Version 11.1

Electromagnetic Physics

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Geant4 Advanced Course

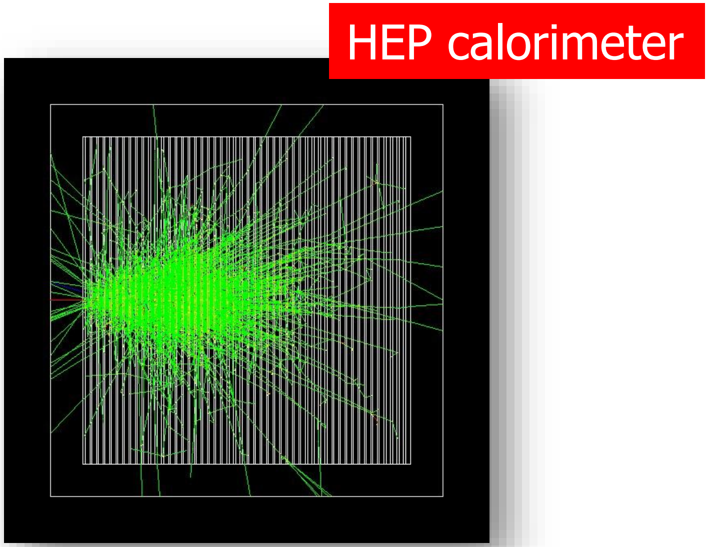
Outline

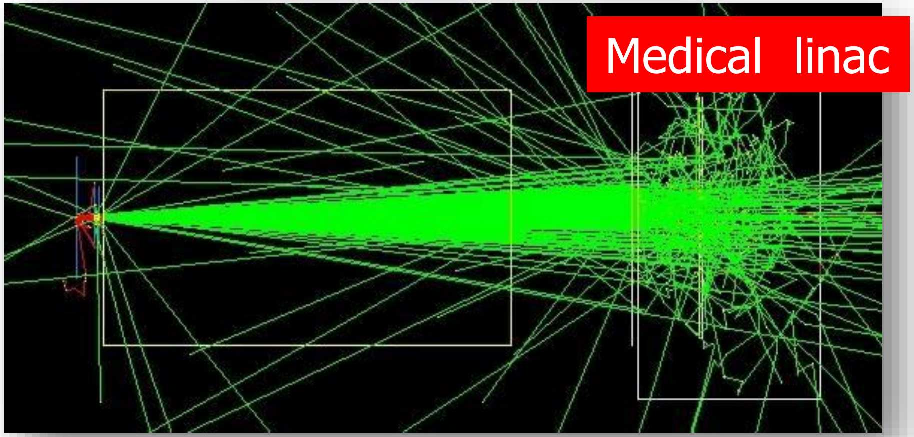
- Electromagnetic physics (EM) overview
- Main Gamma processes
- Main charged particle processes
- Secondary production thresholds
- EM physics constructors
- User interface to EM physics
- Special EM topics

ELECTROMAGNETIC (EM) PHYSICS OVERVIEW

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





Geant4 EM sub-libraries

Located in $G4INSTALL/sources/processes/electromagnetic

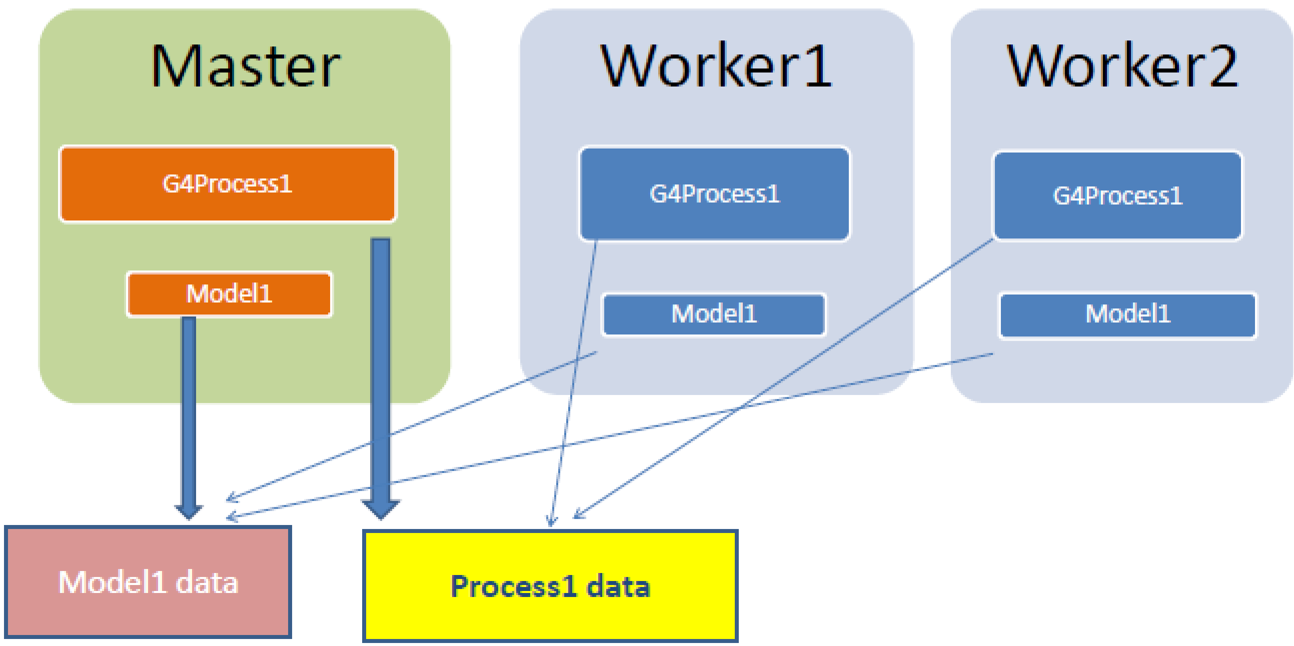
- Standard
  - γ, e up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV
- Muons
  - up to 1 PeV
  - energy loss propagator
- X-rays
  - X-ray and optical photon production processes
- High-energy
  - processes at high energy (E>10GeV)
  - physics for exotic particles
- Polarisation
  - simulation of polarised 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 10 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

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
- **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

