



# Physics in GEANT4 – part 2

Luciano Pandola INFN – Laboratori Nazionali del Sud

pandola@lns.infn.it

The 2<sup>nd</sup> Geant4 School in China, Shandong University, Qingdao, March 25<sup>th</sup>- 29<sup>th</sup>, 2019

# Mixed Monte Carlo: tracking cuts and cut-inrange



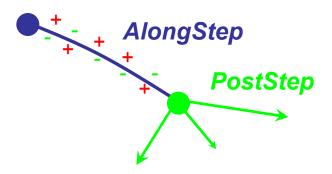
# Solution: the mixed MC

- Simulate explicitly (i.e. force step) interactions only if energy loss (or change of direction) is above threshold W<sub>0</sub>
  - Detailed simulation
  - "hard" interaction (like γ interactions)
- The effect of all sub-threshold interactions is described statistically
  - Condensed simulation
  - soft" interactions
- Hard interactions occur much less frequently than soft interactions
  - Fully detailed simulation restored for W<sub>0</sub>=0

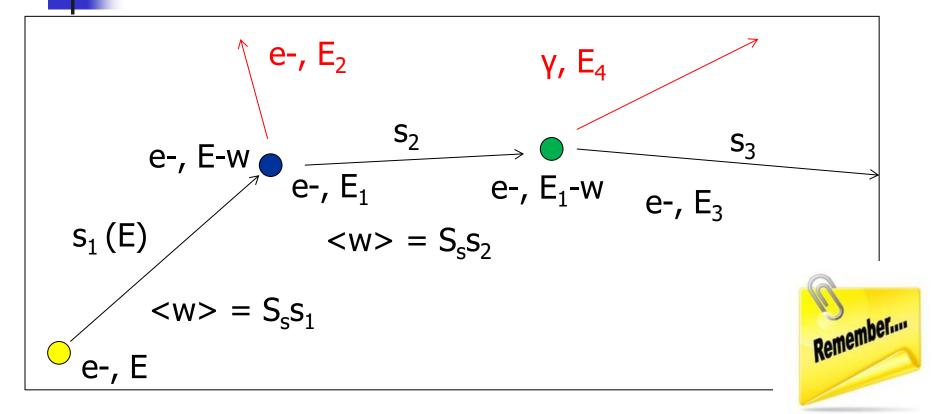


## The G4VProcess

- Physics processes are derived from the G4VProcess base class
- Abstract class defining the common interface of all processes in Geant4, used by all physics processes
- Three kinds of "actions":
  - AtRest actions
    - Decays, e<sup>+</sup> annihilation
  - AlongStep actions
    - To describe continuous (inter)actions, occurring along the path of the particle, i.e. "soft" interactions
  - PostStep actions
    - To describe the point-like (inter)actions, like decay in flight, hadronic interactions, i.e. "hard" interactions

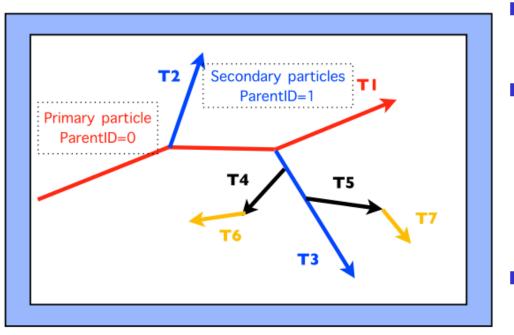


### Particle tracking: mixed recipe



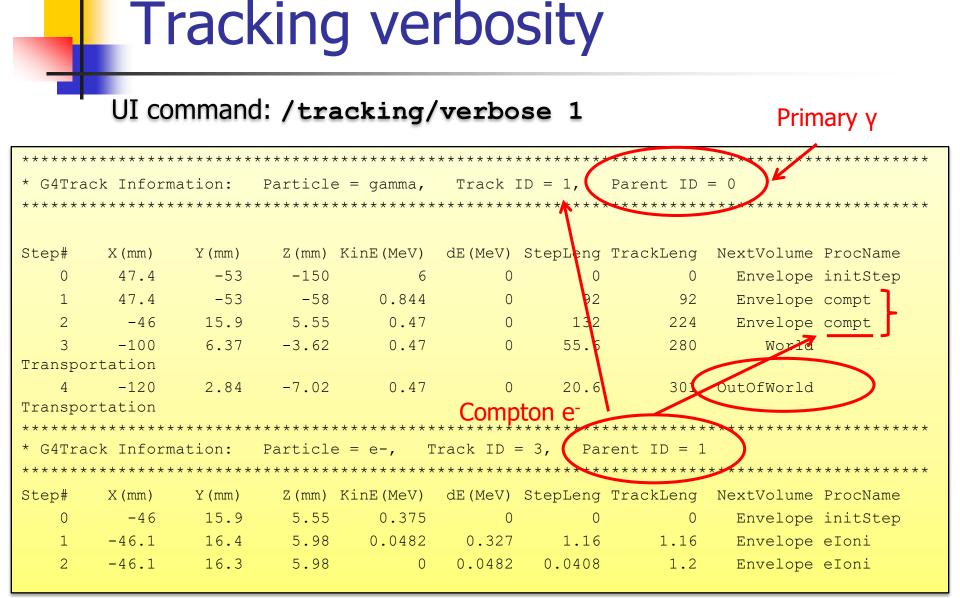
Follow all secondaries, until absorbed or leave volume

