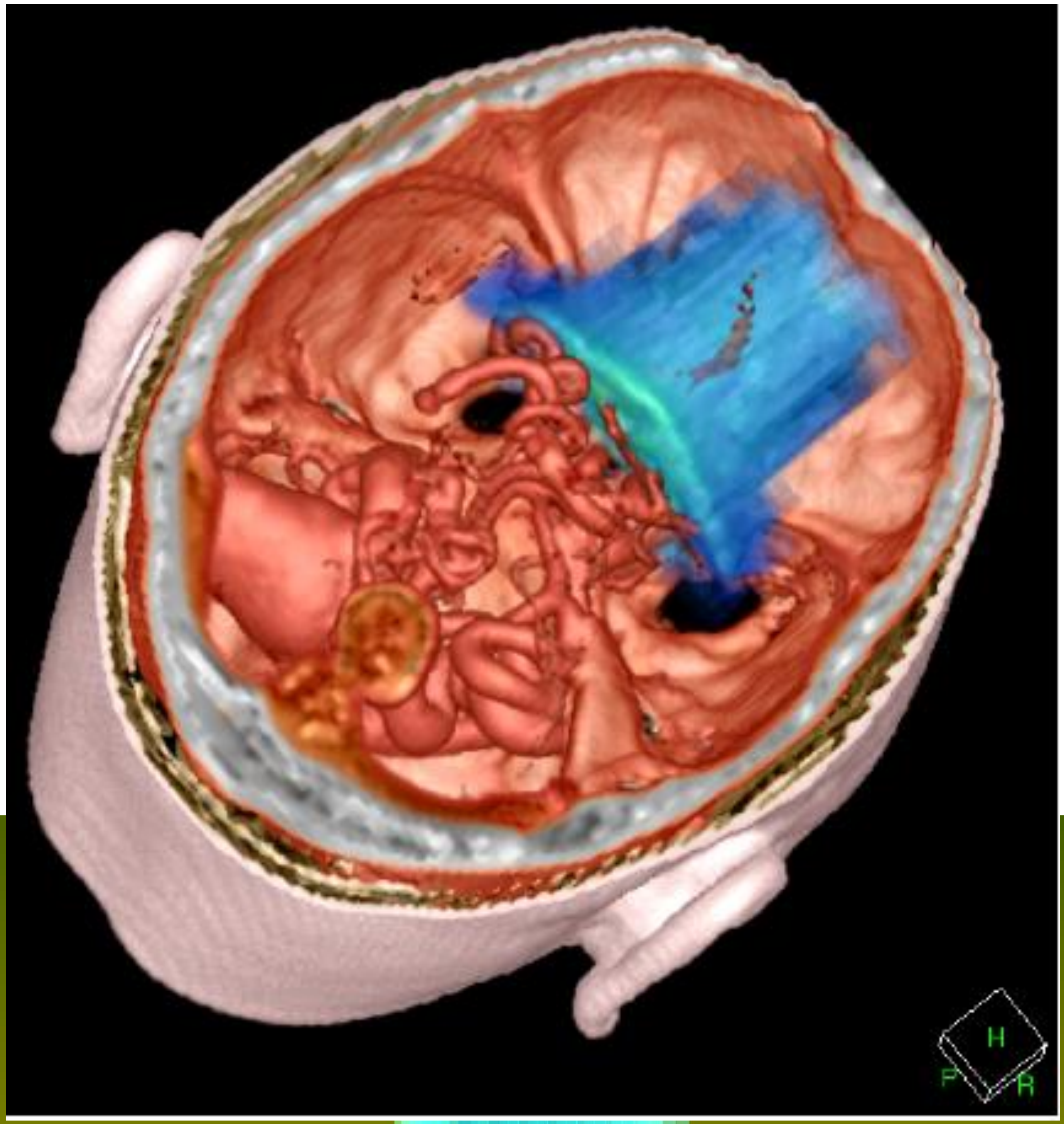
Geant4 Geometry and 523 MeV Neon Event

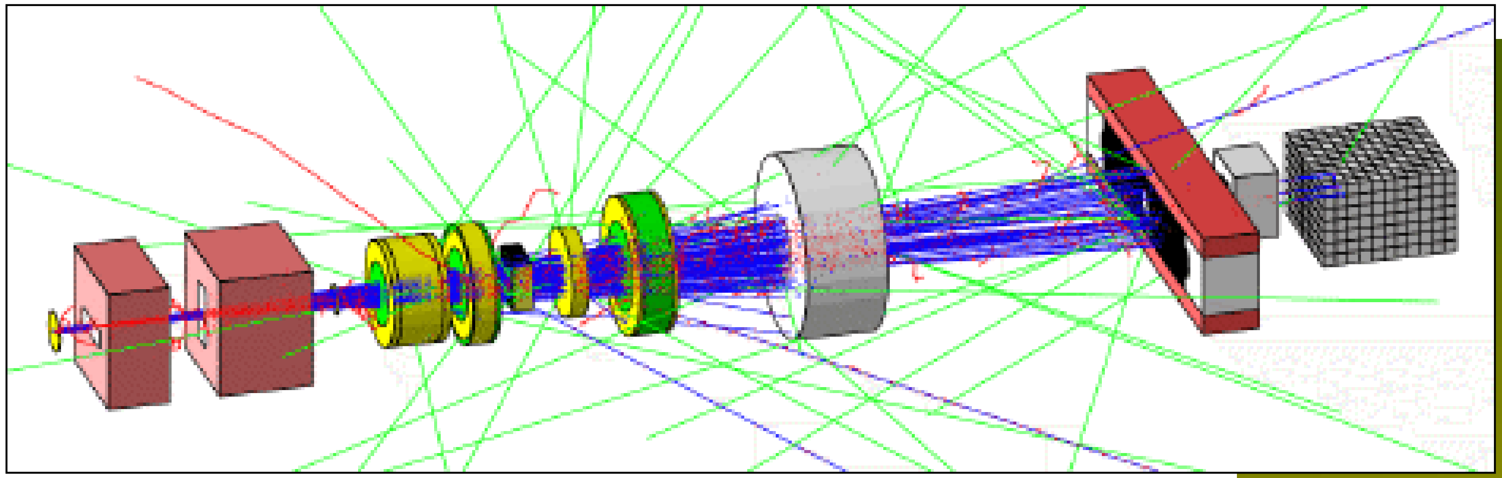


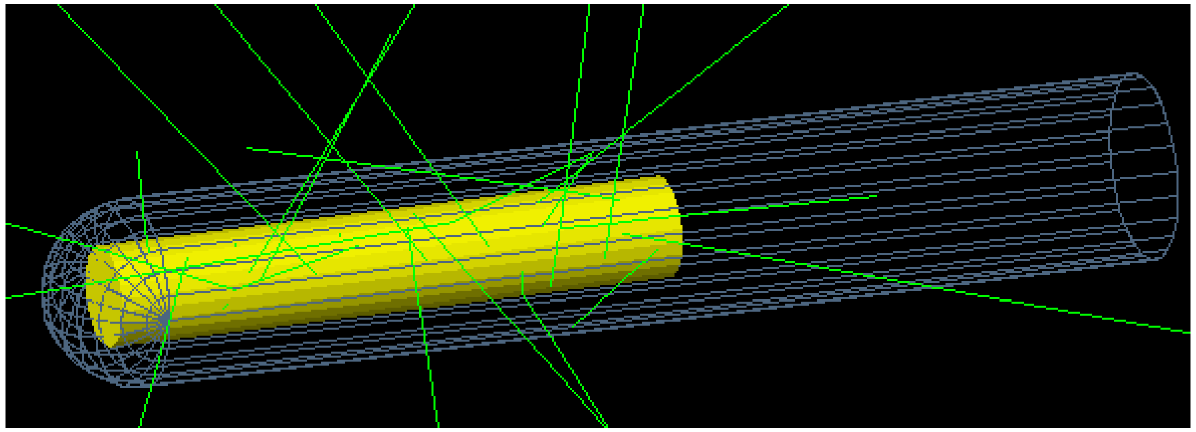
MRED Energy Deposition for 10^8 Events

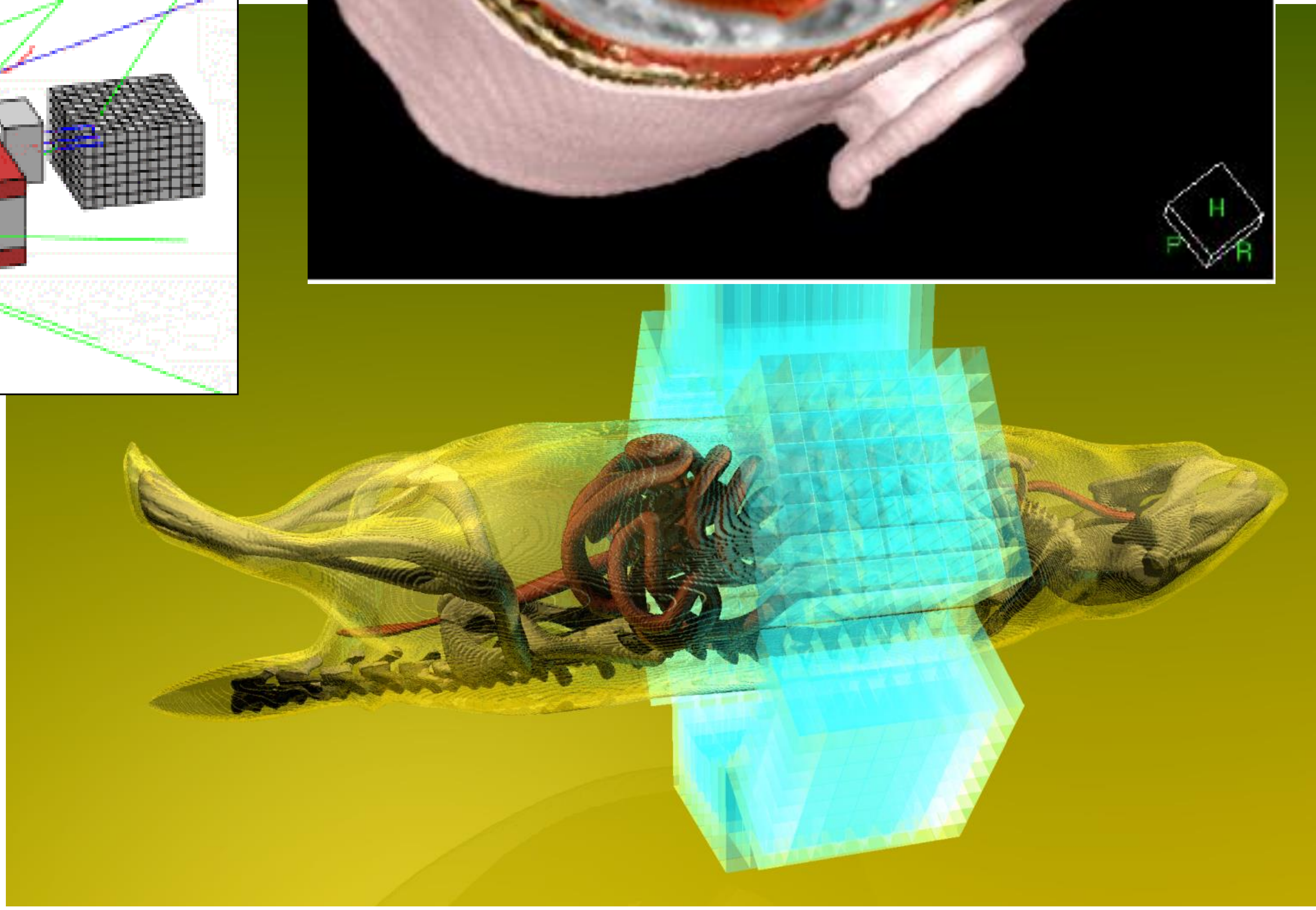
Geant4 @ Medical Science

- Four major use cases
