Summary on Geant4 Electromagnetic Physics

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For Geant4 EM working group

25th Geant4 Collaboration Workshop
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Outline

- Highlights of EM developments for Geant4 10.7
- EPICS2017 and Livermore models update
- Summary of the DPWA-SS model
- Recent updates of infrastructure
- Prospects and plans

This year we carried out important EM developments
Covid-19 slow down some developments

Materials updates

- New methods added for material creation due to ATLAS request
  - G4Material::AddElementByNumberOfAtoms(…)
  - G4Material::AddElementByMassFraction(..)
  - These methods may help to make material definition more easy to users
- Material property extension was described in the D. Sawkey talk

Modifications for 10.7beta

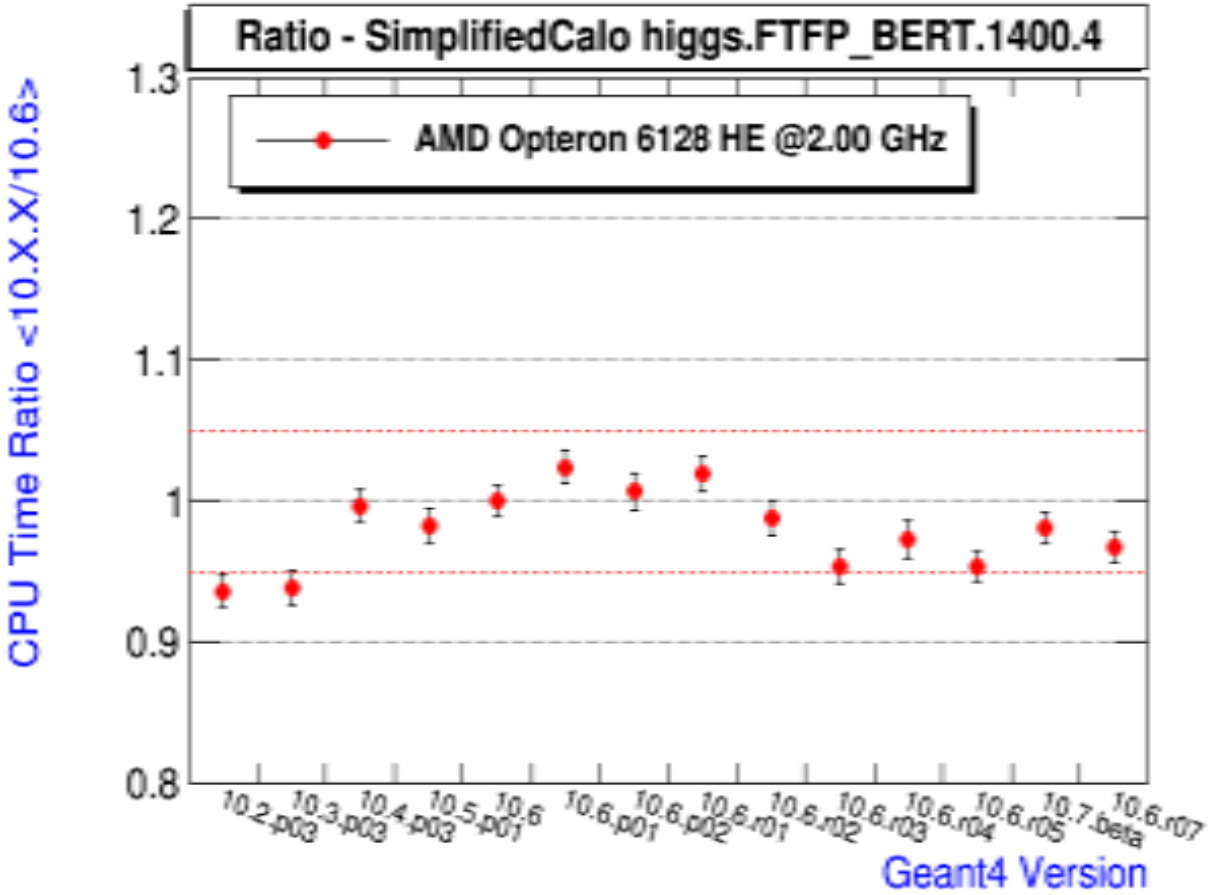
- G4UrbanMscModel – tuning of back-scattering for low-energy e- and e+
- G4Track – use PDG code “-22” instead of check of G4ParticleTable; improved default constructor and removed many “if” from G4Track inline methods
- G4DynamicParticle – added GetBeta() methos
- G4PhysicsVector and G4Physics2DVector – introduce modifications proposed last year by Mihaly