# Geant4 way of tracking



**Force step** at geometry boundaries

- All AlongStep processes co-work, the PostStep compete (= only one selected)
- Call AtRest actions for particles at rest
- Secondaries saved at the top of the stack: tracking order follows 'last in first out' rule: T1 → T3 → T5 → T7 → T4 → T6 → T2



# Geant4 production cuts

- The traditional Monte Carlo solution is to set a tracking cut-off in energy:
  - particles are stopped when this energy is reached and the residual energy is deposited at that point
  - May yield cause imprecise stopping location and deposition of energy
    - Particle and material dependence

#### Geant4 does not have tracking cuts

- All tracks are followed down to zero energy
  - ..or until they leave the world volume or are destroyed in interactions
- Could be implemented manually by the user
- Geant4 uses only a **production cut**  $(\rightarrow W_0)$ 
  - i.e. cuts deciding whether a **secondary** particle to be produced or not
    - AlongStep vs. PostStep
  - Applies only to: γ from bremsstrahlung, e<sup>-</sup> from ionization and lowenergy protons from hadronic elastic scattering

# Geant4 way of cuts: cut-inrange

- Geant4 solution: set a "range" production threshold
  - this threshold is a distance, not an energy
  - default = 1 mm
  - Particles unable to travel at least the range cut value are not produced
    - They contribute to the AlongStep!
- One production threshold is uniformly set
  - Sets the "spatial accuracy" of the simulation
- Production threshold is internally converted to the energy threshold W<sub>0</sub>, depending on *particle* type and *material*
  - Effective energy threshold is different in each material

## Production cut

#### Key ingredient of the mixed MC: energy threshold W<sub>0</sub>

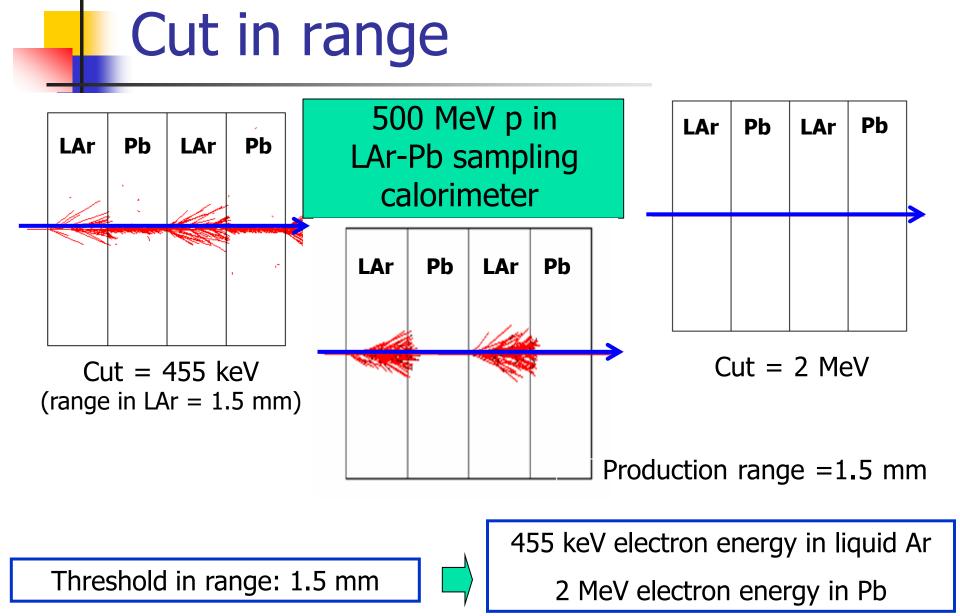
the best compromise

need to go low enough to get the physics you're interested in

accuracy

*can't go too low because some processes have infrared divergence causing huge CPU time* 

performance



# SetCuts()

#### Define all production cuts for gamma and electrons

- Lowest W<sub>0</sub> is 990 eV (but can be changed)
- Remember: this is a production cut, not a tracking cut

```
void MyPhysicsList::SetCuts()
```

```
//G4VUserPhysicsList::SetCuts();
defaultCutValue = 0.5 * mm;
SetCutsWithDefault();
SetCutValue(0.1 * mm, "gamma");
SetCutValue(0.01 * mm, "e+");
G4ProductionCutsTable::GetProductionCutsTable() Lower the possible
```

->SetEnergyRange(100\*eV, 100.\*GeV);

In G4VUserPhysicsList class

#### Cuts – UI commands

# Universal cut (whole world, all particles)
/run/setCut 10 mm

# Override low-energy limit
/cuts/setLowEdge 100 eV

# Set cut for a specific particle (whole world)
/run/setCutForAGivenParticle gamma 0.1 mm

# Set cut for a region (all particles)
/run/setCutForARegion myRegion 0.01 mm

# Print a summary of particles/regions/cuts
/run/dumpCouples



# **G4StepLimiter**

- Alternative to define the level of tracking detail
  Why?
  - you want to see the exact track of the particle
  - you don't trust the chord finder for your magnetic field
- How?
  - Include G4StepLimiter process in your physics list
    - Formally seen as a physics process, competing with all others: always proposing the same step length
    - Can be done by using the Geant4 constructor
       G4StepLimiterPhysics in a modular physics list

physicsList->RegisterPhysics(new G4StepLimiterPhysics());

 Set "user limits" for the logical volumes of interest: SetUserLimits()

logVol->SetUserLimits(new G4UserLimits(1.0 \* mm));