Main Gamma Processes

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

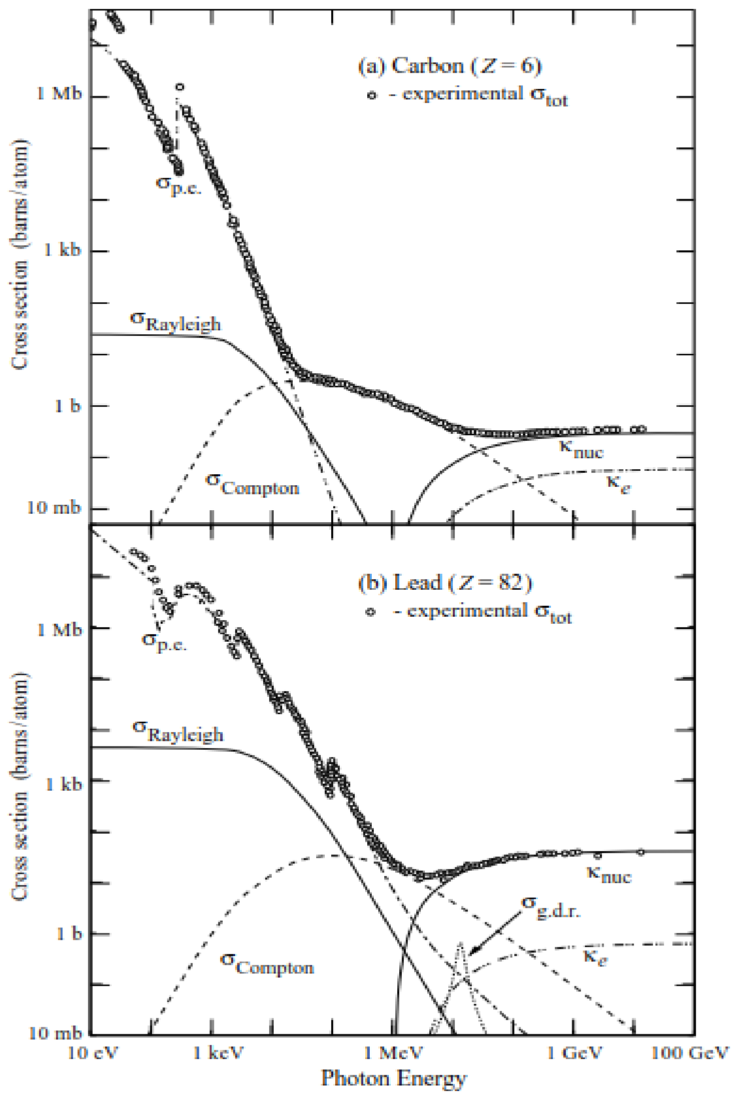
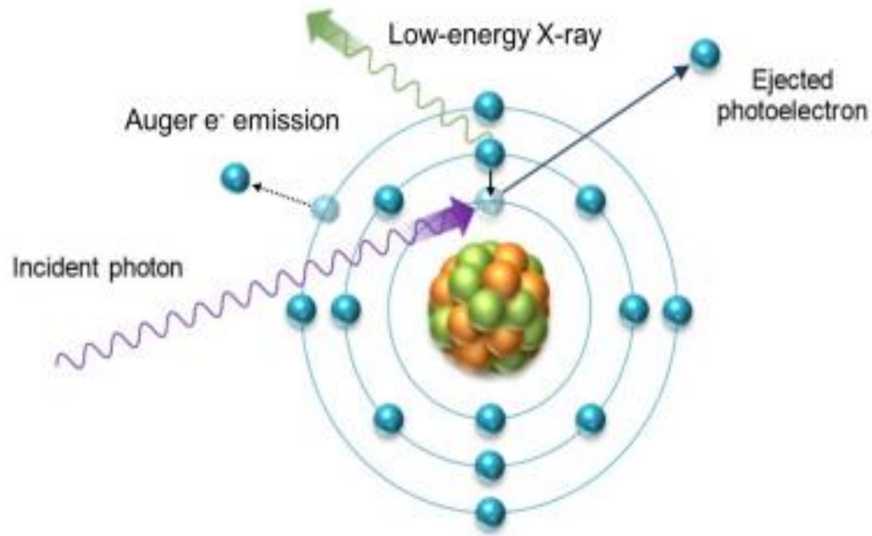


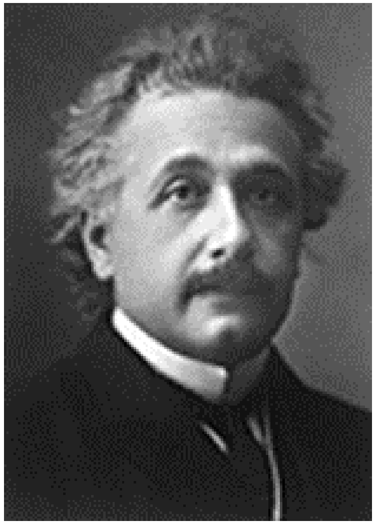
Photo-electric effect – example of gamma process

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

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

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

Atomic de-excitation

- Atomic de-excitation is initiated by other EM physics interactions:
  - photoelectric effect, ionisation (by e- or ions PIXE), Compton scattering,…
  - these interactions leave the target atom in an excited state
- The EADL (Evaluated Atomic Data Library) contains transition probabilities:
  - radiative transition characteristic X-ray emission (fluoressence photon emission)
  - Auger e- emission: initial and final vacancies are in different shells
  - Coster-Kronig e- emission: initial and final vacancies are in the same shells
- Due to a common interface, the atomic de-excitation is compatible with both the standard and the low-energy EM physics categories:
  - can be enabled and controlled by UI command (before initialization):

```
/process/em/fluo true
/process/em/auger true
/process/em/pixe true

/run/initialize
```

  - fluorescence transition is active by default in some EM physics constructor while others (Auger, PIXE) not