  - Beam therapy
  - Brachytherapy
  - Imaging









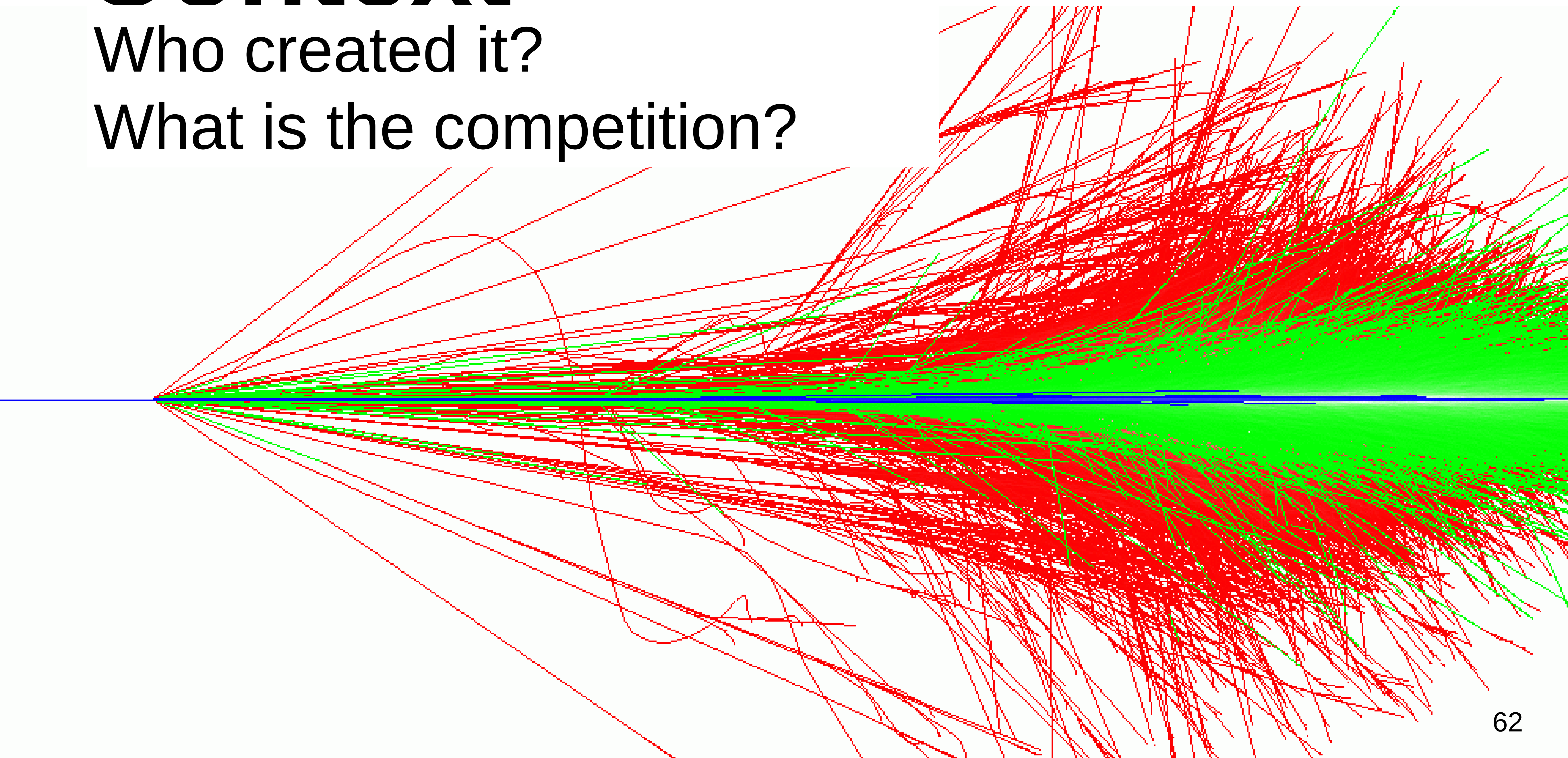
Medical Physic

- Geant4 is used to calculate doses
- but also to design imaging devices (PET, gamma cameras)
- Geant4 is used to validate results obtained with software (fast calculations) to plan therapies
