Keynote: EM aspects in Geant4

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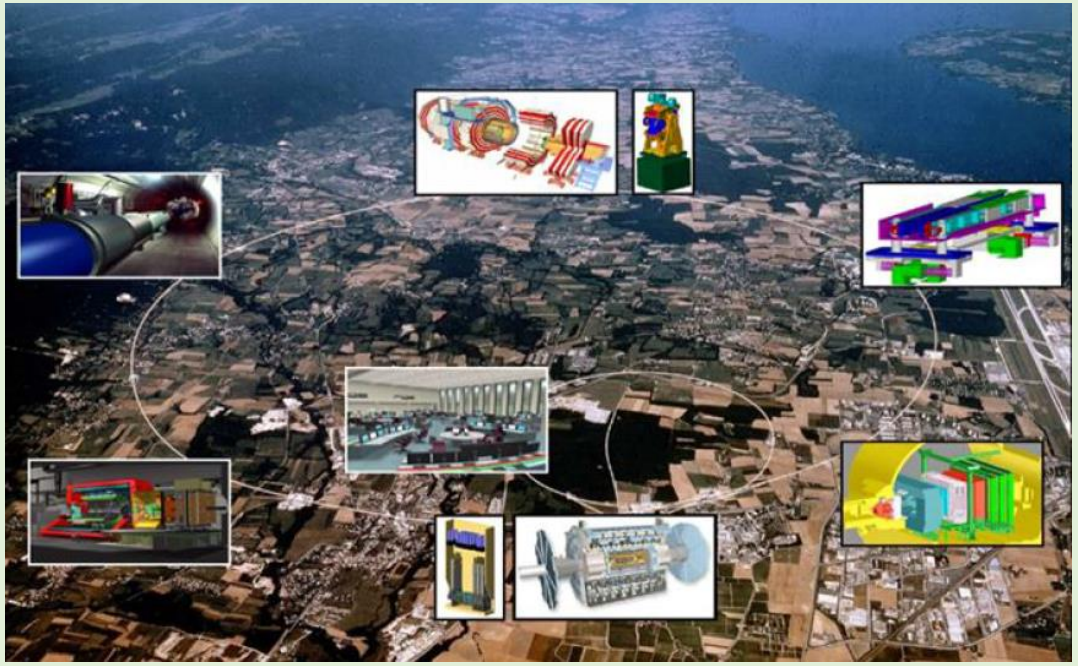
Outline

- Introduction
- Geant4 kernel libraries for EM physics
- Selected EM physics developments
  - Gamma processes
  - Fluctuation of energy loss
  - Ion transport
  - Combined processes
- EM Physics Lists
- Summary



- Release schedule and goals strongly coupled with LHC program
- Phase-2 LHC (2029) required more performant Monte Carlo
- Significant efforts of the Geant4 to redesign the toolkit making it faster
  - For HEP applications 1 % of CPU means a lot
- Production using super-computer facilities with GPU

Introduction

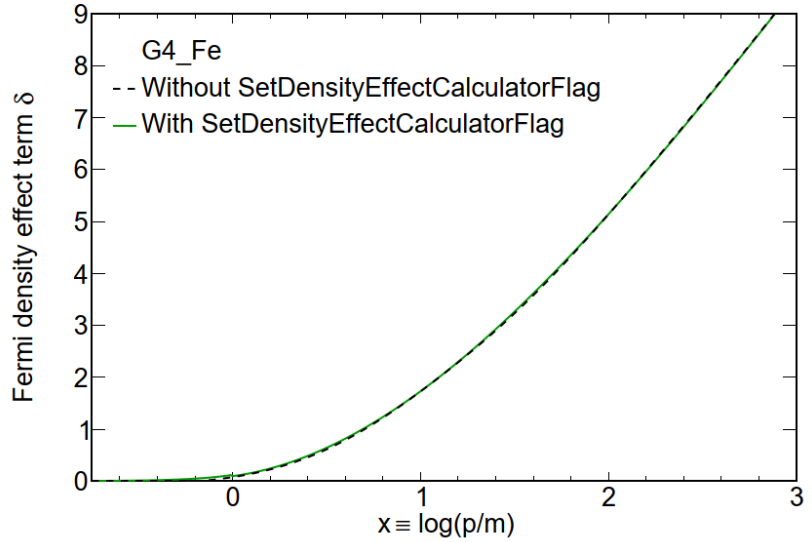
- Geant4 History
  - Early discussions at CHEP 1994 @ San Francisco CERN & Japan seeded R&D proposal
  - Dec ’94 –R&D project start
  - Dec ’98 -First Geant4 public release -version 0.0
  - …..
  - 2004: ATLAS, CMS, and LHCb start using Geant4 in production
  - Dec 2013 – version 10.0 – 1st with multi-threading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