Gamma EM processes in the standard output

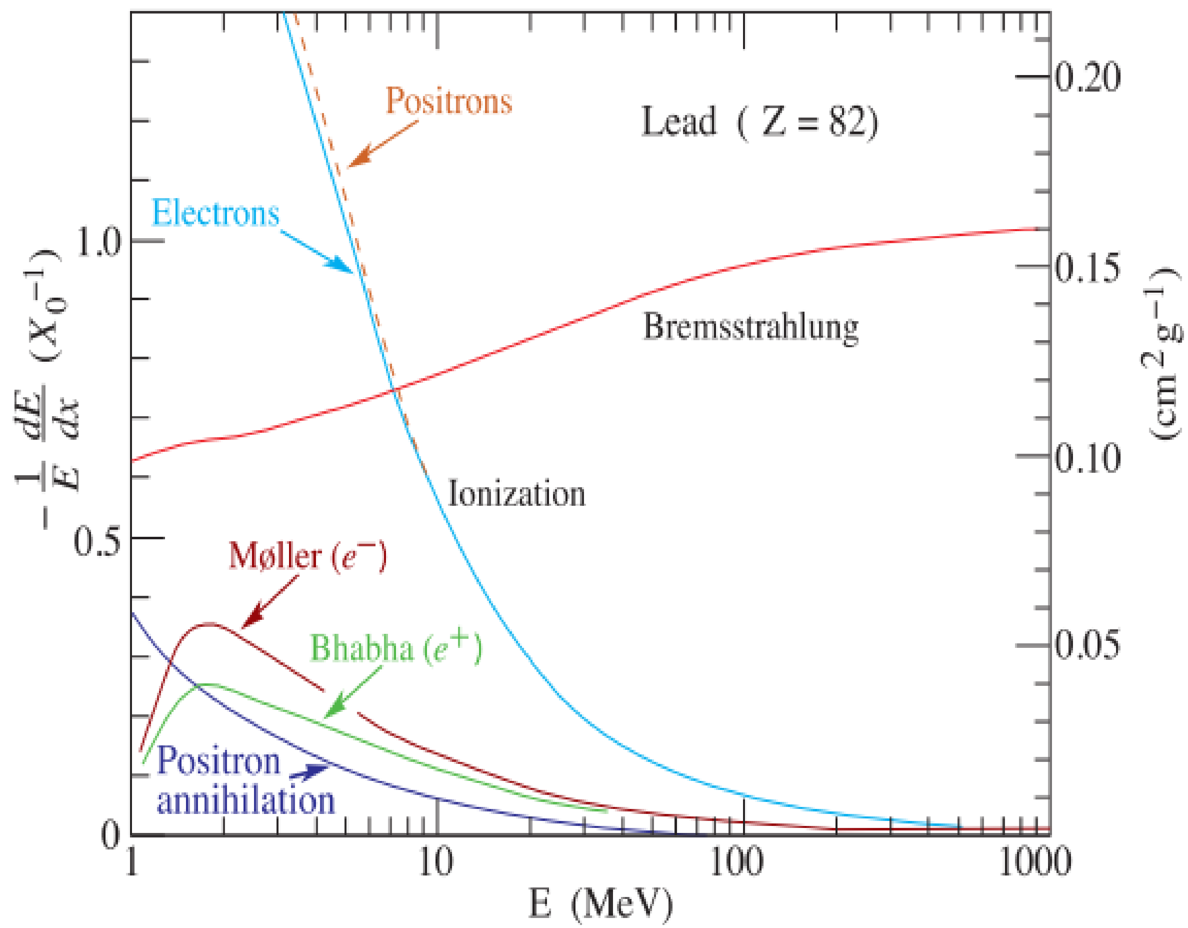
- Geant4 standard EM interactions for:
  - photon (γ) interactions (example):

```
phot:    for  gamma    SubType= 12  BuildTable= 0
      LambdaPrime table from 200 keV to 100 TeV in 61 bins
      ===== EM models for the G4Region  DefaultRegionForTheWorld ======
 LivermorePhElectric :  Emin=       0 eV    Emax=     100 TeV   AngularGenSauterGavrila  FluoActive

compt:    for  gamma    SubType= 13  BuildTable= 1
      Lambda table from 100 eV  to 1 MeV, 7 bins per decade, spline: 1
      LambdaPrime table from 1 MeV to 100 TeV in 56 bins
      ===== EM models for the G4Region  DefaultRegionForTheWorld ======
       Klein-Nishina :  Emin=       0 eV    Emax=     100 TeV

conv:    for  gamma    SubType= 14  BuildTable= 1
      Lambda table from 1.022 MeV to 100 TeV, 18 bins per decade, spline: 1
      ===== EM models for the G4Region  DefaultRegionForTheWorld ======
        BetheHeitler :  Emin=       0 eV    Emax=      80 GeV   AngularGenUrban
     BetheHeitlerLPM :  Emin=      80 GeV   Emax=     100 TeV   AngularGenUrban

Rayl:    for  gamma    SubType= 11  BuildTable= 1
      Lambda table from 100 eV  to 100 keV, 7 bins per decade, spline: 0
      LambdaPrime table from 100 keV to 100 TeV in 63 bins
      ===== EM models for the G4Region  DefaultRegionForTheWorld ======
   LivermoreRayleigh :  Emin=       0 eV    Emax=     100 TeV   CullenGenerator
```

Main Charged Particle Processes

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



Simulation of a step of a charged particle

- Values of mean dE/dx, range, cross section of δ-electron production, and bremsstruhlung are pre-computed at initialisation stage of Geant4 and are stored in a G4PhysicsTable

- At run time for each simulation step, a spline interpolation of tables is used to get mean energy loss

- At each step, a sampling of the energy loss fluctuation is performed
  - The interface to a fluctuation model is G4VEmFluctuationModel

- The cross sections of δ-electron production and bremsstrahlung are used to sample production above the threshold T_{cut} at PostStep

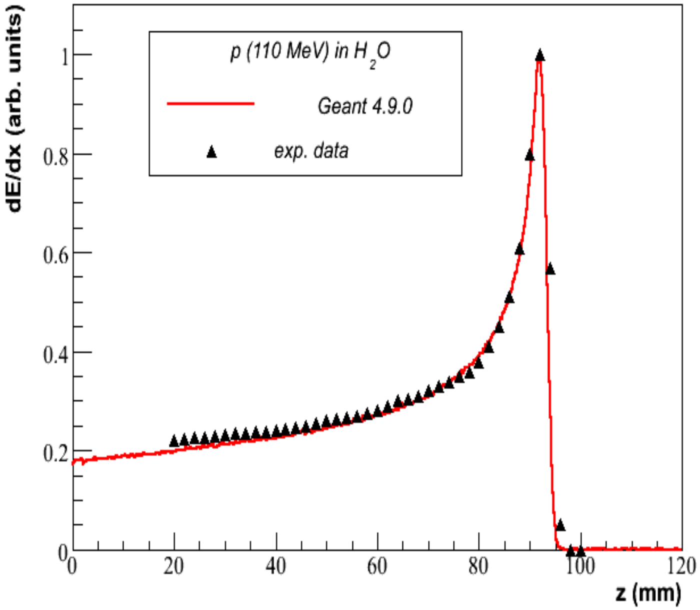
- If atomic de-excitation is active, then fluorescence and Auger electron production is sampled AlongStep and PostStep

Hadron and ion ionisation

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

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

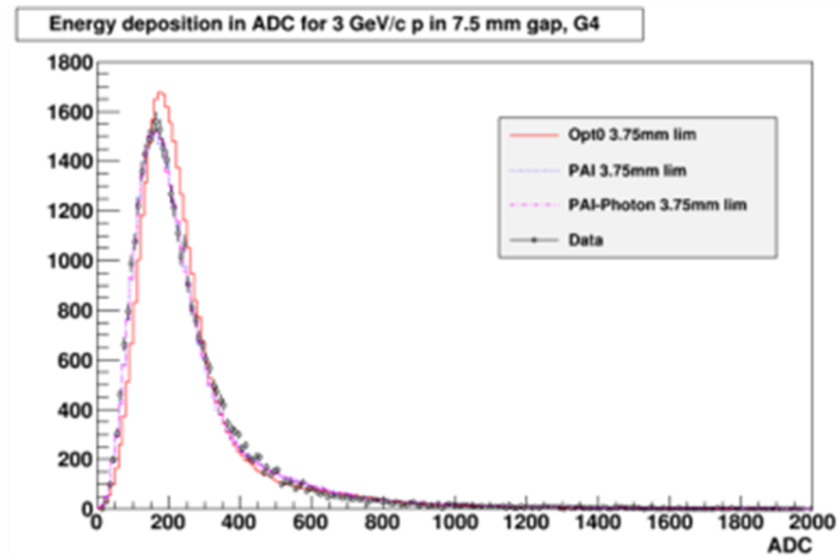
  - C – shell correction
  - G – Mott correction
  - δ – density correction
  - F – finite size correction
  - L_1- Barkas correction
  - L_2- Bloch correction
  - Nuclear stopping
  - Ion effective charge