# Cuts per region

**G4Region** class

- Complex detector may contain many different subdetectors involving:
  - finely segmented volumes
  - position-sensitive materials (e.g. Si trackers)
  - Iarge, undivided volumes (e.g. calorimeters)
  - inert materials
- The same cut may not be appropriate for all of these
- User can define regions (independent of geometry hierarchy tree) and assign different cuts for each region
  - A region can contain a subset of the logical volumes



# Physics processes and models

# Philosophy

- Provide a general model framework that allows the implementation of complementary/alternative models to describe the same process (e.g. Compton scattering)
  - A given model could work better in a certain energy range
- Decouple modeling of cross sections and of final state generation
- Provide **processes** containing
  - <u>Many possible models</u> and cross sections
  - <u>Default cross sections</u> for each model

#### **Models under continuous development**

## **Electromagnetic physics**

# Inventory (and specs) of the models for γ-rays

1 MeV γ in Al

- Many models available for each process
  - Plus one full set of polarized models
- Differ for energy range, precision and CPU speed
  - Final state generators
- Different mixtures available the Geant4 EM constructors

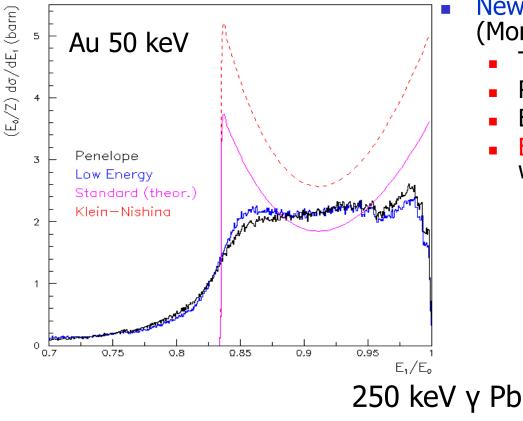
Model	E <sub>min</sub>	$E_{max}$	CPU
G4LivermoreRayleighModel	100 eV	10 PeV	1.2
G4PenelopeRayleighModel	100 eV	10 GeV	0.9
G4KleinNishinaCompton	100 eV	10 TeV	1.4
G4KleinNishinaModel	100 eV	10 TeV	1.9
G4LivermoreComptonModel	100 eV	10 TeV	2.8
G4PenelopeComptonModel	10 keV	10 GeV	3.6
G4LowEPComptonModel	100 eV	20 MeV	3.9
G4BetheHeitlerModel	1.02 MeV	100 GeV	2.0
G4PairProductionRelModel	10 MeV	10 PeV	1.9
G4LivermoreGammaConversionModel	1.02 MeV	100 GeV	2.1
G4PenelopeGammaConversionModel	1.02 MeV	10 GeV	2.2
G4PEEFluoModel	1 keV	10 PeV	1
G4LivermorePhotoElectricModel	10 eV	10 PeV	1.1
G4PenelopePhotoElectricModel	10 eV	10 GeV	2.9

#### Similar situation for e<sup>±</sup>

#### EM concept

- The same physics processes (e.g. Compton scattering) can be described by different models, that can be alternative or complementary in a given energy range
- For instance: Compton scattering can be described by
  - G4KleinNishinaCompton
  - G4LivermoreComptonModel (specialized low-energy, based on the Livermore database)
  - G4PenelopeComptonModel (specialized low-energy, based on the Penelope analytical model)
  - G4LivermorePolarizedComptonModel (specialized low-energy, Livermore database with polarization)
  - G4PolarizedComptonModel (Klein-Nishina with polarization)
  - G4LowEPComptonModel (full relativistic 3D simulation)
- Different models can be combined, so that the appropriate one is used in each given energy range (→ performance optimization)

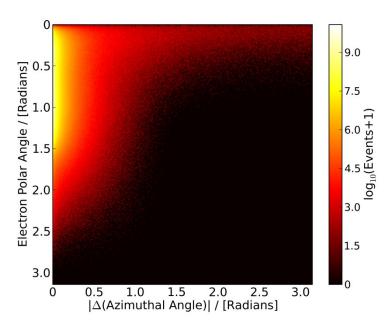
#### For example: Compton scattering



# CPU time is the **price to pay** for better precision

New model: G4LowEPComptonModel (Monash U.)

- Two-body relativistic 3-dim framework
- Relativistic impulse approximation
- Bound atomic electrons
- Electron distribution not uniform in φ wrt photon scattering plane



#### Packages overview

 Models and processes for the description of the EM interactions in Geant4 have been grouped in several packages

Package	Description
Standard	$\gamma$ -rays, e <sup>±</sup> up to 100 TeV, Hadrons, ions up to 100 TeV
Muons	Muons up to 1 PeV
X-rays	X-rays and optical photon production
Optical	Optical photons interactions
High-Energy	Processes at high energy (> 10 GeV). Physics for exotic particles
Low-Energy	Specialized processes for low-energy (down to 250 eV), including atomic effects
Polarization	Simulation of polarized beams

# EM processes for $\gamma$ -rays, e<sup>±</sup>

Particle	Process	G4Process
Photons	Gamma Conversion in e <sup>±</sup>	G4GammaConversion
	Compton scattering	G4ComptonScattering
	Photoelectric effect	G4PhotoElectricEffect
	Rayleigh scattering	G4RayleighScattering
e±	Ionisation	G4eIonisation
	Bremsstrahlung	G4eBremsstrahlung
	Multiple scattering	G4eMultipleScattering
e+	Annihilation	G4eplusAnnihilation