  - Interesting future direction: hadron beams for cancer therapy (C^{12}, p beams)
- Need very precise low energy (keV-MeV) em physics description (at the opposite of the spectra with compared to HEP)

Context

Who created it?

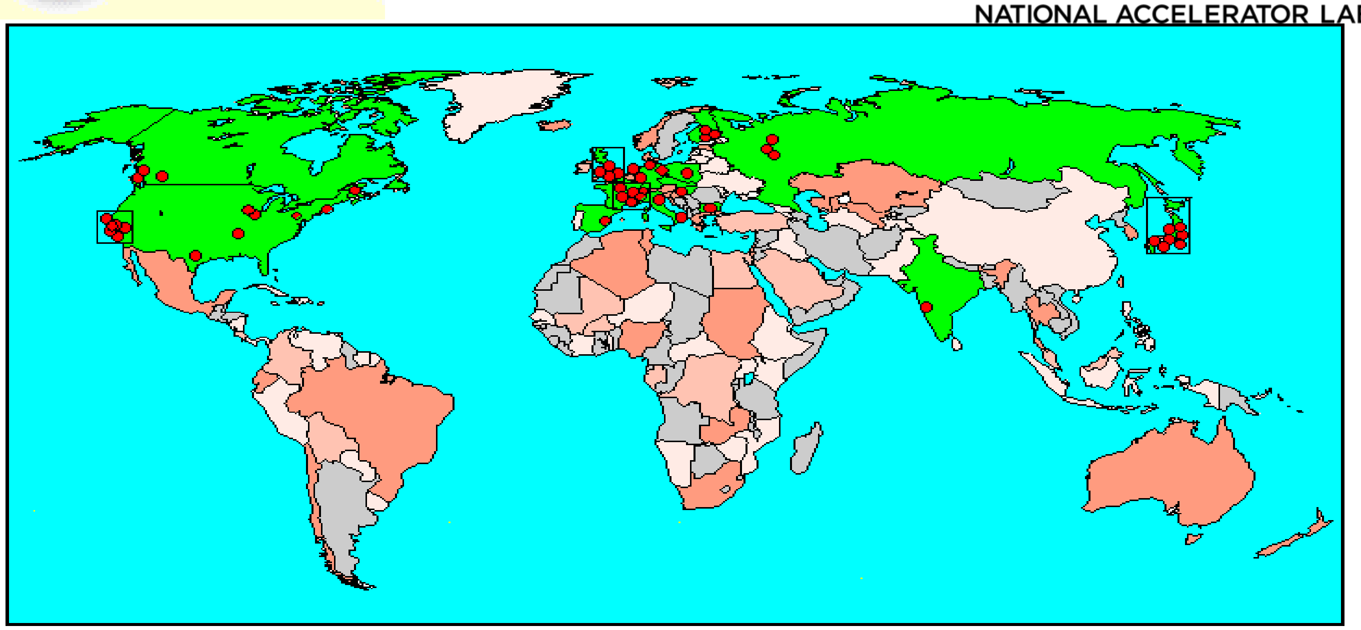
What is the competition?