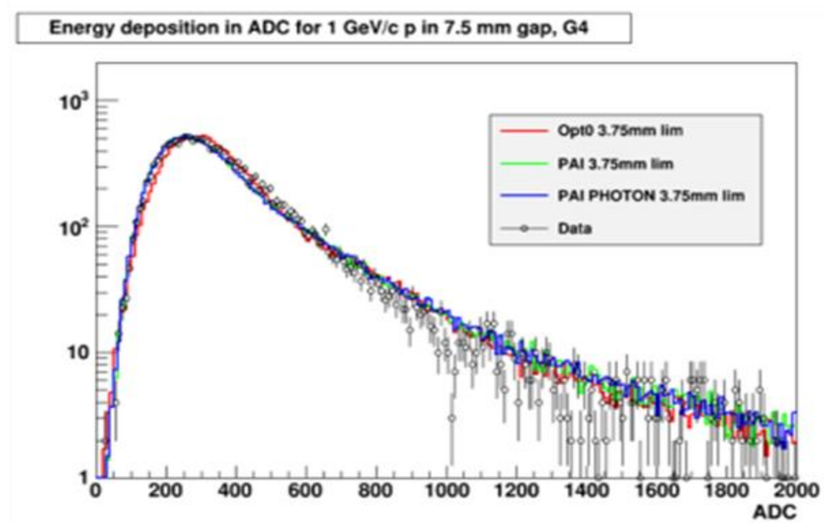


- Bragg peak parameterizations for E< 2 MeV
  - ICRU'49, ICRU'73, ICRU'90, and NIST databases
- Scaling relation for heavy particles:
  - $S_h(E) = S(E^*M_p/M_h)^*Q_h^2$,
  - M_h , Q_h - hadron mass and charge
  - Applicable to any charged particle including exotics and all ions
  - This is possible, because dE/dx depend mainly on β

Geant4 models of energy loss fluctuations

- Urban model based on a simple model of particle-atom interaction
  - Atoms are assumed to have only two energy levels E_1 and E_2
  - Particle-atom interaction can be:
    - an excitation of the atom with energy loss $E = E_1 - E_2$
    - an ionization with energy loss distribution $g(E) \sim 1/E^2$
- PAI model uses photo absorption cross section data
  - Energy transfers are sampled with production of secondary e^- or γ
  - Relativistic model
  - Very slow model, should be applied for sensitive region of detector

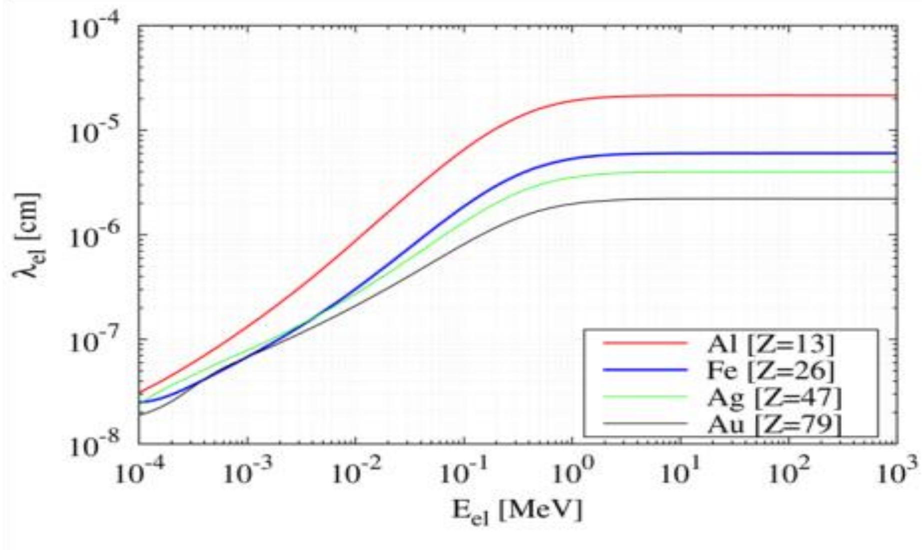




Multiple Coulomb scattering

- Coulomb scattering: elastic scattering of charged particles on the atomic potential
- Event-by-event modelling of elastic scattering is feasible only if the mean number of interactions per track is below few hundred
- this limits the applicability of the detailed simulation model only for electrons with relatively low kinetic energies
    - up to 100 keV or thin targets

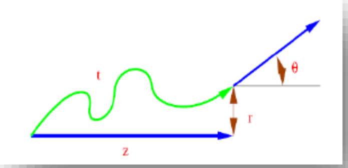
elastic MFP of electrons



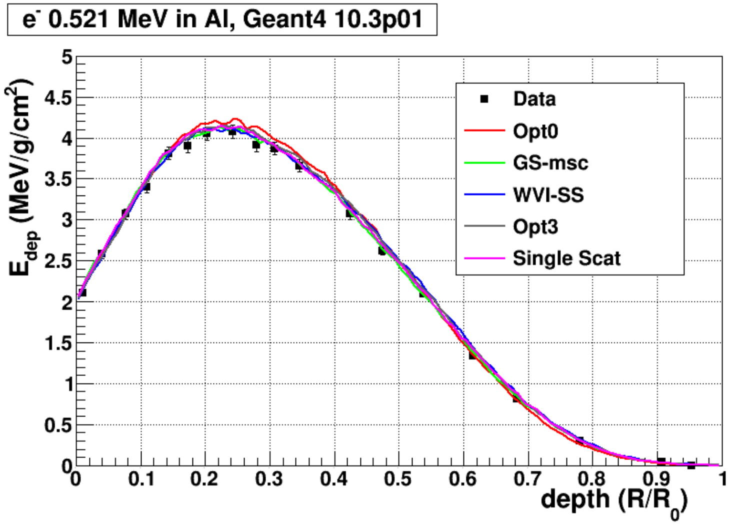
- detailed simulation becomes very inefficient, high energy particle transport simulation codes employ condensed history simulation model
    - multiple scattering (MSC) model is a solution
    - each track is simulated considering many elastic scattering at a step
- A summary effects of high number of elastic interactions is in
    - angular deflection of the particle
    - spatial displacement of the track post step point
    - increased effective track length

Electron/positron Multiple Scattering

- The algorithm performs simulation of many elastic scatterings at a step of a particle
  - The physics processes and the geometry select the step length; MSC performs the t ↔ z transformation only
  - Sampling of scattering angle (θ, Φ)
  - Computing of displacement and relocation of particle AlongStep



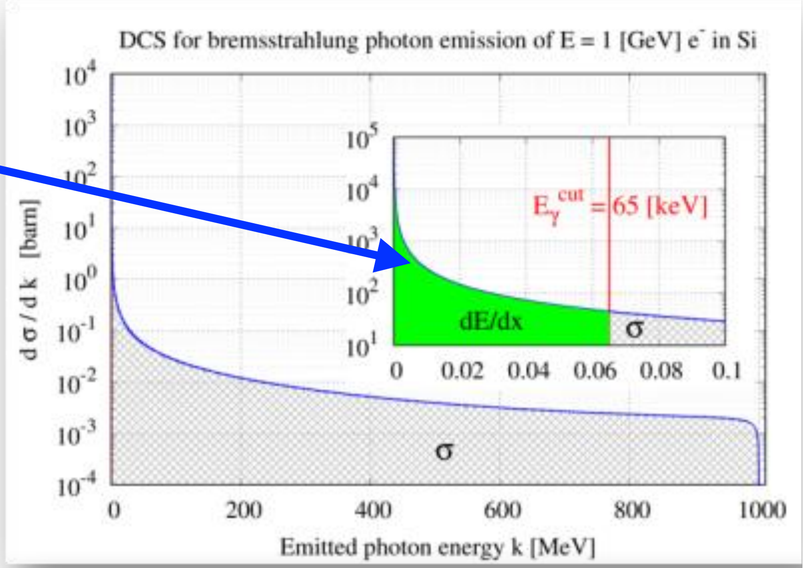
- To provide accurate simulation on geometry interface between different materials MSC step limitation is applied
  - Simple
  - UseSafety
  - UseSafetyPlus
  - UseDistanceToBoundary
- Other step limit parameters:
  - RangeFactor – is the most important
  - Geometry factor
  - Safety factor
  - Skin
  - Lambda limit
- Default MSC parameters are optimized for
  - Accurate simulation of EM showers
  - HEP sampling calorimeters
  - Accurate simulation of shielding