Modifications after 10.7beta

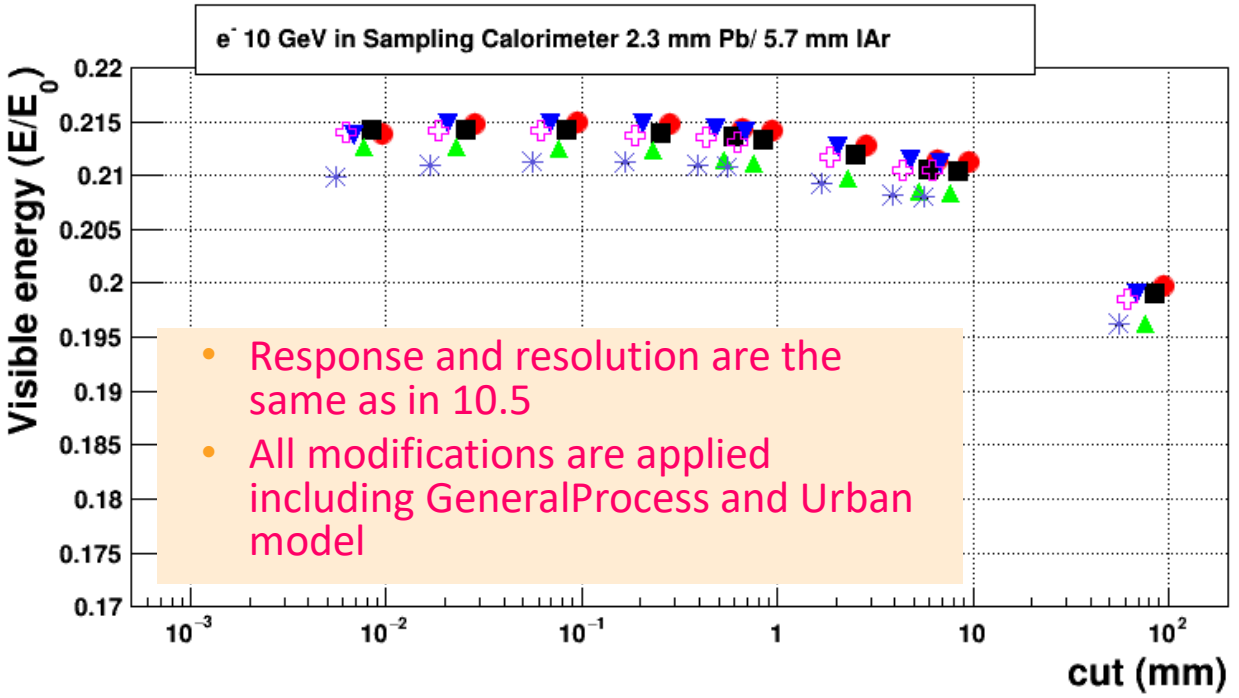
- G4EmParameters – new parameters are added; info output at initialization is improved
- Standard – improve usage of G4Mutex (mutex is used within a method, no call to another methods, when lock is set)
- G4UrbanMscModel – L. Urban tuned backscattering
- G4HadParticles – list of heavy particles for which EM physics should instantiated
- /physics_lists/constructors/electromagnetic:
  - G4EmStandardPhysicsSS – used DPW model
  - G4EmModelActivator – fixed problems #2052 and #2106
  - G4EmBuilder – new utility allowing to remove duplicated code and reduce length of G4EmStandardPhysivcs_optionX

Results of code improvements

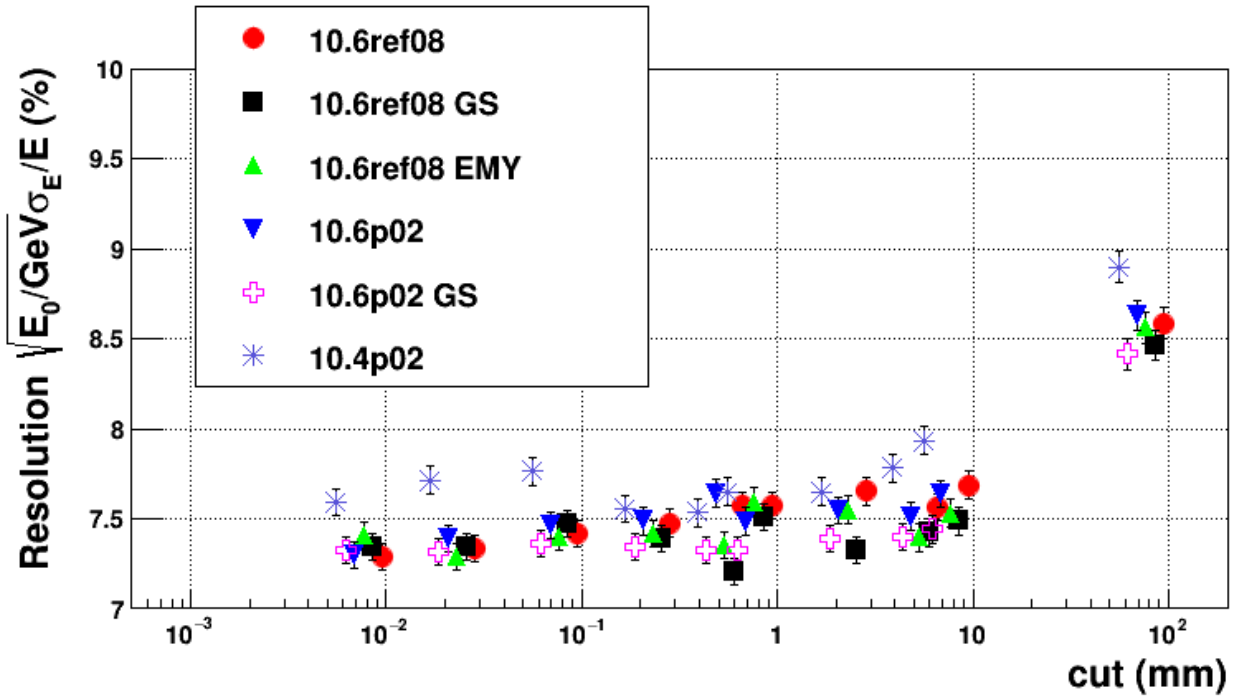
- Copy from FNAL performance monitoring page:



Cut dependence of ATLAS type simplified calorimeter response



- Response and resolution are the same as in 10.5
- All modifications are applied including GeneralProcess and Urban model



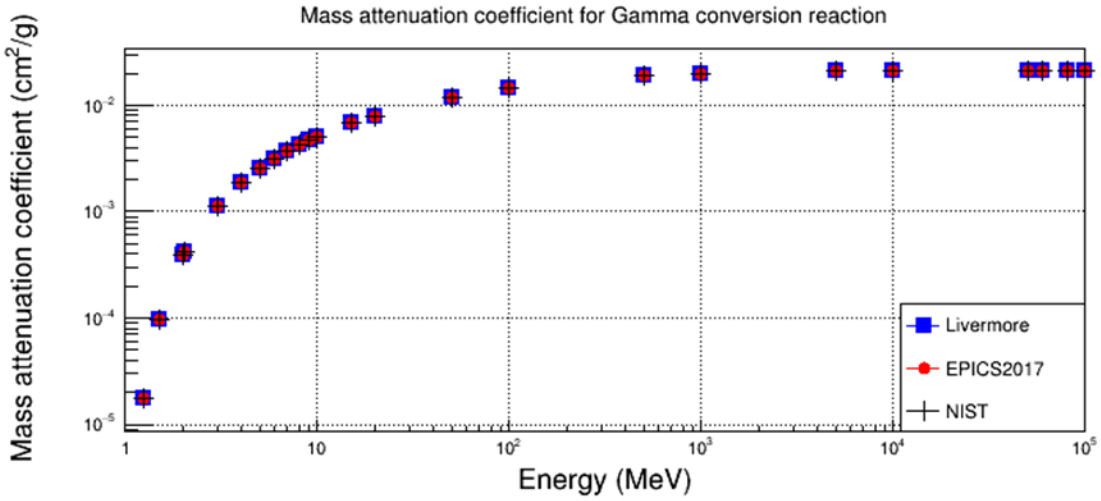
EPICS2017 AND LIVERMORE MODELS UPDATE (ZHUXIN LI)

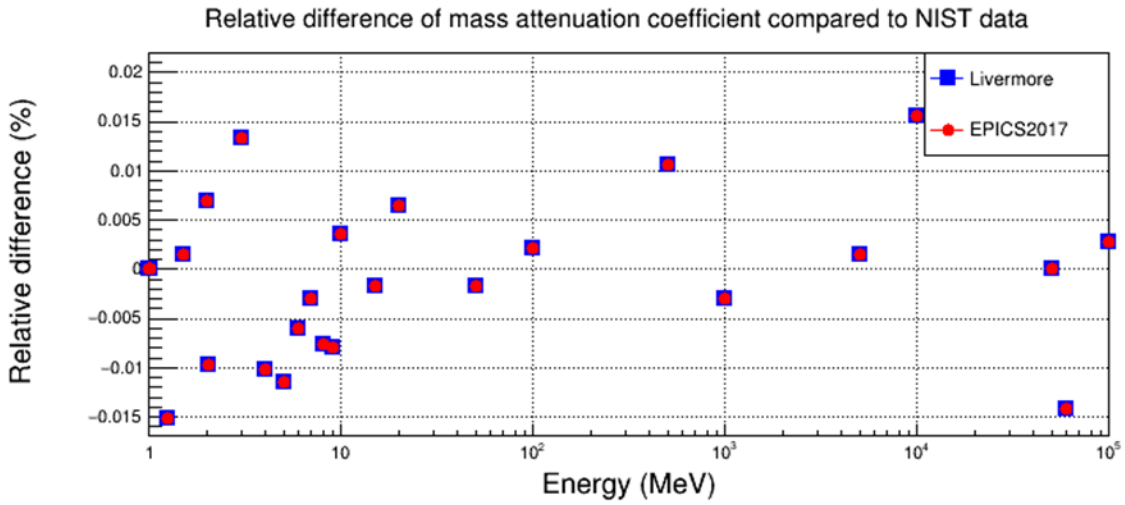
Implementation of EPICS2017 models for photons

- The "Livermore" low-energy electromagnetic models are currently using the databases of EPDL97/2014
- EPICS2017: Electron Photon Interaction Cross Section library
  - Dermott Cullen https://www-nds.iaea.org/epics/
- Update of data and Livermore model implementations for the following photon-matter interaction processes:
  - 1) Gamma conversion
  - 2) Compton effect
  - 3) Photoelectric effect
  - 4) Rayleigh scattering

Gamma Conversion

G4LivermoreGammaConversionModel and G4LivermoreGammaConversionModel5D (new model)