Worldwide collaboration

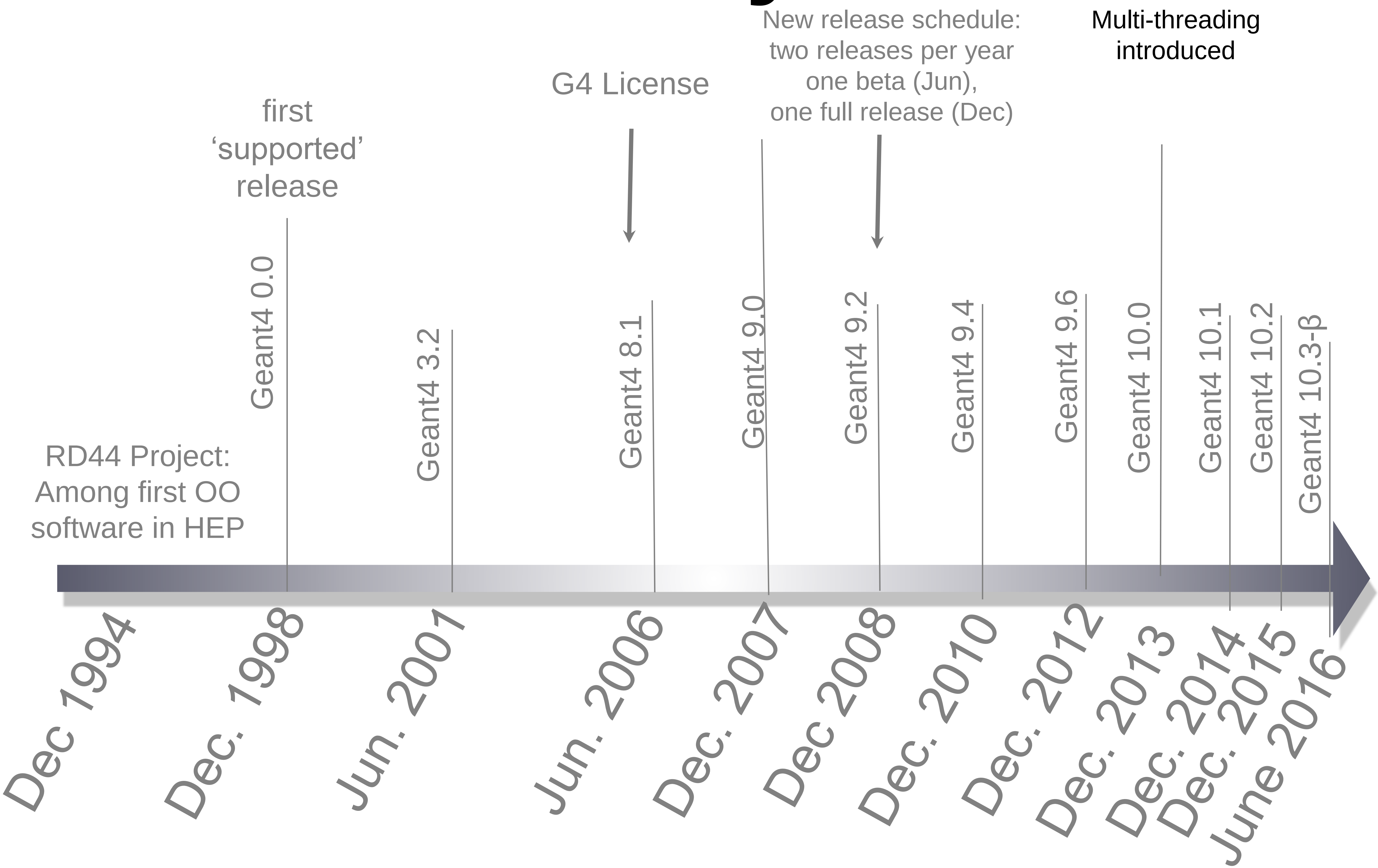
TRIUMF

Lebedev



Collaborators also from non-member institutions, including
IHEP
MEPHI Moscow
Jefferson Laboratory

A bit of history...



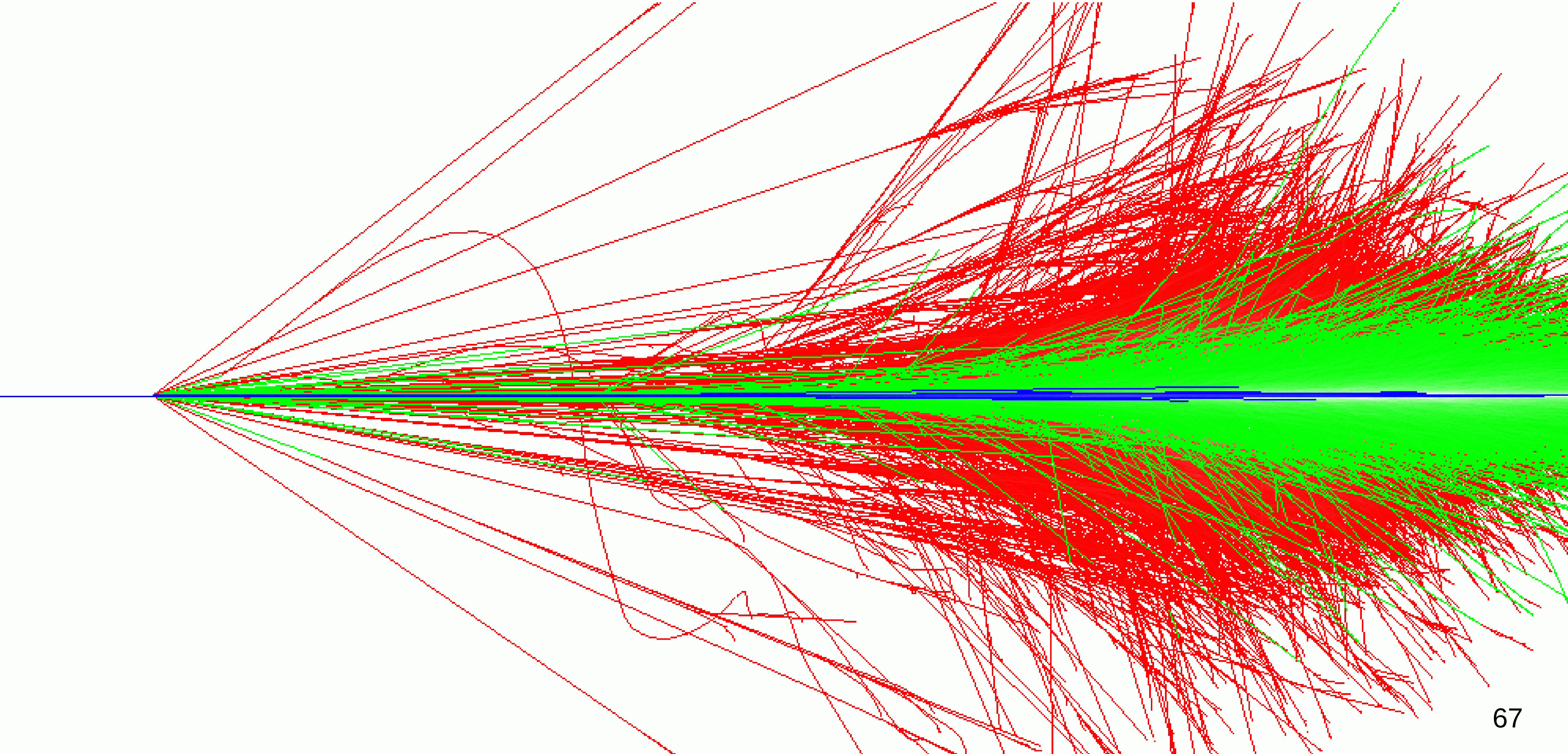
The competition

- A few other 'all-particle' transport tools
  - MCNP (and previously MCNPX) - neutrons/gammas, protons, ..
  - FLUKA (INFN/CERN) - used for shielding, accelerator studies
- Many specialized tools
  - e-/e+/γ simulation (typically at lower energies)
    - Penelope: strong low-energy models
    - EGS4nrc: established precision for medical applications
  - Hadronic shower: MARS, SHIELD
  - Ion simulation: HETC
  - Reactor simulation tools

Comparison

- Each tool has its strengths and weaknesses
  - I will give a personal perspective on those of Geant4
- Geant4 has many advantages
  - the most capable geometry engine
  - ability to check the source code (open source)
  - many tools built on top of it
  - very wide user base in many different application domains
- And some challenges:
  - choosing physics engine (‘list’) and ensuring its validation
  - choosing how to build an application
  - the wide user base means the support effort/load is high.