#### EM processes muons

Particle	Process	G4Process
$\mu^{\pm}$	Ionisation	G4MuIonisation
	Bremsstrahlung	G4MuBremsstrahlung
	Multiple scattering	G4MuMultipleScattering
	e <sup>±</sup> pair production	G4MuPairProduction

Only one model available for these processes (but in principle users may write *their own* models, if needed)

## Standard models

- Complete set of models for  $e^{\pm}$ ,  $\gamma$ , ions, hadrons,  $\mu^{\pm}$
- Tailored to requirements from HEP applications
  - "Cheaper" in terms of CPU
  - Include high-energy corrections (e.g. LPM), assumptions made in the low-energy regime
- Theoretical or phenomenological models
  - Bethe-Bloch, corrected Klein-Nishina, ...
  - Photoabsorption Ionization (PAI)
    - ionization energy loss of a relativistic charged particle in matter
- Specific high-energy extensions available
  - Extra processes, as  $\gamma \rightarrow \mu + \mu$ -, e<sup>+</sup>e<sup>-</sup>  $\rightarrow \mu + \mu$ -
- Dedicated sub-library for optical photons
  - Produced by scintillation or Cherenkov effect

#### Livermore (& polarized) models

- Based on publicly available evaluated data tables from the Livermore data library: e<sup>-</sup>, γ
  - EADL : Evaluated Atomic Data Library, EEDL : Evaluated Electrons Data Library, EPDL97 : Evaluated Photons Data Library, Binding energies: Scofield
  - Mixture of experiments and theories
  - In principle, tables go down to  $\sim 10 \text{ eV}$
- <u>Applications</u>: medical, underground and rare events, space
- Polarized models
  - Same calculation of the cross section, different way to produce the final state
  - Describe in detail the kinematics of polarized photon interactions
  - Application: space missions for the detection of polarized photons

## Penelope models

- Geant4 includes the low-energy models for electrons, positrons and photons from the Monte Carlo code PENELOPE (PENetration and Energy LOss of Positrons and Electrons)
  - Nucl. Instr. Meth. B 207 (2003) 107
  - Geant4 implements v2008 of Penelope
- Physics models specifically developed by the group of F. Salvat et al.
  - Great care dedicated to the low-energy description
  - Atomic effects, fluorescence, Doppler broadening...
- Mixed approach: analytical, parameterized and databasedriven
  - Applicability energy range: 100 eV 1 GeV
- Include positrons
  - Not described by Livermore models

# When/why to use Low Energy Models

- Use Low-Energy models (Livermore or Penelope), as an *alternative* to Standard models, when you:
  - need precise treatment of EM showers and interactions at low-energy (keV scale)
  - are interested in atomic effects, as fluorescence x-rays, Doppler broadening, etc.
  - can afford a more CPU-intensive simulation
  - want to cross-check an other simulation (e.g. with a different model)
- Do not use when you are interested in EM physics > MeV
  - same results as Standard EM models, performance penalty

## EM Physics Constructors for Geant4 10.5 - ready-for-the-use

G4EmStandardPhysics – default G4EmStandardPhysics\_option1 – HEP fast but not precise G4EmStandardPhysics\_option2 – Experimental G4EmStandardPhysics\_option3 – medical, space G4EmStandardPhysics\_option4 – optimal mixture for precision **G4EmLivermorePhysics** G4EmLivermorePolarizedPhysics **Combined** Physics Standard > 1 GeV G4EmPenelopePhysics **LowEnergy** < 1 GeV G4EmLowEPPhysics G4EmDNAPhysics\_option...

 Advantage of using of these classes – they are tested on regular basis and are used for regular validation

. . .

## How to extract Physics ?

- Possible to retrieve physics quantities via G4EmCalculator or directly from the physics models
  - Physics List should be initialized
- Example for retrieving the total cross section (cm<sup>-1</sup>) of a process with name *procName*: for particle *partName* and material *matName*

G4EmCalculator **emCalculator**;

G4Material\* material =

G4NistManager::Instance()->FindOrBuildMaterial("matName);

G4double massSigma = emCalculator.ComputeCrossSectionPerVolume (energy,particle,procName,material);

G4cout << G4BestUnit(massSigma, "Surface/Volume") << G4endl;

#### A good example: \$G4INSTALL/examples/extended/electromagnetic/ TestEm14

## **Optical physics**

#### (some more slides than in my usual Geant4 beginer courses)

# **Optical photons**

- Dedicated particle in Geant4: G4OpticalPhoton
  - Different from G4Gamma
  - No smooth transition between them
  - Polarization information included
- Handling of optical photons in Geant4 requires:
  - Processes able to **produce** optical photons (G4Scintillation, G4Cerenkov, etc.)
  - Processes to **describe** the interaction of optical photons
    - Bulk processes (absorption, elastic scattering, wls)
    - Boundary processes (reflection, refraction, etc.)
    - According to the laws of optics

Same concept applies to G4Phonon (and other exotic)

# **OpPhoton tracking**

- Typically many 1000's of photons per MeV
  - CPU-intensive
  - Track op-photons immediately, to avoid the stack overflow. Specific setting in the parent process(es), e.g.
    - CerenkovProcess->SetTrackSecondaryFirst(true);
- Good tracking requires the accurate knowledge of bulk and surface optical properties
  - Not always available (especially for boundaries)
  - So, tuning from the data
- Make sure that you really need it (!)
- Good examples to start with:
  - examples/extended/optical

#### Processes to create opPhotons

- Optical photons are produced by :
  - G4Cerenkov
  - G4Scintillation
  - G4TransitionRadiation
  - <u>Warning</u>: these processes generate optical photons without energy conservation