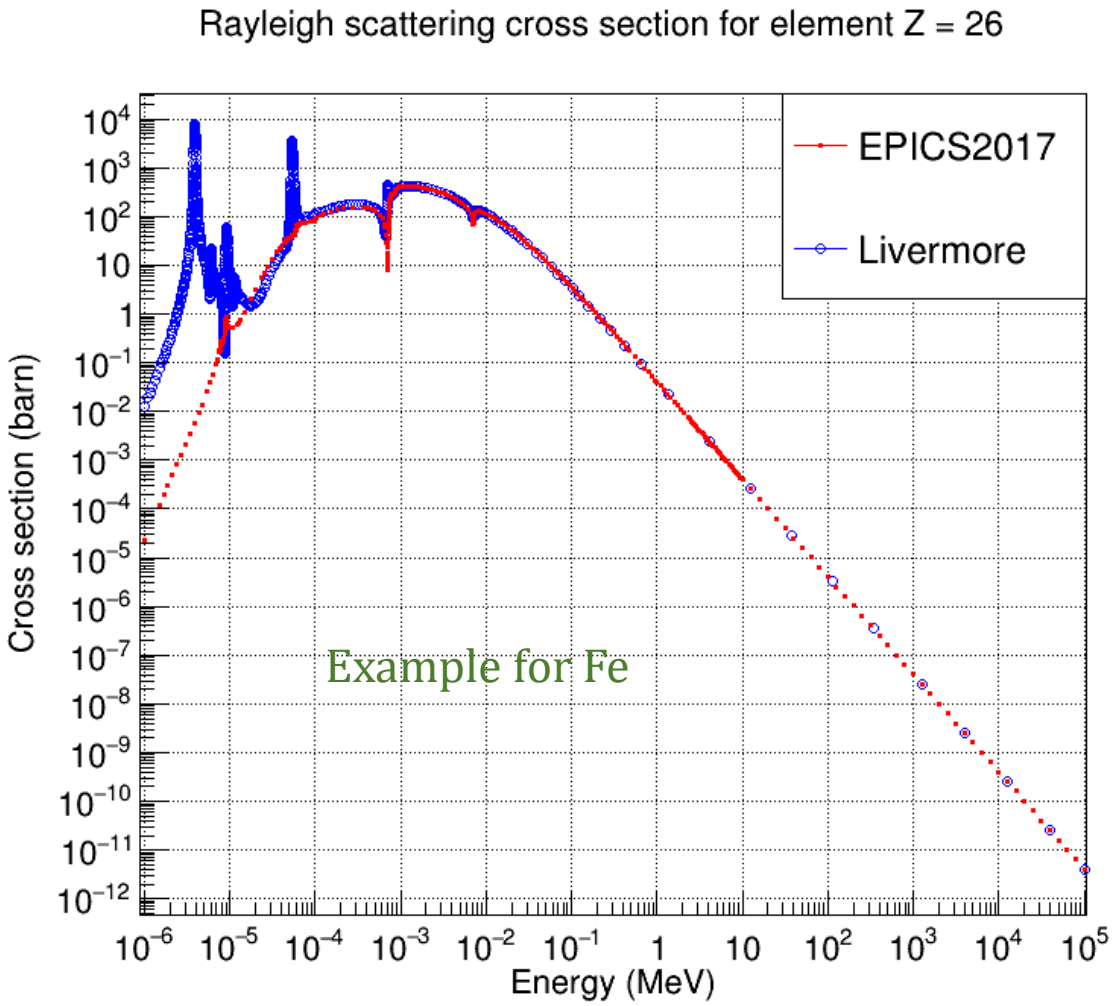


Cross section difference within 1.5 %

Rayleigh scattering

G4LivermoreRayleighModel

- There is an obvious difference in Rayleigh scattering cross section between EPICS2017 and old Livermore
  - There are low-energy data, which supported EPICS2017
- In real media form-factors and material effects significantly change results

