Geant4 Electromagnetic Physics: Status and Perspectives

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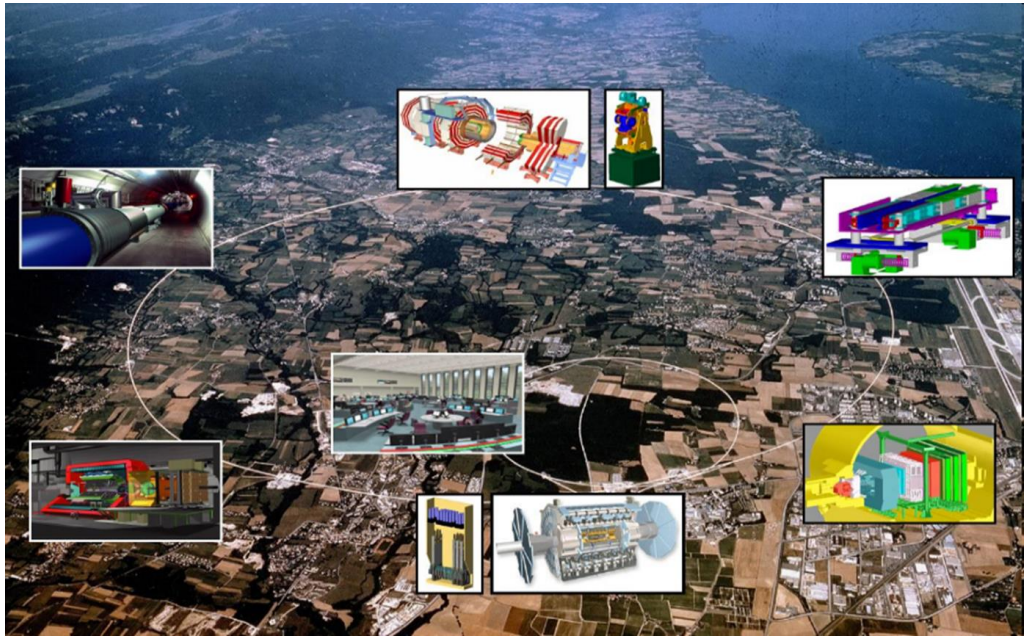
Outline

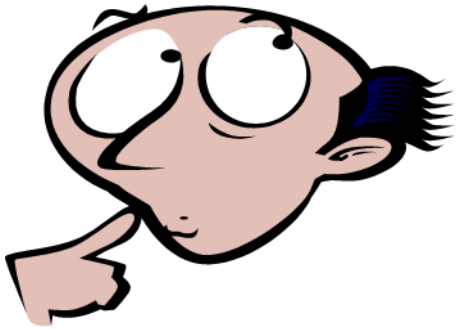
- Introduction
- Electromagnetic (EM) physics sub-libraries in Geant4 10.5
  - New models
  - EM showers simulations
  - Ion ionization
- EM physics developments for Geant4 10.6
  - Optimization and speed-up
  - EM models update
- Selected results
- Configuration of EM physics in Geant4 10.6
- Summary

Introduction



- CERN LHC Run-2 2015-2018 collected data at 13 TeV
  - Geant4 9.6 and Geant4 10.X have been used
  - CMS experiment use 10.4p03
  - Geant4 team was trying to keep stable results between 10.1-10.4
    - Some developments was not in the official release, another – not in main Physics Lists
- Now there is the Large Shutdown of LHC until 2021
  - Geant4 10.5 and 10.6 include all modifications accumulated over last few years
    - We would appreciate if issues in 10.5 or 10.6 will be early reported
  - We may expect some differences in simulation results both in EM and hadronic
    - in particular, in calorimeters and in backscattering and in other observables