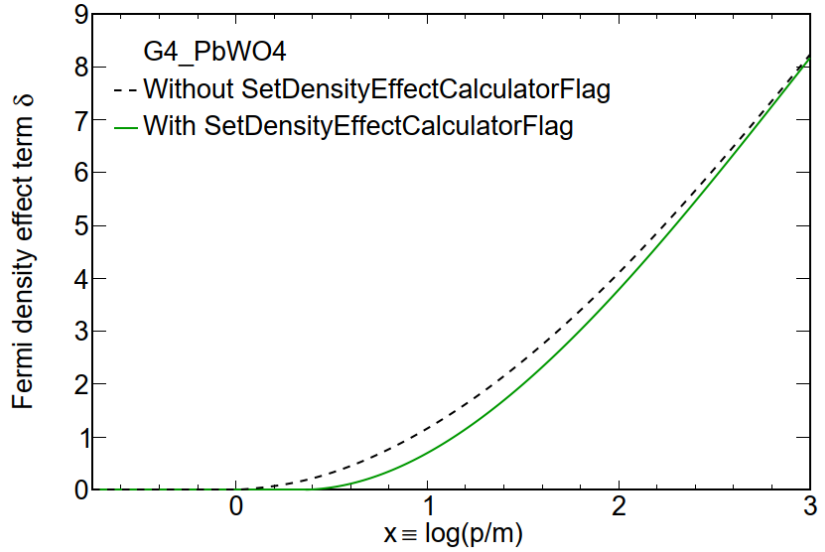
- Object oriented design and C++ allow to have a flexible code organisation
  - New components may be added without affecting other part of exiting code
  - User may be a developer
- Geant4 developments are strongly supported by HEP community
  - Support of the LHC experiments for the Geant4 Collaboration is the top priority
  - Large shutdown of LHC 2019 – 2021
  - The new Run3 is started in 2022
- Limitations from COVID affect Geant4 10.7
  - Recommended version 10.7.4
- For Geant4 11.0 a lot of modifications were introduced
  - Removed many obsolete files related to physics
  - Moved files and directories
  - Geant4 11.0.3 – recommended version

Geant4 kernel libraries for EM physics

Materials category updates

- Matthew Strait proposed several improvements for the density effect computations
  - Initial on-fly computation of the density effect in 10.7 has some problems
  - The algorithm for G4DensityEffectCalculator was improved for 11.0
  - G4DensityEffectData:
    - For 11.1 several typos are fixed in the density effect data table for 8 materials, the most significant fix for G4_Tm, small for G4_Be, G4_Mg, G4_Fe, and G4_Y.
- Mean ionization potential for carbon is changed from 81 to 78 eV
  - Choice what NIST data to take
- New methods to build compound materials
  - void AddElementByNumberOfAtoms(…)
  - void AddElementByMassFraction(…)
  - void AddMaterial(….)
- G4MaterialPropertyVector, G4OpticalMaterialProperties:
  - Insist material property vectors are in increasing order of energy
  - Default verbosity=1 as everywhere in Geant4 physics
  - Use indexes instead of string in run time





Updates of base libraries for Geant4 11.0

- Use C++11 keyword uniformly over EM sub-libraries
  - “virtual” keyword in base classes methods
  - “override” or “final” in derived class methods
  - where possible use advance loop pattern
  - moved initialisation of pointers, Boolean, and simple numbers to headers
  - use “const” variables where possible
  - removed unused variables and headers
  - check interfaces – improve where needed and possible
  - code is C++20 compatible
- Removal of obsolete classes and interfaces
  - the most important is removal of G4EmProcessOptions
- G4PhysicsVector constructor is changed, three type of constructors:
  - G4PhysicsLinearVector
  - G4PhysicsLogVector
  - G4PhysicsFreeVector
  - Spline flag should be enabled in constructor
  - Several spline types - allowing extensions

Updates of EM libraries for Geant4 11.1

- G4VEmProcess, G4VEnergyLossProcess, G4VMultipleScattering:
  - Moved general part of initialization to G4EmTableUtil and G4EmUtility
  - 27-30% class length reduction – easier to navigate inside classes
- EM processes and models was reviewed and updated
  - Spline and integral options belong now to each process and not centrally defined via G4EmParameters
  - Integral approach was reviewed and updated
    - Taking into account cross section change at a step of charged particles
  - G4CrossSectionType is introduced instead of Boolean flag
    - fEmNoIntegral
    - fEmIncreasing
    - fEmDecreasing
    - fEmOnePeak
    - fEmTwoPeacks
    - Implemented integral method for cross sections without precomputed tables
  - Subcut delta-electron production option is removed
    - G4VSubcutProcessor (user hook) interface is available
  - CorrectionAlongStep(..) method is optimized in all ion ionization models
- Number of bins in physics vectors are not anymore part of G4EmParameters but are computed via number of bins per decade

Geant4 model catalog

- Since 2008 we have process subtype
  - G4VProcess::GetSubType()
  - Stable ID for each process
- Separate enumerators for EM, DNA, and hadronics models without overlaps
  - G4EmProcessSubType.hh ID = 1-25
  - G4OpProcessSubType.hh ID = 31-36
  - G4DNAModelSubType.hh ID = 0-5
- There are methods in G4Track:
  - SetCreatorModelID(const G4int)
  - GetCreatorModelID() const
  - GetCreatorModelIndex() const
  - GetCreatorModelName() const
- There is G4PhysicsModelCatalog utility class

