Simulation with Geant4

Владимир Иванченко

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Outline

- Monte Carlo method
- The Geant4 toolkit
- Geant4 kernel
- Geant4 physics
- Geant4 electro-magnetic (EM) physics
- Geant4 hadronic physics
- Geant4 Physics Lists
- How to start and how get help?

Если кто-то думает, что Метод зародился в Монте Карло, то глубоко заблуждается

First application of the Monte Carlo: obtaining value of π (Laplace)

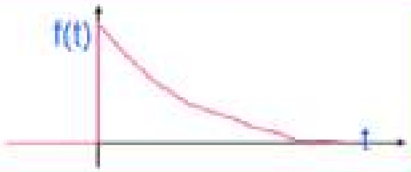
- Let as take a circle with radius R=1
- Let us use random number generator providing a sequence of random numbers in interval (0,1)
  - N – number of pairs of random numbers
  - Two random numbers p and q defines a point
    - (x, y) = (p*2-1, q*2-1)
  - K – number of points with radius < 1
  - The surface of such circle is π
  - The surface of a squared is 4
- As a result, we obtain value π = 4*K/N
  - The statistical uncertainty of the method:
  - $4/\mathrm{N} * \sqrt{(K * (N - K)/N}$

Простейшая задача для метода Монте Карло – распад нестабильной частицы

- Suppose an unstable particle of life time t has initial momentum p (→ velocity v).
  - Distance to travel before decay : d = t v
- The decay 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



- the probability that the particle decays at time t is given by the cumulative distribution function F which is itself is a random variable with uniform probability on [0,1]

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

- Thus, having a uniformly distributed random number r on [0,1], one can sample the value t with the probability density function f(t).

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

What is a particle transport code?

- It is a way to estimate the effects of radiation in a particular region. Given
  - a radiation source or beam,
  - a model of the geometry of a setup or detector
  - a volume or region in which to measure
- The simplest type of task is to estimate
  - Energy deposition in volume (e- displaced) and its variance
  - Dose / volume - weighted by its biological effect
  - Fluxes, e.g. of neutrons (=> nuclear reactions) in a particular region

  and similar 'first order' observable (with estimated errors.)
- It can also estimate complicated observables:
  - distributions of energy deposition, dose, .. Including width
  - correlations between observables or derived quantities - e.g. coincidence of gammas (PET)

Courtesy of GATE

Courtesy of R. Reid, Vanderbilt Univ.

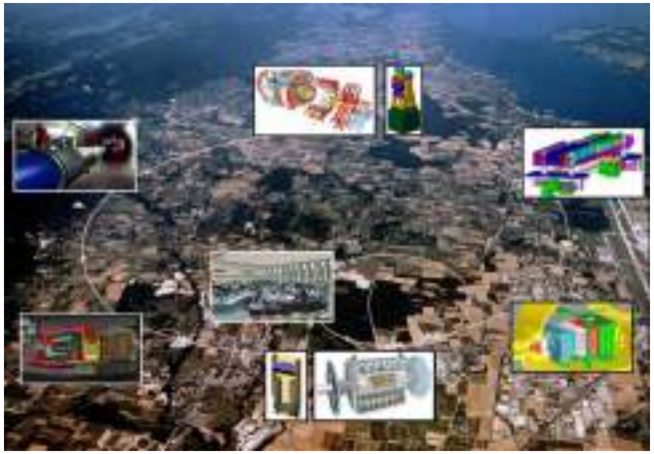
Пакет программ Geant4

Основные принципы Geant4

- In high energy physics a substantial experience in Monte Carlo methods were achieved and many concerns to old codes were accumulated:
  - Non-transparent algorithms
  - Tuning of simulation per each concrete experiment
  - Technical difficulties to extend existing codes for higher energies and new models
    - Problems in HEP with Geant3 extensions and FLUKA
- For preparation of experiments at LHC CERN started R&D project (1994)
  - Experts from different countries joined
  - They agreed to create the Geant4 toolkit
- As a result of start of the R&D it was decided
  - To use object-oriented style of programming
  - To adopt programming in C++
  - Make it open source
  - Do not tune physics model parameters to the data of complex experiments
  - Tune only for publish data for thin target experiments
- Later the Geant4 Collaboration was established

Этапы развития пакета программ

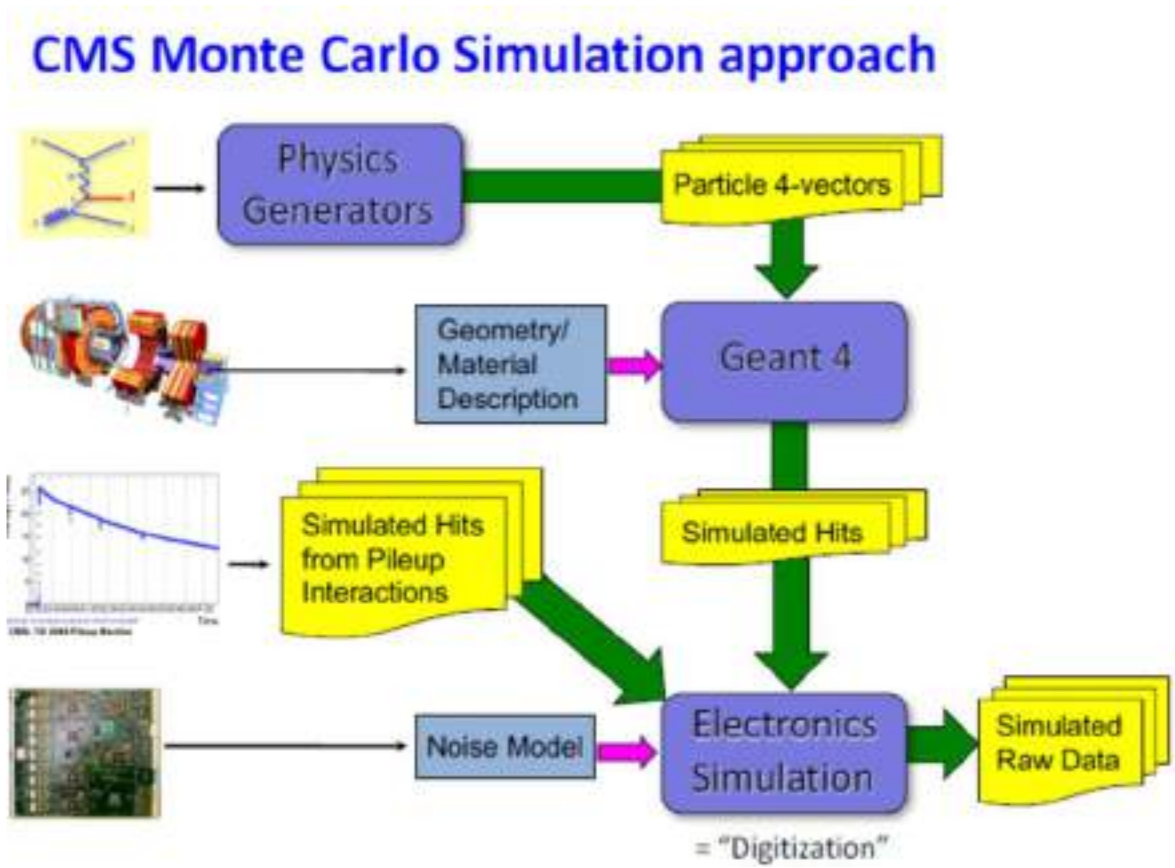
- Geant4 History
  - Early discussions at CHEP 1994 @ San Francisco CERN & Japan seeded R&D proposal
  - Dec ’94 –R&D project start
  - Dec ’98 -First Geant4 public release -version 0.0
  - …..
  - 2004: ATLAS, CMS, and LHCb start using Geant4 in production
  - Dec 2013 – version 10.0 – 1st with multi-threading
  - Dec 2020 - version 10.7 completed 10 series
  - Dec 2021 – Geant4 11.0 – start of the new series
  - Dec 2022 – Geant4 11.1 – recent public version
  - Dec 2023 – Geant4 11.2 is expected
- Main publications
  - Nucl. Instr. Meth. **A 506**, 250-303 (2003) – 15499 citations.
  - IEEE Trans. Nucl. Sci. **53**, 270-278 (2006) – 4094 citations.
  - Nucl. Instr. Meth. **A 835**, 186-225 (2016) – 1620 citations.
  - Med. Phys., **48**, 19-56 (2021) – 50 citations.



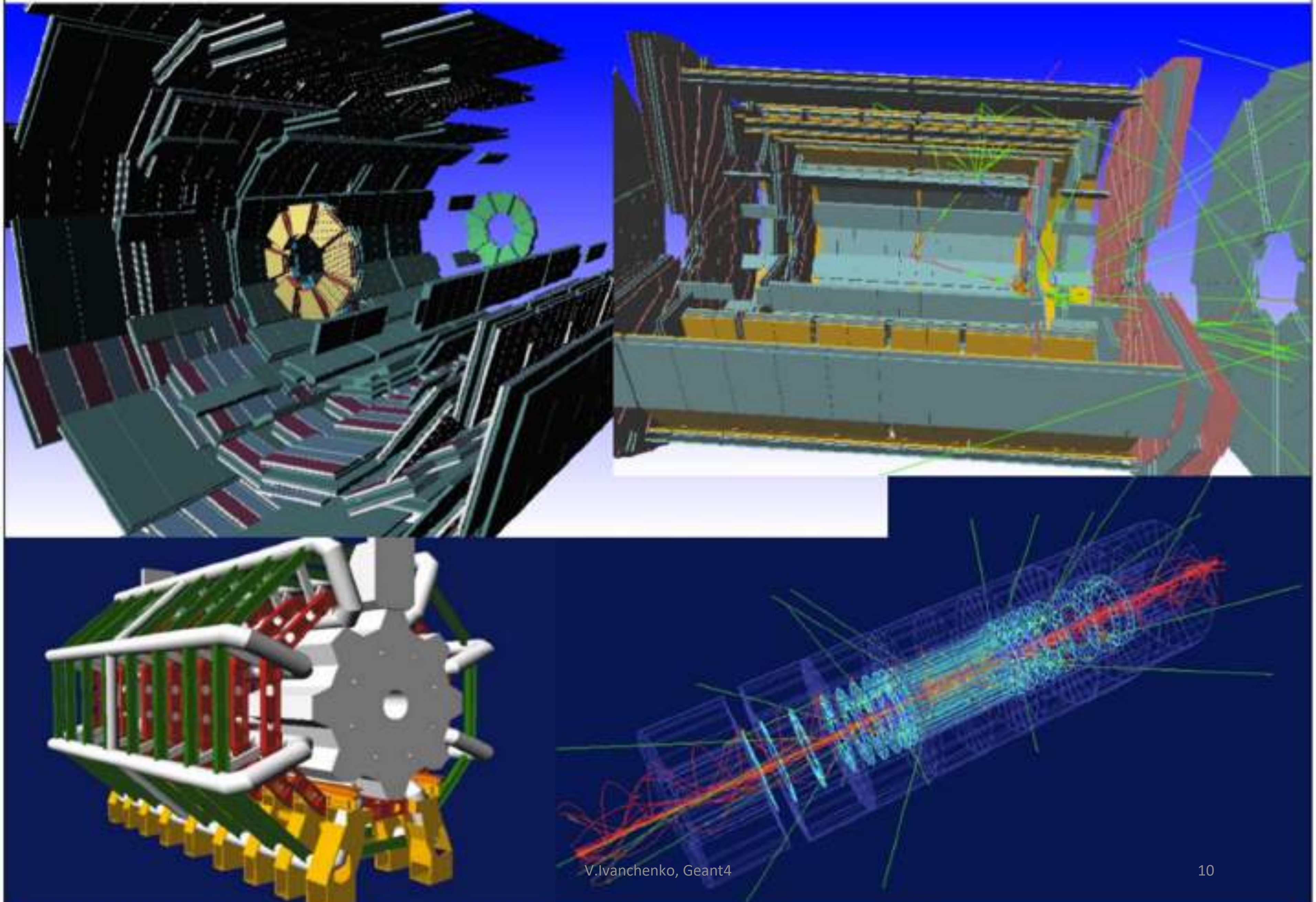
- Object oriented design and C++ allow to have a flexible code organisation
  - New components may be added without affecting other part of exiting code
  - User may be a developer
- Geant4 developments are strongly supported by HEP community
  - Support of the LHC experiments for the Geant4 Collaboration is the top priority
  - The new Run3 was started in 2022
- Requirements from other scientific domains are also considered
  - Space science
  - Radiation medicine
  - Nuclear physics

Geant4 for HEP experiments

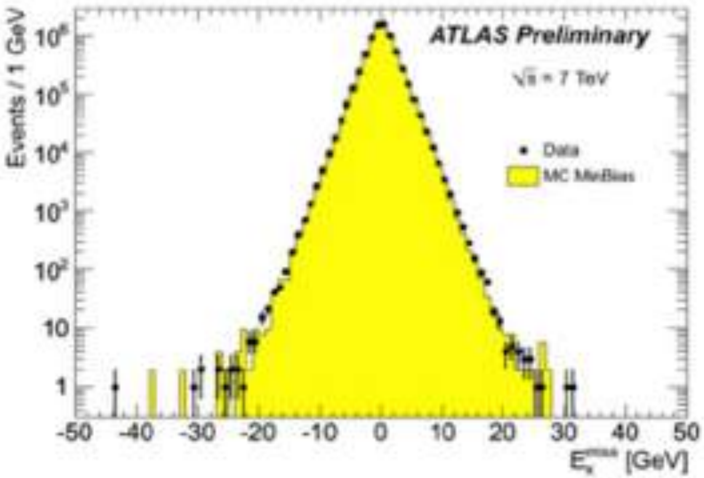
- Monte Carlo simulation of particle interaction in pp collision at LHC or collisions at other accelerators is performed by special Monte Carlo tools
  - For example, PHYTHIA
- Geant4 is responsible for Monte Carlo simulation of particle transport in experimental setup
  - Hits in detectors
- Simulation of electronics and pileup is performed by specialized user code
  - DIGI step