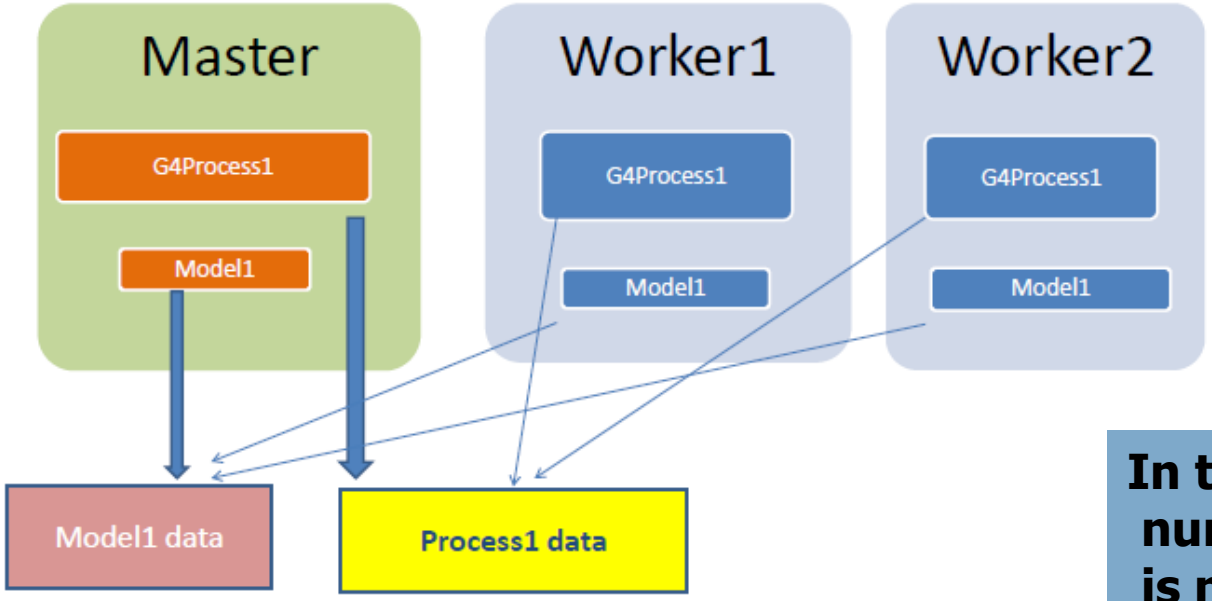
Geant4 EM libraries



- Low-energy
  - Livermore library γ, e- from 10 eV up to 1 GeV
  - Livermore library based polarized processes
  - PENELOPE code rewrite , γ, e- , e+ from 100 eV up to 1 GeV (2008 version)
  - hadrons and ions up to 1 GeV
  - atomic de-excitation (fluorescence + Auger)
- Geant4-DNA
  - micro dosimetry models for radiobiology (Geant4-DNA project) from 0.025 eV to 10 MeV
- Adjoint
  - Reverse Monte Carlo processes and models to track from the volume of interest back to source of radiation
- Utils
  - general EM interfaces
- 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 circular polarized beam transport
- Optical
  - optical photon interactions

EM Data Sharing for Geant4 MT

- The scalability of Geant4 10.X 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

Electromagnetic (EM) physics sub-libraries in Geant4 10.5

Updated standard EM models

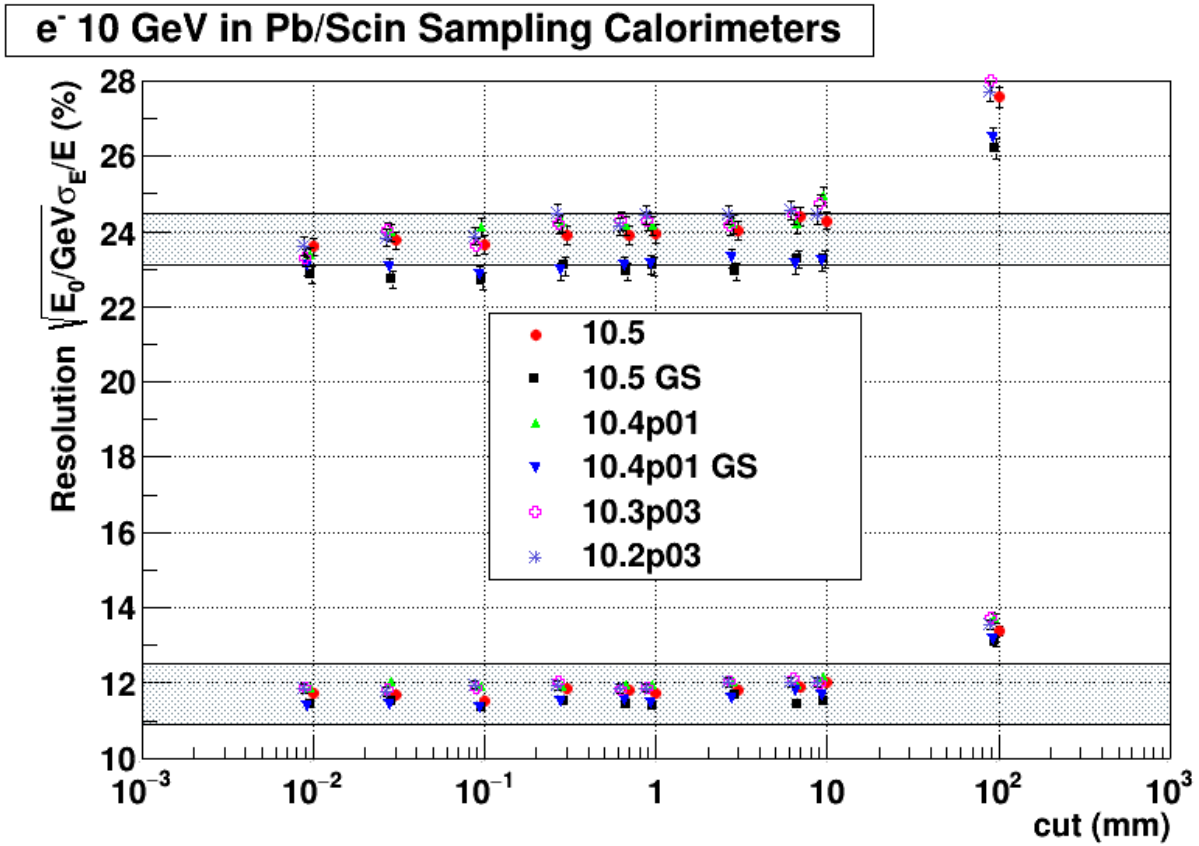
- Models of single and multiple scattering for e+-
  - Improved sampling of displacement for the G4UrbanMscModel
  - Added Mott corrections to G4WentzelVIModel used for simulation of multiple scattering of e+- above 100 MeV
  - G4ScreenedMottCrossSection – use G4MottData shared between threads and implemented more optimal computations
  - G4GoudsmithSoundersonMscModel – fix initialisation and added extra access method to transport cross section
- Gamma models and bremsstrahlung
  - G4ModifiedTsai – use as a default for bremsstrahlung and pair production, added new method SamplePairDirection, improved performance
  - G4BetheHeitlerModel, G4PairProductionRelModel – improved screening function approximation, LPM function approximation, selection of elements in compounds
  - G4SeltzerBergerModel – added optional mechanism of sampling final state using sampling table

