What's new in 11.1: Electromagnetic physics

V. Ivantchenko, CERN & Princeton University

for the Geant4 Collaboration

2 February 2023

Outline

- Update of infrastructure for EM physics
- Selected model developments
- EM Physics Lists
- Geant4-DNA developments
- New approaches for EM physics
- Summary

For the release 11.1 general updates of EM libraries started for previous release were completed. Significant focus of new developments toward R&D on alternative methods for EM physics.

Not all names of developers are shown

Updates for materials

- Mean ionization potential for carbon is changed from 81 to 78 eV
  - Choice, which NIST data to take
- G4MaterialPropertyVector, G4OpticalMaterialProperties:
  - Insist material property vectors are in increasing order of energy (PR #42);
  - default verbosity=1 as everywhere in Geant4 physics
- Updated bio-materials
  - the material descriptions for G4_ADENINE, G4_GUANINE, G4_CYTOSINE, G4_THYMINE and G4_DEOXYRIBOSE have been updated and G4_PHOSPHORIC_ACID has been added.
- Problems #2346, #2474, #2486 are fixed
  - handling of complex materials and parameterization of density effect correction
- G4DensityEffectData:
  - Matthew Strait fix typos in the density effect data table (#2423) for 8 materials, the most significant fix for G4_Tm, small for G4_Be, G4_Mg, G4_Fe, and G4_Y.

Updates in kernel libraries for physics

- Added virtual GetCrossSection(…) method for G4VDiscreteProcess to be used for initialisation
  - Needed for the integral method
- Added virtual GetCreatorProcess(…) method for G4VProcess
  - Needed for combined processes
- For particle change
  - G4VParticleChange, G4ParticleChangeForLoss, G4ParticleChangeForGamma, G4ParticleChangeForMSC:
    - SetNumberOfSecondaries(..) is not mandatory anymore
    - Improved diagnostic for wrong energy/momentum/time (useful for studies on #2353, #2368)
    - Substitute severity “EventShouldBeAborted” by “JustWarning”
- For G4SteppingManager:
  - Removed unused “ApplyCuts” facility
  - Updated code to identify CreatorProcess pointer having in mind combined processes
    - Important for gamma general, neutron general, transportation with msc

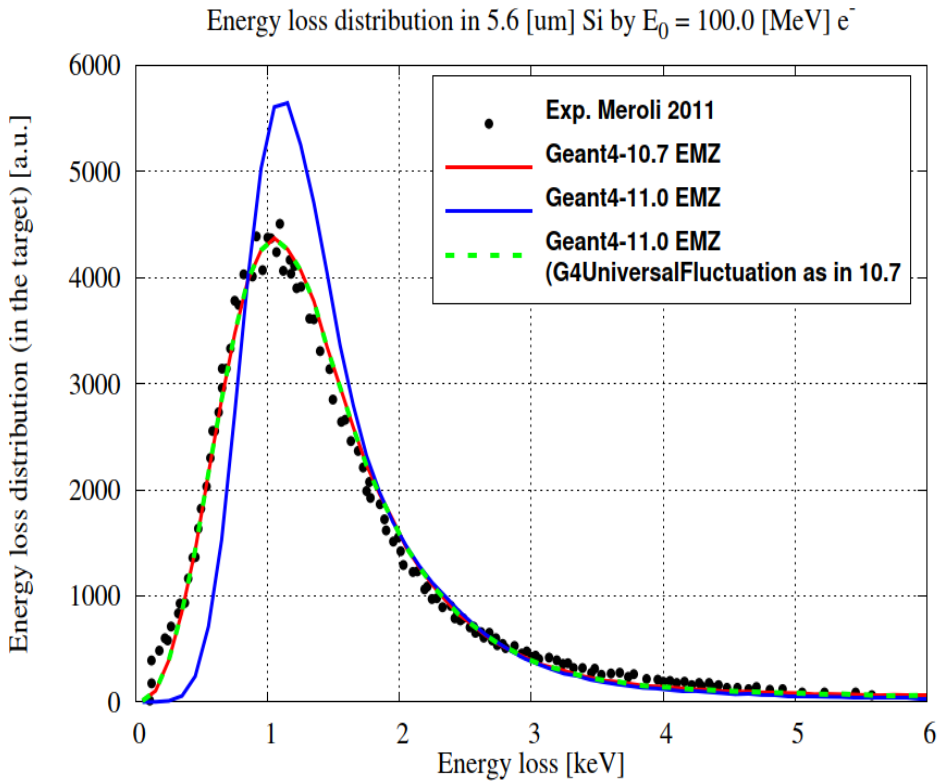
Updates in EM libraries

- G4VEmProcess, G4VEnergyLossProcess, G4VMultipleScattering:
  - Moved general part of initialisation to G4EmTableUtil and G4EmUtility
    - 27-30% class length reduction – easier to navigate inside classes
  - Updated integral method for charged particles:
    - Implemented for processes without precomputed cross section tables
    - Allowed up to 3 maximum in cross section
- Updated data set
  - G4EMLOW8.2
  - Change the default Livermore DB from EPDL97 to EPICS2017
- Fixed problems:
  - #2495, #2492, #2480

Updates in standard EM processes/models

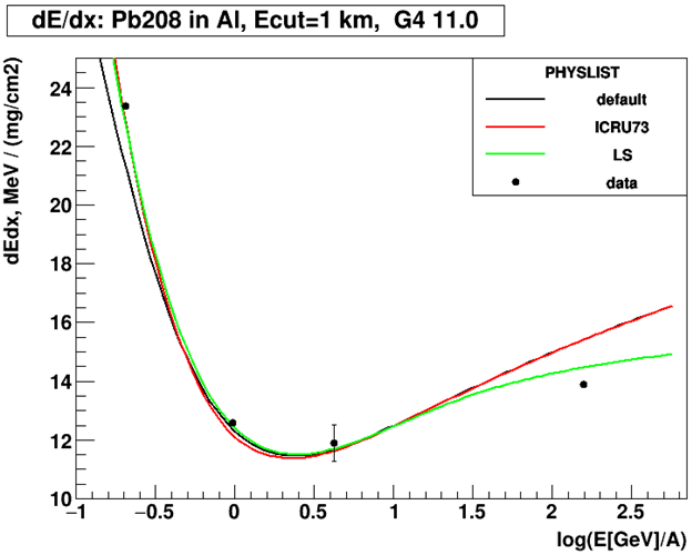
- Review was done of all processes and helper classes
  - Linear interpolation of tables are used for smooth cross sections
- Introduced choice of model of fluctuations
  - G4UniversalFluctuation – default fast
  - G4UrbanFluctuation – most accurate model
    - used in Opt0, Opt3, Opt4, LIV, and PEN EM physics
  - G4IonFluctuations
  - G4LossFluctuationDummy
  - Also, an external model of fluctuation may be used
- G4UrbanMscModel – technical improvements
  - Extended precomputed data structure
  - Reduced number of instructions