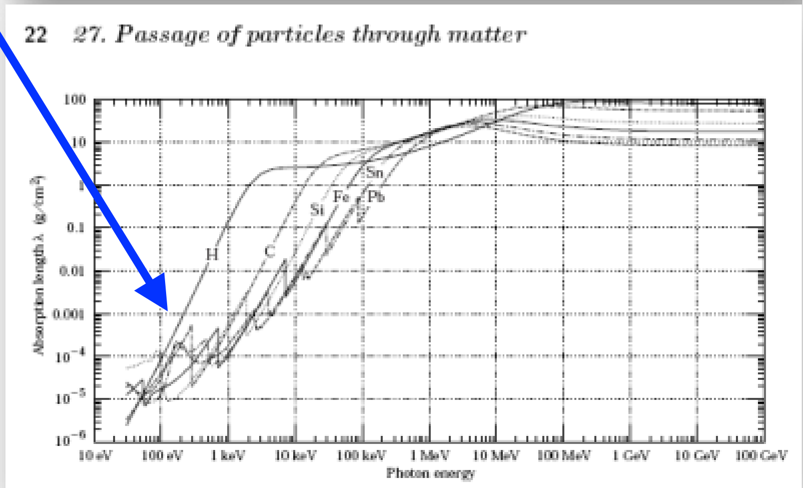


Secondary production thresholds

Secondary production threshold for bremsstrahlung

- Bremsstrahlung photon emission:
  - low energy photons (k) will be emitted with high rate DCS ~ 1/k
  - generation and tracking of all these low energy photons would not be feasible (CPU time)
  - but low energy photons has a very small absorption length
  - If the detector spacial resolution is worst than this length then the followings are *equivalent*:
    - *a*: generating and tracking these low energy photons till all their energy will be deposited
    - *b*: or just depositing the corresponding energy at the creation point (at a trajectory point)
  - note, that we think in energy scale at the model level that translates to length (spacial) at the transport level
  - a secondary production threshold might be introduced (either in energy or length)

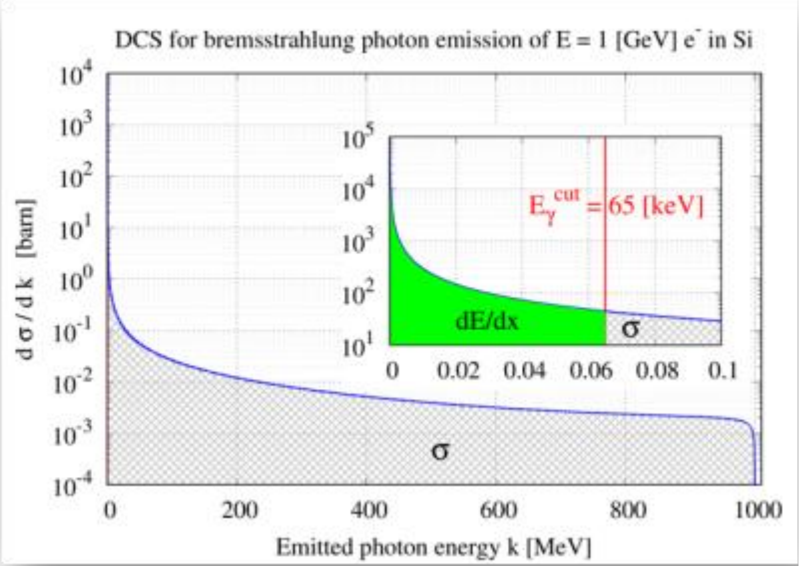




Secondary production threshold technique

- 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*)

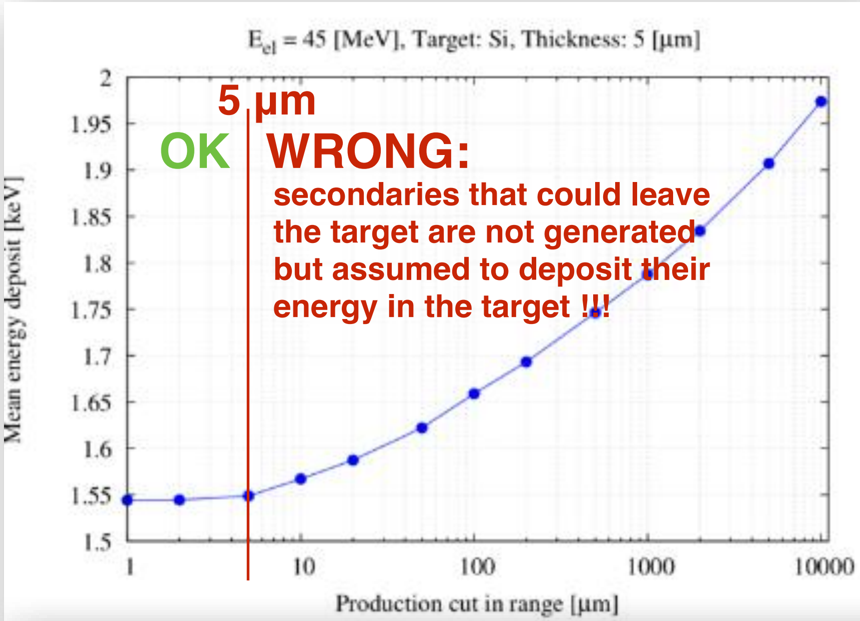
- the emission rate is determined by the corresponding (restricted) cross section(σ)

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

Secondary production threshold in Geant4

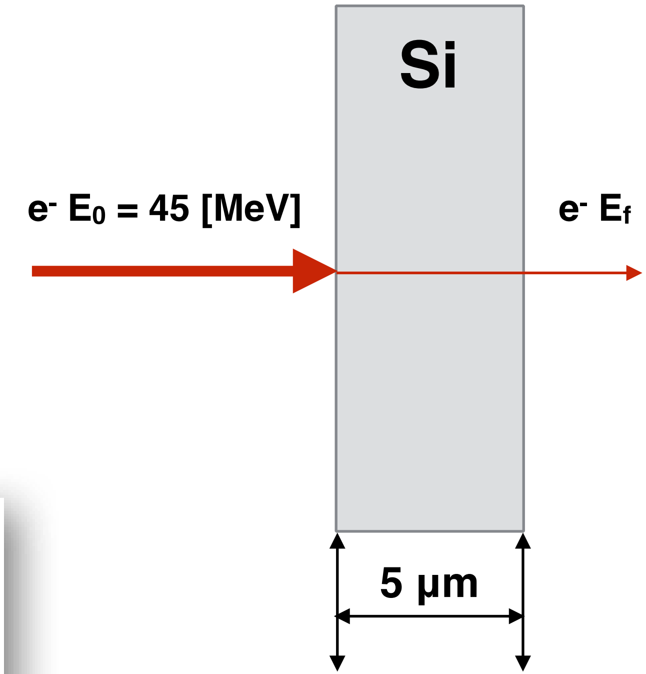
- Secondary production thresholds in Geant4:
  - user needs to provide them in length (the default value of 0.7 [mm] for the reference physics lists)
  - its proper value application dependent (size of the sensitive volume, CPU)
  - UI command: /run/setCut 0.1 mm
    - /run/setCutForAGivenParticle e- 0.1 mm
  - internally translated to energies at initialisation (depending on material and particle type)
  - the corresponding energy has a minimum value: default 1 keV but the user can set it
    - UI command: /cuts/setLowEdge 500 eV
  - production threshold defined for gamma, e^-, e^+ and proton secondary particle types
    - gamma production threshold is used in bremsstrahlung while the e^- in ionization
    - e^+ production threshold might be used in case of e-/e+ pair production
    - proton production threshold is used as a kinetic energy threshold for nuclear recoil in case of elastic scattering of *all hadrons and ions*
    - gamma and e^- production thresholds might be used (optionally: `/process/em/applyCuts true`) in all discrete EM interactions producing such secondaries - Compton, Photoelectric, etc.
  - it's not mandatory to use production thresholds
  - however, high energy physics simulation would not be feasible without them !