New EM models

- G4BetheHeitler5DModel
  - Accurate sampling of final state (~100 slower)
  - Nuclear recoil and polarisation are taken into account
- Proton/hadron ionisation
  - Added possibility to use ICRU90 data for stopping powers
  - Geant4/GATE project
- Ion ionisation based on Lindhard-Sorensen theory
  - G4LindhardSorensenModel – parameterisation above 10 MeV
  - G4AtimaEnergyLossModel – implementation of ATIMA code in C++
  - G4AtimaFluctuations – relativistic ion energy loss fluctuations
- 3-gamma annihilation model
  - G4eplusTo2GammaOKVIModel and G4eplusTo3GammaOKVIModel implements 2-gamma and 3-gamma positron annihilation in fly and at rest
  - Probability of 3-gamma final state depends on cut to gamma energy

Resolution of Pb/Sc calorimeters

Bernardi E. et al. 1987 Nucl. Instrum. Meth. A **262**, 229



- A classical benchmark (ZEUS test-beam) for two sampling calorimeters with different sampling fractions
  - The same simulation conditions for two setups
- Geant4 results are stable between different releases
  - Goudsmit-Saunderson (GS) model of multiple scattering predicts less width within experimental uncertainty

ICRU73 Ion Ionisation Model

- A. Lechner, V. N. Ivanchenko, J. Knobloch, Nucl. Instrum. and Meth. B 268 (2010) 2343-2354
- G4IonParameterisedLossModel implements ion ionisation using ICRU73 stopping power tables
  - Initially we used only tables from the report
  - Later we get full set of projectile/target tables computed specially for Geant4
    - We have all targets for pure elements up to Uranium
    - Additionally for G4_WATER
  - A table for stopping power is uploaded by request for each new projectile/target combination
    - A user can add a custom table
  - Energy interval E/A from 0.025 keV to 1 GeV
  - In Geant4 10.6 ICRU90 data will be available as an alternative

Stopping Power of Relativistic Ions

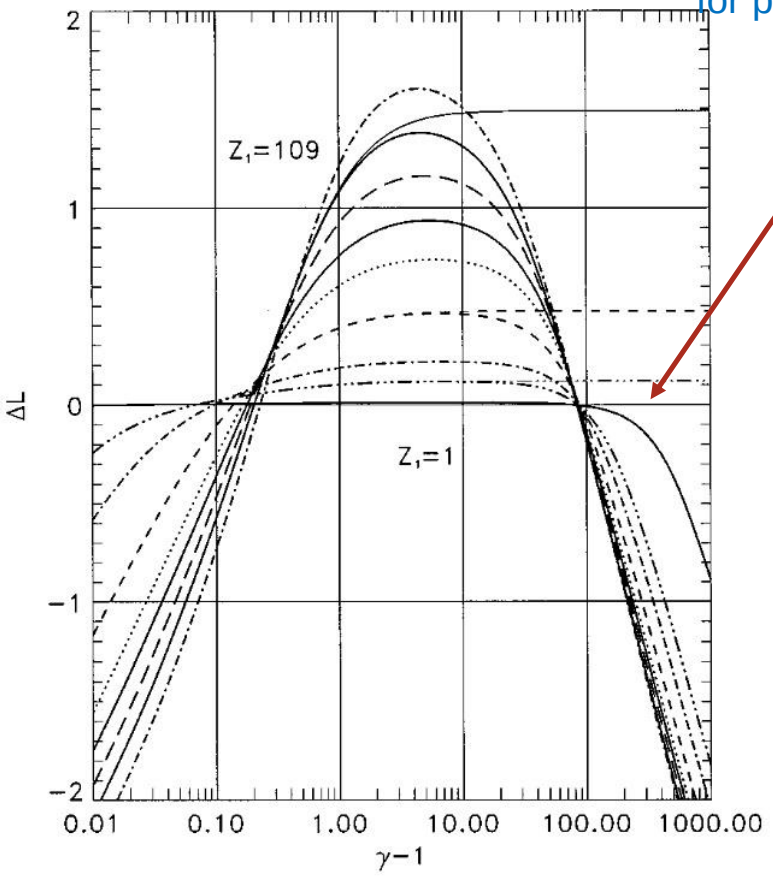
Lindhard J., Sorensen A.H., Relativistic theory of stopping for heavy ions.
Phys. Rev. A 53 (1996) 2443

$$-\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{mv^2} N Z_2 L$$

$$L_{stand} = ln\left(\frac{2mv^2}{I}\right) - \frac{v^2}{c^2} - \frac{1}{2}\delta$$

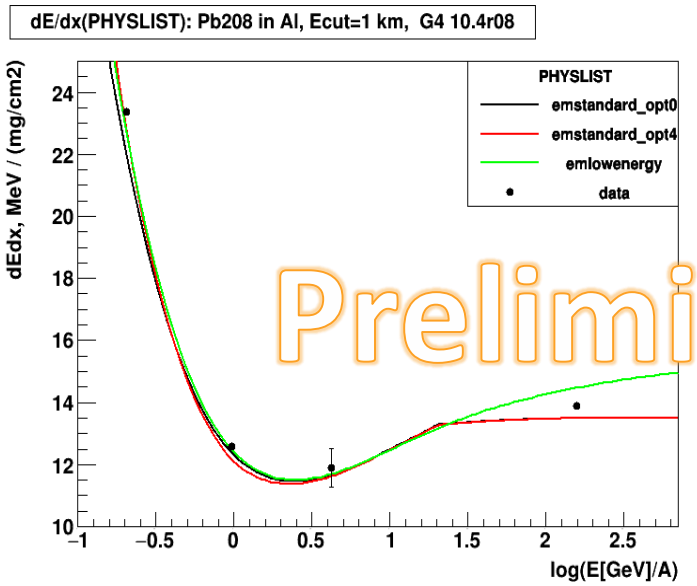
$$L - L_{stand} = \Delta L + \delta L_{shell} + L_{Barkas} + L_{scr}$$