#### Pure "AlongStep" processes

- Average number according to ΔE in the step: actual number sampled from Poisson distribution
- Still can limit the step in special cases (e.g. refraction index drops below Cerenkov threshold)
- Emission position sampled uniformly along the step
- Scintillation yield, spectrum and time can be set from the user
  - slow/fast component, different yields per particles

Processes to handle opPhotons

- Optical photons are handled by :
  - bulk absorption (G4OpAbsoption)
  - Rayleigh scattering (G4OpRayleigh)
  - wavelength shifting (G4OpWLS)
  - refraction and reflection at medium boundaries (G4OpBoundary)
  - All "discrete" processes
- Geant4 keeps track of polarization
  - but not overall phase → no interference
- User can supply
  - WLS emission spectrum and decay time
  - Reflectivity, surface properties (roughness, specular, metal vs. dielectric, etc.) of all boundaries
  - Mean free path for Rayleigh and absorption

# **Optical properties**

- Bulk properties stored as G4MaterialPropertiesTable and attached to G4Material
  - Refraction index, absorption length, Rayleigh mfp vs.  $\lambda$
  - Scintillation yield, spectra and time constants
  - WLS properties
- Boundary properties stored as G4MaterialPropertiesTable attached to G4OpticalSurface, which in turn belongs to
  - G4LogicalBorderSurface (ordered pair of logical volumes)
  - G4LogicalSkinSurface (skin of a logical volume)
  - Include reflectivity and absorbance (vs. λ), surface polishing (polished or rough), dielectric vs. metal, specular lobe vs. spike reflectivity, rms roughness, ...
- <u>Typical case</u>: properties are unknown (esp. surface) and have to be tuned from data

# Hadronic physics

(a very quick overview)

# **Hadronic Physics**

- Data-driven models
- Parametrised models
- Theory-driven models

# Hadronic processes

- At rest
  - Stopped muon, pion, kaon, anti-proton
  - Radioactive decay
  - Particle decay (decay-in-flight is PostStep)
- Elastic
  - Same process to handle all long-lived hadrons (multiple models available)
- Inelastic
  - Different processes for each hadron (possibly with multiple models vs. energy)
  - Photo-nuclear, electro-nuclear, mu-nuclear
- Capture
  - Pion- and kaon- in flight, neutron
- Fission

# Hadronic physics challenge

#### Three energy regimes

- < 100 MeV</p>
- resonance and cascade region (100 MeV 10 GeV)
- > 20 GeV (QCD strings)
- Within each regime there are several models
- Many of these are phenomenological

Reference physics lists for Hadronic interactions

#### Two families of builders for the high-energy part

- QGS, or list based on a model that use the Quark Gluon String model for high energy hadronic interactions of protons, neutrons, pions and kaons
- FTF, based on the FTF (FRITIOF like string model) for protons, neutrons, pions and kaons
- Three families for the cascade energy range
  - **BIC**, binary cascade
  - BERT, Bertini cascade
  - INCLXX, Liege Intranuclear cascade model

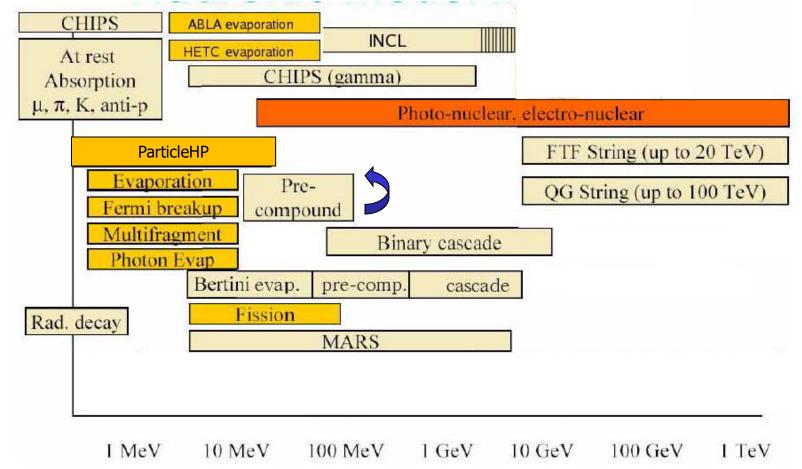


## **ParticleHP Models**

- Since Geant4 10.2  $\rightarrow$  ParticleHP
  - Data-driven approach for *inelastic* reactions for n (in place since many years, named NeutronHP) p, d, t, <sup>3</sup>He and a
  - Data based on TENDL-2014 (charged particles) and ENDFVII.r1 (neutrons). Compressed binary files
    - For neutrons, includes information for *elastic* and *inelastic scattering, capture, fission* and *isotope production*
  - Range of applicability: from thermal energies up to 20 MeV
  - Very precise tracking, but also very slow
  - Use it with care: thermal neutron tracking is very CPU-demanding
    - A thermal neutron can have 100's of thermal scatterings before being captures
    - No cut applied on low-energy protons from elastic scattering
- **NeutronHP** fully merged with ParticleHP since 10.3
  - NeutronHP headers are still included the release 10.3 for backwards compatibility, but they will be removed
- Neutron models debugged since a long while, but it is a fresh development for the other particles