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

EM PHYSICS CONSTRUCTORS

EM Physics Lists Components

- A Physics list is the mandatory user class making the general interface between the physics the user needs and the Geant4 kernel
- List of particles: for which EM physics processes are defined
  - γ, $e^{\pm}$, $\mu^{\pm}$, $\pi^{\pm}$, $K^{\pm}$, p, $\Sigma^{\pm}$, Ξ^{-}, Ω^{-}, anti($\Sigma^{\pm}$, Ξ^{-}, Ω^{-})
  - $\tau^{\pm}$, $B^{\pm}$, $D^{\pm}$, $D_s^{\pm}$, Λ_c^{+}, Σ_c^{+}, Σ_c^{++}, Ξ_c^{+} , anti(Λ_c^{+}, Σ_c^{+}, Σ_c^{++}, Ξ_c^{+})
  - d, t, He3, He4, GenericIon, anti(d, t, He3, He4)
  - 12 light hyper- and anti-hyper- nuclei

- The G4ProcessManager of each particle maintains a list of processes

- Geant4 provides several configurations of EM physics lists called constructors (G4VPhysicsConstructor) in the physics_lists library of Geant4

- These constructors can be included into a modular Physics list in a user application (G4VModularPhysicsList)

Standard EM Physics Constructors

Geant4 standard EM Physics Constructors for HEP applications

- Description of Coulomb scattering:
  - $e^{\pm}$: Urban - MSC model below 100 [MeV] and the Wentzel - WVI + Single scattering (mixed simulation) model above 100 [MeV]
  - muon and hadrons: Wentzel - WVI + Single scattering (mixed simulation) model
  - ions: Urban - MSC model
- Different MSC stepping algorithms and/or parameters: speed v.s. accuracy

Constructor	Components	Comments
`G4EmStandardPhysics`	Default: nothing or _EM0 (QGSP_BERT, FTFP_BERT,…)	for ATLAS and other HEP simulation applications
`G4EmStandardPhysics_option1`	Fast: due to simpler MSC step limitation, cuts used by photon processes (FTFP_BERT_EMV)	similar to one used by CMS; good for crystals but not good for sampling calorimeters (with more detailed geometry)
`G4EmStandardPhysics_option2`	Experimental: similar to option1 with updated photoelectric model but no-displacement in MSC (FTFP_BERT_EMX)	similar to one used by LHCb

EM Physics Constructors for medical applications

Combined Geant4 EM Physics Constructors

- The primary goal is more the physics accuracy over the speed
- Combination of standard and low-energy EM models for more accurate physics description
- More accurate models for $e^{\pm}$ MSC (Goudsmit-Saunderson(GS)) and more accurate stepping algorithms (compared to HEP)
- Stronger continuous step limitation due to ionisation (as others given per particle groups)
- Recommended for more accuracy sensitive applications: medical (hadron/ion therapy), space

Constructor	Components	Comments
`G4EmStandardPhysics_option3`	**Urban** MSC model for all particles	proton/ion therapy
`G4EmStandardPhysics_option4`	most accurate combination of models (particle type and energy); GS MSC model with Mott correction and error-free stepping for $e^{\pm}$)	the goal is to have the most accurate EM physics description
`G4EmLivermorePhysics`	**Livermore models** for e^-, γ below 1 GeV and standard above; same GS MSC for $e^{\pm}$ as in option4)	accurate Livermore based low energy e^- and γ transport
`G4EmPenelopePhysics`	**PENELOPE** models for $e^{\pm}$, γ below 1 GeV and standard above; same GS MSC for $e^{\pm}$ as in `option4`)	accurate PENELOPE based low energy e^-, e^+ and γ transport

EM Physics Constructors for testing of new models

Experimental Geant4 EM Physics Constructors

- Supposed to be used only by the developers for validations and model developments
- The main difference is in the description of the Coulomb scattering (GS, WVI, SS)

Constructor	Components	Comments
G4EmStandardPhysicsGS	standard EM physics and the GS MSC model for $e^{\pm}$ with HEP settings	may be considered as an alternative to EM0 i.e. for HEP
G4EmStandardPhysicsWVI	WentzelWVI + Single Scattering mixed simulation model for Coulomb scattering	high and intermediate energy applications
G4EmStandardPhysicsSS	single scattering (SS) model description of the Coulomb scattering	validation and verification of the MSC and mixed simulation models
G4EmLowEPPhysics	Monarsh University Compton scattering model, 5D gamma conversion model, WVI-LE model	testing some low energy models
G4EmLivermorePolarized	polarized gamma models	a (polarized) extension of the Livermore physics models

USER INTERFACE TO EM PHYSICS

EM parameters

- EM parameters of any EM physics list may be modified at initialization of Geant4 using C++ interface to the G4EmParameter class or via UI commands
- Example of interfaces of G4EmParameters:
  - SetMuHadLateralDisplacement()
  - SetMscMuHadRangeFactor()
  - SetMscMuHadStepLimitType()
- Corresponding UI commands:
  - /process/msc/MuHadLateralDisplacement
  - /process/msc/RangeFactorMuHad
  - /process/msc/StepLimitMuHad
- Some other UI commands:
  - /process/em/deexcitationIgnoreCut true
  - /process/eLoss/UseAngularGenerator true
  - /process/em/lowestElectronEnergy 50 eV
  - /process/em/lowestMuHadEnergy 100 keV
  - ....

User Interfaces and Helper Classes

- Geant4 UI commands to define cuts and other EM parameters
- G4EmCalculator
  - easy access to cross sections and stopping powers (TestEm0)
- G4EmParameters
  - C++ interface to EM options alternative to UI commands
- G4EmSaturation
  - Birks effect (satuaration of response of sensitive detectors)
- G4ElectronIonPair
  - sampling of ionisation clusters in gaseous or silicon detectors
- G4EmConfigurator
  - add models per energy range and geometry region
- G4NIELCalculator
  - Helper class allowing computation of NIEL at a step, which should be added in user stepping actions or sensitive detector (TestEm1)

How to extract Physics ?