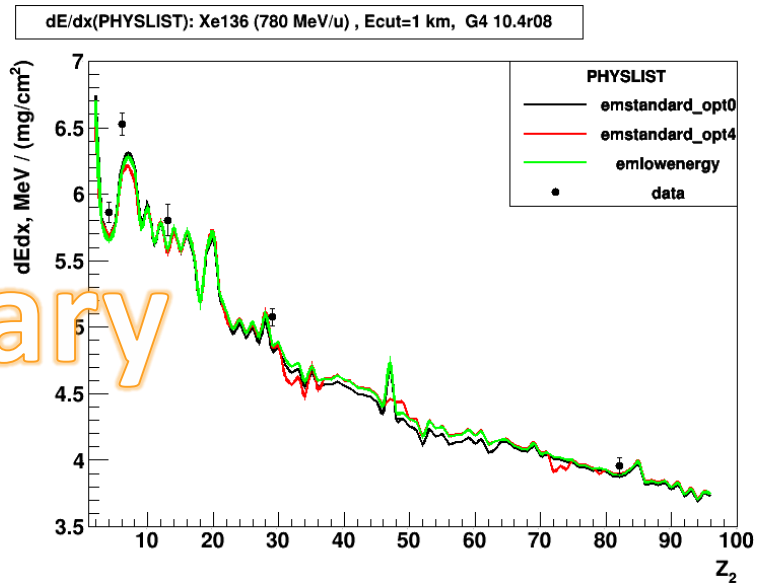
ΔL is the function of energy and projectile ion size
It has been parameterized in the form f(γ, Z)



Stopping for finite nuclear size. The curves display the values of ΔL for atomic numbers Z1 = 1, 10, 18, 36, 54, 66, 79, 92, and 109

Validation Results





- LS model can describe stopping power of heavy relativistic ions
- Additionally to ionization we need to take into account radiation losses of heavy ions: bremsstrahlung and e^+e^- pair production
  - It is possible reusing proton processes
  - Energy limit will be E/A ~0.2 GeV

Low Energy EM & DNA Physics

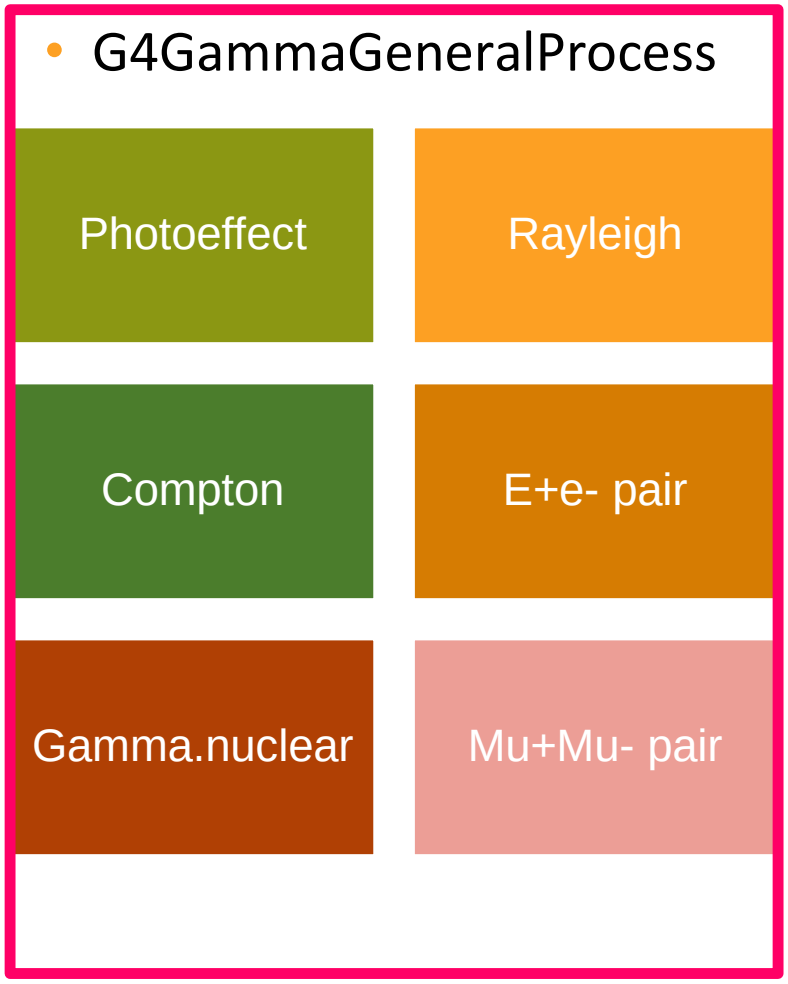
- Added new JAEA model of gamma elastic scattering (M.Omer and R.Hajima)
- Geant4-DNA
  - Published Special Report in Medical Physics journal describing all physics models and applications for track structure simulations (covers 2008-2018 period)
    - Med. Phys. 45, e722-e739 (2018)
  - New constructors
    - Physics (G4EMDNAPhysics_option8) – electron elastic scattering based on CPA100 approach
    - Chemistry (G4EmDNAChemistry_option1) – alternative set of values (diffusion constants, reaction rates) from RITRACKS / NASA software
  - New examples
    - **splitting**: illustrating computing speedup in ionisation
    - Updated **svalue** example for the calculation of S values in nuclear medicine
- Making chemistry more accurate and faster for 10.6:
  - Influence of phyiscs models and chemistry parameters on the simulation of radiochemical yields Wook Geun Shin et al.
  - Porting of TOPASnBio IRT & alternative versions to Geant4 is on-going in collaboration with TOPAS developers
  - New constructor G4EmDNAChemistry_option2