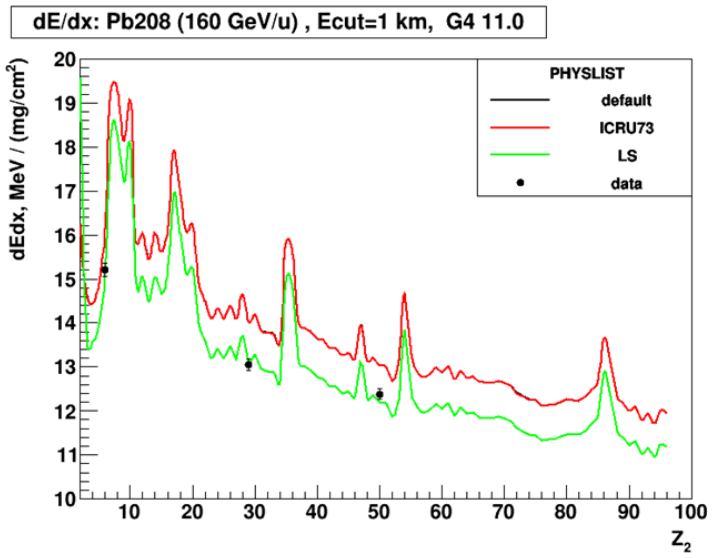
M. Novak

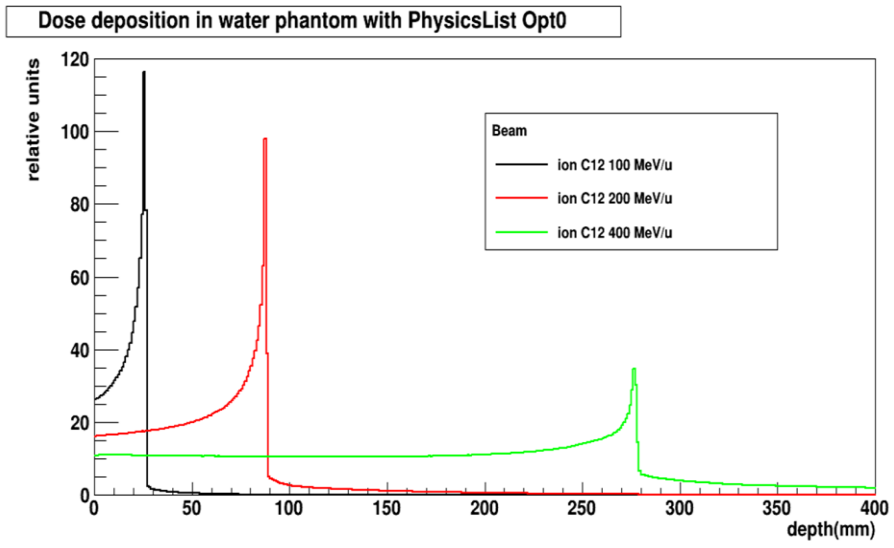


Lindhard-Sorensen ion ionization model

- G4LindhardSorensenIonModel is a combined models for the full energy range
  - Lindhard-Sorensen model above (*J. Lindhard & A.H. Sorensen, Phys. Rev. A 53 (1996) 2443-2455*)
  - Data are shared between threads, optimization of data access
    - Initialisation before the run and lazy initialization during the run
  - Is significantly faster than the old G4ParametrizedIonModel and includes extended data
    - ICRU73 and ICRU90 data at low energy below 2 MeV/amu