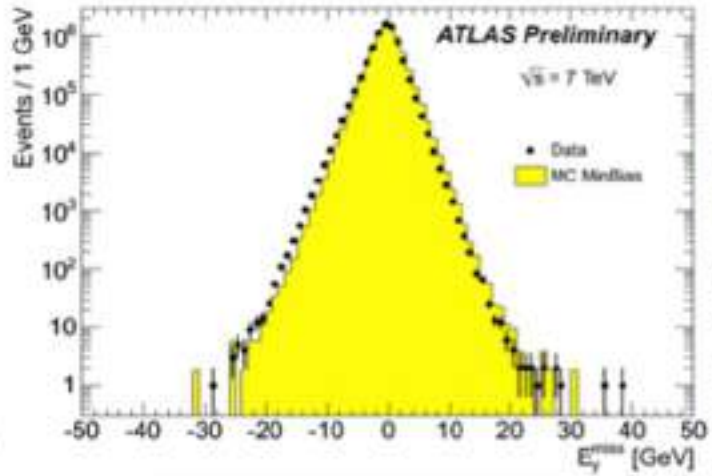


Geant4 in High Energy Physics (ATLAS at LHC)



Моделирование потерянной энергии

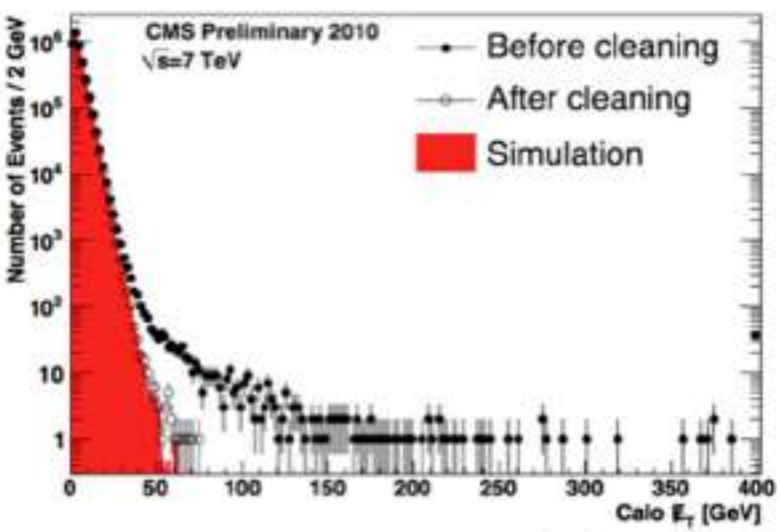


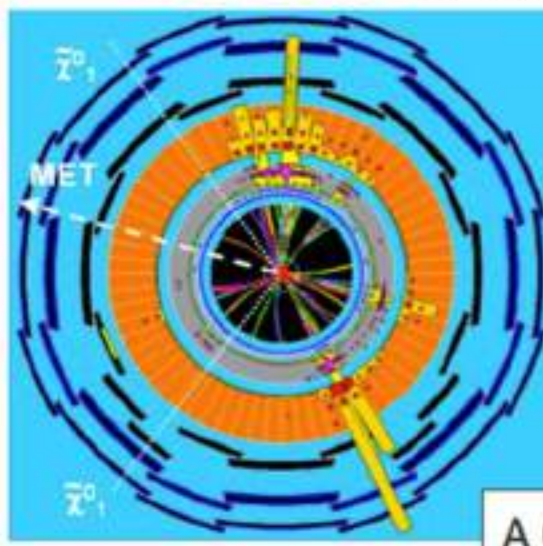


This is one of the hardest things to get right. MET incorporates everything measured in the detector and attempts to identify non-interacting particles, such as neutrinos or dark matter.

Agreement is astounding.

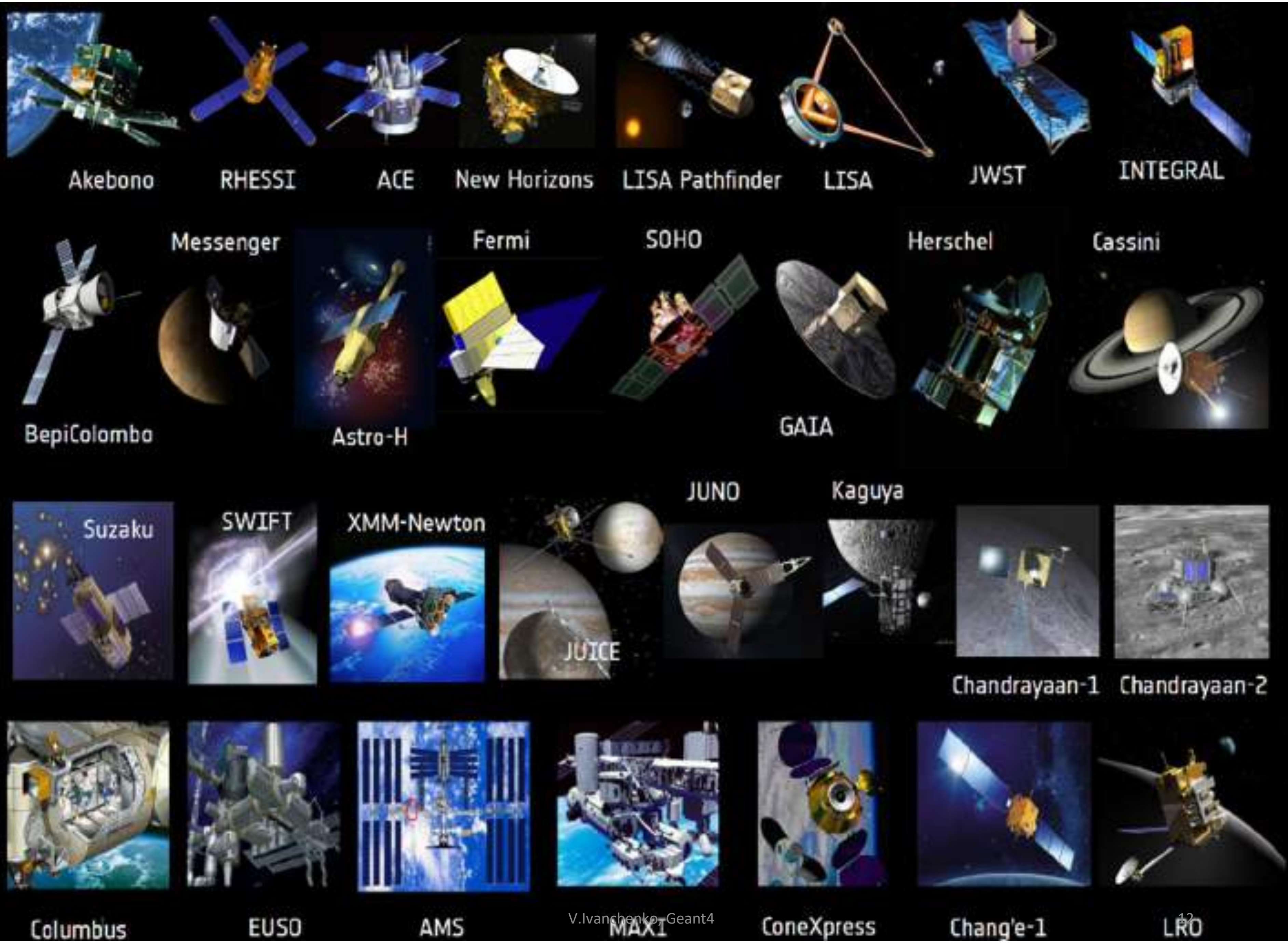
You can even see that the ATLAS detector is not quite centered – in both data and MC.





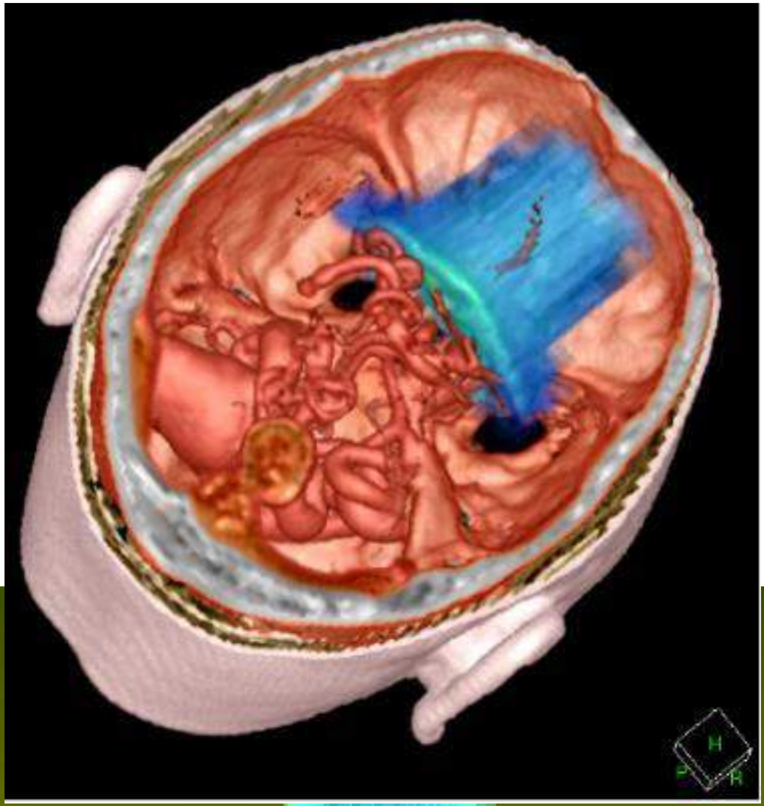
A GEANT4 event.

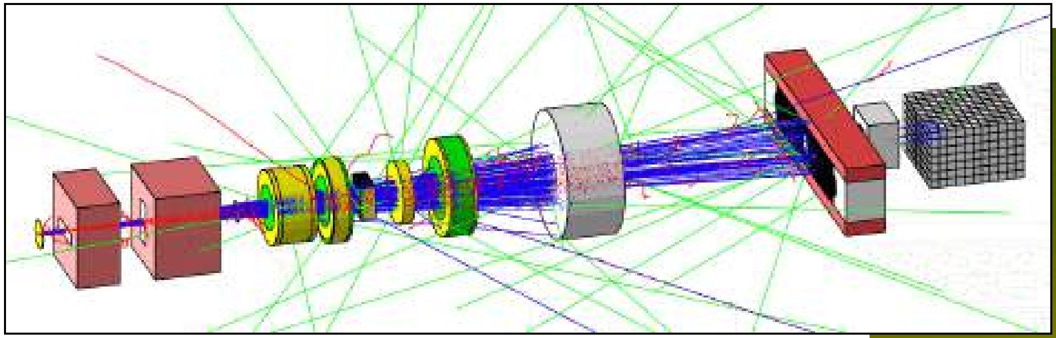
Both ATLAS and CMS plots are made from a tiny piece of the very earliest data.

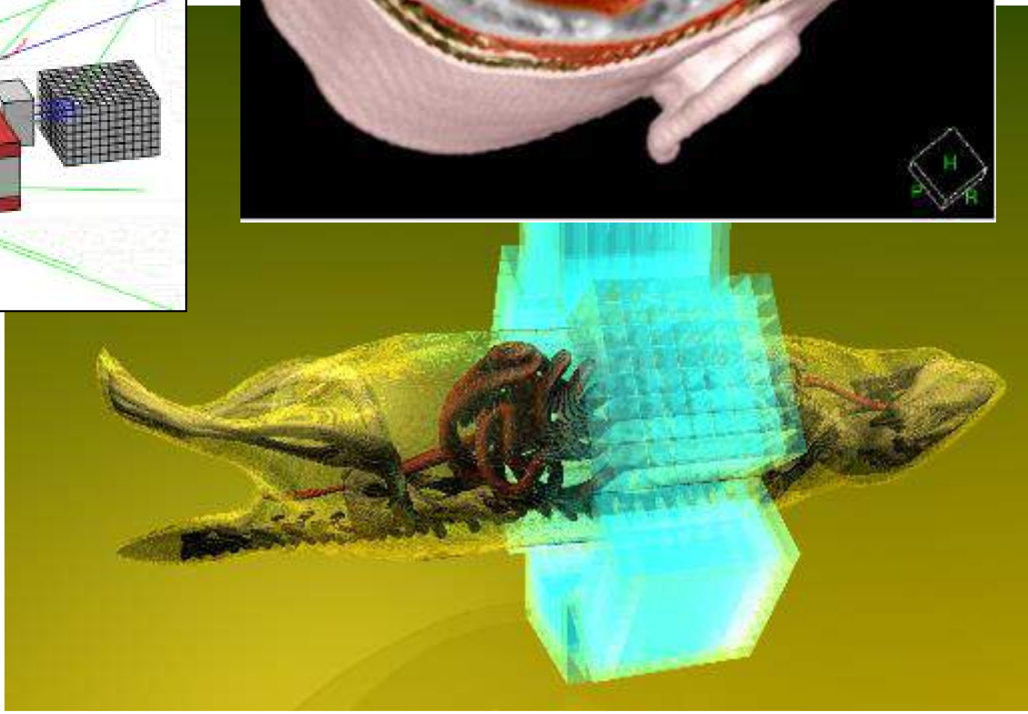

Akebono
RHESSI
ACE
New Horizons
LISA Pathfinder
LISA
JWST
INTEGRAL
BepiColombo
Messenger
Astro-H
Fermi
SOHO
GAIA
Herschel
Cassini
Suzaku
SWIFT
XMM-Newton
JUICE
JUNO
Kaguya
Chandrayaan-1
Chandrayaan-2
Columbus
EUSO
AMS
MAXI
ConeXpress
Chang'e-1
LRO