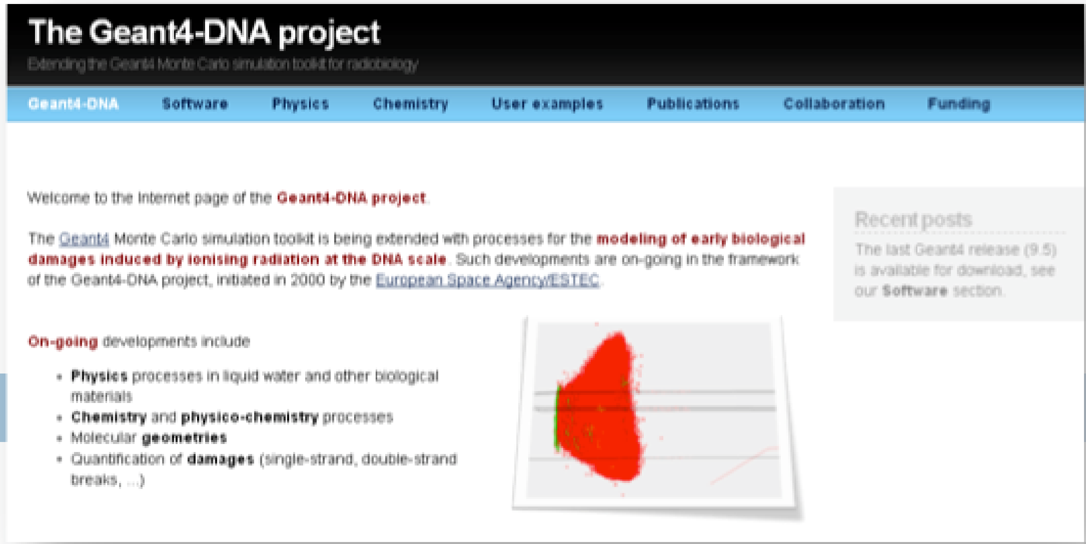
Recent developments & future directions



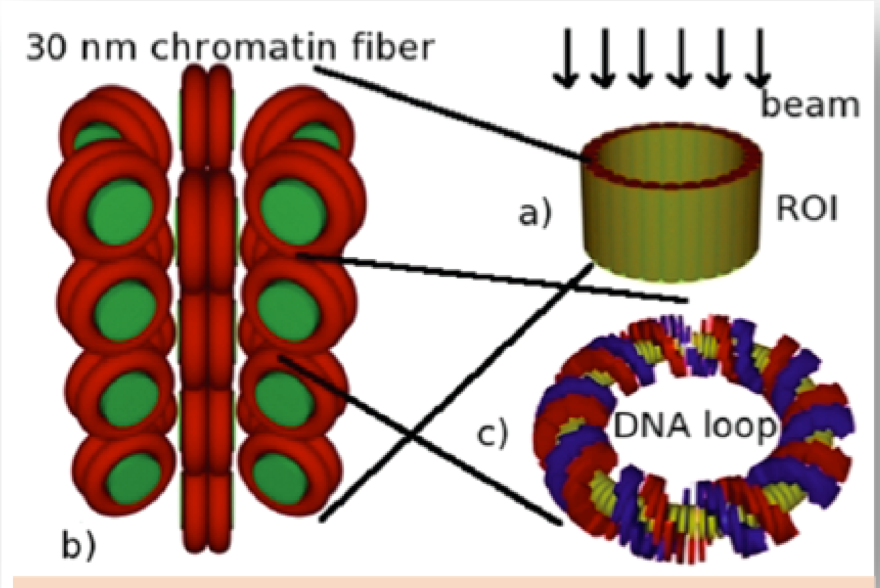
The Geant4-DNA project

http://geant4-dna.org

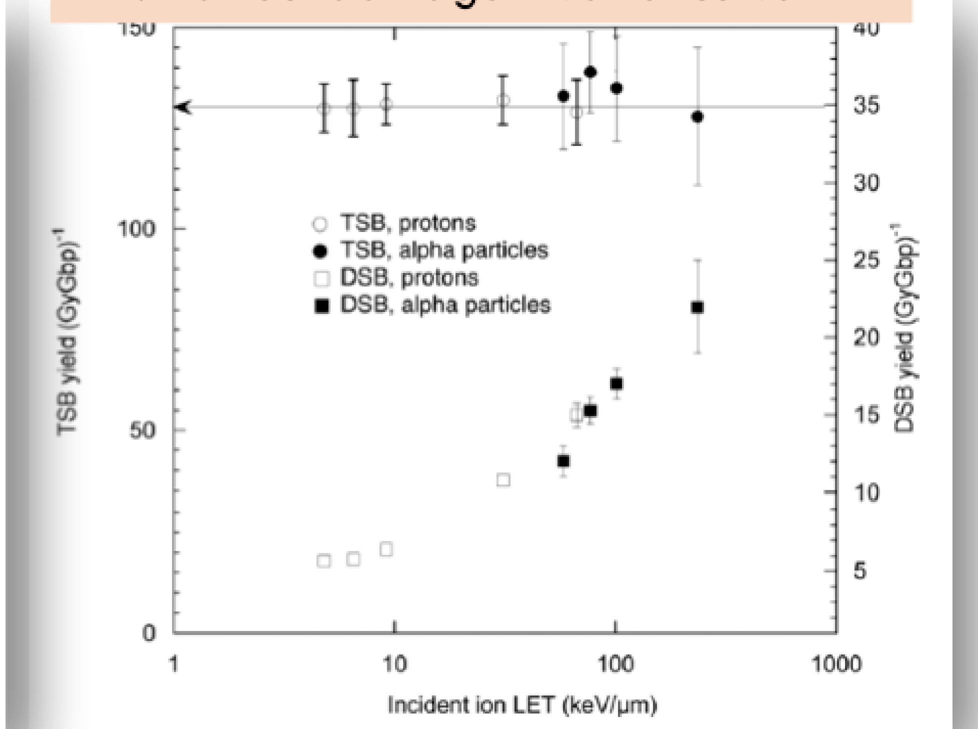
1



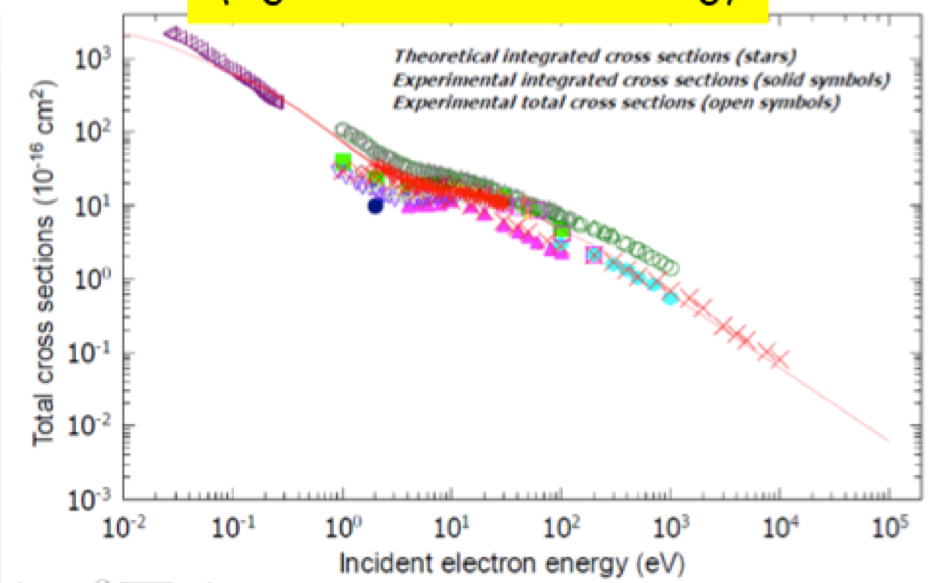
- Initiated in 2001 by the European Space Agency
- Purpose
  - extend Geant4 capabilities for the modelling of early DNA damages from ionising radiation in biological cells
  - including physical and physico-chemistry processes
    - water radiolysis
  - down to the eV and nanometer scales
- Status
  - A full component of the Geant4 toolkit