#### Hadronic model inventory

#### http://geant4.cern.ch/support/proc\_mod\_catalog/models



## **Cross sections**

- Default cross section sets are provided for each type of hadronic process:
  - Fission, capture, elastic, inelastic
- Can be overridden or completely replaced
- Different types of cross section sets:
  - Some contain only a few numbers to parameterize cross section
  - Some represent large databases (data driven models)
- Cross section management
  - GetCrossSection ()  $\rightarrow$  sees last set loaded for energy range

# Geant4 extensions / exotic

- The tracking implemented in Geant4 is very general and transparent
  - Possible to accommodate for custom particles and processes
  - Possible to accommodate for alternative models, also to be used together with the Geant4 ones
- <u>Recent development</u>: add the possibility to simulate solid state effects (e.g. channeling)



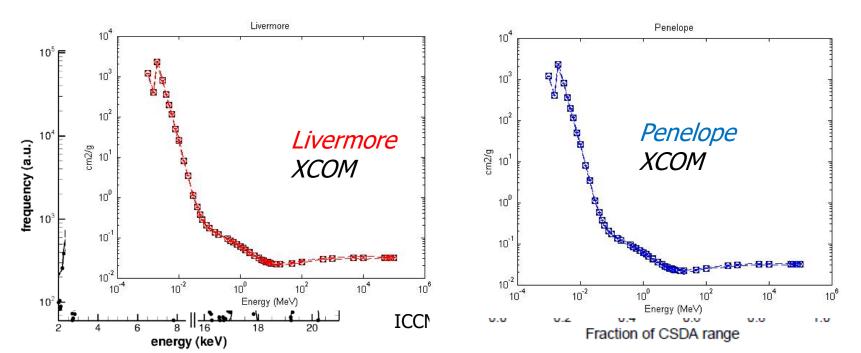
- Extension of the G4Material to include lattice properties
  - E.g. unit cell
- Framework generic enough to include other kinds of auxiliary material properties
- See examples/extended/exoticphysics

## Quick overview of validation

-

# EM validation - 1

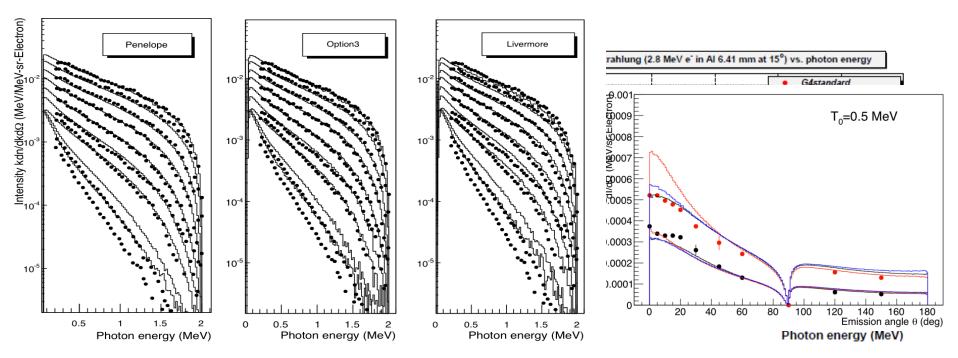
- Tens of papers and studies available
  - Geant4 Collaboration + User Community
- Results can depend on the specific observable/reference
  - Data selection and assessment critical

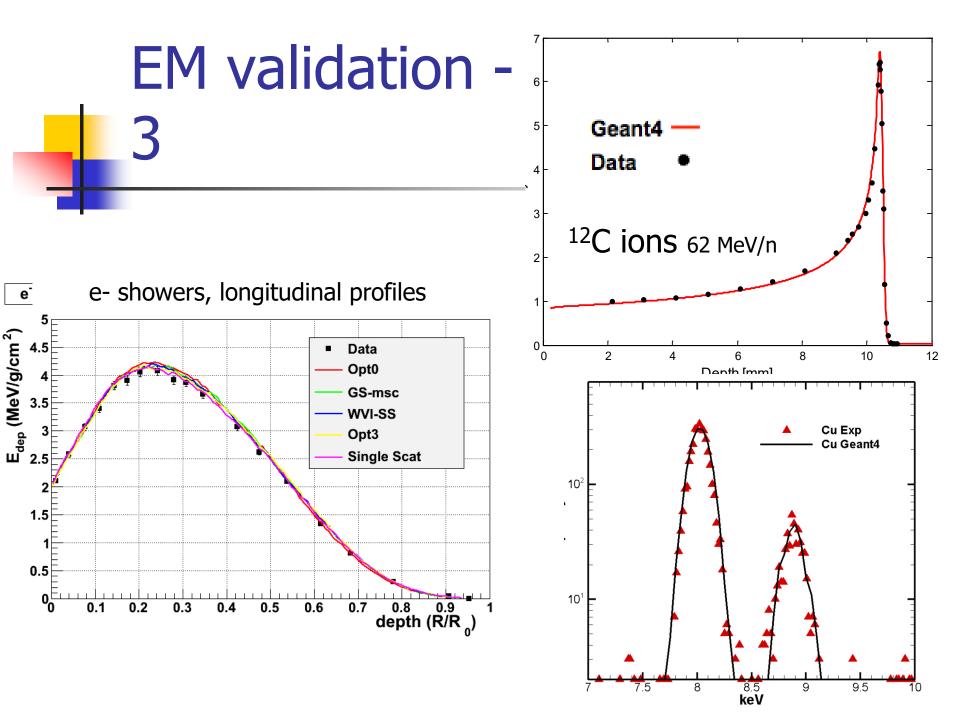


# EM validation – 2

- In general satisfactory agreement
- Validation/verification repository available on web