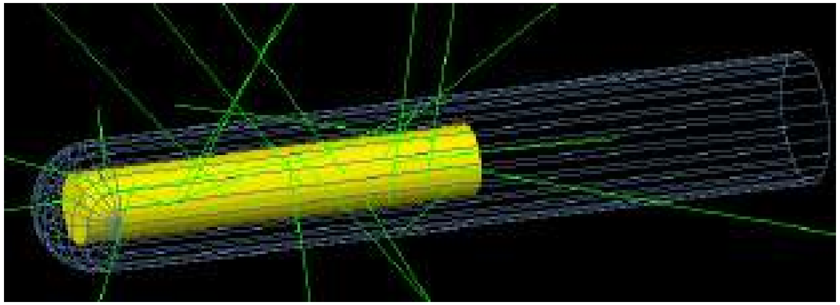
Geant4 для медицины

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





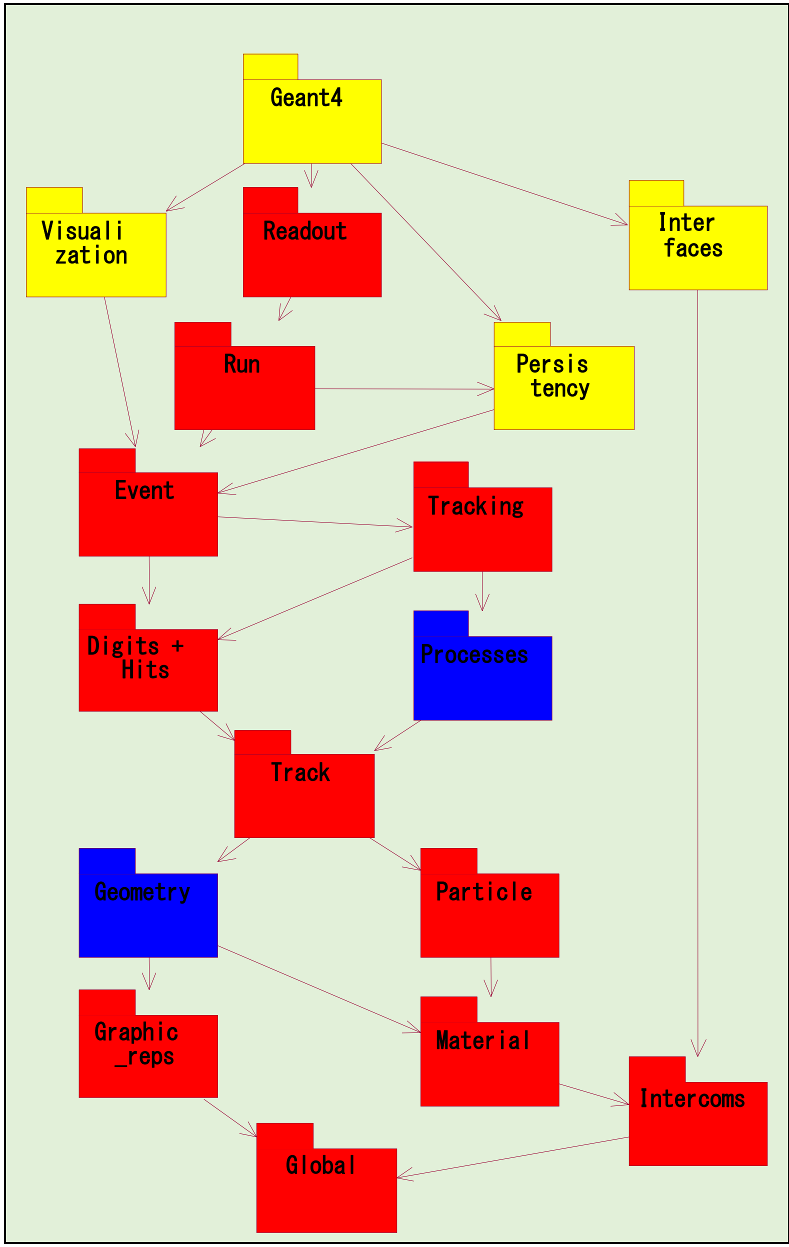




Geant4 Kernel

Geant4 kernel

- Geant4 consists of 17 categories.
  - Independently developed and maintained by WG(s) responsible to each category.
  - Interfaces between categories (top level design) are stable since the version of Geant4
- Geant4 Kernel
  - Handles run, event, track, step, hit, trajectory.
  - Provides frameworks of geometrical representation and physics processes.



How define your geometry?

- Derive your own concrete class from G4VUserDetectorConstruction abstract base class
  - This one of mandatory user classes
- Implement Construct() and ConstructSDandField() methods
  - Construct all necessary materials
  - Define shapes/solids
  - Define logical volumes
  - Place volumes of your detector geometry
- Optional actions
  - Associate (magnetic) field to geometry
  - Instantiate sensitive detectors / scorers and set them to corresponding logical volumes
  - Define visualization attributes for the detector elements
  - Define regions
- Alternatively, geometry may be defined in XML file exchange format
  - For Geant4 gdml format should be used
  - There are built-in dump and upload methods

Geometry shapes in Geant4

CSG (Constructed Solid Geometry) solids

- G4Box, G4Tubs, G4Cons, G4Trd, G4Para, G4Trap,
  G4Torus, G4CutTubs, G4Orb, G4Sphere

Specific solids (CSG like)

- G4Polycone, G4Polyhedra, G4Hype, G4Ellipsoid,
  G4EllipticalTube, G4Tet, G4EllipticalCone, G4Hype,
  G4GenericPolycone, G4GenericTrap, G4Paraboloid

Tessellated solids

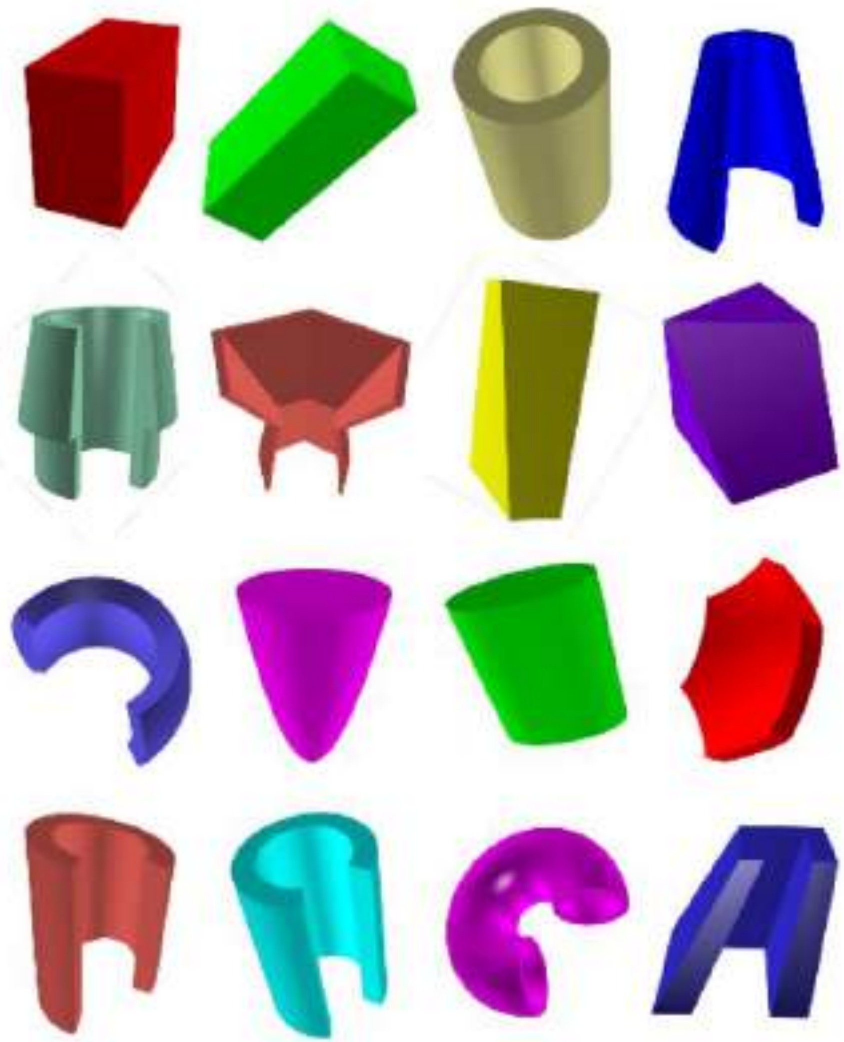
- G4TessellatedSolid, G4ExtrudedSolid

Boolean & scaled solids

- G4UnionSolid, G4SubtractionSolid,
  G4IntersectionSolid, G4MultiUnion, G4ScaledSolid

Twisted shapes

- G4TwistedBox, G4TwistedTrap, G4TwistedTrd,
  G4TwistedTubs



Geant4 data base for materials

- The data base includes more than 3000 isotopes
- Isotopic composition of elements (Z = [1-108]) with their natural isotopic abundance: using the NIST Atomic Weights and Isotopic Compositions data base
- NIST elements can be obtained easily from the Geant4 NIST data base by using their `symbol` or `Z - atomic number:`
  - the corresponding *G4Isotope* objects will be automatically built
  - "find or build" i.e. avoids duplication of element objects

```
// get the carbon G4Element object from the NIST data base: by its symbol
G4Element* elC  = G4NistManager::Instance()->FindOrBuildElement("C");
// get the silicon G4Element object from the NIST data base: by its Z
G4Element* elSi = G4NistManager::Instance()->FindOrBuildElement(14);
```

- Large collection of pre-defined materials:
  - pre-defined: density, elemental composition (with the pre-defined natural isotopic composition), mean ionization energy, density effect parameters, etc.

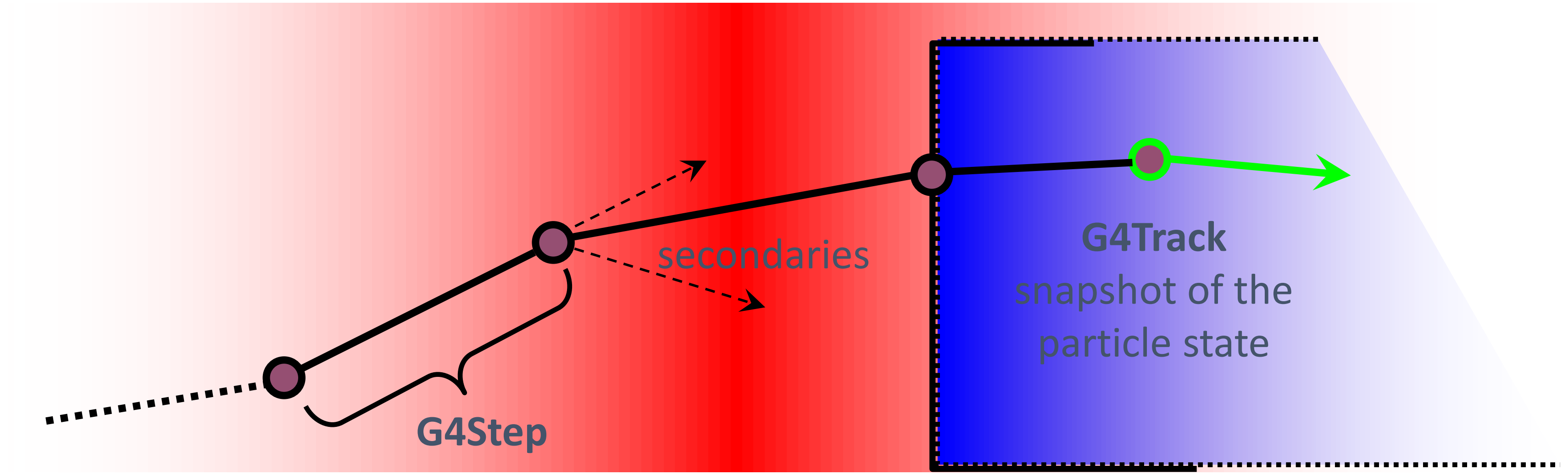
Complex material is built from components

- `G4Material` object definition as mixture:
  - mixture of element(s) and material(s) example: using the `AddElement` and `AddMaterial` methods

```
// Create aerogel material as 62.5 % silicon dioxide (SiO2), 37.4 % water (H2O)
// materials and 0.1 % carbon elemet. Assumimg that the materials (matSiO2 and
// matH2O) as well as the carbon elemnt (elC) have already been created.
//
// create the aerogel material (name, density, number of components):
G4Material* matAerog = new G4Material(name        = "Aerogel",
                                      density     =  0.2 * g/cm2,
                                      ncomponents =  3);
// add the elements to the material with their fractional mass
matAerog->AddMaterial(matSiO2, fractionmass = 62.5 * perCent);
matAerog->AddMaterial(matH2O , fractionmass = 37.4 * perCent);
matAerog->AddElement (elC    , fractionmass =  0.1 * perCent);
```

Geant4 tracking

- **`G4Track`** is the object "pushed" step by step by the tracking :
- Moving by one step is the responsibility of the "stepping"
  - Which is the core engine of the "tracking" machinery



- These moves/steps are defined by physics or by geometry
  - Step length limit is a result of competition of processes
  - Processes involved at a step may change the **`G4Track`**
  - By default, G4Transportation stops track at the volume boundary
    - There are special methods how to skip boundaries during tracking
    - Implementation was recently introduced for gamma tracking in ATLAS calorimeter