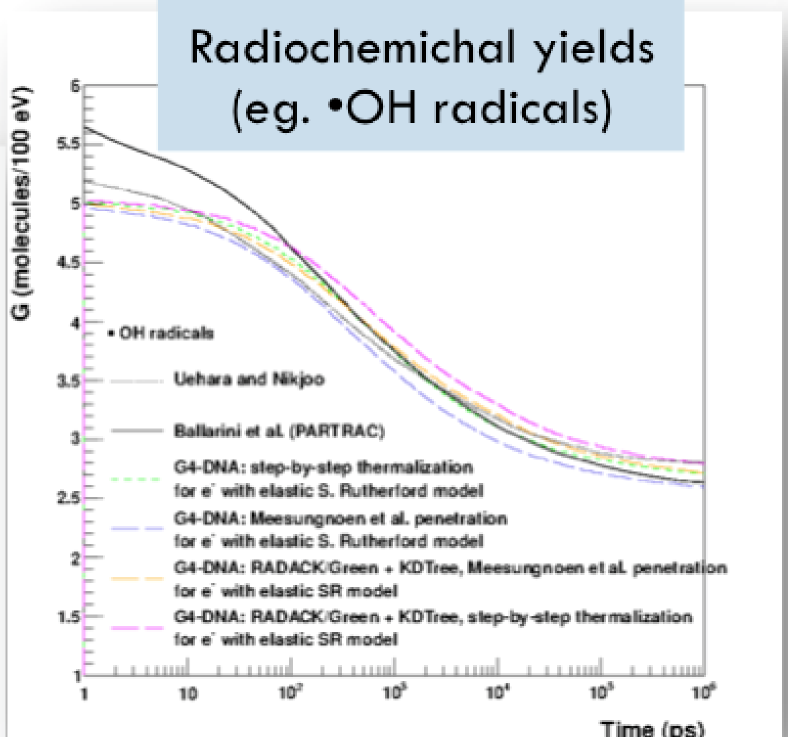
DNA direct damage invariance vs LET



Accurate physics models (eg. e- elastic scattering)



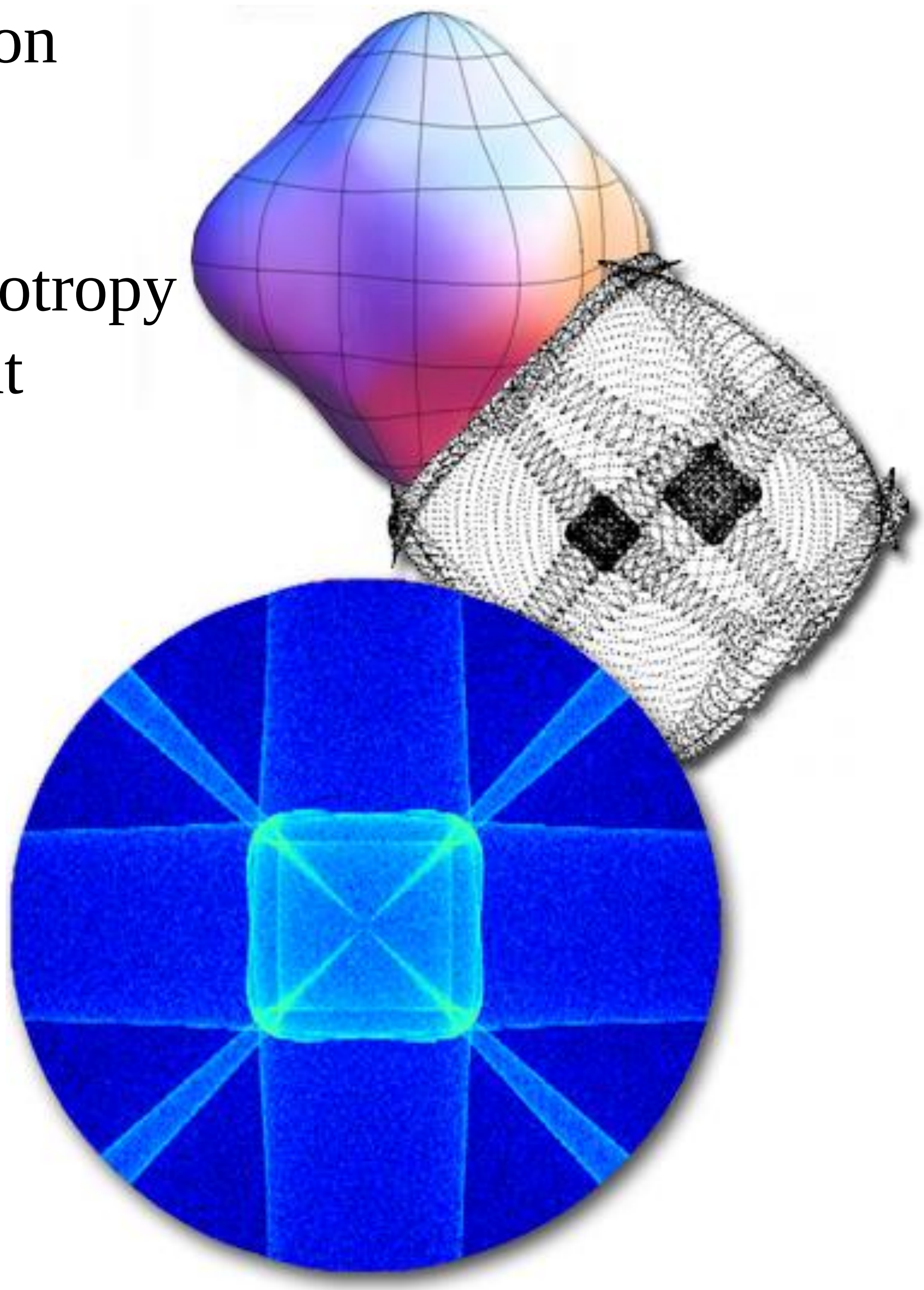
Radiochemichal yields (eg. •OH radicals)