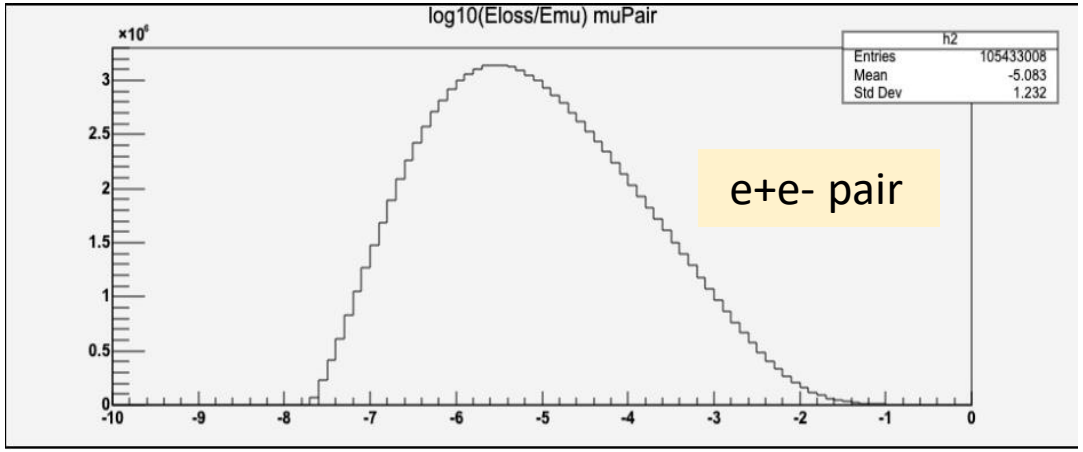


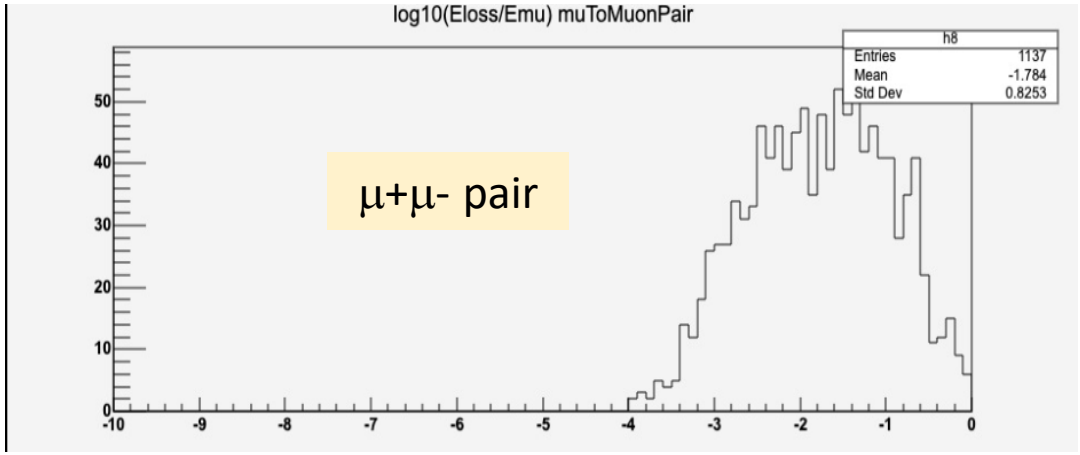




Updates in muons processes/models

- Review was done of all processes
  - Linear interpolation of tables are used for smooth cross sections
- Reduced low-energy limits
  - G4MuBetheBlochModel – down to 0.2 MeV (was 100 MeV)
  - G4MuBremsstrahlungModel – down to 100 MeV (was 1 GeV)
  - G4MuPairProductionModel – down to 850 MeV (was 1 GeV)
- New process/model (*CERN summer student S. Yajaman*)
  - G4MuonToMuonPairProduction
  - G4MuonToMuonPairProductionModel
  - Cross section is ~10^{-5} of e+e- pair production
  - Spectrum of muons is much harder
    - High energy muon pair may be produced by energetic muon is a calorimeter