Geant4 Physics

Geant4 интерфейс к физике

- The interface of Geant4 kernel to physics is abstract
- Base physics abstract classes are following:
  - The **G4ParticleDefinition** objects shared between threads
  - The **G4VProcess** thread local objects
  - The **G4ProcessManager** thread local interface class
- Configuration of physics is prepared in the G4VUserPhysicsList mandatory user class
- These interfaces are stable for >20 years allowing users to work with different Geant4 versions and providing a basis for new developments
  - Concrete physics is implemented in physics models and cross section classes
  - Alternative models and cross sections are provided in Geant4 libraries
  - A user may be also a developer of a custom particle, process, physics model, or cross section

Geant4 particles

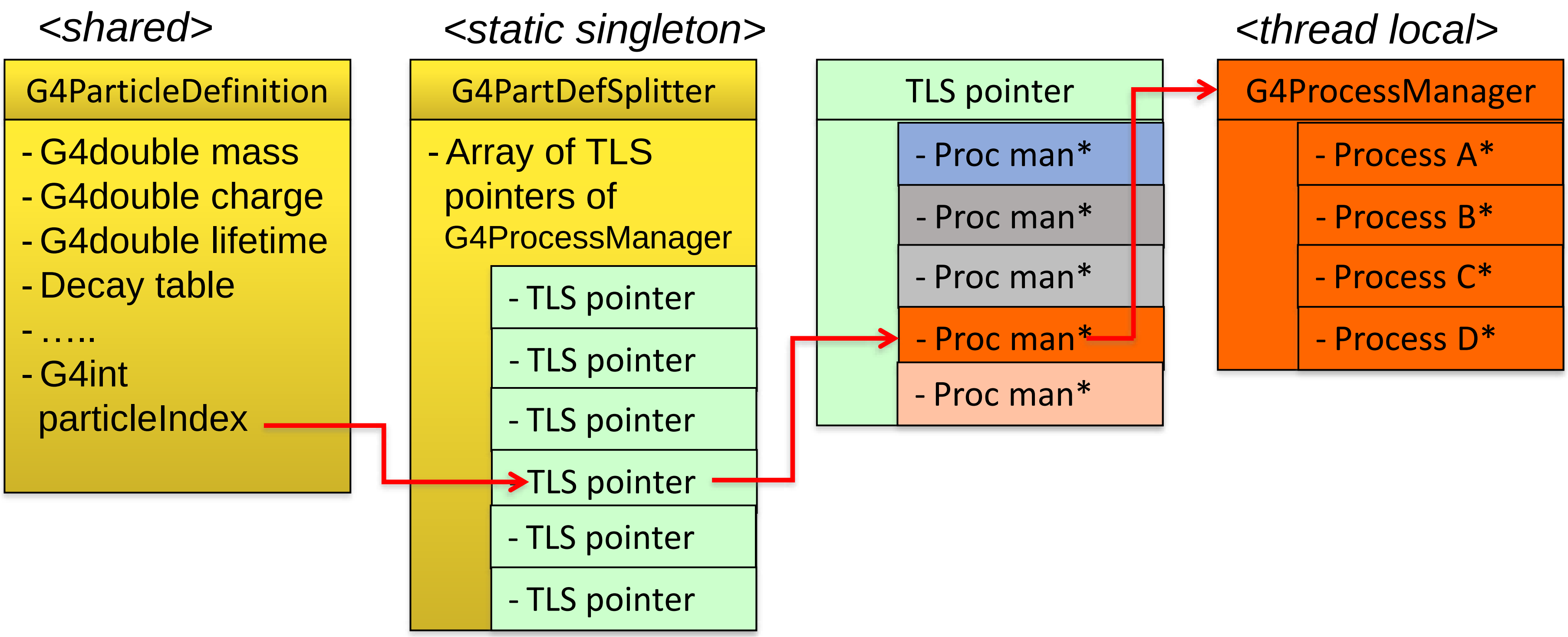
- G4ParticleDefinition is the main object keeping static information about particles
  - Name, mass, charge, quantum numbers, decay table….
- "Stable" particles
  - Leptons: $e^{\pm}$, $\mu^{\pm}$, ….
  - Bosons: G4Gamma, G4OpticalPhoton, ….
  - Geantino is a particle without any interaction
  - "Stable" hadrons: $\pi^{\pm}$, $K^{\pm}$, ….
  - Light ions: d, t, ^{3}He, ^{4}He, and anti-ions
  - 12 hyper- and anti-hyper- nuclei are added in Geant4 11.0
- "ShortLived" hadrons normally do not tracked by Geant4 but used internally by hadronic models
  - Quarks, di-quarks, ρ(770), ω(783)…

Geant4 Approach for Ions

- Light ions are individual Geant4 particles:
  - **G4Deuteron**
  - **G4Triton**
  - **G4He3**
  - **G4Alpha**
  - **anti-light ions**
- Generic ion serves all other ions:
  - **G4GenericIon** - only one particle
  - Not a real particle (charge = +1, mass = Mp)
  - Serving for any kind of ion with Z>2 (>3000 known isomeres)
  - All concrete ions peak up processes and cross sections of the G4GenericIon
    - Scaling relations for electromagnetic interactions are used in run time
- Ion names
  - "**C12**" means that the carbon ion is in the ground state
  - "**Co60**[58.590]" is the first excitation state of Co60
  - Extra information about atomic shell may be filled to any ion

Split class – case of particle definition

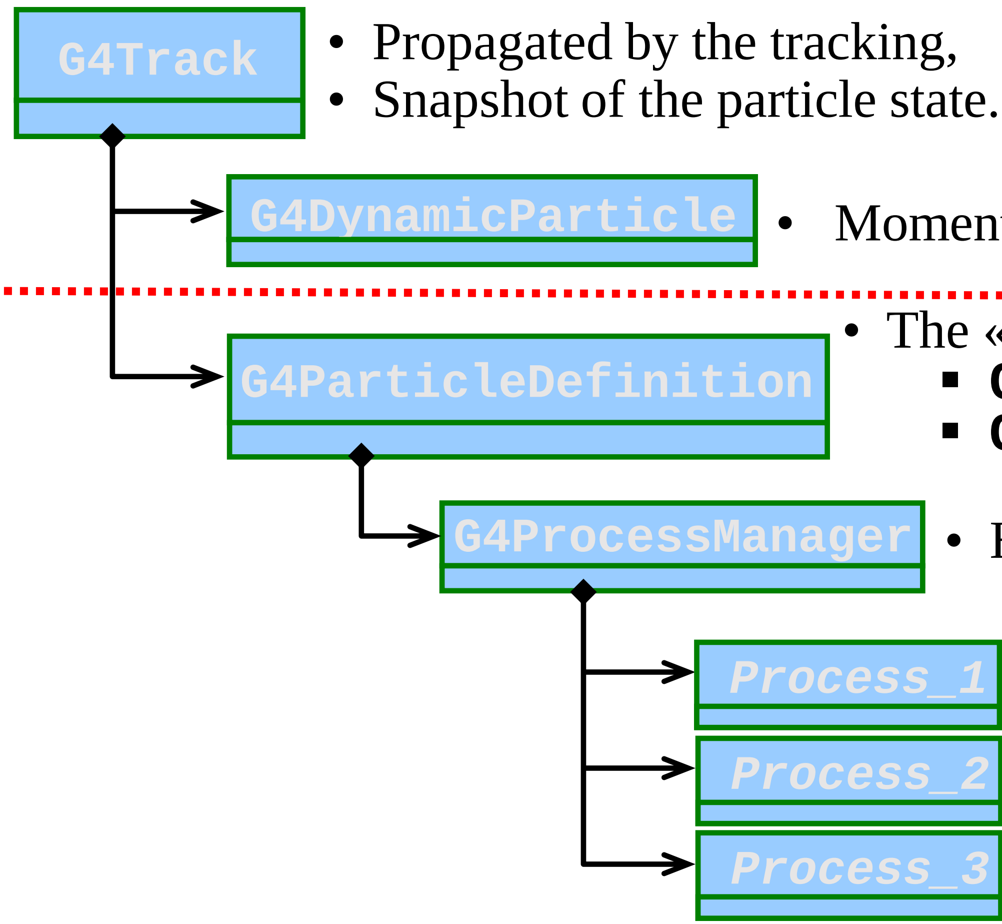
- In Geant4, each particle type has its own dedicated object of G4ParticleDefinition class.
  - Static quantities : mass, charge, lifetime, decay channels, etc.,
    - Are shared by all threads
  - Dedicated object of G4ProcessManager : list of physics processes which this particle undertakes.
    - Physics process object must be thread-local
    - Thread local storage is used (TLS)



G4VProcesses – main interface to physics

- Processes are classified as:
  - Electromagnetic
  - Hadronic
  - Decay
  - Parameterized
  - Transportation
  - ……..
- Any process has process has type and sub-type
  - const G4String& G4VProcess::GetProcessType();
  - G4int G4VProcess::GetProcessSubType();
    - This method is recommended to be used for MC truth
    - The list of sub-types is stable since introduced and only extended with new processes
- Any process may be initialized using virtual methods:
  - **G4bool IsApplicable(const G4ParticleDefinition &);**
    - Used to check if a process can handle given particle type
  - **void PreparePhysicsTable**(const G4ParticleDefinition&);
  - **void BuildPhysicsTable**(const G4ParticleDefinition&);
    - Used for initialization of internal data of a process before run

From G4Track to processes



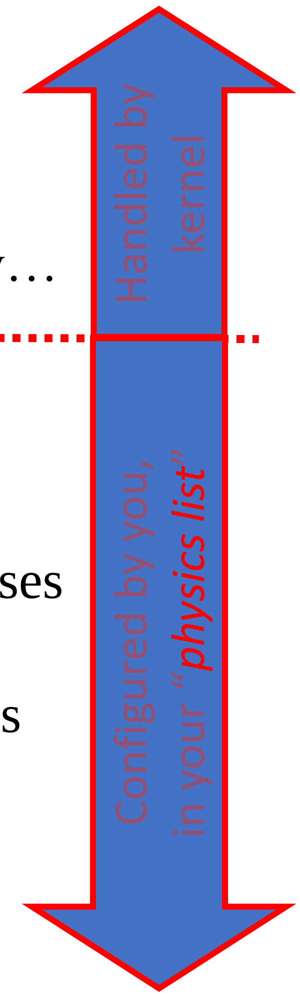
- Propagated by the tracking,
- Snapshot of the particle state.

- Momentum, pre-assigned decay…

- The « particle type »:
  - **G4Electron**,
  - **G4PionPlus**…

- Holds pointers to processes

- Implementing physics processes



How tracks are created and killed

- G4Track can be created
  - By **G4VUserPrimaryGeneratorAction**
  - By any **G4VProcess**
- Geant4 particle is tracked until it is killed by one of Geant4 processes:
  - Transport out of the world volume
  - Inelastic interaction
  - Decay
  - Tracking low energy cut in the ionization process
  - **G4NeutronKiller** or **G4UserLimits**
  - If during tracking kinetic energy become zero and there is no processes **AtRest** the particle is killed by the stepping manager
- Any particle may be also killed by user action classes
- Geant4 introduced conception of "**cut in range**"
  - Physically this means required spatial accuracy of simulation
  - At initialization for each material a production threshold for kinetic energy of secondary particles is computed
    - This means different production thresholds for different materials
  - This is the main difference between Geant4 and other simulation tools, which implement only tracking cuts and cuts per volume

Geant4 Physics: Decay, Parameterized and Transportation

- Decay processes includes:
  - weak decay (leptonic, semi-leptonic decay, radioactive decay of nuclei)
  - electromagnetic decay (π^0, Σ^0, etc.)
  - strong decay not included by default
    - they are part of hadronic models
    - may be assigned by a user to a particle
- Parameterized process:
  - assigned to G4LogicalVolume
  - instead of step-by-step simulation provides hits in the logical volume and list of particles living the volume
  - for example, EM shower generation in a calorimeter based on parameters obtained from detailed simulation of the calorimeter response
- Transportation process:
  - responsible for propagating a particle through the geometry in electromagnetic or gravitational field
  - needs to be assigned to each “stable” particle

Geant4 EM and hadronic physics

- The EM physics sub-libraries are used in all kind of applications
  - For e+-, mu+-, charged hadrons, and ions
  - Full energy interval from 10 eV to 1 PeV
- Hadronic physics sub-libraries are used for simulation of interactions with atomic nuclei
  - Hadrons and ions in full energy range
  - Capture of neutrons and negatively charged muons and hadrons
  - Leptons
  - Neutrinos