http://cern.ch/vnivanch/verification/verification/electromagnetic/



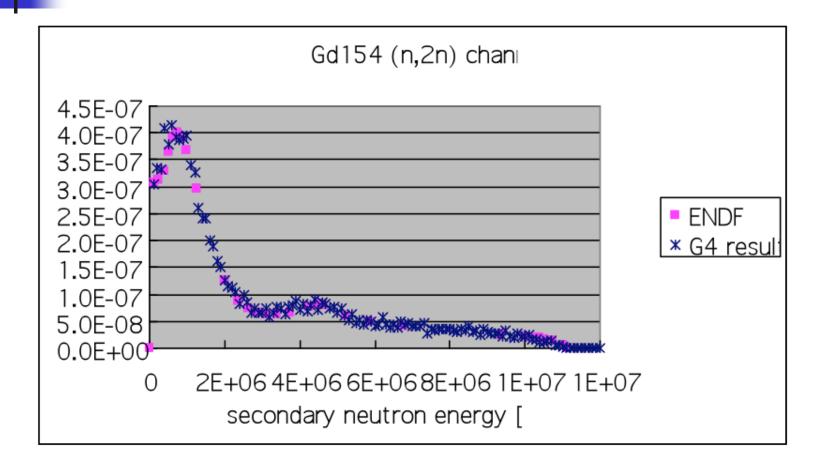


#### Hadronic validation

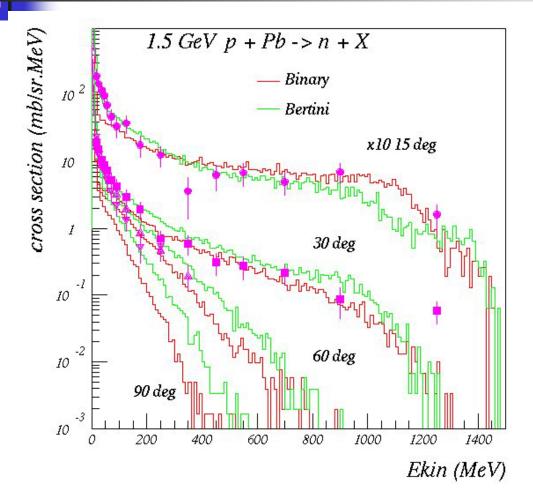
 A website is available to collect relevant information for validation of Geant4 hadronic models (plots, tables, references to data and to models, etc.) http://geant4.cern.ch/results/validation\_plots.htm http://g4validation.fnal.gov:8080/G4ValidationWebApp/

- Several physics lists and several use-cases have been considered (e.g. thick target, stopped particles, lowenergy)
- Includes final states and cross sections

# Some verification: secondary energy spectrum

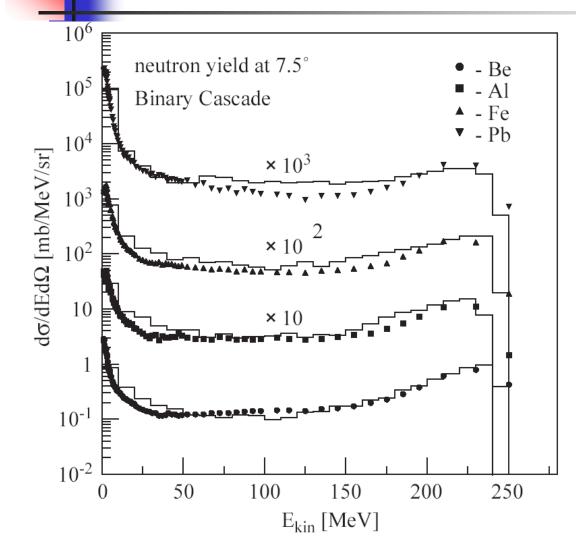


#### Nuclear fragmentation



Bertini and Binary cascade models: neutron production vs. angle from 1.5 GeV protons on Lead

#### Neutron production by protons



Binary cascade model: double differential cross-section for neutrons produced by 256 MeV protons impinging on different targets

# Hands-on session Task3c

#### http://202.122.35.42/task3



## EM concept - 2

- A physical interaction or process is described by a process class
  - Naming scheme : « G4ProcessName »
  - Eg. : « G4Compton » for photon Compton scattering
- A physical process can be simulated according to several models, each model being described by a <u>model class</u>
  - The usual naming scheme is: « G4ModelNameProcessNameModel »
  - Eg. : « G4LivermoreComptonModel » for the Livermore Compton model
  - Models can be alternative and/or complementary on certain energy ranges
  - Refer to the Geant4 manual for the full list of available models

#### **NeutronHP Models**

- Dedicated NeutronHP models in Geant4 since many years
  - HP = high-precision
- Cross sections and final state information based on ENDF/BVII.1 tabulated data (G4LEND)
  - Includes information for *elastic* and *inelastic scattering, capture, fission* and *isotope production*
- Applicable from thermal energies to 20 MeV
  - Very precise tracking, but also very slow
  - Use it with care: thermal neutron tracking is very CPU-demanding
    - A thermal neutron can have 100's of thermal scatterings before being captures
- Included in all physics lists ending with <u>HP</u> and <u>Shielding</u>

Cuts per region – C++ code

MyPhysicsList::SetCuts()