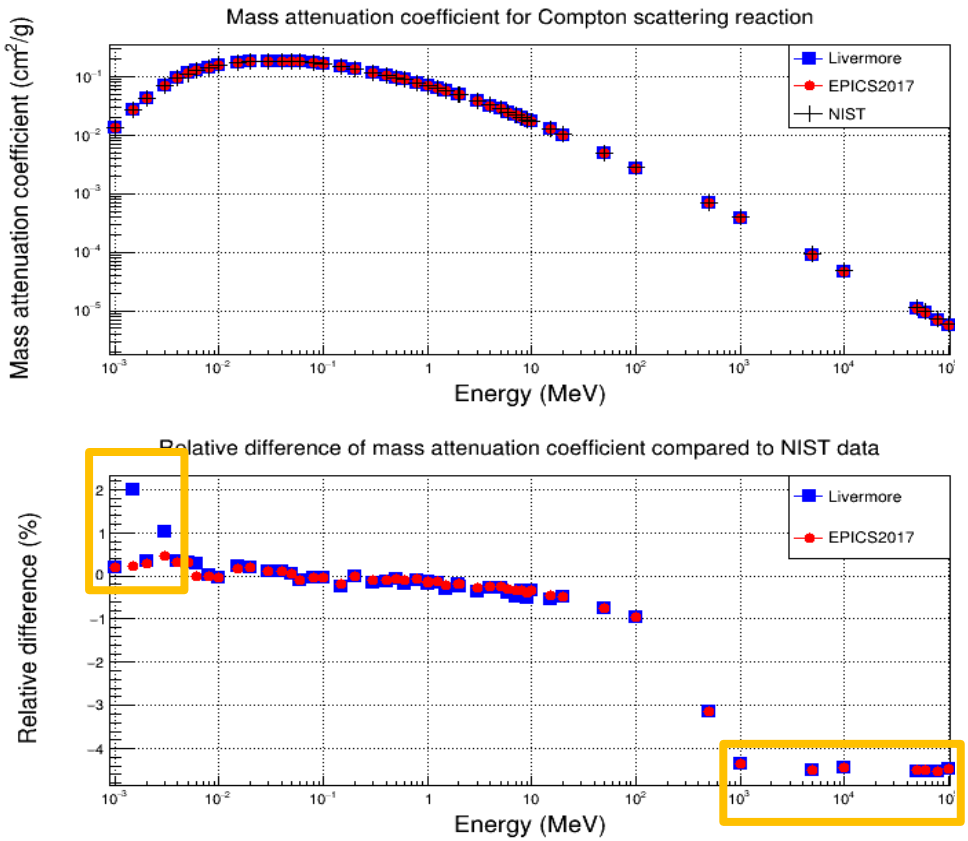


Compton effect

G4LivermoreComptonModel

- Calculation of mass attenuation coefficient
- Comparison with NIST reference data
- Smaller energy intervals in EPICS2017 lead to an improvement in low energy range
- A good agreement is obtained considering the energy limit used in Geant4 (E ≤ 1 GeV)

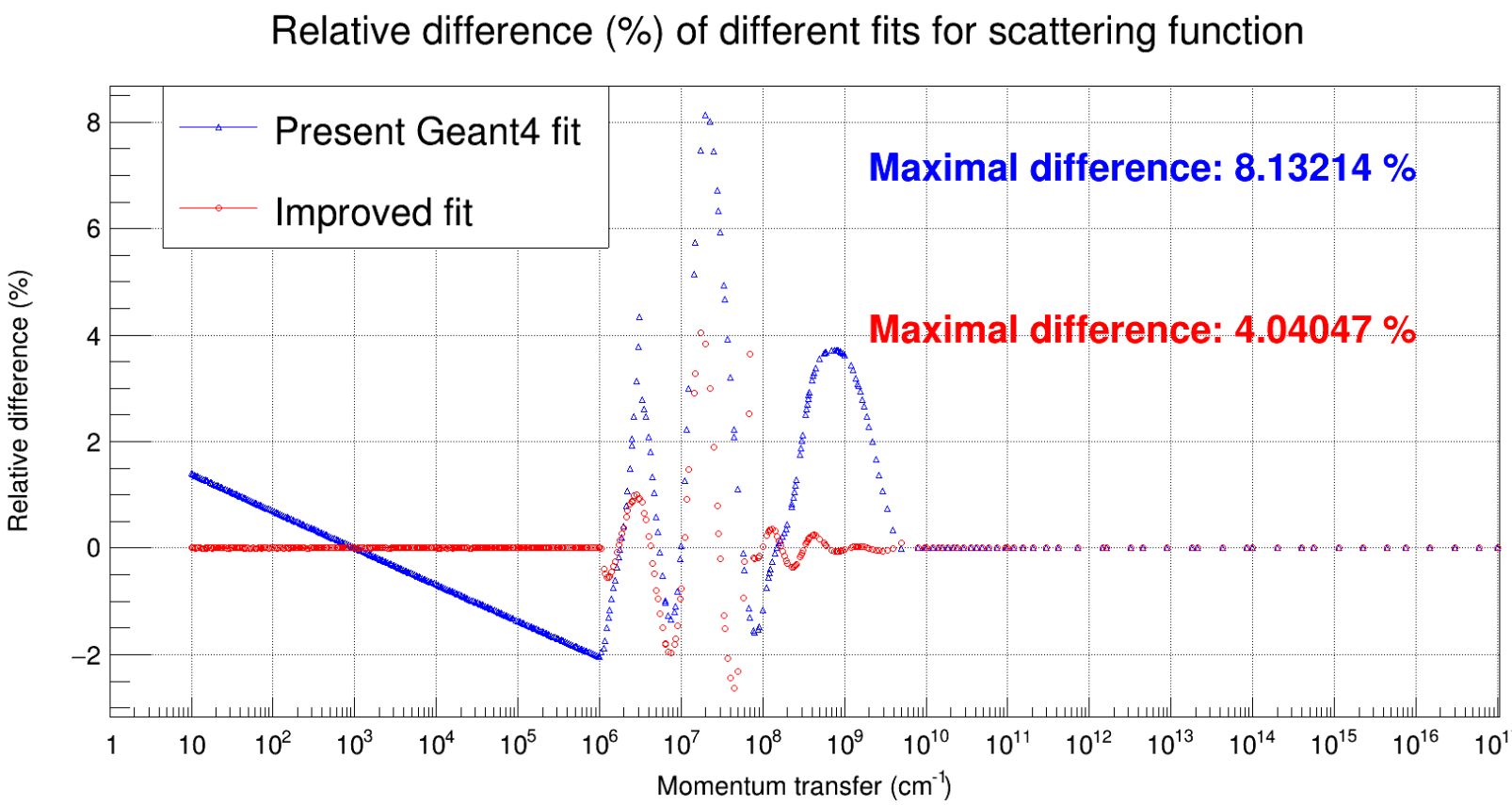
Example for water



Compton effect

- Fit of scattering function is improved

Example for Fe



SUMMARY OF THE DPWA-SS MODEL (M. NOVAK)