Geant4 EM physics

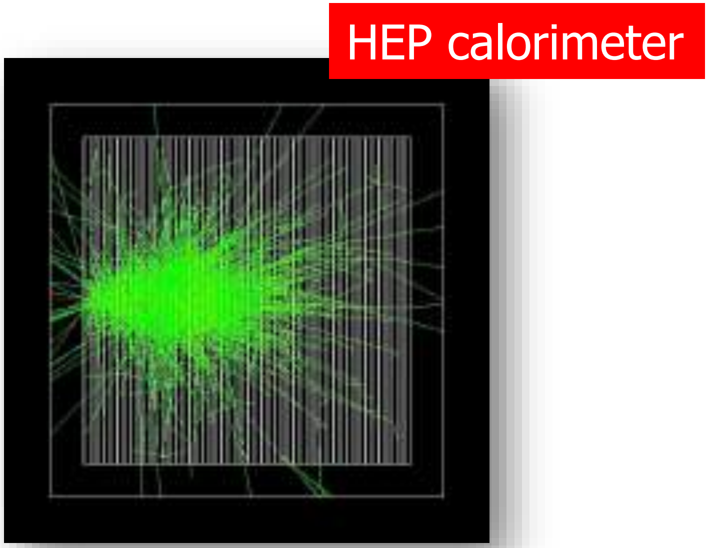
Geant4 EM sub-libraries

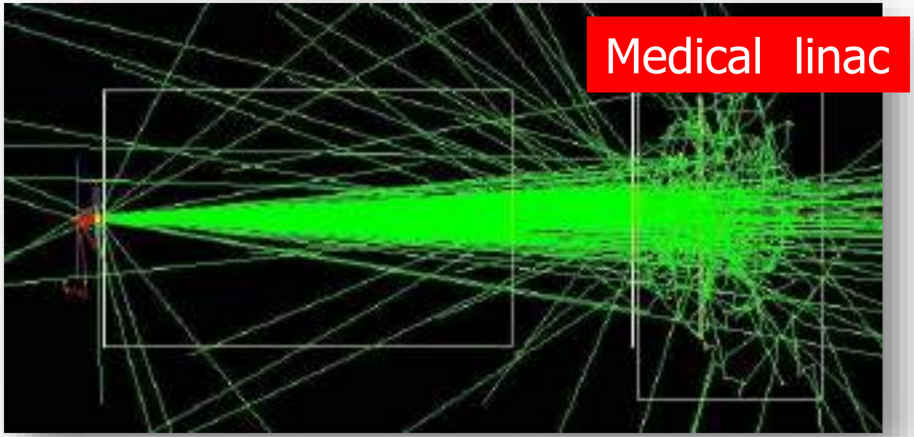
Located in $G4INSTALL/sources/processes/electromagnetic

- 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 processes
- 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 2008 code rewrite , γ, e- , e+ from 250 eV up to 6 GeV
  - hadrons and ions up to 1 GeV
  - atomic de-excitation (fluorescence + Auger)
- DNA
  - Geant4 DNA modes and processes
  - Micro-dosimetry models for radiobiology
  - rom 0.025 eV to 300 MeV
  - many of them material specific (water)
  - Chemistry in liquid water
- Adjoint
  - sub-library for reverse Monte Carlo simulation from the detector of interest back to source of radiation
- Utils : general EM interfaces and helper classes

Gamma and electron transport

- Photon processes
  - γ conversion into e+e- pair
  - Compton scattering
  - Photoelectric effect
  - Rayleigh scattering
  - *Gamma-nuclear interaction in hadronic sub-library*
- Electron and positron processes
  - Ionization
  - Coulomb scattering
  - Bremsstrahlung
  - Production of e+e- pair
  - *Nuclear interaction in hadronic sub-library*
  - Positron annihilation
- Suitable for HEP & many other Geant4 applications with electron and gamma beams



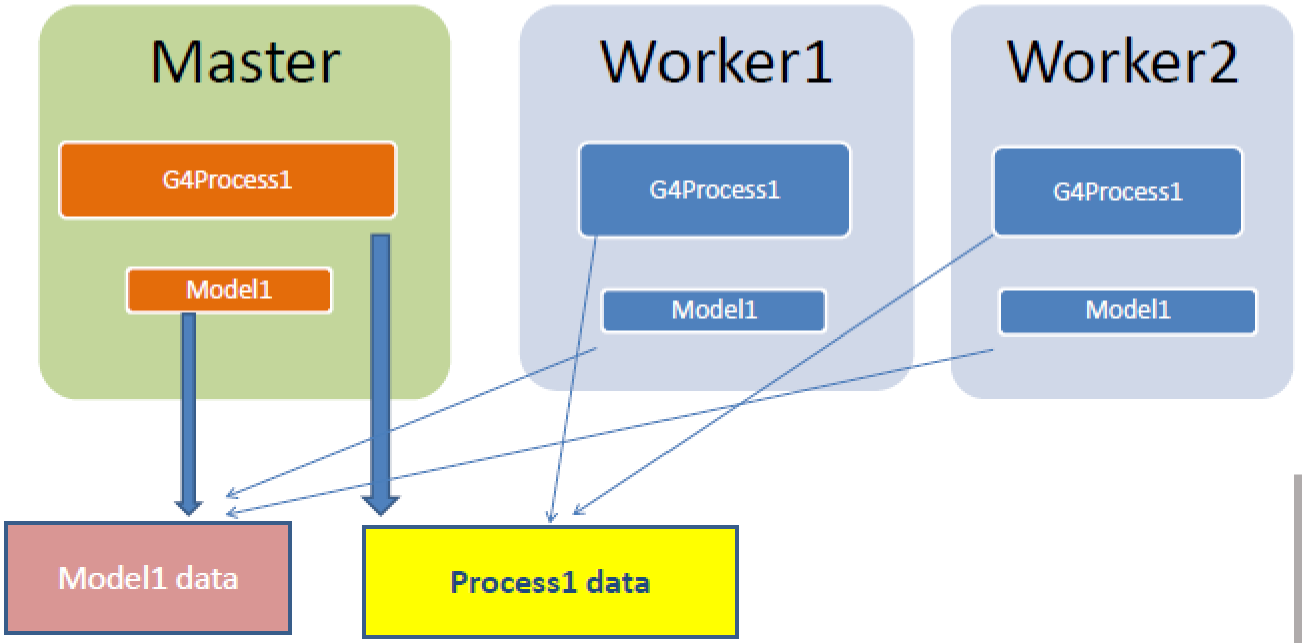


Software Design of EM Physics

- The uniform coherent approach for all EM packages
  - low energy and high energy models may work together
- A physical interaction or process is described by a process class
  - For example: **G4ComptonScattering**
    - Assigned to Geant4 particle types in Physics List
  - Three EM base processes:
    - **G4VEmProcess**
    - **G4VEnergyLossProcess**
    - **G4VMultipleScattering**
- A physical process can be simulated according to several models
  - each model being described by a model class
  - Naming scheme : « G4ModelNameProcessNameModel »
    - For example: G4LivermoreComptonModel
  - Models can be assigned to certain energy ranges and G4Regions
  - Inherit from **G4VEmModel** base class
- Model classes provide the computation of
  - Cross section and stopping power
  - Sample selection of atom in compound
  - Final state (kinematics, production of secondaries, …)

EM Data Sharing for Geant4 MT

- The scalability of Geant4 application in the MT mode depends on how effectivly data management is performed
  - Geant4 10.X is the multi-threaded toolkit
- **Shared EM physics data:**
  - tables for cross sections, stopping powers and ranges are kept by processes
  - Differential cross section data are kept by models
  - Material propertes are in material data classes
  - EM parameters established for Physics Lists in the G4EmParameters class



Tables are filled by Master and have read-only access in run time

In this scheme number of threads is not limited

Gamma processes

- Photo-effect is the main process for absorption of low-energy gamma
  - Rayleigh scattering should not be neglected if an accurate dosimetry simulation is needed
- At high energy gamma conversion dominates
- Gammas may be absorbed by nuclei due to giant dipole resonance
  - Producing neutrons, protons, and gamma

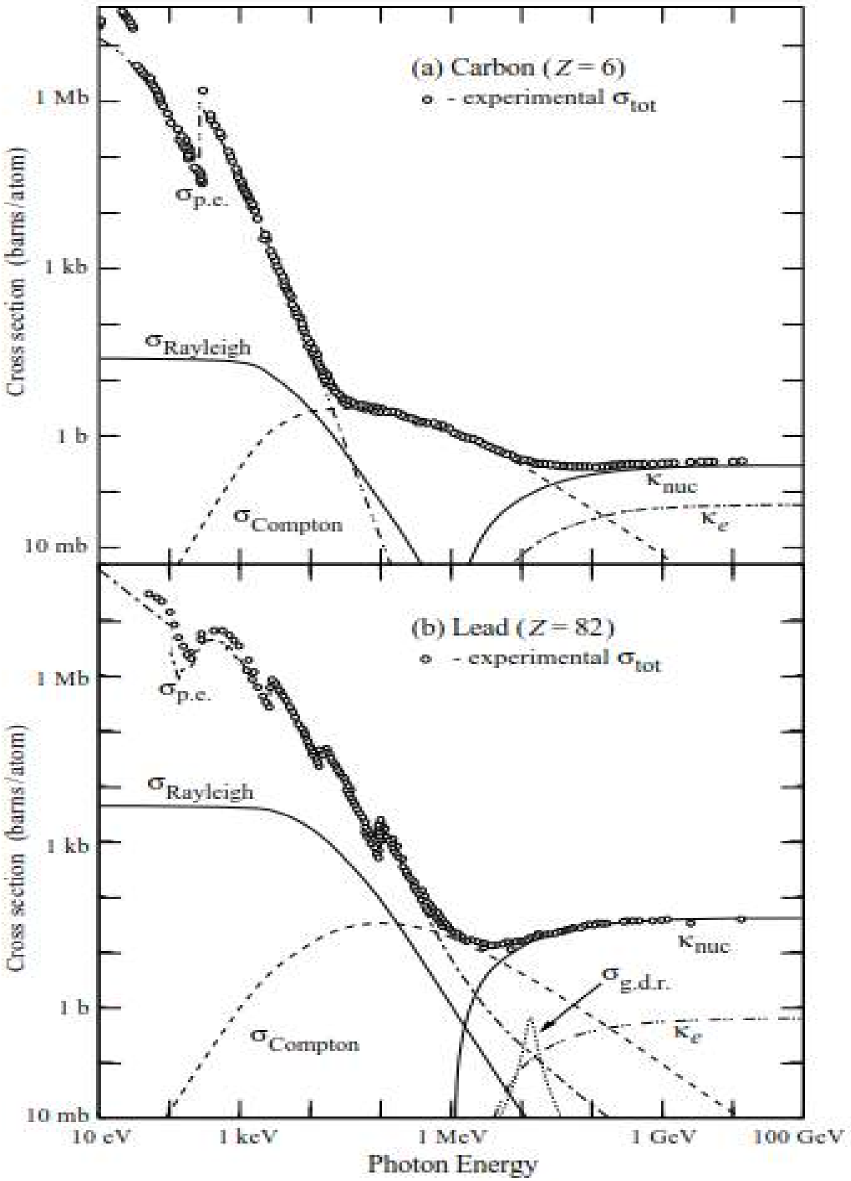
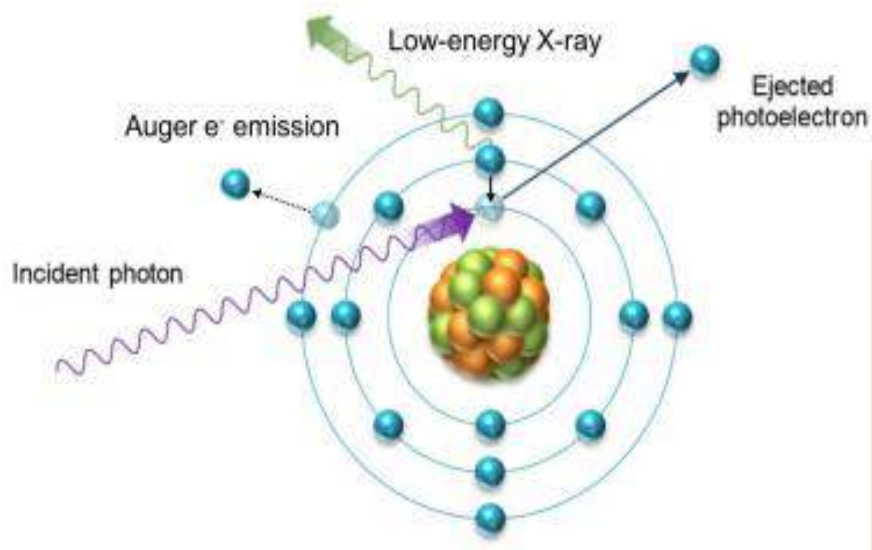


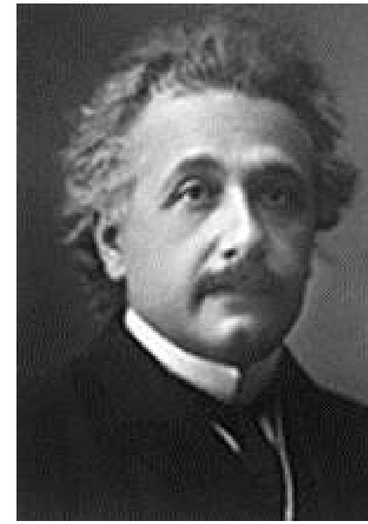
Photo-electric effect – example of gamma process

In the photo-electric absorption process a **photon is absorbed** by an atom and an **electron is emitted** with an energy:

$$E_{photoelectron} = E_{\gamma} - B_{shell}(Z_i) \tag{1}$$

The atom, left in an excited state with a vacancy in the ionized shell, decays to its ground state through a cascade of radiative and non-radiative transitions with the **emission of characteristic x-rays** and **Auger and Coster-Kronig electrons**.





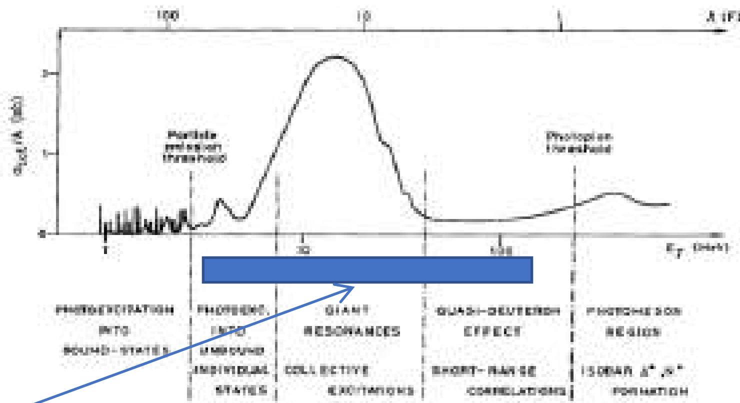
Primary gamma may be polarized, photoelectron angular distribution will be affected.