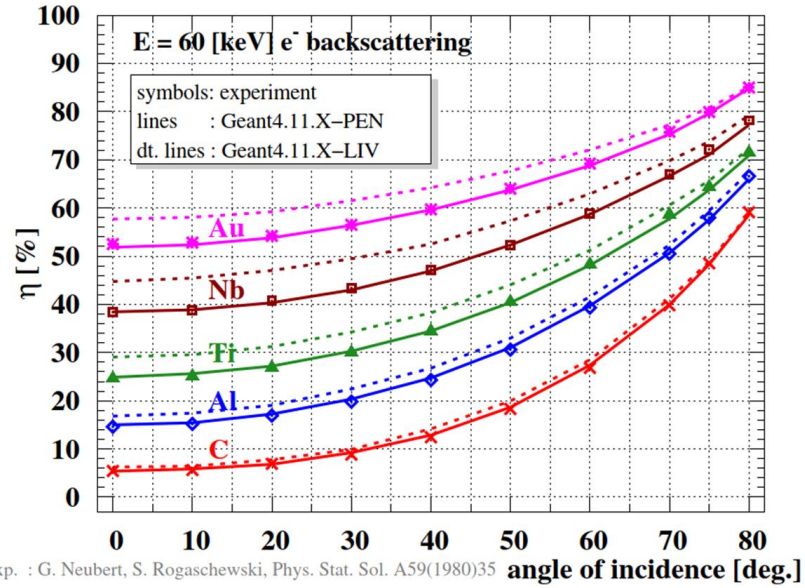


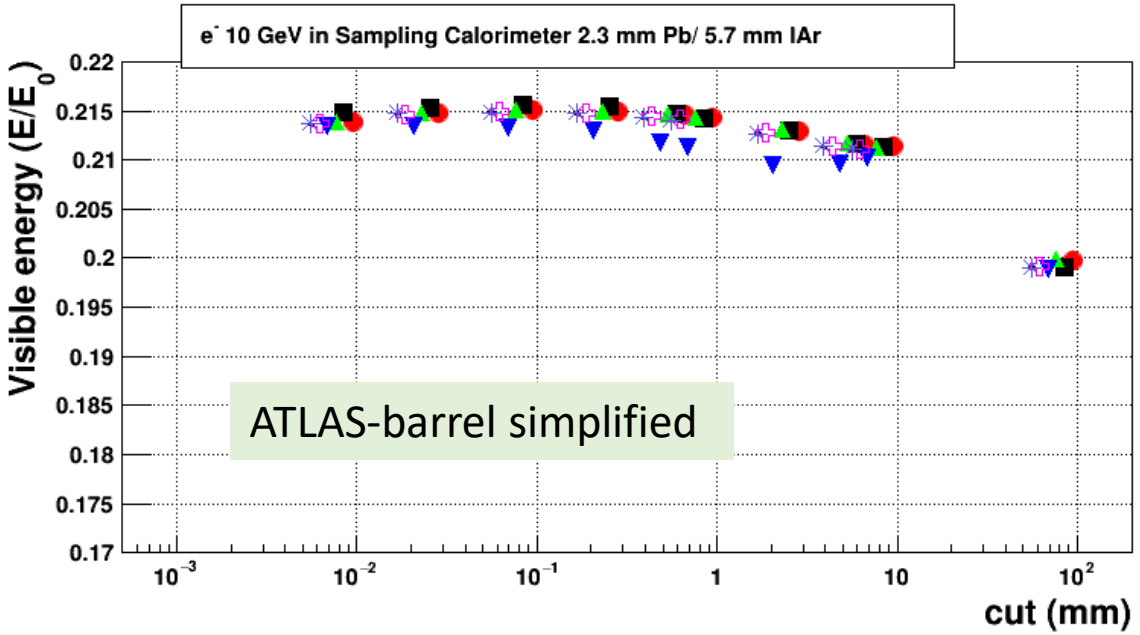


Modifications in EM physics for 11.1

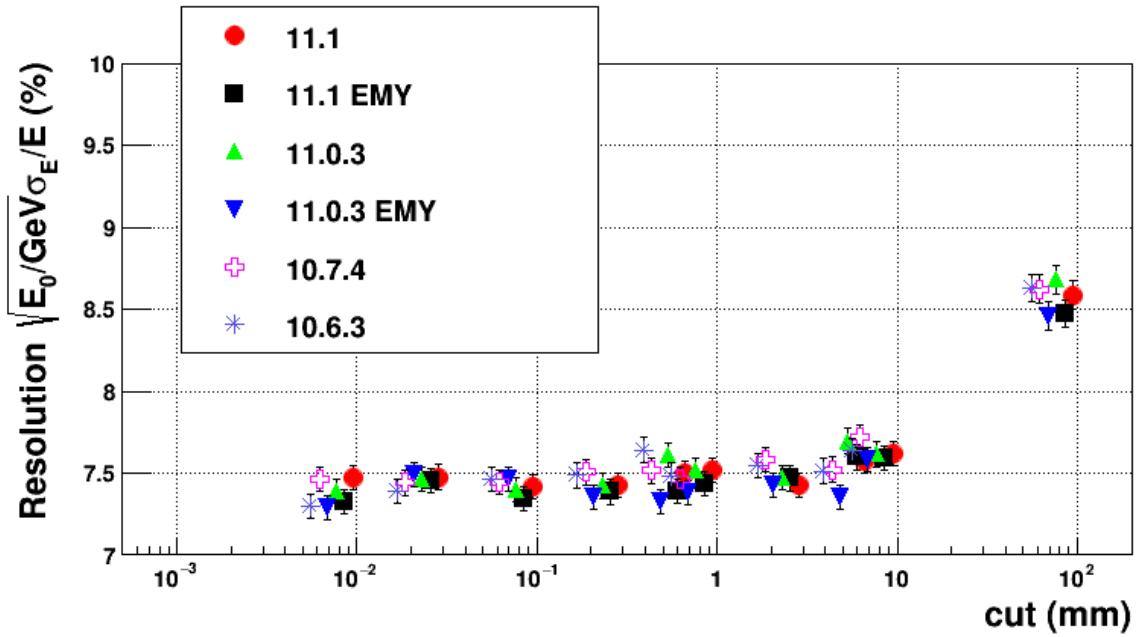
- G4EmStandardPhysics
  - Gamma general process
  - G4UrbanFluctuation
- G4EmStandardPhysics_option1
  - G4TransportationWithMsc
- G4EmStandardPhysics_option3
  - Gamma general process
  - G4UrbanFluctuation
  - G4LinhardSorensen ion ionisation model
  - MSC RangeFactor=0.03
- G4EmStandardPhysics_option4
  - Gamma general process
  - Penelope (instead of Livermore) ionisation for e- below 100 keV
  - G4UrbanFluctuation
  - G4LinhardSorensen ion ionisation model

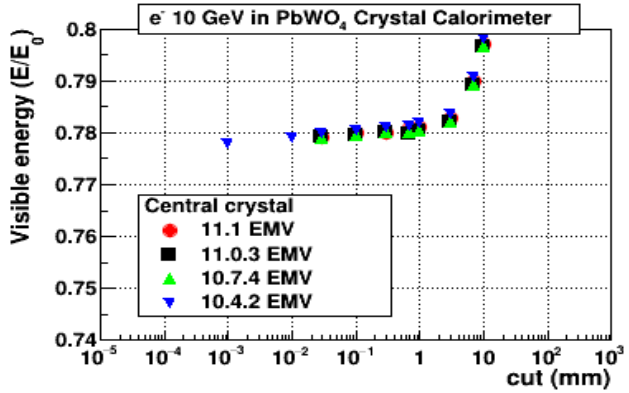
- G4EmLivermorePhysics
  - G4UrbanFluctuation
  - G4LinhardSorensen ion ionisation model
  - EPICS2017 gamma cross sections
- G4EmPenelopePhysics
  - G4UrbanFluctuation
  - G4LinhardSorensen ion ionisation model