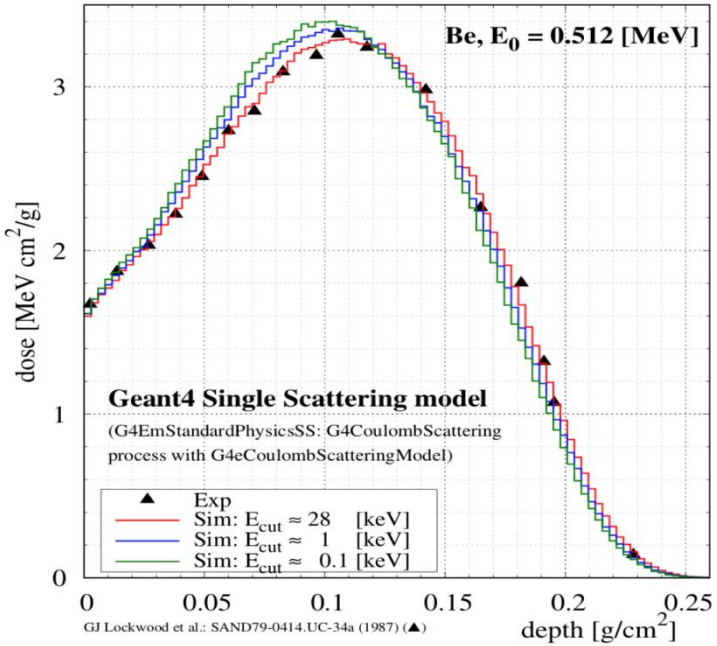
The new model:

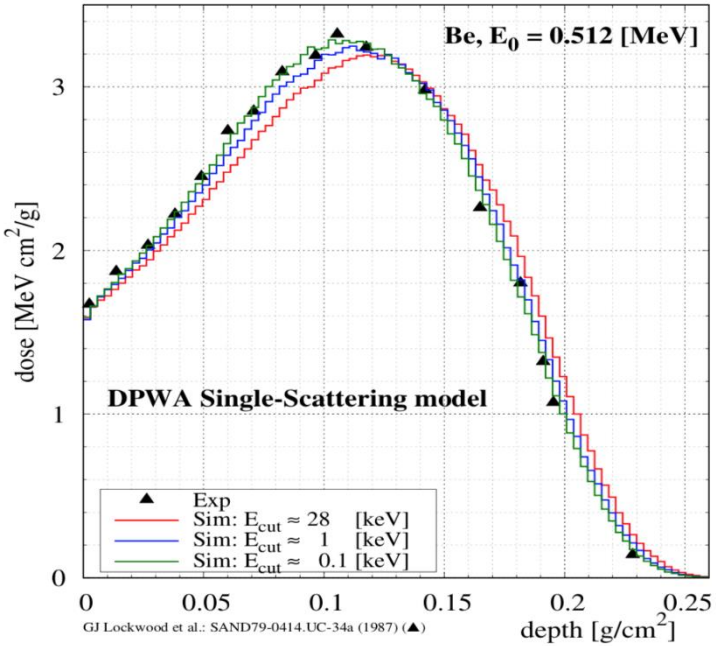
G4eDPWACoulombScatteringModel

- New model for e-/e+ single Coulomb scattering based on numerical Differential Cross Section (DCS) computed by ELSEPA: Dirac Partial Wave Analysis (DPWA)
  - scattering on the **static-field** of the nucleus **screened** by the atomic electrons
  - using **Fermi charge distribution** of the nucleus and **Dirac-Fock electron densities** of the atoms
  - ***exchange*** (only for e- of course), ***correlation-polarization*** (for E<10 [keV]) were applied on the top of the above ***static-field*** approximation
  - **for electrons** and **positrons** scattering on *free atoms* (described by the above scattering potential) with atomic numbers of **Z = 1-103** and **primary kinetic energies of 10eV - 100MeV**
  - **see more at** https://indico.cern.ch/event/937007/contributions/3937722/attachments/2070119/3475015/MNovak_DPWAElasticModel.pdf
- **NOTE**:
  - ***absorption correction*** **was not included** in the computation (since it's an inelastic channel)
  - most accurate **free atoms DCS**: **accuracy** might be **limited** when **aggregation effects** become **important** (i.e. E < ~keV)
  - the 10 eV low energy limit of the model is only for completeness

Production threshold dependence of the energy profile

- **Production threshold dependence of the shower shape**:
  - the new DPWA-SS model was used to simulate **depth dose profiles** (together with condensed history simulation for ionisation and bremsstrahlung)
  - strong **production threshold dependence** was observed in case of **all EM standard constructors** (except **Opt4**) **in low Z materials**
  - the example below compares the standard SS with the new DPWA-SS model
    - the new **DPWA-SS model converges to the experimental data** when l**owering the secondary production threshold** (as expected in all cases)