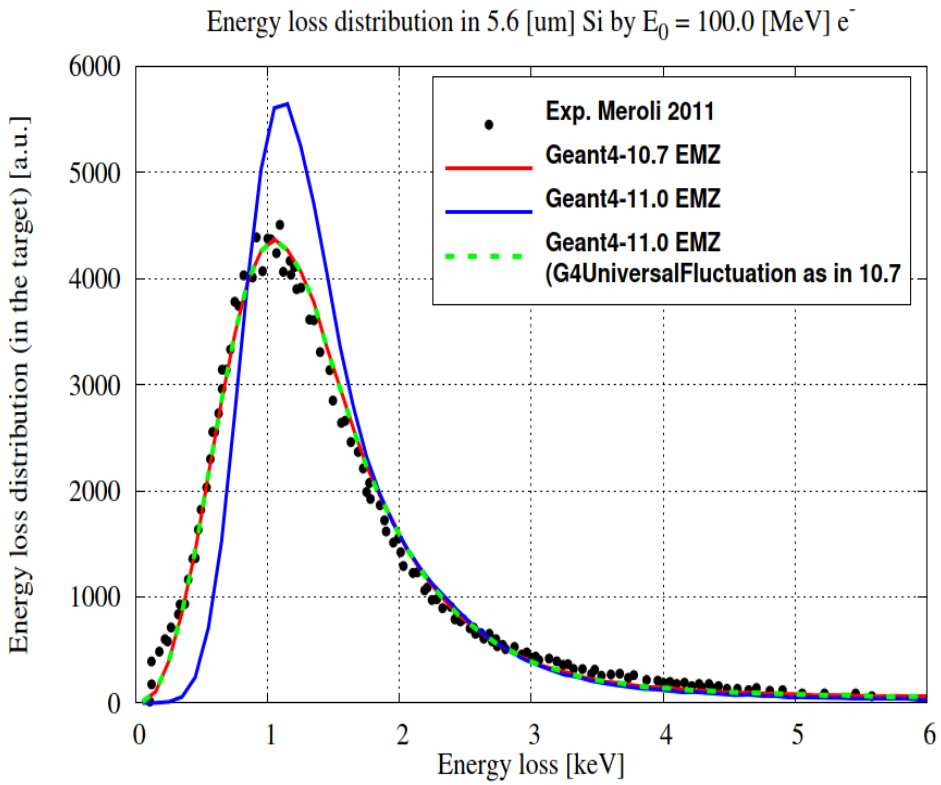
- EM models IDs and names
  - 10000 EMunknown // any EM model
  - 10010 DeltaElectron // ionisation
  - 10011 DeltaEBelowCut // sub-cutoff production
  - 10012 TripletElectron //
  - 10013 AugerElectron // from any process
  - 10020 Bremmstrahlung
  - 10021 SplittedBrem
  - 10022 TripletGamma // from any process
  - 10023 Fluorescence // from any process
  - 11000 DNAModel // any DNA model
  - 11001 Ritchie1994eSolvation
  - ..... 5 more DMA models

Selected EM physics developments for Geant4 11.1

Updates in standard EM processes/models
electromagnetic/standard

- 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
  - G4IonFluctuations
  - G4LossFluctuationDummy
  - An extension of the model list is possible
- G4UrbanMscModel – technical improvements
  - Main model for HEP
  - Extended precomputed data structure
  - Reduced number of instructions
- G4GoudsmitSandersonMscModel is stable