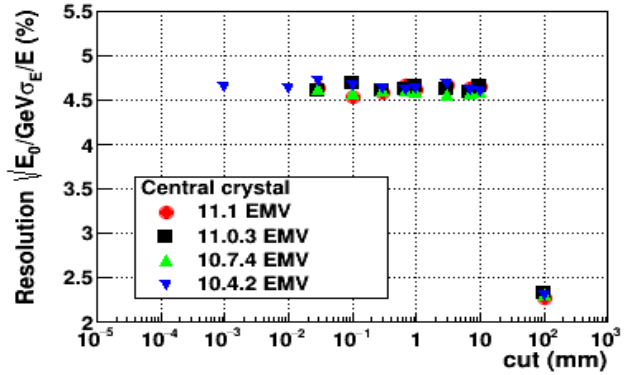


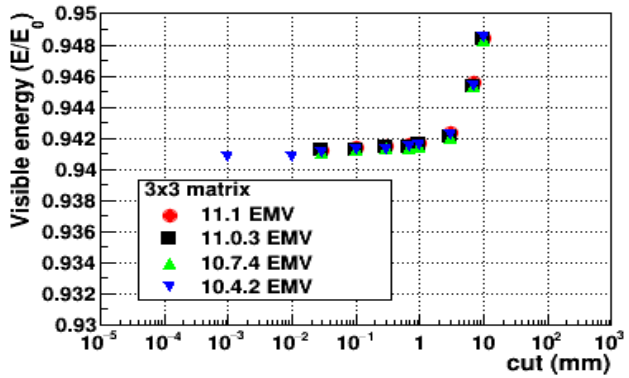


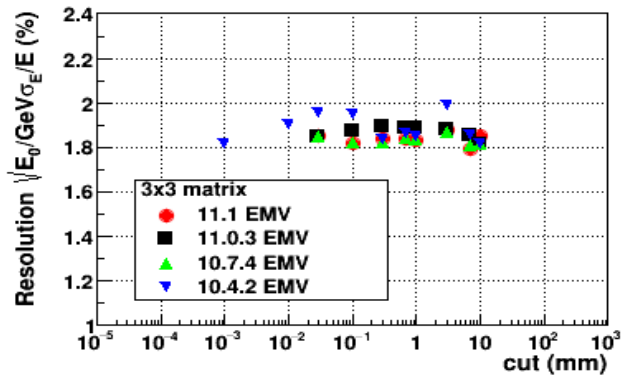
ATLAS-barrel simplified

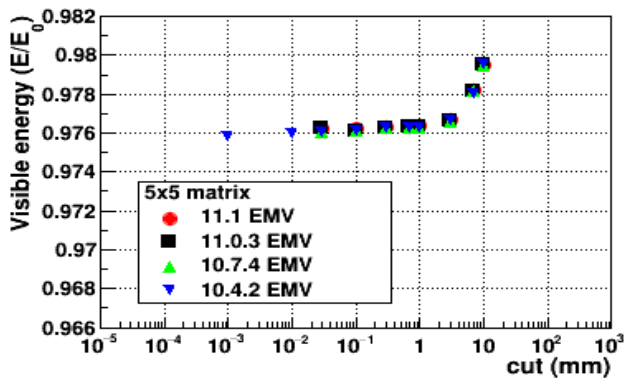


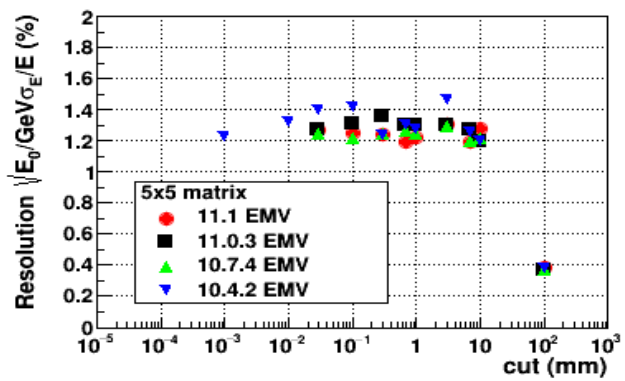




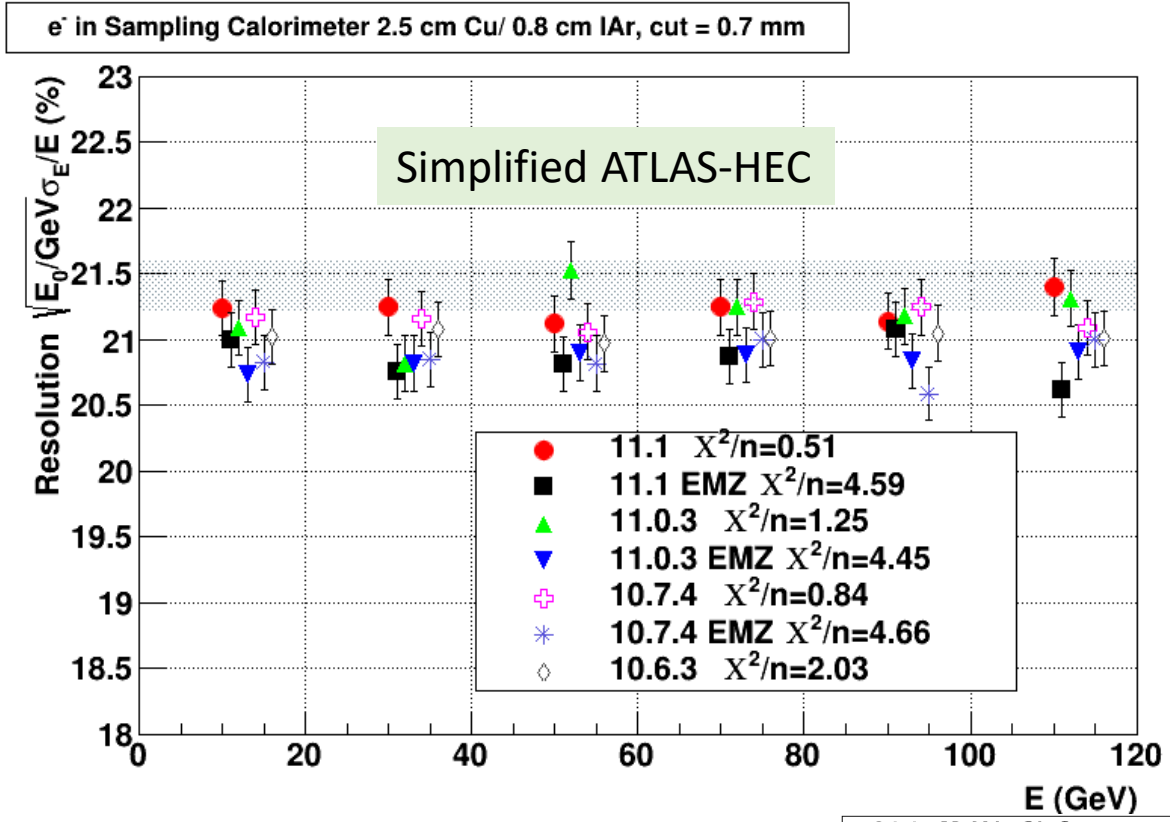


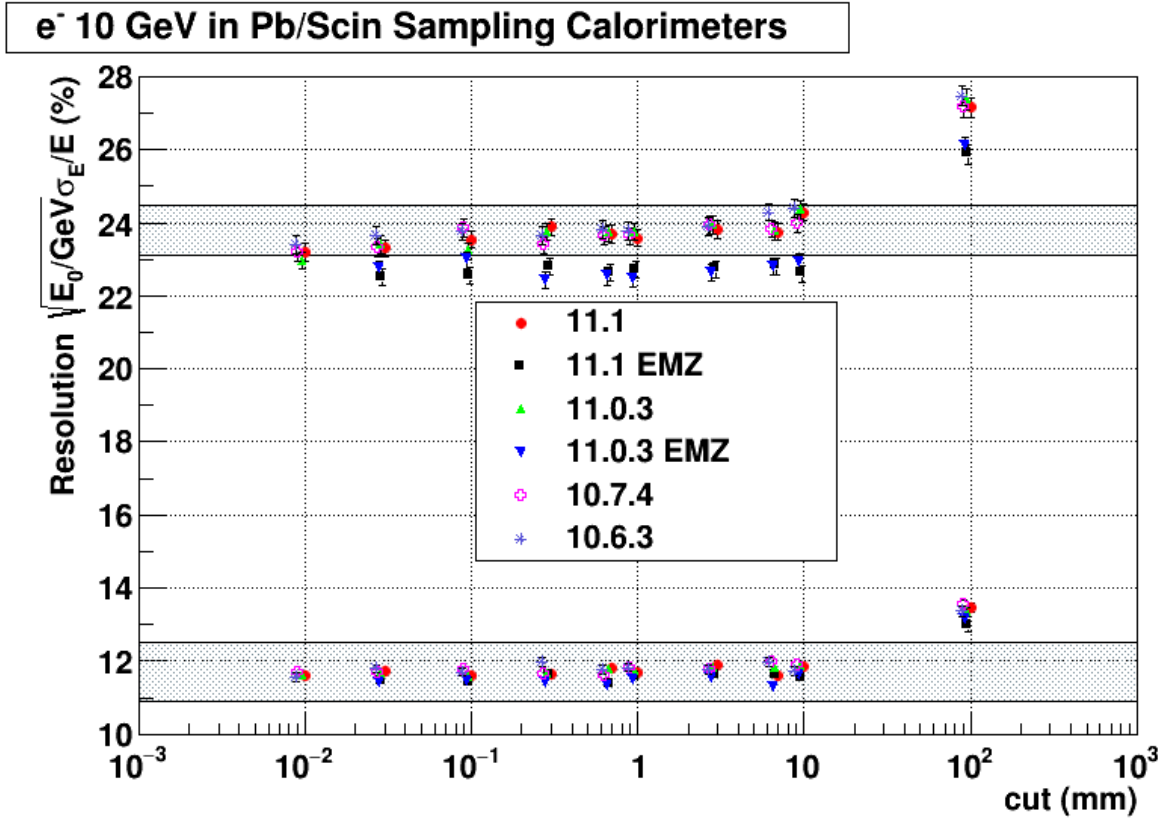


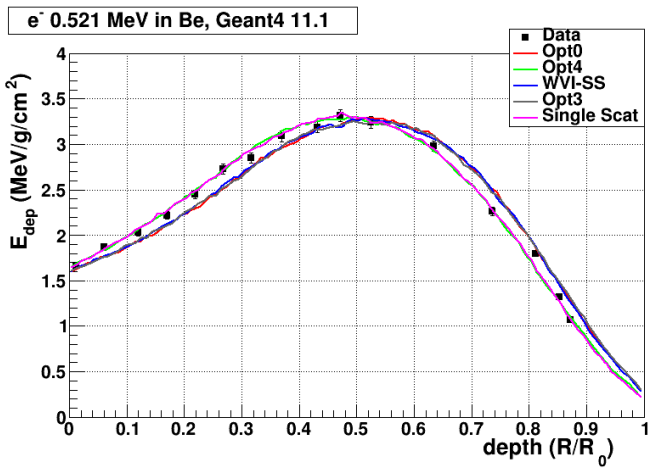


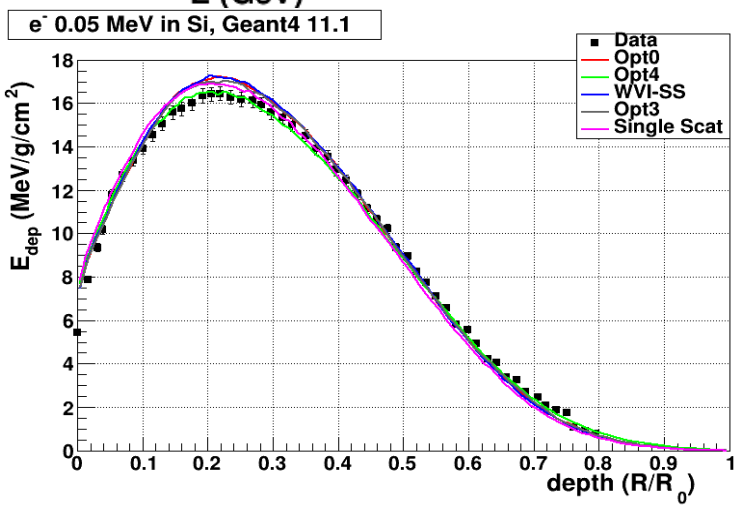


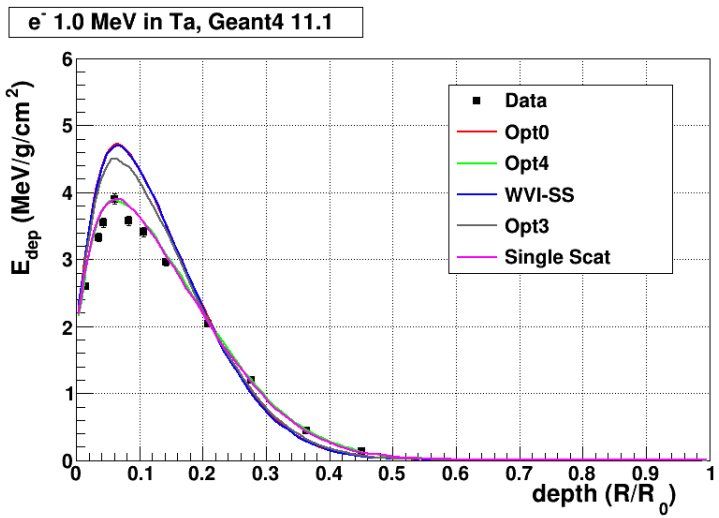
CMS ECAL simplified


e⁻ in Sampling Calorimeter 2.5 cm Cu/ 0.8 cm lAr, cut = 0.7 mm
Simplified ATLAS-HEC
Resolution $\sqrt{E_0}/\mathrm{GeV}\,\sigma_E/E$ (%)
E (GeV)
11.1 X^2/n=0.51
11.1 EMZ X^2/n=4.59
11.0.3 X^2/n=1.25
11.0.3 EMZ X^2/n=4.45
10.7.4 X^2/n=0.84
10.7.4 EMZ X^2/n=4.66
10.6.3 X^2/n=2.03


e⁻ 10 GeV in Pb/Scin Sampling Calorimeters
Resolution $\sqrt{E_0}/\mathrm{GeV}\,\sigma_E/E$ (%)
cut (mm)
11.1
11.1 EMZ
11.0.3
11.0.3 EMZ
10.7.4
10.6.3


e⁻ 0.521 MeV in Be, Geant4 11.1
Data
Opt0
Opt4
WVI-SS
Opt3
Single Scat
E_{dep} (MeV/g/cm^2)
depth (R/R$_0$)


e⁻ 0.05 MeV in Si, Geant4 11.1
Data
Opt0
Opt4
WVI-SS
Opt3
Single Scat
E_{dep} (MeV/g/cm^2)
depth (R/R$_0$)


e⁻ 1.0 MeV in Ta, Geant4 11.1
Data
Opt0
Opt4
WVI-SS
Opt3
Single Scat
E_{dep} (MeV/g/cm^2)
depth (R/R$_0$)