Transition energies are available in several DB, which may be differ on eV level, should be selected depending on use case.

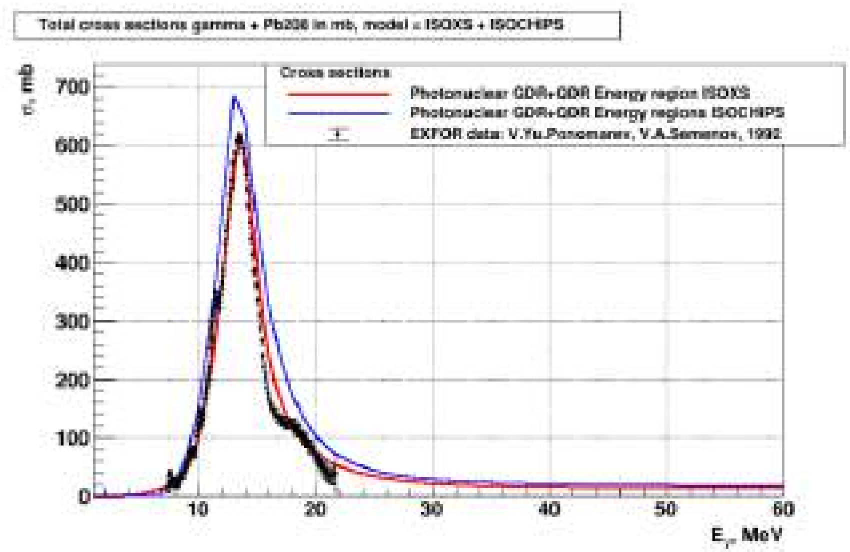
Gamma-nuclear cross section

https://cds.cern.ch/record/2778865/files/Kutsenko_report.pdf

- Several different mechanisms are responsible for gamma-nuclear cross section
  - For a long time in Geant4 CHIPS parameterization was used for full energy range above 10 MeV (NIM A 835, 186-225 (2016))
- Recently a new evaluation of the data was published (T. Kawano et al, IAEA photo nuclear data library2019.Nuclear Data Sheets,163,109-162 (2020))
  - A new data set has been included into Geant4 11.0 per natural isotope
  - Low energy limit defined by data (was 10 MeV before)
  - Data tables from threshold to 130 MeV
  - CHIP interpolation above 150 MeV
  - Linear interpolation in the transition energy range

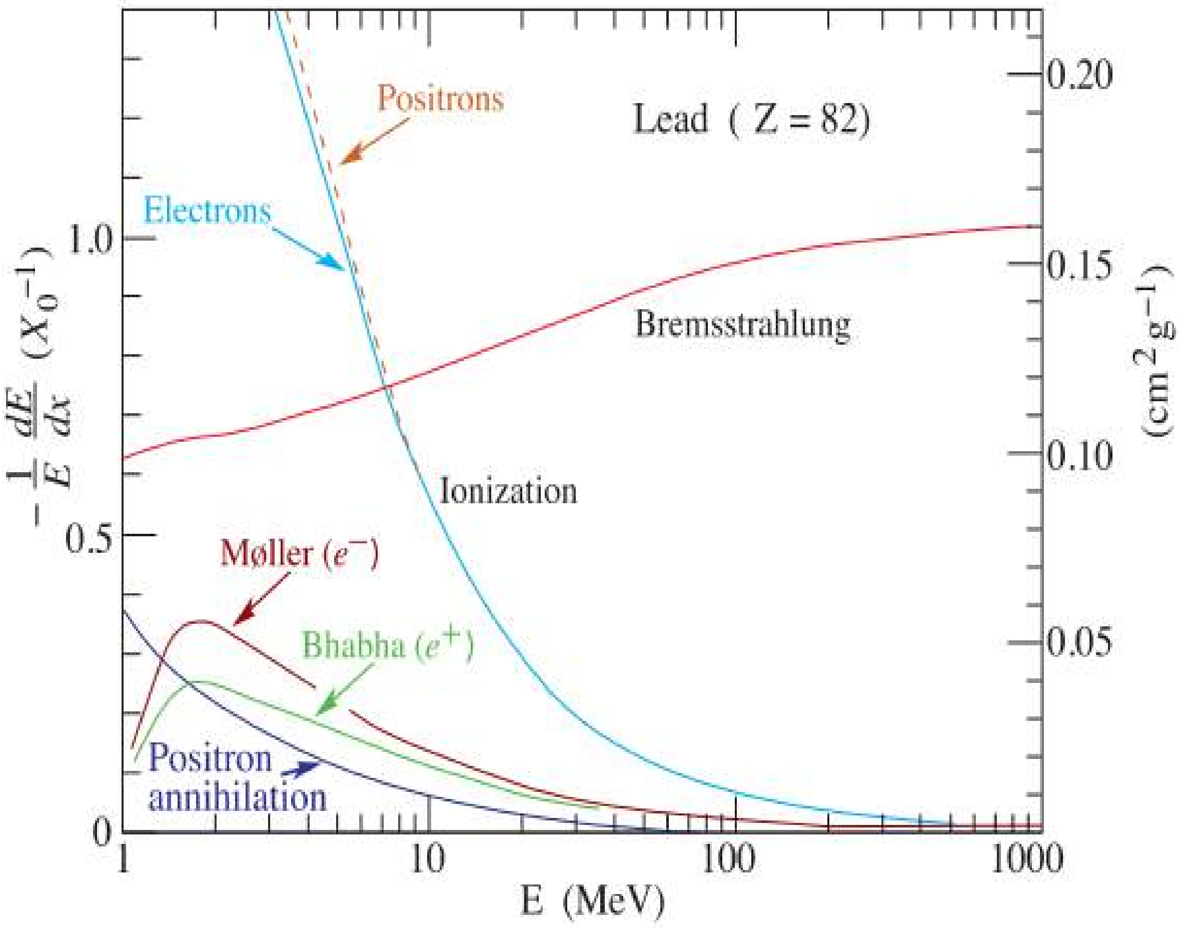


Geant4 gamma nuclear X-section versus EXFOR data



Electron and positron processes

- At low energies ionisation dominates for e-
  - For e+ annihilation dominates at very low energy
- Above critical energy bremsstrahlung is the main process
  - Radiation energy loss exceed ionization energy loss
  - Process of e+e- pair production has much less cross section
- Difference between electrons and positrons increased for low energy
  - Is practically negligible above critical energy

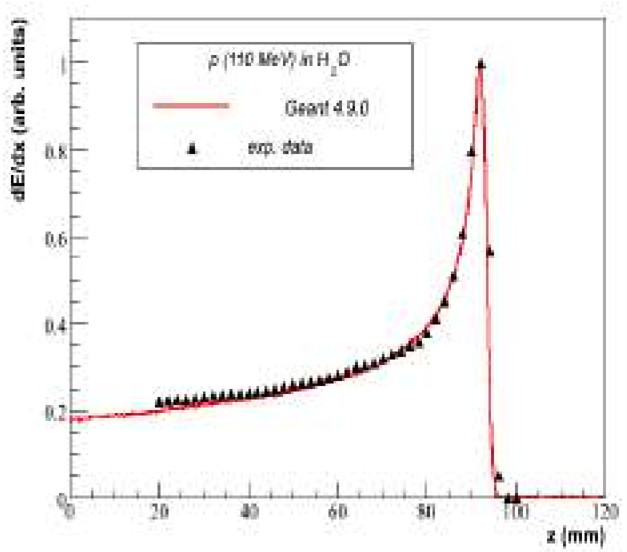


Hadron and ion ionisation

- Bethe-Bloch formula with corrections used for E>2 MeV

$$-\frac{dE}{dx} = 4\pi N_e r_0^2 \frac{z^2}{\beta^2}\left(\ln\frac{2m_e c^2\beta^2\gamma^2}{I} - \frac{\beta^2}{2}\left(1-\frac{T_c}{T_{max}}\right) - \frac{C}{Z} + \frac{G-\delta-F}{2} + zL_1 + z^2L_2\right)$$

  - C – shell correction
  - G – Mott correction
  - δ – density correction
  - F – finite size correction
  - L_1- Barkas correction
  - L_2- Bloch correction
  - Nuclear stopping
  - Ion effective charge

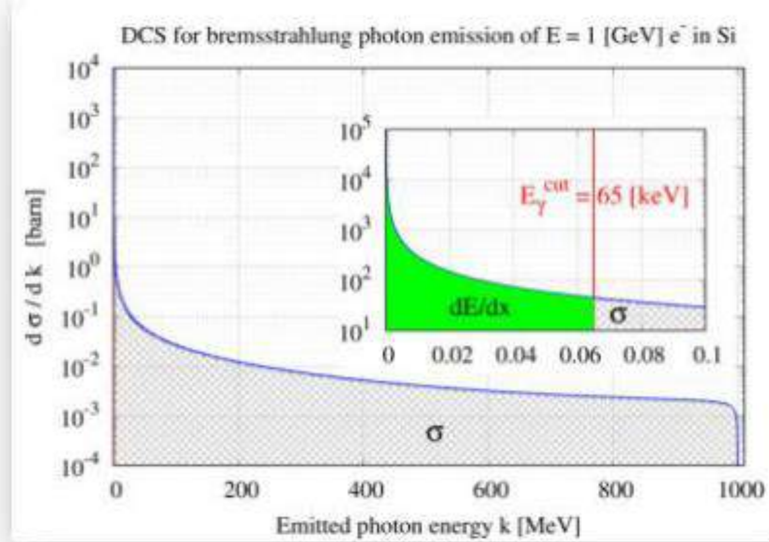


- Bragg peak parameterizations for E< 2 MeV
  - ICRU'49, ICRU'73, ICRU'90, and NIST databases
  - Data for elements and materials

- Scaling relation for heavy particles:
  - $S_h(E) = S(E*M_p/M_h)*Q_h^2$,
  - M_h , Q_h - hadron mass and charge
  - Applicable to any charged particle including exotics and all ions
  - This is possible, because dE/dx depend mainly on β

Secondary production threshold technique

- Introduce secondary photon production threshold:
  - *secondary photons*, with initial energy below a gamma production threshold($k<E_\gamma^{cut}$), are not generated
  - the corresponding energy (that would have been taken away from the primary) is accounted as *CONTINUOUS* energy loss of the primary particle along its trajectory



- Electron makes a step with a given length *L*, one can compute the mean energy loss (due to sub-threshold photon emissions) along the step as *L* x *dE/dx* (would be true only if *E* = *const* along the step)

$$\frac{dE}{dx}(E, E_\gamma^{cut}, Z) = \mathcal{N}\int_0^{E_\gamma^{cut}} k\frac{d\sigma}{dk}(E,Z)dk$$

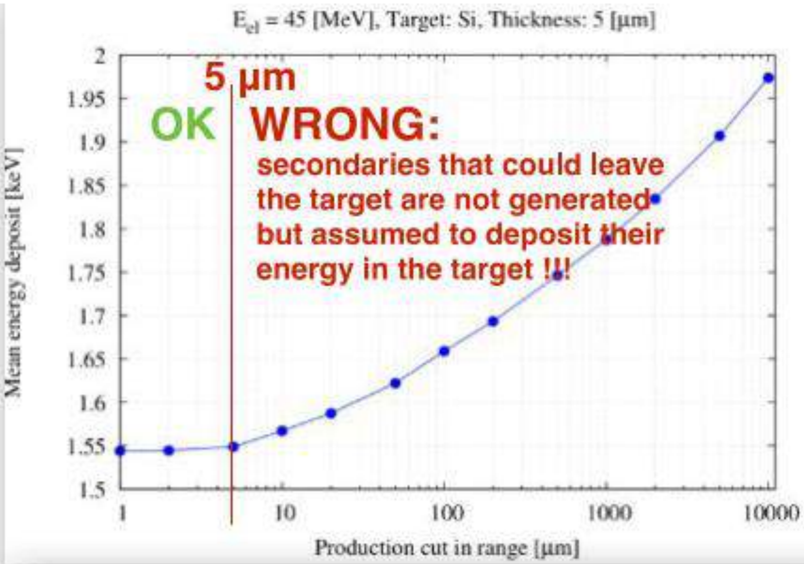
- *Secondary photons*, with initial energy above a gamma production threshold ($k>E_\gamma^{cut}$), are generated (*DISCRETE*)
- the emission rate is determined by the corresponding (restricted) cross section(σ)

$$\sigma(E, E_\gamma^{cut}, Z) = \int_{E_\gamma^{cut}}^{E} \frac{d\sigma}{dk}(E,Z)dk$$