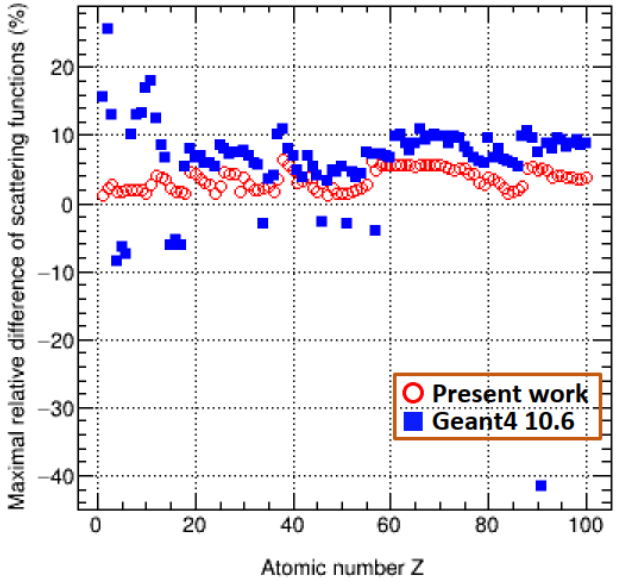
M. Novak



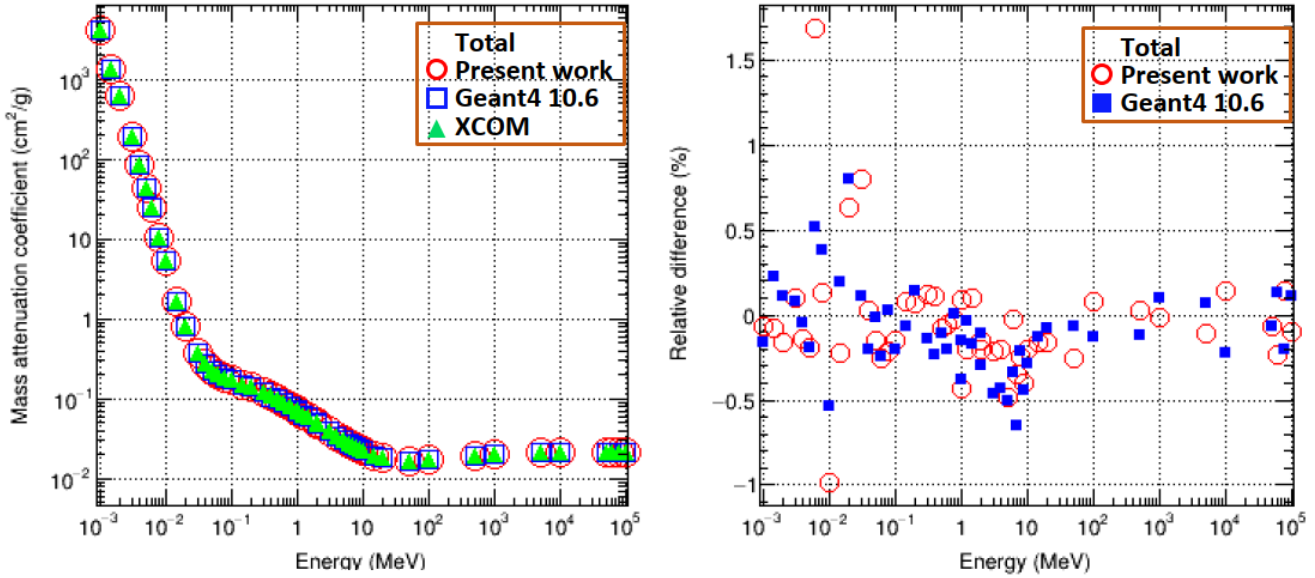
Implementation of the EPICS2017 database for photons in Geant4

Zhuxin Li et al., Physica Medica 95, 94-115 (2022)