Updates in DNA processes/models

- DNA sub-library dependences are resolved (H. Tran)
- G4Pow, G4Log, G4Exp are used in DNA models (P. Dondero)
- Many updates for chemistry models (H. Tran)
- A new extended example “moleculardna” in Geant4 11.1 (H. Tran)
  - Full chain DNA example
  - Simulation of physics, physics-chemistry and chemistry processes in DNA geometries
  - Improvements of molecularDNA are on-going in context of ESA/BioRad3 project including combination with muti-scale framewok for DNA damage prediction
    - GRAS / Geant4 / Geant4-DNA : GCR, SPE -> lunar habitat -> ICRP human phantoms -> organs -> cells -> molecularDNA
- Extension proton transport to 300 MeV (M. A. Cortes-Girardo)
  - G4DNARPWBAExcitationModel, G4DNARPWBAIonisationModel

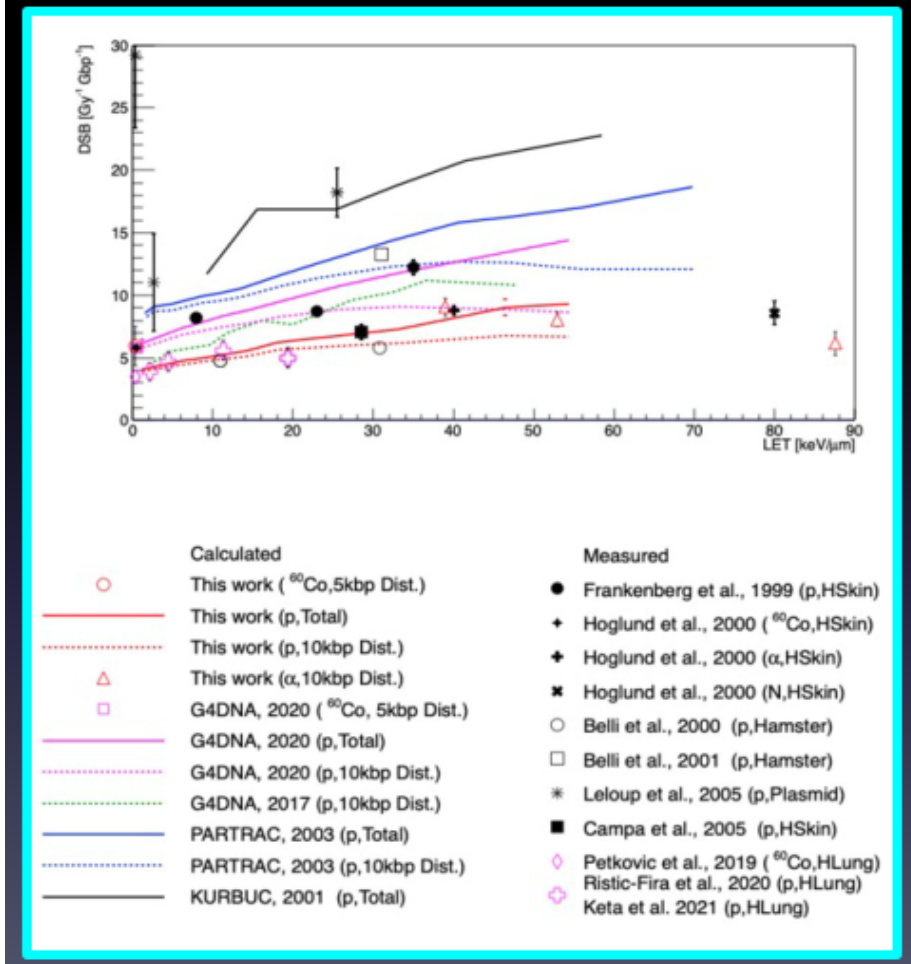
Extended utility classes to build EM physics

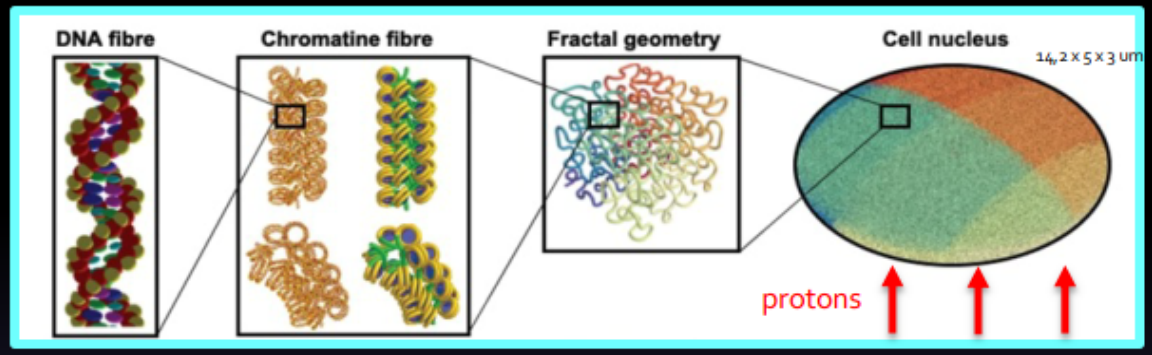
- G4EmBuilder
  - Added instantiation of G4TransportationWithMsc
- G4EmModelActivator
  - Fixed instantiation of PAI model per region
  - Fixed light ion instantiation per region
- All G4EmDNAPhysics_X are inheriting of G4EmDNAPhysics
  - Common method ConstructParticle()
  - ConstructProcess() is now implemented via G4EmDNABuilder utility
    - Set of parameters for G4EmDNABuilder is different for each X
    - Classes become much more compact; maintenance become significantly easier
  - Standard models are used for particle type and energy interval, where DNA models are not available
  - Upper energy limit is extended to 300 MeV
- G4EmDNAPhysicsActivator
  - Provides DNA physics configuration on top of any standard Physics List
  - G4EmDNABuilder utility are used in the same way as inside G4EmDNAPhysics_X