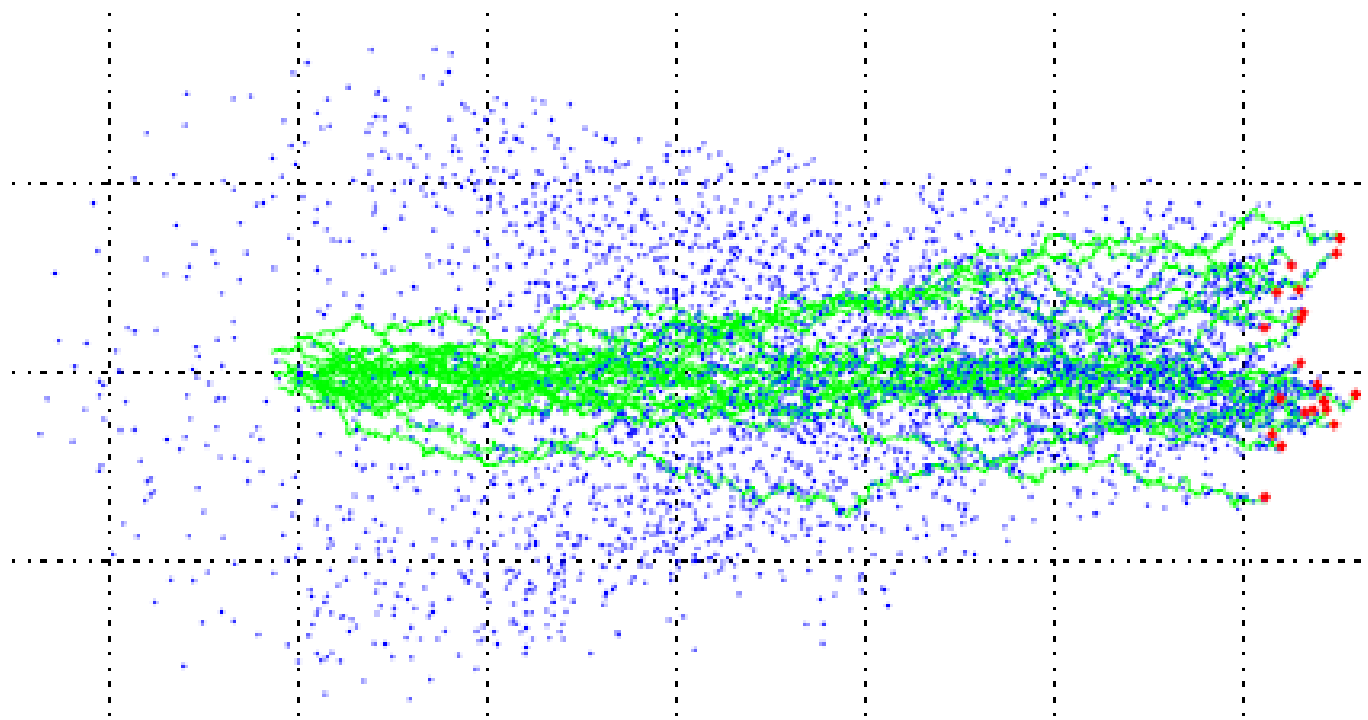


Condensed Matter Physics in Geant4

- Phonon propagation, including focusing based on elasticity tensor (right)

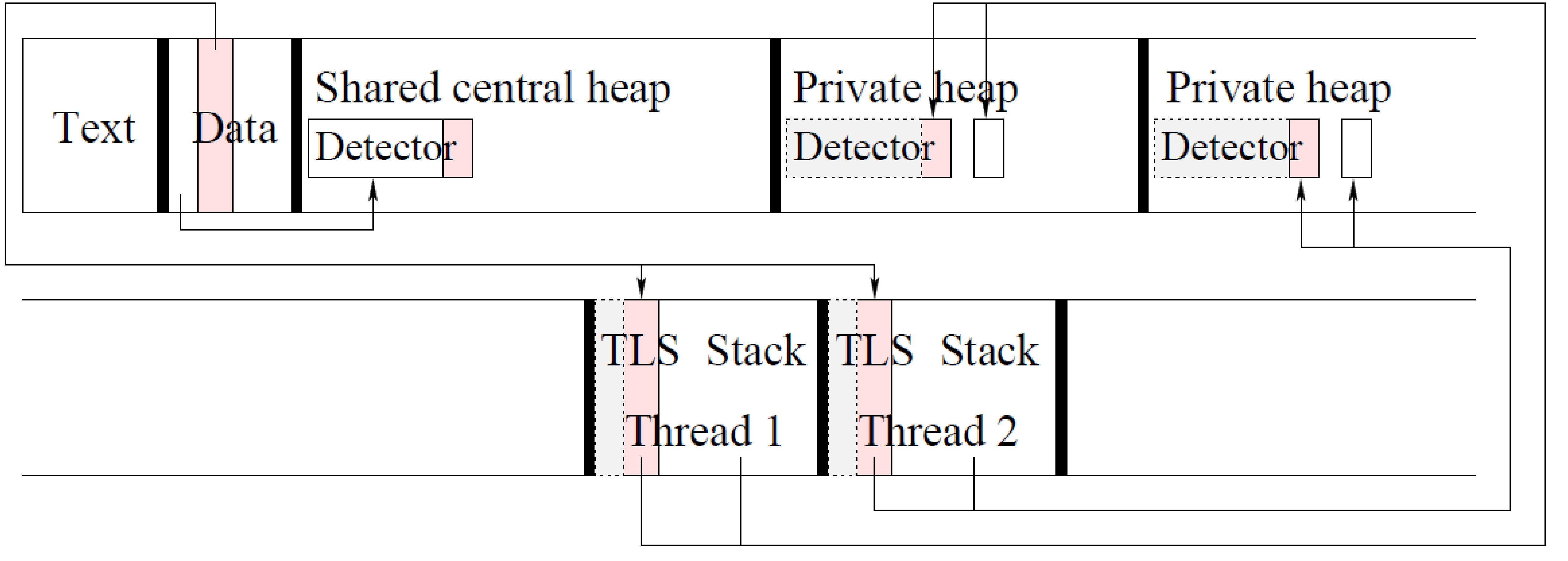
- e-/h+ transport, including conduction band anisotropy and Luke-Neganov emission, under development (below)