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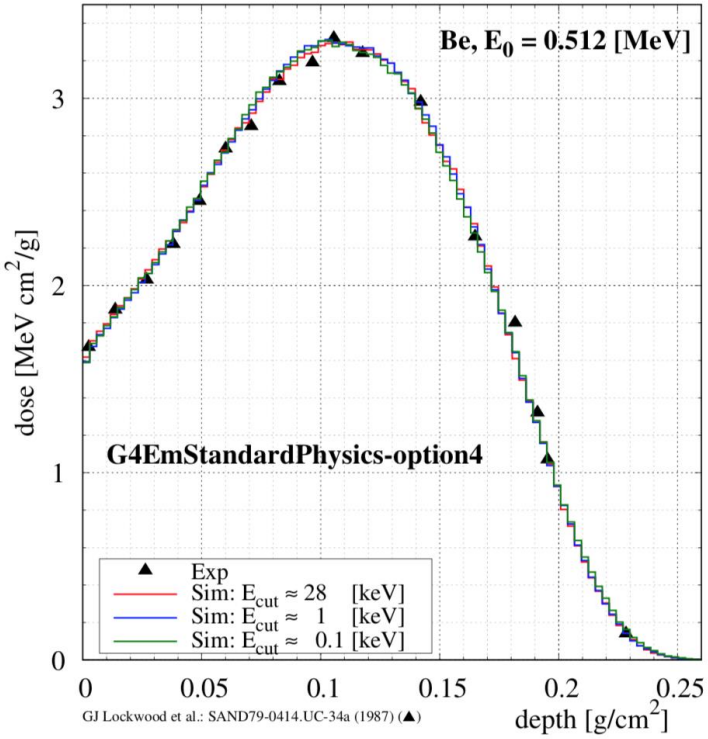
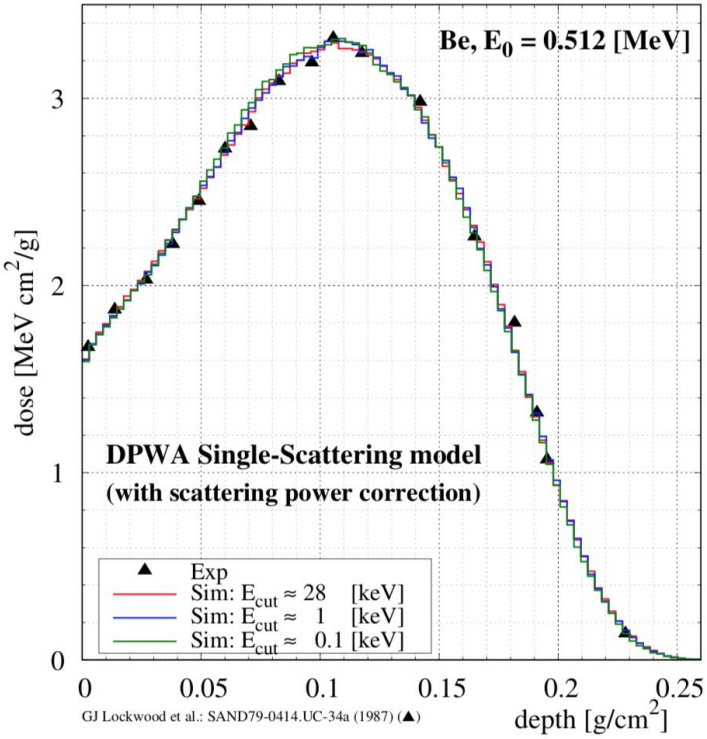
  - the example below compares the standard SS with the new DPWA-SS model
    - the new **DPWA-SS model converges to the experimental data** when l**owering the secondary production threshold** (as expected in all cases)
  - **Opt4** is the only standard EM constructor that **is not effected**:
    - a **scattering power correction** has been implemented (and activated in Opt4) in the corresponding **`G4GoudsmitSaundersonMsc`** model
    - this correction accounts the (otherwise neglected) deflections caused by the sub-threshold ionisations
  - a similar scattering power correction has been **added to** the n**ew DPWA-SS model** (**NOTE**: should be active in case of condensed history ionisation!)
  - see the results on the next slide

Energy profile in a light media

- This work demonstrates, that Option4 EM physics provides unbiased energy profile for low-energy electron transport
- High energy electron shower consists of many profiles, so Option4 may be recommended for cross checks of high energy shapes