EM physics developments for Geant4 10.6

Optimization and speed-up

- EM physics software was reviewed and several optimizations were introduced into the toolkit:
  - At any step of each track EM energy loss, ranges, cross sections are recomputed using internal tables
  - Energy scales of tables are logarithmic over particle kinetic energy
    - Main optimization is in computing logarithm only once if the energy is the same
    - This also allows substantial simplify interpolation code reducing number of lines of code used at a step practically in 10 times
- Benchmark results for CMS geometry without hit creation:
  - ~8% for Mac Book Pro (Mac OS 10.13.2) 2.8 GHz i7
  - ~5 % for AMD (SLC6 gcc8.2.0) 3.5 GHz

G4GammaGeneralProcess



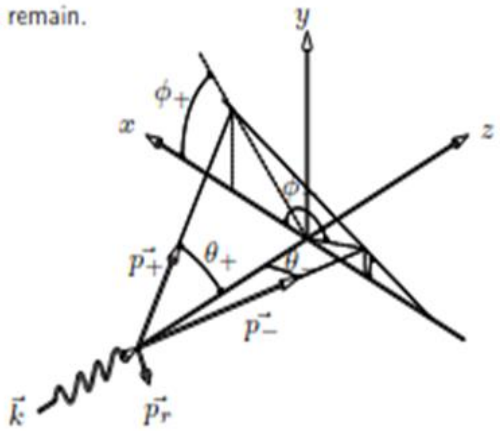
- SteppingManager see only 1 physics process
  - Only 1 mean free path
  - Plus transportation
- Enabled via UI command
  - In 10.6 will be optional in general, UI command may be used to enable
  - Will be defaults for Opt1 EM physics
- Reduced number of instructions
  - Advantage in CPU ~5% for calorimeters
  - Extra PhysicsTables shared between threads – a bit more memory
- Final numbers for CPU/memory should be checked by users

Gamma conversion to lepton pair model

by D. Bernard and I. Semeniouk (LLR, CNRS/IN2P3, Ecole Polytechnique)

A 5D phase space

- 3 particle final state, $4 - 1 = 3$ free parameters for each one.
- energy-momentum conservation fixes 4 of them.
- $3 \times 3 - 4 = 5$ variables remain.



- $+, -, r$ = positron, electron, recoil. ϕ azimuthal, θ polar angles.
- $\Omega \equiv (\phi_+,\ \phi_-,\ \theta_+,\ \theta_-,\ x_+ \equiv E_+/E_\gamma)$

The model was developed for e+e- pair production but is applicable to muon pair production

Linear polarization of incoming gamma, nuclear recoil, and triplet production are taken into account

Can be applied for full energy range from threshold (M.Novak, CERN)

- List of publications (+references inside)
  - P. Gros and D. Bernard, Astropart. Phys. 88, 60 (2017)
  - D. Bernard, Nucl. Instrum. Meth. A 899, 85 (2018
  - V. Ivanchenko et al., EPJ Web of Conferences 214 02046 (2019)

NIEL Calculator For Radiative Background Studies

- As a result of several discussion inside CERN-SFT group and with FLUKA developer it was decided to provide more support for LHC users
- We introduced G4NIELCalculator helper class
  - This class calculate NIEL at a step independently on cuts
  - Example how to use is in TestEm1
  - This class uses G4VEmModel which provides NIEL computation
  - The default model – G4ICRU49NuclearStoppingModel
- Alternatively user should correctly combine tracking cuts and production thresholds in EM physics definition
  - In that case, NIEL will be available from the G4Step
  - This method seems to be much more complicate and less obvious to a user