Compton scattering



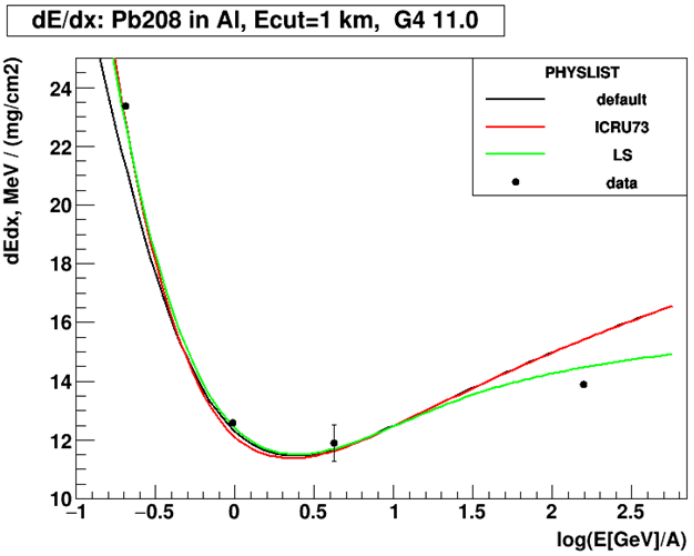
Gamma attenuation

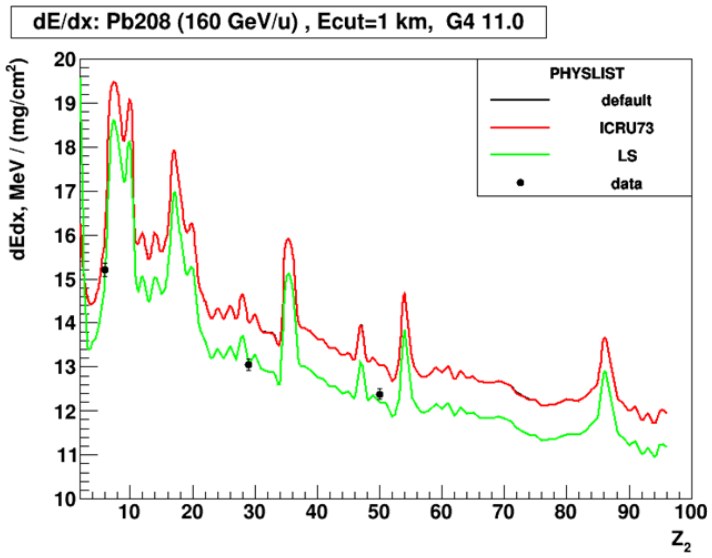


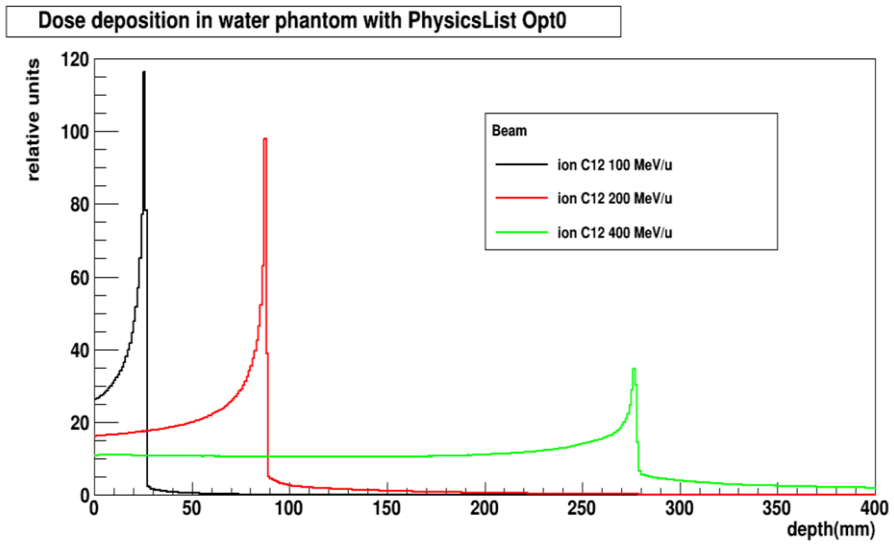
- EPICS-2017 data for cross sections and form factors are parameterized or used as a data table
  - In average accuracy of the new parameterisation total χ^2 is better for about 30%
- Validation performed versus XCOM and SCOFIELD
  - D.E. Cullen, A survey of photon cross section data for use in EPICS2017. IAEA-NDS-225, rev 1, 2018
- For Geant4 11.1 is the default for the Livermore models