Cut definition

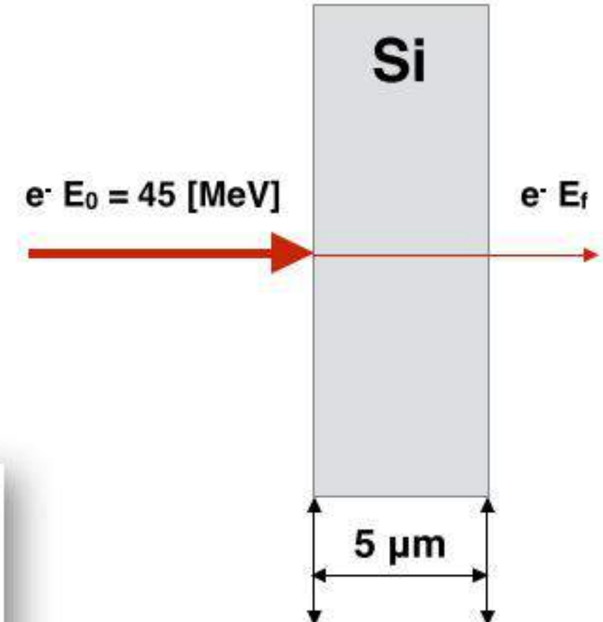
- In past cuts were defined in SetCuts() method of physics list
  - After migration to the MT mode, we recommend not doing this
  - Cuts may be defined via UI commands
  - Details on Geant4 cuts will be described below
- Using UI interface Geant4 kernel change cuts and try to count number of steps in the same run
  - /run/setCut 0.01 mm
  - /run/beamOn 100
- Define cuts only for electrons
  - /run/setCutForAGivenParticle e- 10 um
  - /run/setCutForRegion GasDetector 0.1 mm
  - /run/dumpCouples
- How to change low-energy limit of production threshold
  - /cuts/setLowEdge 0.1 keV
  - /cuts/setHighEdge 5 GeV
  - The highEdge limit cannot be above 10 GeV
    - Until now there was no need to increase this limit

Example demonstrating importance of cuts



cut [μm]	mean E_{dep}	rms E_{dep}	prod. thres. [keV]		mean num. sec.	
			γ	e^-	γ	e^-
1	1.54423	0.000573911	0.99	0.99	0.0006811	0.1018230
2	1.54443	0.000583879	0.99	2.9547	0.0006843	0.0316897
5	1.54882	0.000605834	0.99	13.1884	0.0006857	0.0068261
10	1.56717	0.000665733	0.99	31.9516	0.0006730	0.0028232
20	1.58734	0.000743473	1.08038	47.8191	0.0006651	0.0018811
50	1.62223	0.000912408	1.67216	80.7687	0.0006557	0.0011304
100	1.65893	0.001108240	2.32425	121.694	0.0006518	0.0007536
200	1.69338	0.001342180	3.2198	187.091	0.0006465	0.000477
500	1.74642	0.001774670	5.00023	337.972	0.0006184	0.0002617
1000	1.78751	0.002219870	6.95018	548.291	0.0006054	0.0001622
2000	1.83440	0.002861020	9.66055	926.09	0.0005786	9.3e-05
5000	1.90700	0.004243030	14.9521	2074.3	0.0005427	4.07e-05
10000	1.97378	0.006036600	20.6438	4007.59	0.000521	2.22e-05

Compute the mean of the energy deposit in the target: E_0 - primary, E_f - final energy



Golden rule:
For transport in solid/liquid media cut in range should be below minimal geometry size

Geant4-DNA Project

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

- Excited water molecules
- Ionized 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

t=0

DIRECT DNA DAMAGE

INDIRECT DNA DAMAGE

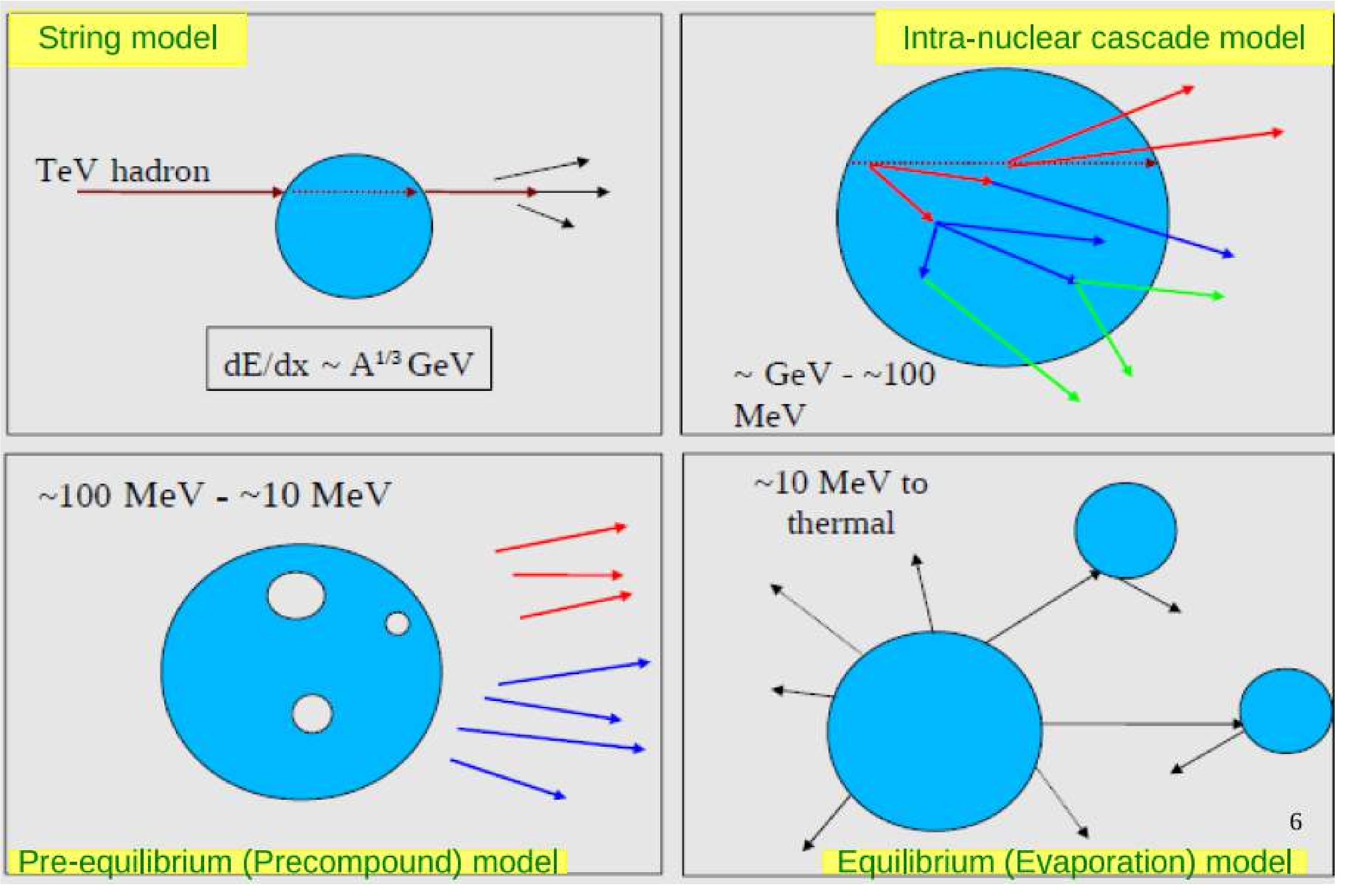
repair

Geant4 hadronic physics

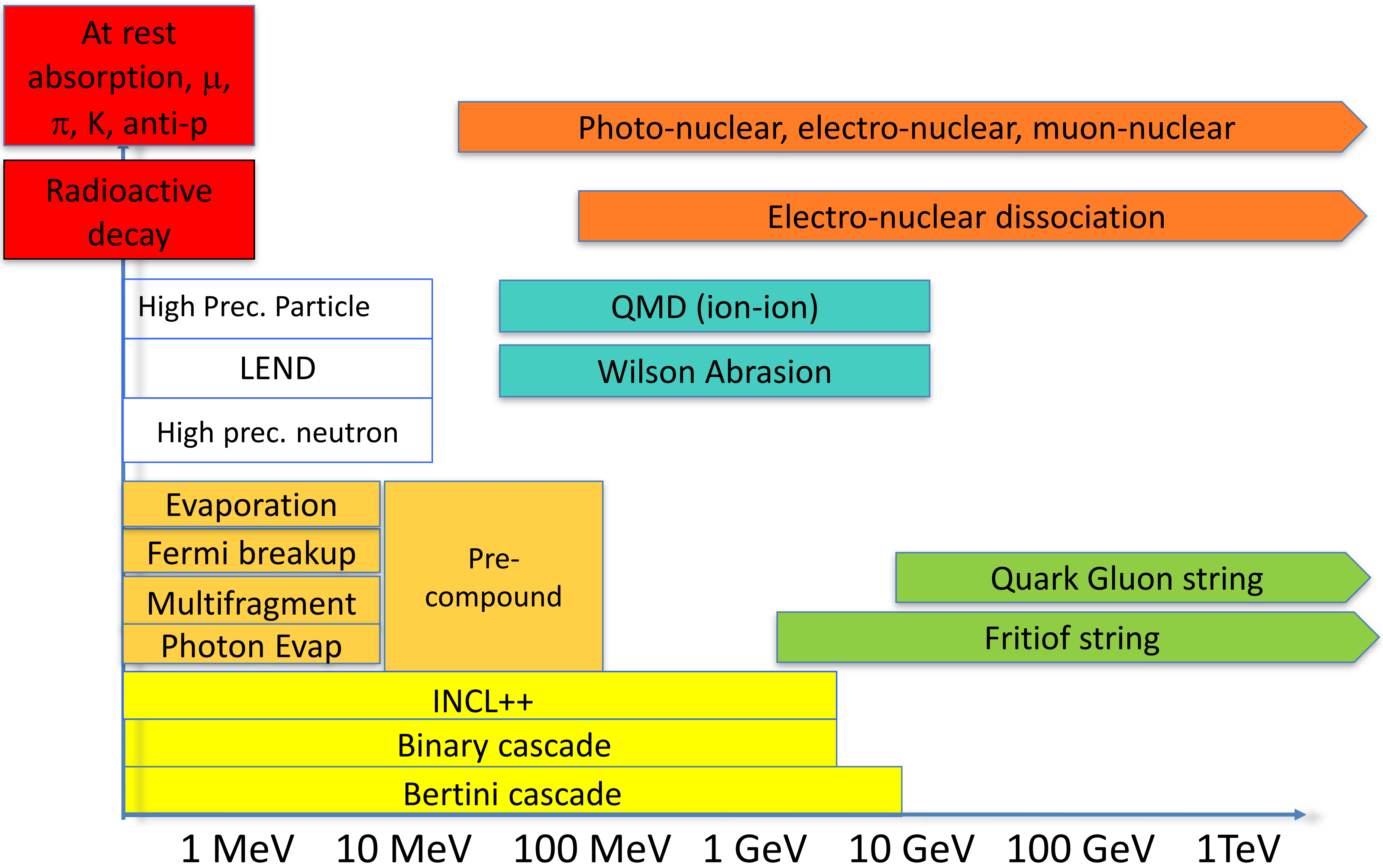
Hadronic Physics components

- Hadron elastic physics
  - Default set for hadron elastic interactions
  - There are few alternative constructors
- Hadron inelastic physics
  - Many different constructors
    - String models for high energy
    - Cascade models for moderate energy
    - Precise data driven models for low-energy neutron transport may be added
- Ion physics
  - Light ions and G4GenericIon
  - Elastic and inelastic interactions
- Capture processes
  - Neutron capture below 15 MeV
  - μ^-, negatively charged meson and baryons capture at rest