Ready to use extended example in Geant4 11.1

New « molecularDNA » extended example : simulation chain on a fractal cell nucleus model

« molecularDNA » example





- A full fractal geometrical model of a cell has been developed from realistic pieces of chromatin fibers (0.012 bp/nm³) – straight, turned and turned-twisted segments (75 nm, 38 histones)
- The simulation of physics, physico-chemistry and chemistry (IRT) are combined with such a geometry in a single Geant4-DNA application fully controlled by macro files
- Early DNA damage can be simulated reasonable agreement with simulations and experiments (protons)

Parameters
- Geant4-DNA Physics: option2 + ELSEPA
- R_{direct}: 3,5 A°
- E_{direct}: 5 eV – 37,5 eV
- Geant4-DNA Chemistry: option3
- P_{OH}: 0.405
- Histone as absorber
- d_{kill}: 9 nm
- Δt_{chem}: 0.5 ns
- t_{chem}: 5 ns
- **Output: Nikjoo (Nikjoo, 1997), SDD**

PhD thesis of N. Lampe (2017)
PhD thesis of W. G. Shin (2020)
D. Sakata et al.
K. Chatzipapas et al.
M. Dordevic et al.
Hoang Tran et al.

Phys. Med. 62 (2019) 152-157 (link)
Cancers 2021, 13 (2021) 4940 (link)

19

New approaches for EM physics

- How to speed-up simulation without compromise of physics?
  - Perform less number of computations at a step and less number of steps
- G4GammaGeneralProcess
  - Adopted by both ATLAS and CMS
  - In Geant4 11.1 is the default for Opt0, Opt3, Opt4, Liv, Pen physics
- G4TransportationWithMSC (J. Hahnfeld)
  - A new combined process
  - User may enable this process via UI command and/or C++ interface
  - Cannot work with G4CoupleTransportation
- Custom tracking manager (J. Hahnfeld)
  - Simplified gamma, e+- transport
- G4HepEm external library (M.Novak + J.Hanhfeld, B. Morgan)
  - Optimized gamma, e+- transport
  - https://github.com/mnovak42/g4hepem
  - https://g4hepem.readthedocs.io/en/latest/
  - Gateway for GPU use for EM physics

The Problem

```
*****************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
*****************************************************************************************

Step#  [...]     KineE         dEStep    StepLeng   TrakLeng    Volume      Process
    0  [...]     10 MeV          0 eV       0 fm       0 fm     World    initStep
    1  [...]     10 MeV  1.214e-15 meV       4 cm       4 cm     World    Transportation
    2  [...]  9.469 MeV      530.7 keV  442.5 um   4.044 cm     G4_Pb          msc
    3  [...]   8.78 MeV      689.5 keV  549.8 um   4.099 cm     G4_Pb          msc
    4  [...]  8.167 MeV      612.5 keV  576.7 um   4.157 cm     G4_Pb          msc
    5  [...]  7.287 MeV      678.7 keV  535.8 um    4.21 cm     G4_Pb        eBrem
    6  [...]  3.789 MeV      4.844 keV  5.203 um   4.211 cm     G4_Pb        eBrem
    7  [...]  3.089 MeV      699.9 keV  560.4 um   4.267 cm     G4_Pb          msc
    8  [...]  2.912 MeV      177.5 keV  160.5 um   4.283 cm     G4_Pb        eBrem
    9  [...]  2.412 MeV          500 keV  490.5 um   4.332 cm     G4_Pb          msc
   10  [...]  1.938 MeV      473.7 keV    503 um   4.382 cm     G4_Pb          msc
   11  [...]  1.304 MeV      633.7 keV  502.7 um   4.433 cm     G4_Pb          msc
   12  [...]  796.1 keV      508.2 keV  437.5 um   4.476 cm     G4_Pb          msc
   13  [...]  173.7 keV      622.4 keV  462.1 um   4.523 cm     G4_Pb          msc
   14  [...]     0 eV       173.7 keV  65.48 um   4.529 cm     G4_Pb        eIoni
```

The Solved Problem (with Internal MSC Stepping)

```
*****************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
*****************************************************************************************

Step#  [...]     KineE         dEStep    StepLeng   TrakLeng    Volume      Process
    0  [...]     10 MeV          0 eV       0 fm       0 fm     World    initStep
    1  [...]     10 MeV  1.214e-15 meV       4 cm       4 cm     World    TransportationWithMsc
    2  [...]  7.461 MeV      2.406 MeV  2.105 mm    4.21 cm     G4_Pb        eBrem
    3  [...]  6.518 MeV      723.9 keV  597.6 um    4.27 cm     G4_Pb        eBrem
    4  [...]  3.433 MeV      1.807 MeV  1.304 mm   4.401 cm     G4_Pb        eBrem
    5  [...]  1.911 MeV      1.412 MeV  1.434 mm   4.544 cm     G4_Pb        eBrem
    6  [...]  566.5 keV      1.345 MeV  1.372 mm   4.681 cm     G4_Pb        eIoni
    7  [...]  102.8 keV      463.7 keV  245.9 um   4.706 cm     G4_Pb        eBrem
    8  [...]     0 eV       102.8 keV  28.64 um   4.709 cm     G4_Pb        eIoni
```

- No steps limited by msc, directly go to discrete interaction (or volume boundary)!

Summary

- Active developments were carried out in different EM physics domains
  - Improved EM related code quality
  - Fixed problems in EM sub-libraries
  - Improvement of CPU efficiency for HEP applications
  - New model for ions
  - New model of muon pair production by muons
  - Addition of new models and examples for DNA physics
    - DNA models up to 300 MeV
  - Improved Physics List configurations
- Geant4 EM inside 11.1 is in a good shape
  - There are no bug reports required prompt fixing
- EM physics in 11.1 allows different opportunities application specific
  - LHC experiments may benefit from existing new features
  - The G4HepEm library may be used together with 11.1
    - GPU and other R&D developments may be performed more effectively
- ATLAS and CMS already using these new developments