Lindhard-Sorensen ion ionization model

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



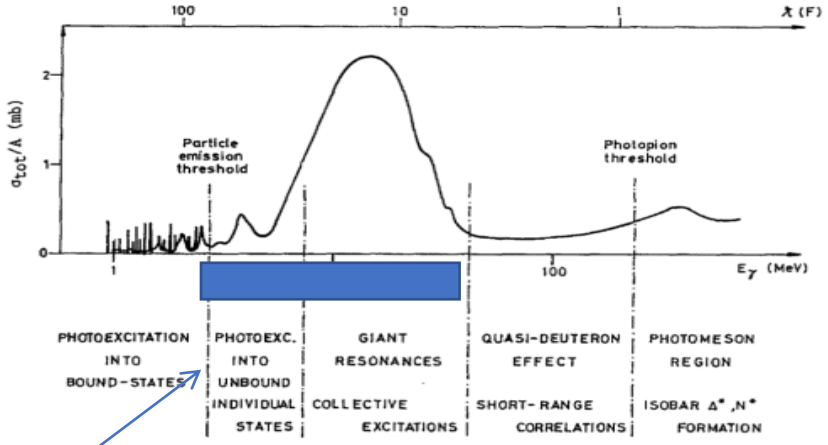


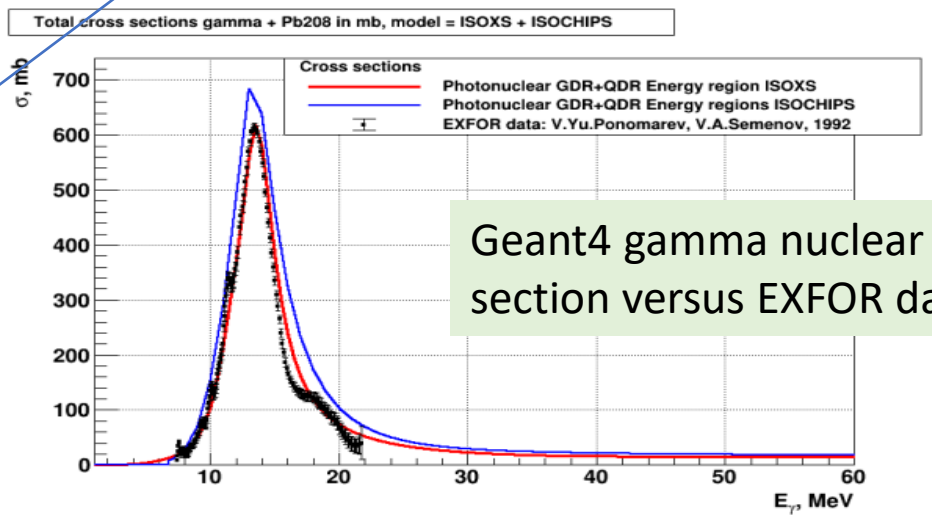


Gamma-nuclear cross section

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

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

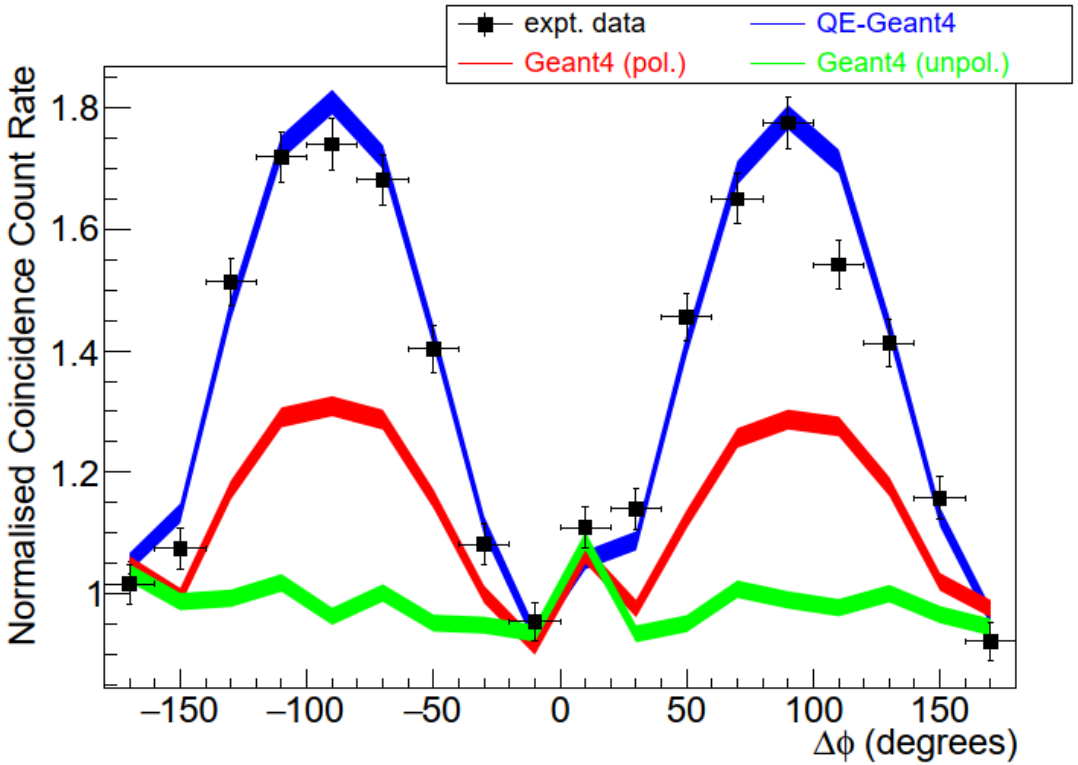


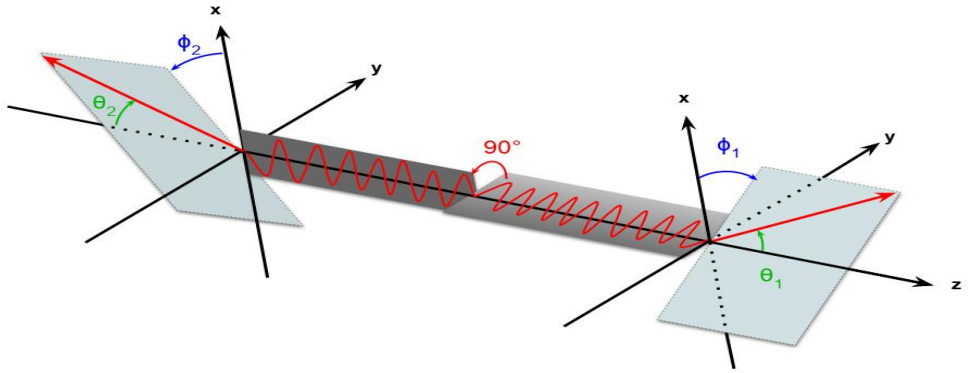


Geant4 gamma nuclear X-section versus EXFOR data

Quantum entanglement in positron annihilation

D.P. Watts et al. Nature Commun. 12 (2021) 1, 2646; arXiv: 2012.04939v1





- There is angular correlation for Compton scattering of two photons in PET device
- The developed method may be potentially used in HEP (Higgs->2 decay) and other applications

New approaches for EM physics

- How to speed-up simulation without compromise of physics?
- G4GammaGeneralProcess
  - Adopted both by ATLAS and CMS
  - Is the Geant4 default for 11.1
  - Use spline interpolation of x-section tables below 150 keV and above 100 MeV
- G4TransportationWithMSC (J. Hahnfeld)
  - New combined process
  - User may enable this process via UI command and/or C++ interface
  - Cannot work with G4CoupleTransportation
- Custom tracking manager (J. Hahnfeld, M. Novak)
  - Simplified gamma, e+- transport
- G4HepEm external library (M.Novak)
  - Optimized gamma, e+- transport
  - https://github.com/mnovak42/g4hepem
  - https://g4hepem.readthedocs.io/en/latest/

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)