High energy hadron-nucleus inelastic reaction



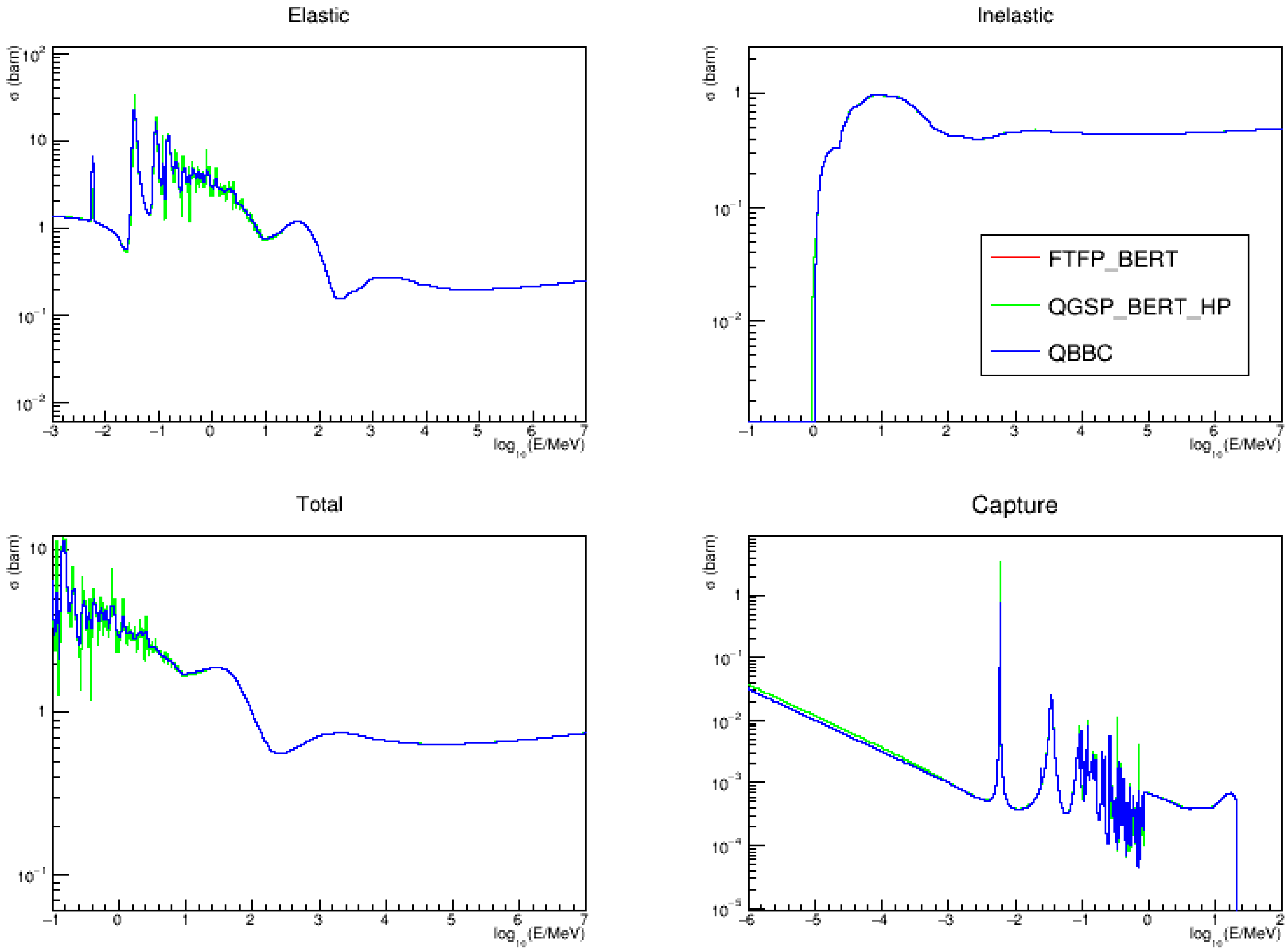
Hadronic Model Inventory



Geant4 High Precision (HP) Sub-library

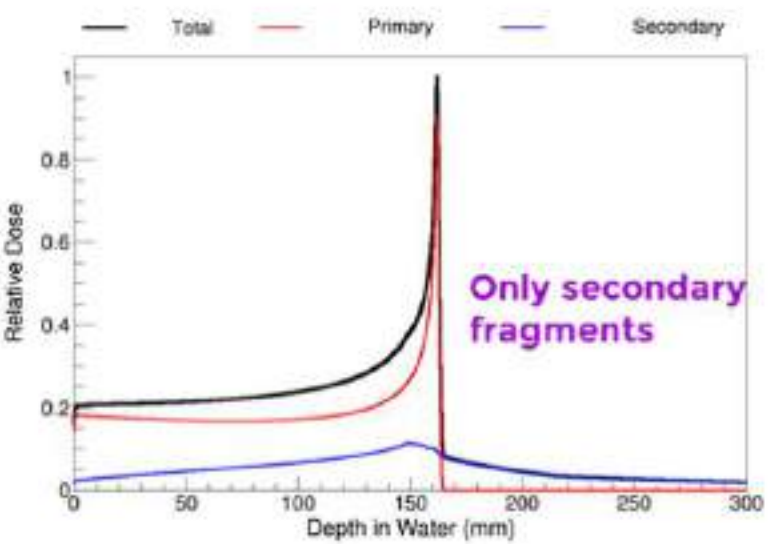
- Currently supported final states are (nA) nγs (discrete and continuum), np, nd, nt, n 3He, nα, nd2α, nt2α , n2p, n2α, np , n3α, 2nα, 2np, 2nd, 2nα, 2n2α, nX, 3n, 3np, 3nα, 4n, p, pd, pα, 2p d, dα, d2α, dt, t, t2α, 3He, α, 2α, and 3α.
- Secondary distribution probabilities are supported
  - isotropic emission
  - discrete two-body kinematics
  - N-body phase-space distribution
  - continuum energy-angle distributions
    - Legendre polynomials and tabulation distribution
    - Kalbach-Mann systematic   A + a → C → B + b, C:compound nucleus
  - continuum angle-energy distributions in the laboratory system
- Cross sections and final state models are based on world databases
  - G4PARTICLEHPDATA – includes all neutron and light ion low-energy data derived from JEFF-3.3 data library
  - G4PARTICLXSDATA – derived from G4PARTICLEHPDATA
  - G4LEVELGAMMADATA – data on nuclear levels and transition probabilities

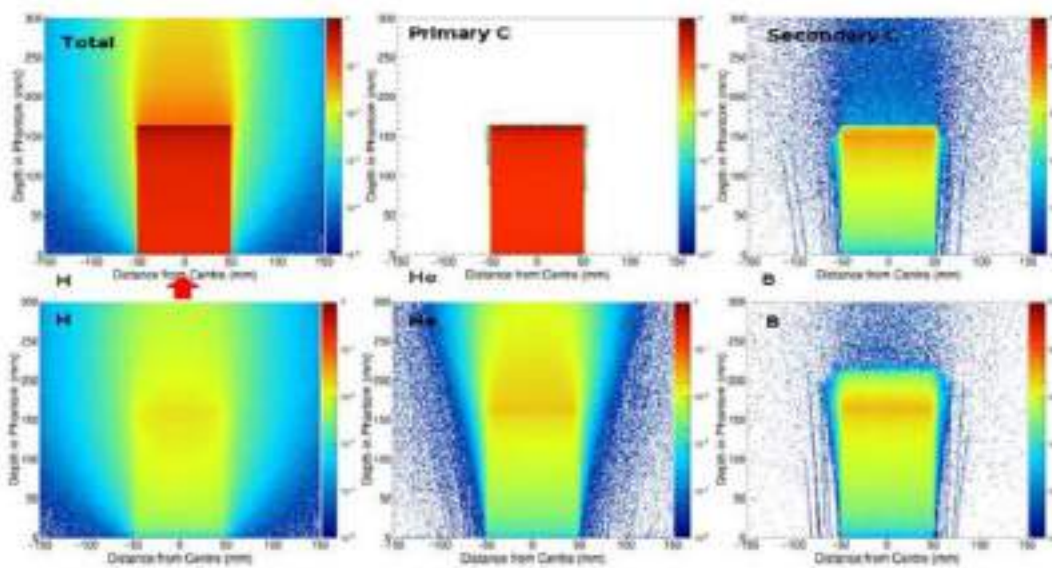
Neutron x-sections in Aluminum



Carbon ion therapy

- Methods of usage of proton and carbon beam for cancer treatment have been established in recent ~20 years in Japan
- Geant4 was validated using HIBMC facility, which provides high quality beam allowing to measure of Bragg peak position in water with accuracy 0.1 mm.
  - Mixed radiation field produced by a Carbon Ion Beam with clinical energy (290 MeV/u)
  - This and other studies confirms, that nuclear fragmentation make a significant contribution to the radiation field





Radioactive decay

- To simulate decay of radioactive nuclei
- Empirical and data-driven models
- Models of α, $\beta^{\pm}$ decays, and e^- capture are implemented
- Data derived from Evaluated Nuclear Structure Data File (ENSDF)
  - Nuclear half-lives, level structure, nuclear decay branching ratio, Q-value of decays, the data directory $G4RADIOACTIVEDATA
- If the daughter of a nuclear decay is an excited isomer, its prompt nuclear de-excitation is treated using photon evaporation code – data-base of γ lines and nuclear levels in $G4LEVELGAMMADATA
- G4RadioactiveDecayPhysics constructor can be added on top of any Physics List
  - Necessary options for time limit and internal gamma-electron conversion will be defined automatically

Geant4 Physics Lists

Physics Lists

- Physics List is an object that is responsible to:
  - specify all the particles that will be used in the simulation application
  - together with the list of physics processes assigned to each individual particles
- One out of the 3 mandatory objects that the user needs to provide to the G4RunManager in case of all Geant4 applications:
  - it provides the information when, how and what set of physics needs to be invoked
- Provides a very flexible way to set up the physics environment:
  - the user can chose and specify the particles that they want to be used
  - the user can chose the physics (processes) to assign to each particle
- Geant4 distribution includes the "physics_list" sub-library with many components and many predefined "reference" Physics Lists
  - Simulation results between different group of users may be compared

Modular Physics Lists

- Current recommendation to use Physics List via inheritance from G4VModularPhysicsList which derives from G4VUserPhysicsList
- Main public methods:
  - **G4VModularPhysicsList::RegisterPhysics**(G4VPhysicsConstructor*)
    - Addition of physics constructor
  - **G4VModularPhysicsList::ReplacePhysics**(G4VPhysicsConstructor*)
    - Replacement of the same type of physics constructor
- Constructor types:
  - Electromagnetic, EM extra (lepton-nuclear)
  - Decay, Radioactive Decay
  - Hadron elastic, hadron inelastic
  - Ion elastic and inelastic
  - Stopping of negatively charged particles
  - Step limiters (tracking cuts)
  - Optical
  - User may add custom constructor
- Physics List and its components are unique objects, which called in each thread two methods
  - **G4VPhysicsConstructor::ConstructParticle**()
  - **G4VPhysicsConstructor::ConstructProcess**()
  - Only const class members are allowed

Instantiation and ownership of physics objects

- G4PhysicsListHelper provides correct ordering for all processes from Geant4 libraries
  - **G4PhysicsListHelper*** helper = **G4PhysicsListHelper::GetPhysicsListHelper();**
  - helper->**RegisterProcess**(G4VProcess*, G4ParticleDefinition*);
- Custom process should be instantiated with defined ordering
  - **G4ParticleDefinition*** particle;
  - **G4ProcessManager*** man = particle->**GetProcessManager();**
  - man->**AddDiscreteProcess**(G4VDiscreteProcess*); // added to the end
  - man->**AddProcess**(G4VProcess*, idxAtRest, idxAlongStep, idxPostStep);
- Ownership of classes is not belonging to the Physics List class
  - **G4ParticleDefinition** classes are static shared between threads
  - **G4VProcess** classes are registered in process thread local store
  - Model classes for EM and hadronic physics are also registered in thread local stores
  - Hadronic cross sections are registered in another thread local store
  - All registrations and destructions are done automatically
- All processes, models, and cross section classes should be instantiated via "new"
  - Allowing sharing of processes/models between particles
  - Should not be included by object in any class
    - Does not guaranteed correct destruction order at different platforms

Choosing appropriate physics list

- There are groups of physics lists oriented to different application domains:
  - HEP experiments: FTFP_BERT, QGSP_FTFP_BERT, FTFP_BERT_ATL,….
  - Space applications: QBBC,….
  - Medical applications: QGSP_BIC,…
  - Radiation protection: Shielding,….
- There is no strong limitation for an application domain to use or not to use a particular physics lists for a given use case
  - We would always suggest to start from the default FTFP_BERT and to choose an alternative if there are special requirement:
    - More accurate models are needed: try FTFP_BERT_EMZ
    - Faster models are needed: try optimizing cut in range first

Naming convention

- Some Hadronic options:
  - "QGS" Quark Gluon String model (> ~15 GeV)
  - "FTF" FRITIOF String model (> ~5 GeV)
  - "BIC" Binary Cascade model (< ~10 GeV)
  - "BERT" Bertini Cascade model (< ~10 GeV)
  - "P" G4Precompound model used for de-excitation
  - "HP" High Precision neutron model (< 20 MeV)
- Some EM options:
  - No suffix: standard EM i.e. the default G4EmStandardPhysics constructor
  - EMV, EMX, EMY, EMZ, LIV, PEN, WVI, GS, SS – various EM physics
- Name decoding: String_Cascade_Neutron_EM
- The complete list with description see in the web page "Guide for Physics Lists"): http://geant4-userdoc.web.cern.ch/geant4-userdoc/UsersGuides/PhysicsListGuide/html/index.html

How to start and how get help?

Is Geant4 easy to use toolkit?

- Geant4 initially designed as a toolkit
  - This means that it is assumed to be a part of bigger software framework
  - Geant4 does not provide its native framework
- The set of examples allowing easy start for beginners but cannot serve complicated use cases
  - We always recommend users to study Geant4 examples
  - > 300 extended and advanced examples
- In medical domain there are specific setups used in radiation medicine
  - Linac
  - Brachytherapy
  - PET
  - Imaging
  - Geant4 Collaboration do not have enough manpower to provide support for all kind of simulations
- Usage of dedicated tools on top of Geant4 allows involvement more medical users and real practical oncologists in simulation

Software tools on top of Geant4

- GATE – simulation of preclinical and clinical scans in emission tomography, transmission tomography, and radiation therapy
  - http://www.opengatecollaboration.org/
- GAMOS is a GEANT4-based framework
  - http://fismed.ciemat.es/GAMOS/
  - Use plug-in mechanism to add modules to the system, which significantly increase flexibility
- TOPAS is a user-friendly simulation software layered upon the general-purpose Geant4 particle transport toolkit.
  - https://gray.mgh.harvard.edu/software/256-topas
  - It was designed specifically for medical physics applications by MGH, Stanford and UCSF
- Usage of external software also bring some disadvantages:
  - One must study both Geant4 and extra tool
  - Extra tool sometime uses not the most recent Geant4
  - Some features may be not well implemented

WEB resources

- Main Geant4 web https://geant4.web.cern.ch/ includes references to
  - Download page
  - Documentation
  - Main Geant4 publications
    - we ask to cite these publications in your articles
  - User forum
    - This is a place to discuss problems with developers and other users
  - Bug report system
  - Announcements
  - Open-source license
- Geant4 virtual machine https://geant4.lp2ib.in2p3.fr/
  - It is possible to install a player and ready to use virtual machine to your PC

How to start?

- Read documentation
- Install Geant4 according to manual
  - Compile Geant4 and examples of interest
- Alternatively install virtual machine
  - Geant4, ROOT, and QT visualization driver will be pre-installed for you
- Try to use Geant4 examples
  - Basic $G4INSTALL/example/basic
  - Electromagnetic
    - $G4INSTALL/examples/extended/electromagnetic/TestEm5
      - It is possible to used macro files from the example directory or use you own
      - Study penetration of particles via target – various histograms built-in
    - $G4INSTALL/examples/extended/electromagnetic/TestEm7
      - Study profile of energy deposition in the target for various particle type
      - Observe the Bragg peak of ionization
  - Hadronic
    - $G4INSTALL/examples/extended/hadronic/Hadr01
      - Study profile of energy deposition in the target
      - Study production of secondary particles
      - Study neutron flux after the target

Спасибо за внимание