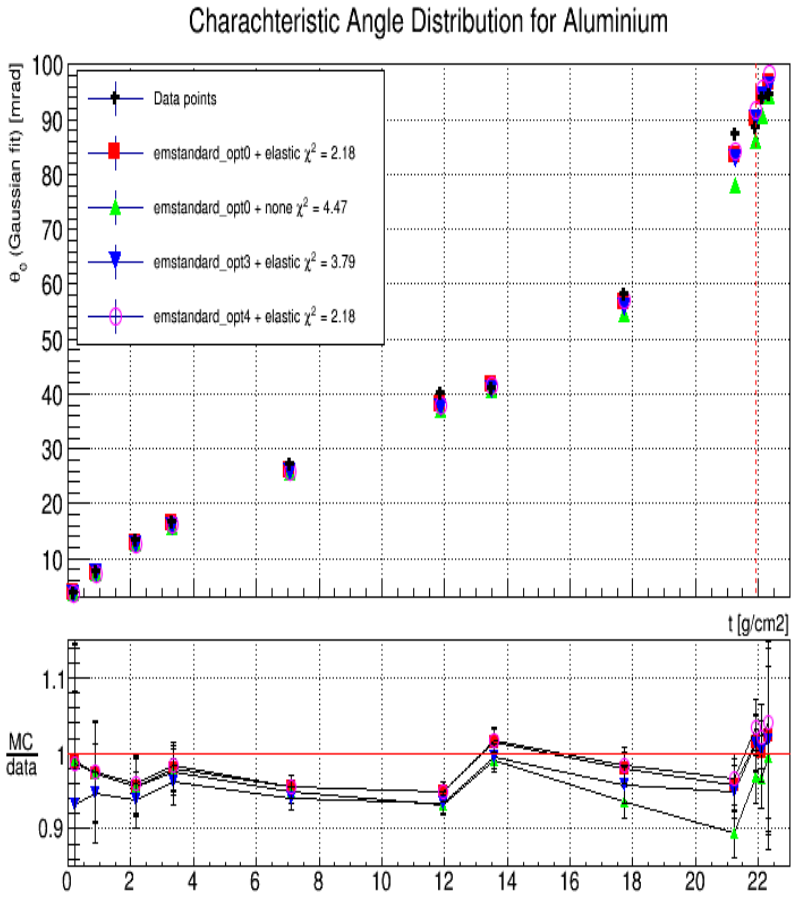
Low Energy EM & DNA Physics

- Extension Geant-val GRID validations with many EM tests
  - https://geant-val.cern.ch/
  - Medical physics benchmark and new fine W/Si calorimeter are included
- Low energy models:
  - New models for electrons in DNA material
- Making chemistry more accurate and faster for 10.6:
  - Influence of phyiscs models and chemistry parameters on the simulation of radiochemical yields (Wook Geun Shin et al.)
  - Porting of TOPASnBio IRT & alternative versions to Geant4 is on-going in collaboration with TOPAS developers
  - Evaluation of DNA damage in a fractal nucleus geometry
  - New examples:
    - Evaluation of proximity functions "microprox"
    - Various DNA geometries "dnadamage1"
  - New constructor G4EmDNAChemistry_option2

Selected results

Geant4 Multiple and Single Scattering

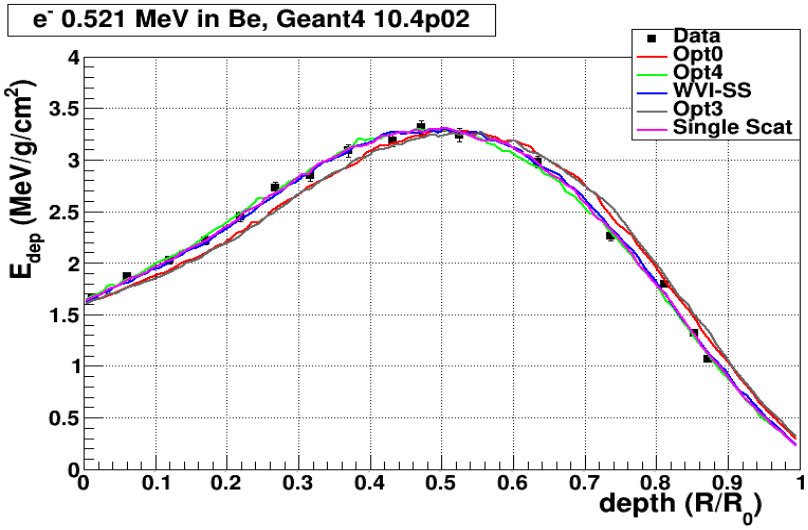
- Combined multiple and single scattering Wentzel-VI models
  - Single scattering for large angles
  - Multiple scattering for small angles
  - For muons and hadrons
  - For e+- above 100 MeV
- Urban multiple scattering
  - By default for e+- below 100 MeV by default
  - For ions
- New GS model
  - Used for e+- below 100 MeV
  - Used single scattering regime in vicinity of geometry boundary
  - Mott corrections since 10.4