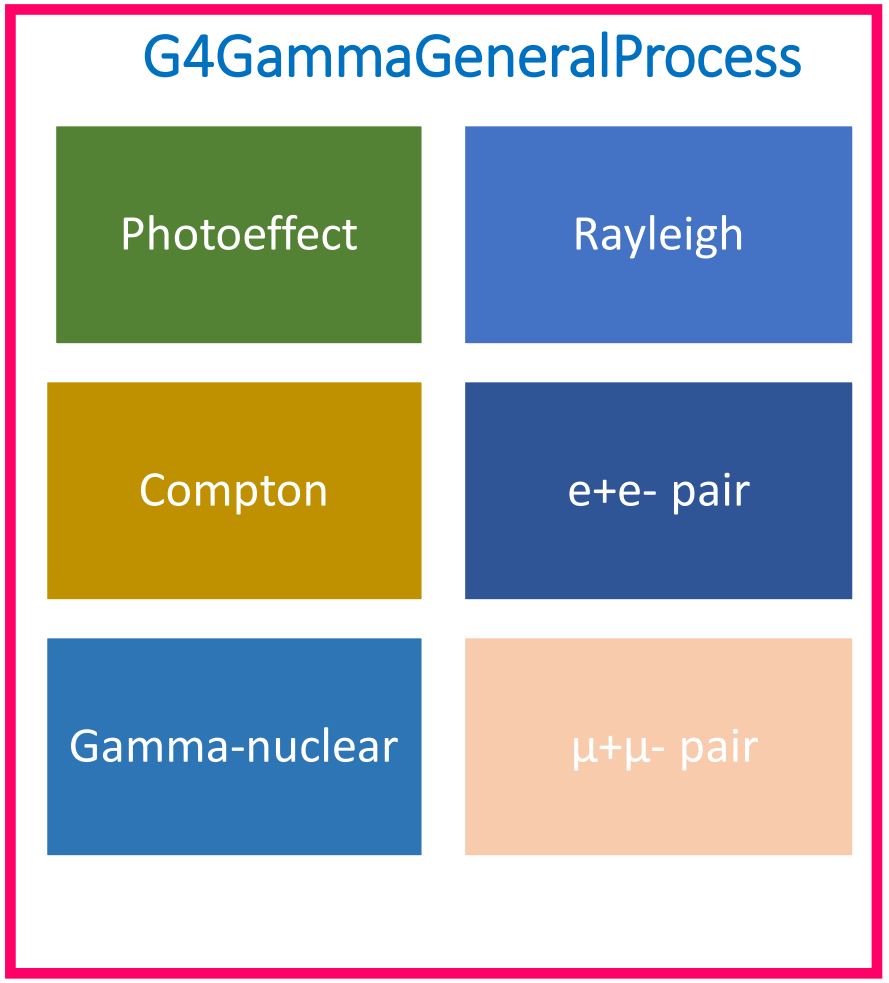
```
*****************************************************************************************
* G4Track Information:   Particle = e-,   Track ID = 1,   Parent ID = 0
*****************************************************************************************

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)!

G4GammaGeneralProcess

EPJ Web Conf. 214 (2019) 02046



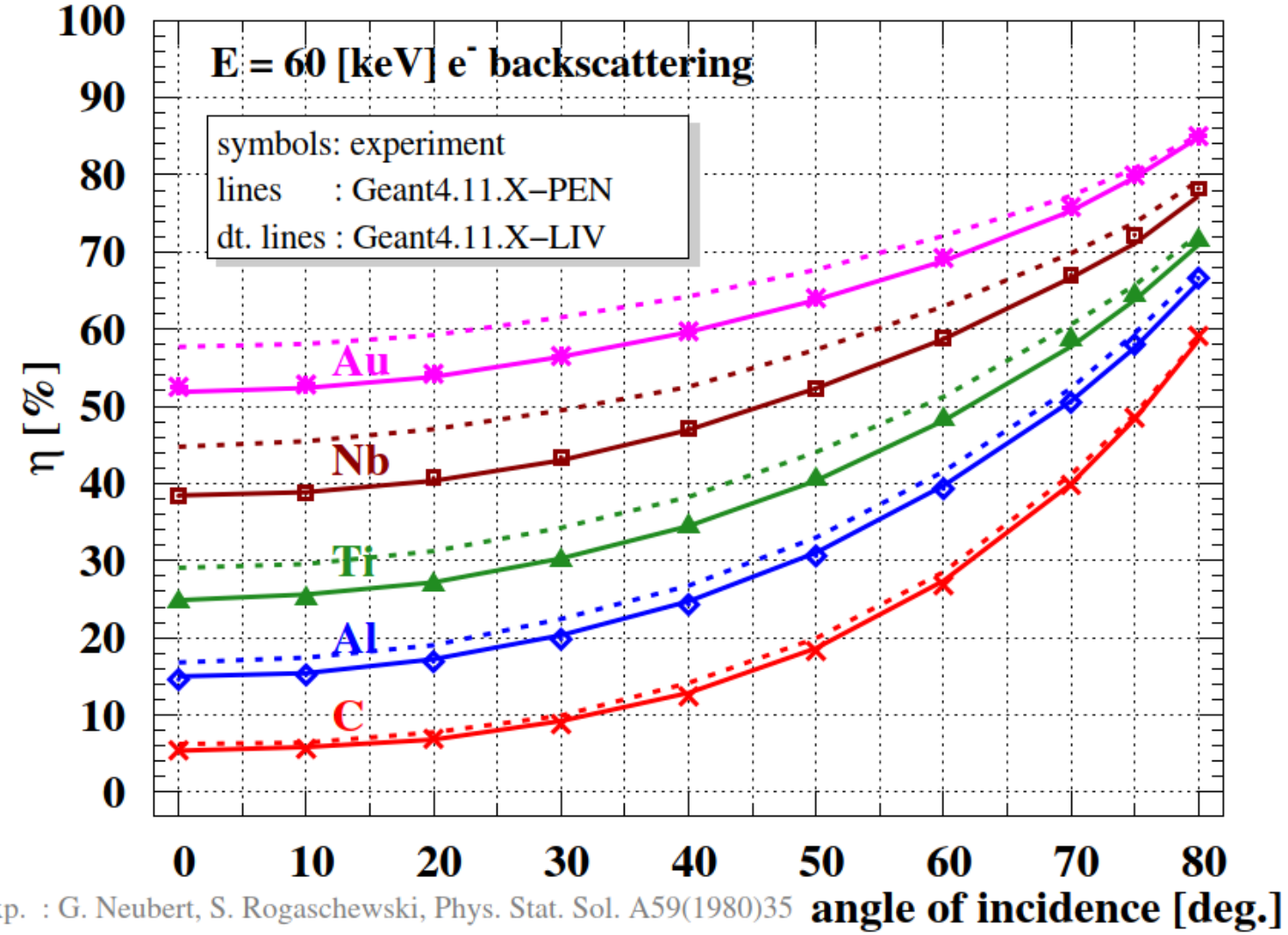
- SteppingManager see only 1 physics process
  - Only 1 mean free path
  - Plus transportation
- Enabled via UI command
  - In 11.1 is the default, UI command may be used to enable/disable
- Reduced number of instructions
  - Advantage in CPU ~5%
  - Extra PhysicsTables shared between threads – a bit more memory
- Final numbers for CPU/memory should be checked by users
- Woodcock tracking for ATLAS is implemented using inheritance

EM Physics Lists

Modifications in EM physics for Geant4 11.1

- G4EmStandardPhysics
  - Gamma general process
  - G4UrbanFluctuation
- G4EmStandardPhysics_option1
  - G4TransportationWithMsc
- G4EmStandardPhysics_option3
  - Gamma general process
  - G4UrbanFluctuation
  - G4LindhardSorensen ion ionisation model
  - MSC RangeFactor=0.03
- G4EmLowPPhysics
  - Gamma linear polarization is enabled by default
  - J. M. C. Brown and M. R. Dimmock, NIM B, 502, 2021, 176-182
- G4EmStandardPhysics_option4
  - Gamma general process
  - Penelope (instead of Livermore) ionisation for e- below 100 keV
  - EPICS2017 gamma cross sections for photo-effect and Rayleigh scattering
  - G4UrbanFluctuation
  - G4LindhardSorensen ion ionisation model