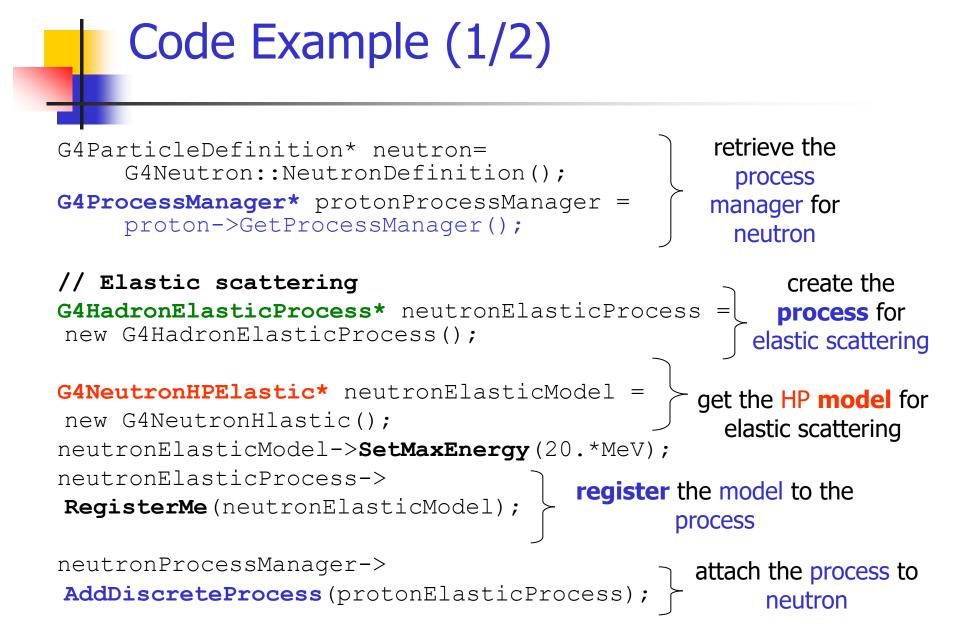
// default production thresholds for the world volume
SetCutsWithDefault();

// Same cuts for all particle types
G4Region\* region = G4RegionStore::GetInstance()->GetRegion("myRegion1");
G4ProductionCuts\* cuts = new G4ProductionCuts;
cuts->SetProductionCut(0.01\*mm); // same cuts for gamma, eregion->SetProductionCuts(cuts);

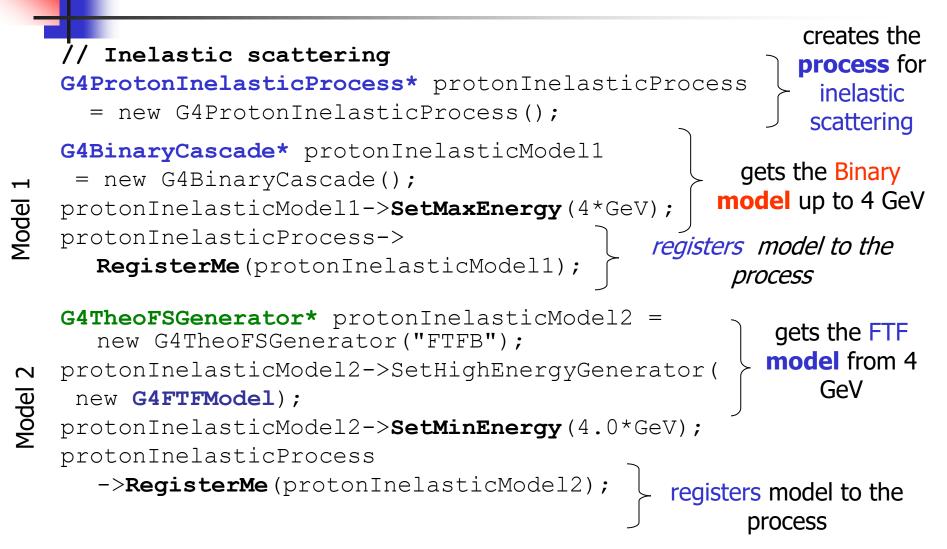
// individual production thresholds for different particles
region = G4RegionStore::GetInstance()->GetRegion("myRegion2");
cuts = new G4ProductionCuts;
cuts->SetProductionCut(1 \* mm, "gamma");
cuts->SetProductionCut(0.1 \* mm, "e-");
region->SetProductionCuts(cuts);

// ... or (simpler)
SetCuts(0.01 \* mm, "gamma", "absorber");

7



#### Code example (2/2)



## **Example:** PhysicsList, γ-rays

G4ProcessManager\* pmanager = G4Gamma::GetProcessManager(); pmanager->AddDiscreteProcess(new G4PhotoElectricEffect); pmanager->AddDiscreteProcess(new G4ComptonScattering); pmanager->AddDiscreteProcess(new G4GammaConversion); pmanager->AddDiscreteProcess(new G4GammaConversion);

• Use AddDiscreteProcess because γ-rays processes have only PostStep actions

• For each process, the default model is used among all the available ones (e.g. G4KleinNishinaCompton for G4ComptonScattering)

## Alternative cross sections

- To be used for specific applications, or for a given particle in a given energy range, for instance:
- Low energy neutrons
  - elastic, inelastic, fission and capture (< 20 MeV)</li>
- Neutron and proton inelastic cross sections
  - 20 MeV < E < 20 GeV</p>
- Ion-nucleus reaction cross sections (several models)
  - Good for E/A < 1 GeV
- Isotope production data
  - E < 100 MeV
- Photo-nuclear cross sections

Information on the available cross sections at http://geant4.cern.ch/support/proc\_mod\_catalog/cross\_sections/