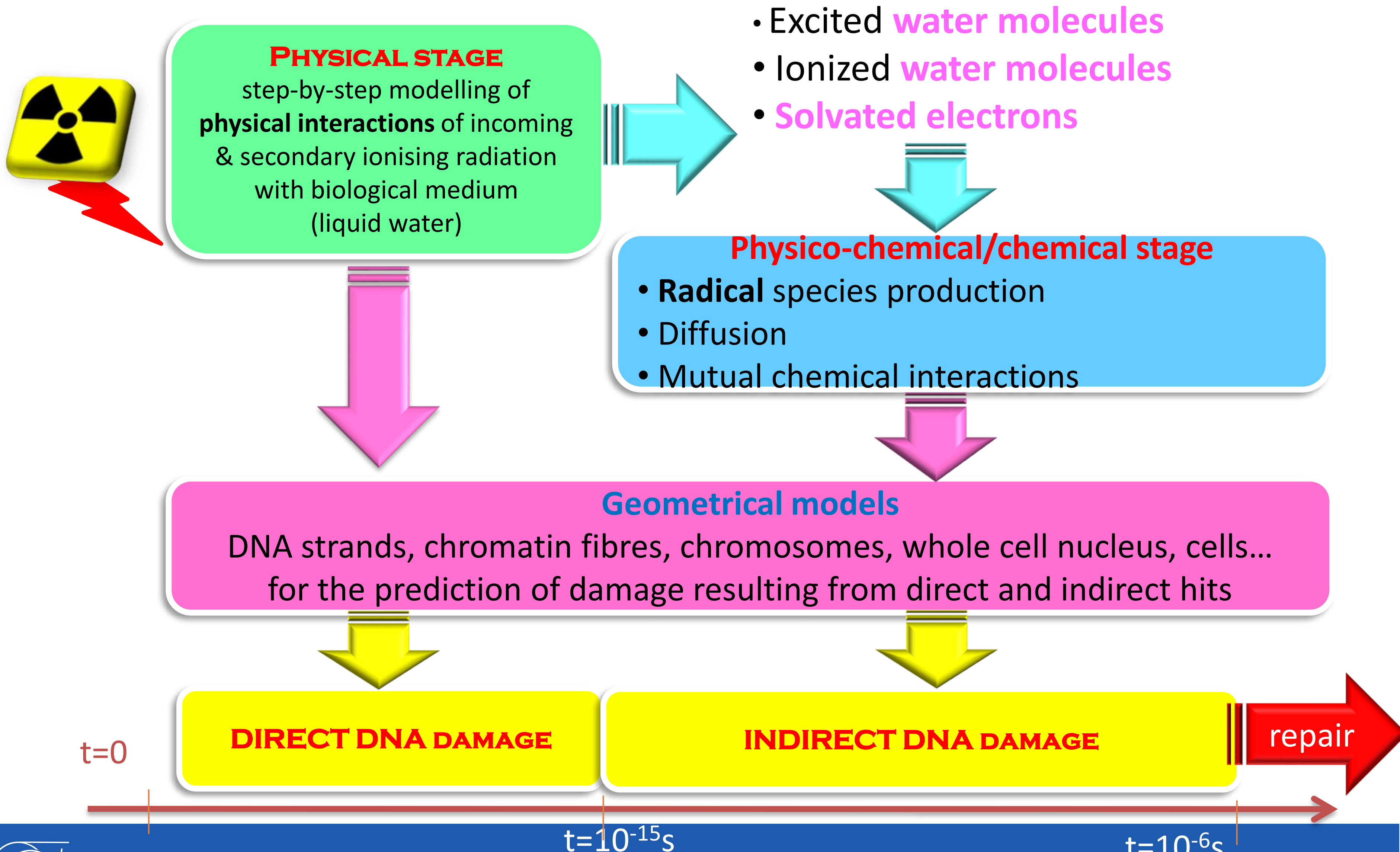
- Possible to retrieve Physics quantities using a G4EmCalculator object
- Physics List should be initialized
- Example for retrieving the total cross section of a process with name procName, for particle and material matName

```
#include "G4EmCalculator.hh"
...
G4EmCalculator emCalculator;

G4Material* material =
  G4NistManager::Instance()->FindOrBuildMaterial(matName);
G4double density = material->GetDensity();
G4double massSigma = emCalculator.ComputeCrossSectionPerVolume
     (energy, particle, procName, material)/density;
G4cout << G4BestUnit(massSigma, "Surface/Mass") << G4endl;
```

- A good example: $G4INSTALL/examples/extended/electromagnetic/TestEm0
  Look in particular at the RunAction.cc class

SPECIAL EM TOPICS

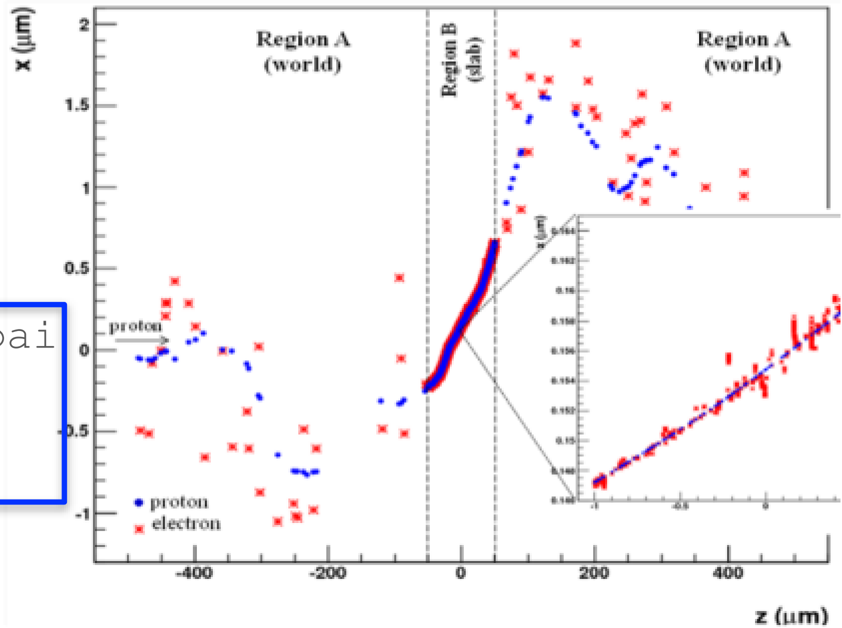
Geant4-DNA Project



Special EM topics: EM models per region

- Special EM models can be set to be used only in a given detector `G4Region`
- Example to use Geant4-DNA physics in a given detector region on the top of the standard EM physics:
  - the **`G4EmConfigurator`** can be used to add Geant4-DNA models
  - the DNA models are used only in the region B. for energies below 10 MeV
  - makes possible CPU and physics performance optimisation
  - the more accurate CPU intense simulation is done only in the region of interest
  - UI commands are available from Geant4 10.2 that allow easy configuration of some models per-region on the top of any EM constructor:

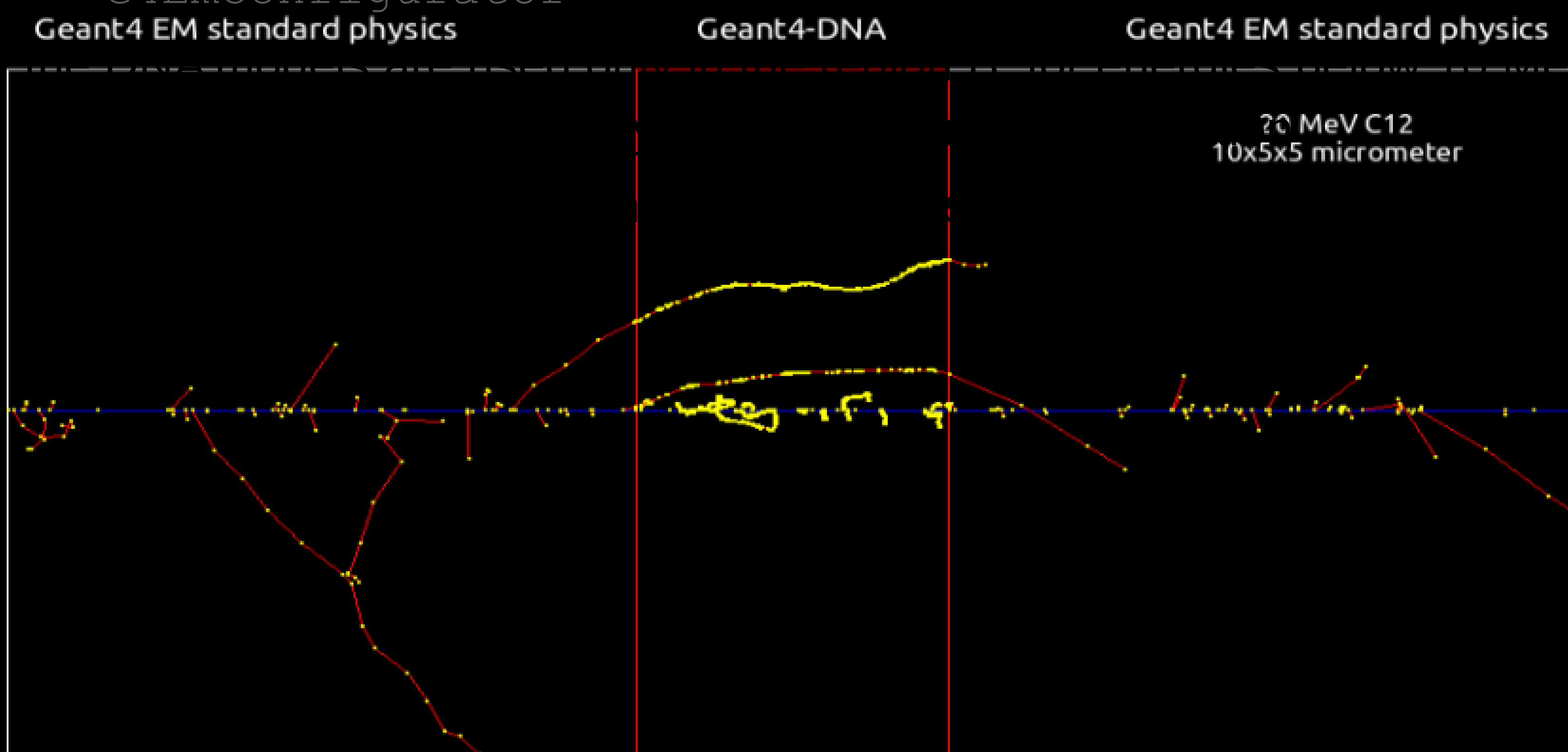
```
/process/em/AddPAIRegion proton MYREGION pai
/process/em/AddMicroElecRegion MYREGION
/process/em/AddDNARegion MYREGION opt0
```



Special EM topics: EM models per region

- Special EM models can be set to be used only in a given detector `G4Region`
- Example to use Geant4-DNA physics in a given detector region on the top of the standard EM physics:

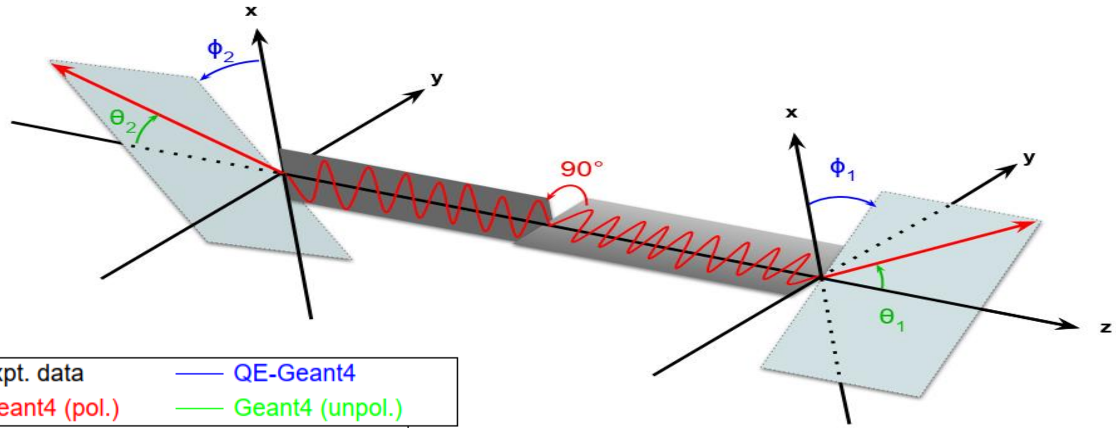
the `microdosimetry` extended example: `G4EmConfigurator`

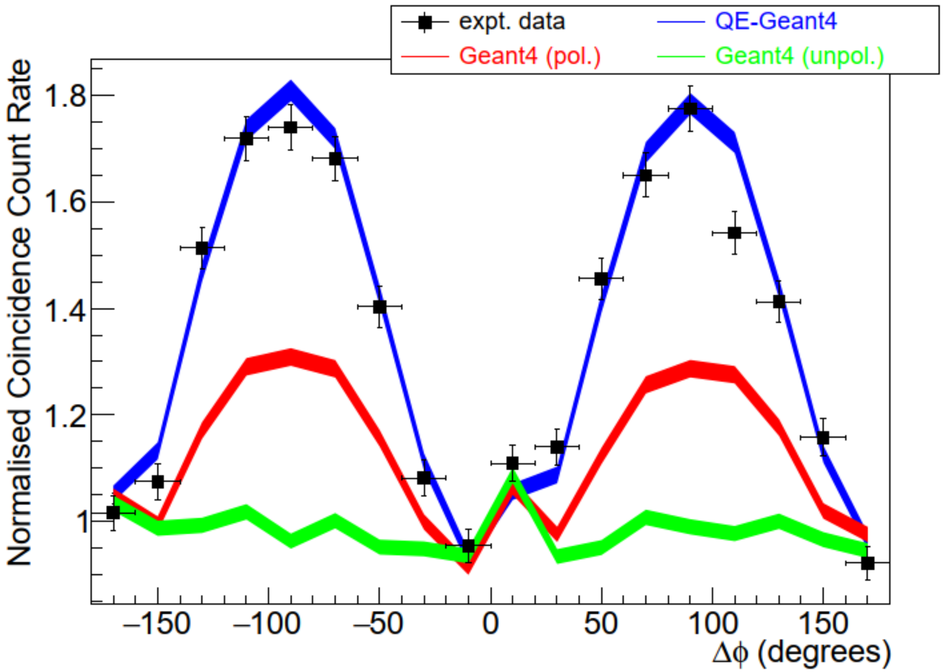


Nucl. Instrum. and Meth. B 273 (2012) 95
Prog. Nucl. Sci. Tec. 2 (2011) 898

Quantum entanglement in positron annihilation

(arXiv: 2012.04939v1)





- There is angular correlation for Compton scattering of two photons in PET device
- Geant4 method how simulate quantum effects has been developed by J. Allison
- The developed method may be potentially used in HEP

THANK YOU