- G4EmLivermorePhysics
  - G4UrbanFluctuation
  - G4LindhardSorensen ion ionisation model
  - EPICS2017 gamma cross sections
- G4EmPenelopePhysics
  - G4UrbanFluctuation
  - G4LindhardSorensen ion ionisation model

Backscattering MC/data (M. Novak)



Penelope ionisation below 100 keV allows reproduce backscattering of electrons with higher accuracy as it was in Geant4 10.6

Extended utility classes to build EM physics

- G4EmBuilder
  - Provided initialization of basic EM particles
  - Added instantiation of G4TransportationWithMsc
- G4EmModelActivator
  - Fixed instantiation of PAI model per region
  - Fixed light ion instantiation per region
- G4EmDNABuilder utility for DNA physics
  - DNA processes instantiation
- All G4EmDNAPhysics_X are inheriting of G4EmDNAPhysics
  - Common method ConstructParticle()
    gamma, e+, e-, p, hydrogen, alpha, alpha+, GenericIon
  - 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 upper energy limit 300 MeV
    - For processes without DNA implementation standard processes/models are used
- G4EmDNAPhysicsActivator
  - Provides combined standard/DNA physics configuration on top of any standard Physics List
  - G4EmDNABuilder utility is used

Summary

- Active developments were carried out for Geant4 11.1
  - Improved code quality
  - Improvement of CPU efficiency
  - Addition of new models for DNA physics
  - Improved Physics List configurations
- Recommendation for users for recent releases
  - Geant4 10.7.4 and 11.0.3
- Geant4 11.1 is in a good shape
  - Number of pending problems are resolved
  - Several new features to speed-up simulation

THANK YOU, NAPOLI!