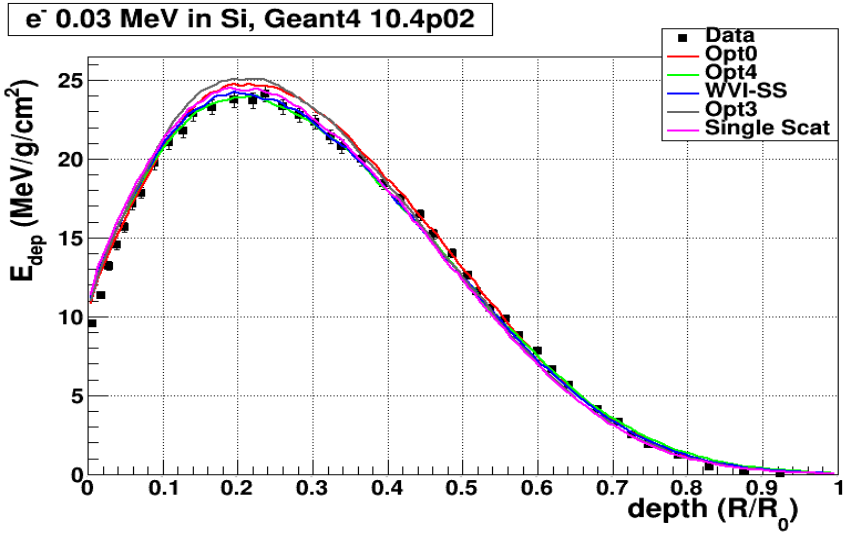


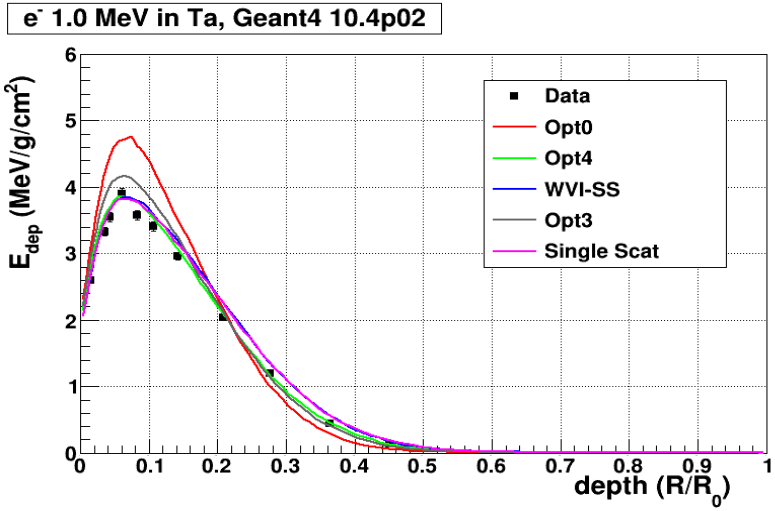
Proton multiple scattering benchmark
Nucl. Instr. Meth. B 74, 467 (1992)

Energy deposition in semi-infinite media

SANDIA REPORT SAND79-0414.UC-34a



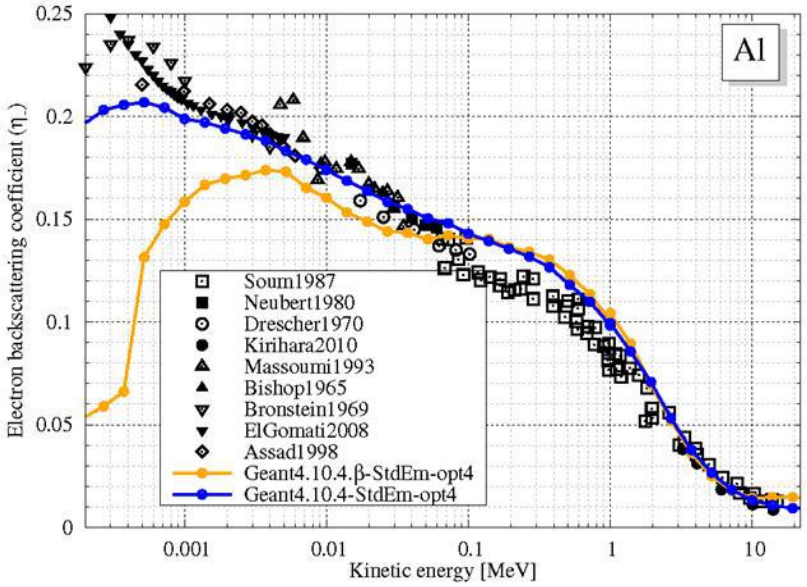


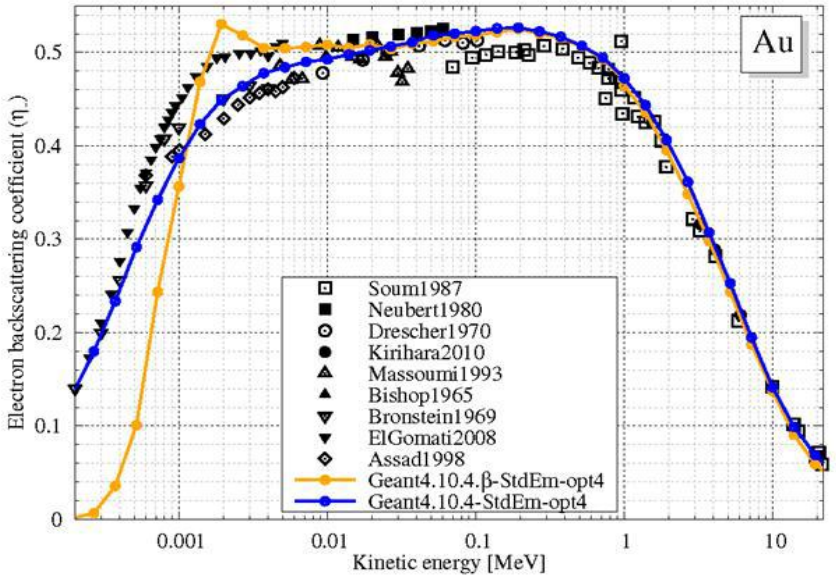


- Recent GS model now describes data for both low and high density media
- Opt0 (default) is not so accurate but is fast
- Opt4 (EMZ) is recommended as an alternative if increased precision is needed but is slower