RECENT UPDATES OF INFRASTRUCTURE

Configuration of EM physics

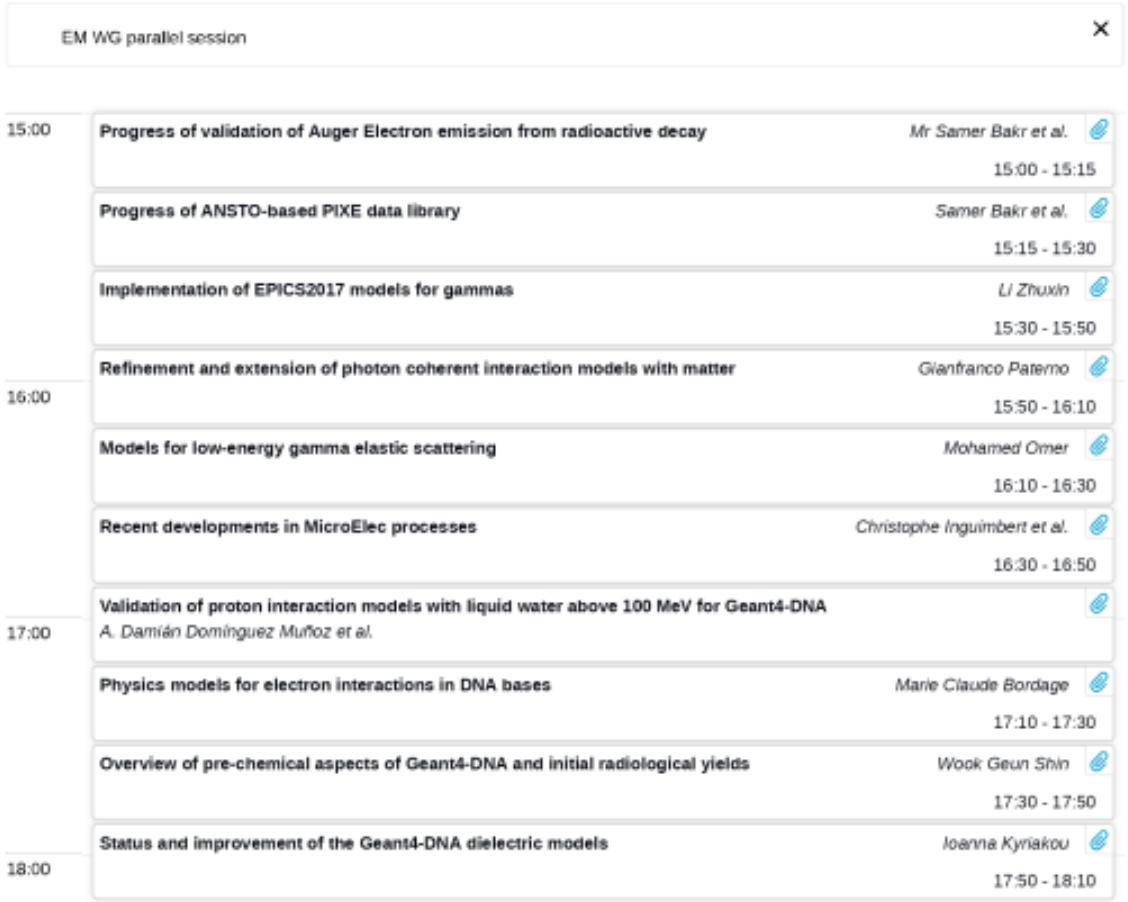
- Number of fixes were introduced in EM physics configurations
  - Resolved problem in definition of EM options when Radioactive decay is enabled
    - EM options may be changed in two builders and via UI commands
  - Resolved problems of G4EmModelActivator
    - Activation of model per region should not change base EM parameters definitions
  - The alternative Opt4 (EMZ) physics is combination of the most accurate EM models
    - ICRU90 data are enabled by default
- G4EmDNAmodelActivator has been extended to include all DNA options
  - This is a contribution from external group in Poland
  - Very accurate and correct code was provided

EM physics for HEP is now coherent with hadronic physics

- Now the list of particles is used from G4HadParticle utility
  - Ionisation and multiple scattering are defined for the list of particles provided by the utility
  - Added b-particles EM interactions
- Initialisation is improved
  - G4HadronicParameters class is used to identify if EM physics should be defined for heavy hadrons
  - Printout at initialisation is improved
  - Improved and fixed messeger classes
  - User interface unchanged
  - DNA parameters are printed if DNA physics ins
- Added separate step fuction parameters for light and heavy ions
  - Useful for medical applications

PROSPECTS AND PLANS

Ongoing developments



EM WG parallel session

15:00	Progress of validation of Auger Electron emission from radioactive decay	*Mr Samer Bakr et al.*	15:00 - 15:15
	Progress of ANSTO-based PIXE data library	*Samer Bakr et al.*	15:15 - 15:30
	Implementation of EPICS2017 models for gammas	*Li Zhuxin*	15:30 - 15:50
	Refinement and extension of photon coherent interaction models with matter	*Gianfranco Paterno*	15:50 - 16:10
16:00	Models for low-energy gamma elastic scattering	*Mohamed Omer*	16:10 - 16:30
	Recent developments in MicroElec processes	*Christophe Inguimbert et al.*	16:30 - 16:50
	Validation of proton interaction models with liquid water above 100 MeV for Geant4-DNA	*A. Damián Domínguez Muñoz et al.*	
17:00	Physics models for electron interactions in DNA bases	*Marie Claude Bordage*	17:10 - 17:30
	Overview of pre-chemical aspects of Geant4-DNA and initial radiological yields	*Wook Geun Shin*	17:30 - 17:50
	Status and improvement of the Geant4-DNA dielectric models	*Ioanna Kyriakou*	17:50 - 18:10
18:00			

- Majority of development focused on medical physics
- We will try to integrate new models in 10.7 and try to optimize Option4 EM physics for the next major release

Summary

- We expect faster simulation due to clean-up of kernel classes
- We improve initialization and user interface
- Some part of our development is slowed down due to covid-19
  - Will be completed in 2021
- Shower shape in 10.7 is very similar to 10.6
- New models and examples are integrated in 10.7
  - Expected improved physics for medical applications in 2021
  - Mihaly single scattering model validation demonstrates that energy profile is defined by elastic scattering and not by fluctuations
- We will contribute to R&D efforts for LHC Run-4 in 2021

THANK YOU