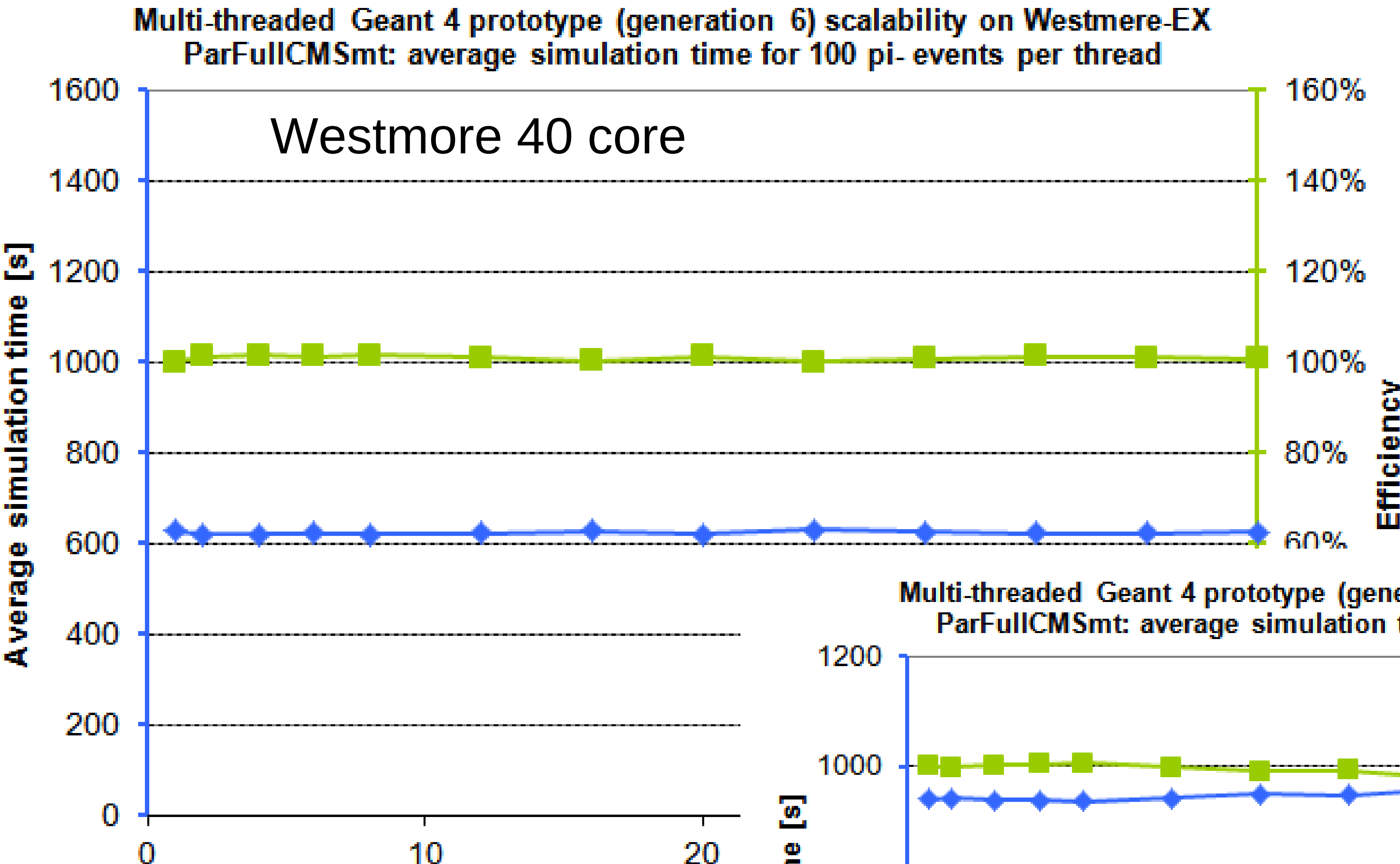




Multi-threaded Geant4

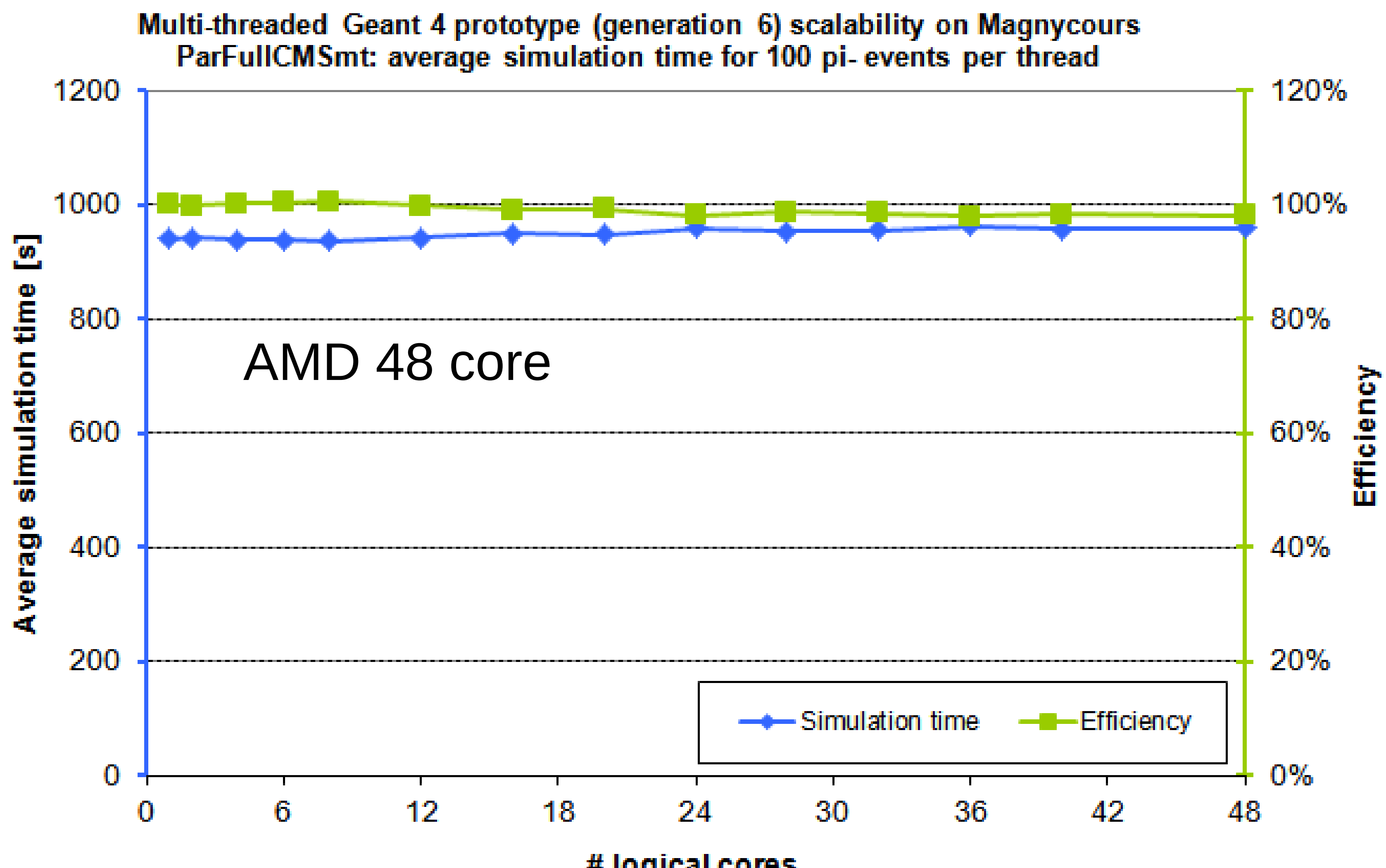
- Offers event-level parallelism within one job with many threads.
- Uses the many-core machine in a memory-efficient scalable manner.
- Shares “relatively read-only data” among threads for memory footprint reduction.
  - Relatively read-only data : data written at initialization phase but kept unchanged during the event loop
- Allocates thread-local heap for transient objects.
  - Full-CMS benchmark showed only 25MB of memory per thread.





Courtesy of Andrzej Nowak (OpenLab)

Note: scaling was still perfect with using 80 threads on Westmore (2 threads per core).
Note: G4MT shows perfect scalability for Intel MIC prototype as well.



Even more performance

- Some applications want 10x speedup
  - Medical & HEP applications need more events per CPU or $
- Explored adapting Geant4 for GPUs
  - Challenging, but successful for ‘narrow’ application areas (typically medical phantoms), observable & beam/source type (limited physics)
- One project is restarting from scratch - GeantV
  - This ‘vector’ prototype targets today’s CPUs & GPUs
  - Aims to greatly improve cache use & leverage vector instructions
  - A number of improvements created already (VecGeom, better Multiple scattering) are/will be fed back to Geant4