Backscattering validation results

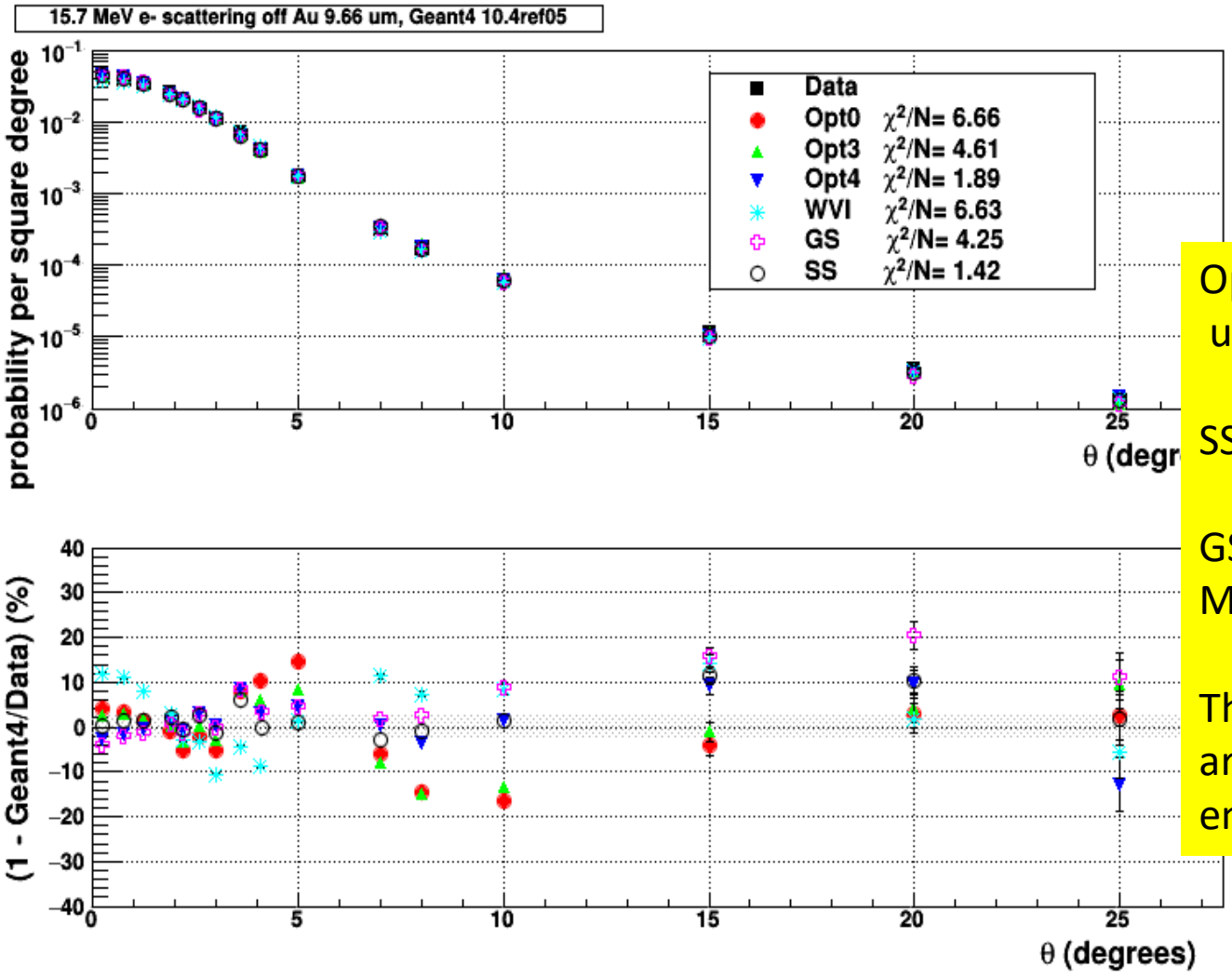
CHEF-2017 Conference (JINST 13 C02054, 2018)





- Validation of electron backscattering from light (Al) and heavy (Au) targets versus data from different experiments.
- Old Opt4 (EMZ) EM configuration uses the Urban model (yellow), the final variant of Opt4 uses GS with “error-free” stepping (blue)
- Simulation with GS is substantially more accurate below 10 keV

Hanson data for electron scattering off Gold target (*Phys. Rev.* **84**, 634-637, 1951)



Opt4 Physics List uses the GS model

SS is single scattering

GS and SS are using Mott corrections

These improvements are also valid for all energies

Configuration of EM physics

Physics List Choice

- A set of EM physics constructors are provided together with each recent Geant4 version
  - The default (Opt0) EM physics is optimized for use in HEP
  - There are variants Opt1 (EMV) and Opt2 (EMY) with simplified multiple scattering and other options for HEP
  - The alternative Opt4 (EMZ) physics is combination of the most accurate EM models
    - Is recommended for R&D and detector performance studies
    - For 10.6 will use 5D gamma conversion model
- Opt3, Livermore and Penelope Physics constructors may be considered as an intermediate variant between Opt0 and Opt4
  - They are faster than Opt4
- Other EM constructors are not recommended for production
  - They are used to study new models

EM Parameters in Geant4 10.6

- On top of any EM physics configuration it is possible to customize EM parameters via UI commands and C++ interface
  - G4EmParameters class may be called
  - The list of available parameters is printed in log file or may be printed via UI command
  - Part of parameters may be changed only in PreInit_State
  - Another part also can be changed in the Idle_State
- Following customization options for EM physics are recommended:
  - Production thresholds (cuts in range) per G4Region
  - Tracking cuts per particle type
  - General process for gamma may be enabled
- G4EmConfigurator helps defining models for G4Region
  - PAI, MicroElec and DNA models may be defined for or more G4Region(s)
  - There are UI commands for such configurations

Custom EM Physics

- User may created custom EM physics
  - It is recommended to start from one of EM constructors from Geant4 distribution
  - CMS at LHC is based on Opt1
  - ALICE at LHC is based on Opt0
- Different multiple scattering parameters may be tuned per G4Region (per sub-detector)
  - Range Factor
  - Geom Factor
  - Safety Factor
  - Lambda Limit
  - Stepping algorithm
  - Lateral displacement
- User may design EM physics constructor with multiple scattering models separately defined per G4Region or use G4EmConfigurator interface

Summary

- Several new models were included in Geant4 10.5
  - Extended interface to configure EM physics per detector region
- With Geant4 10.6 several new features will be provided
  - Default EM physics become faster
  - General gamma process option may be applied
  - NIEL calculator allows making various studies of radiation damage
- Several EM physics models were updated
  - Improvements are available in the default and in other EM physics including Opt4 (EMZ) EM physics constructors
    - Calorimeter response may be slightly changed (<1%)
- Reports on Geant4 10.6 performance are very welcome