Status of Electromagnetic Physics

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For Geant4 EM working group

24th Geant4 Collaboration Workshop
Jefferson Lab, Virginia (US), 23-27 September 2019

Outline

- EM working groups merge
- Highlights of EM developments for Geant4 10.6
  - Materials update
  - Optimization of G4PhysicsVector
  - GeneralProcess for gamma
  - UrbanMscModel update
  - Other EM physics model updates
  - Geant4-DNA developments
- Special topics for HEP
  - Gamma factory requirement
  - Radiation background simulation for LHC
- Recent updates of infrastructure
- Prospects and plans

This year EM developments for LHC were focused on improvements of CPU speed and memory reduction

Merging EM-standard and Low-E EM working groups

Objectives

- For several years EM working groups coordinators discussed a possibility to merge the standard and the low energy electromagnetic working groups into a single EM working group
  - The merge was approved by the Steering Board at July,12 meeting
- Physical reasons:
  - We were not able defining a real boundary energy between two groups
  - In the default EM physics, in EM option4 (EMZ), and other physics constructors both standard and low-energy physics models are used
- Technical reasons:
  - We use common design of EM physics even for DNA physics
- Organizational reasons:
  - We have common EM meetings and common EM sessions at Geant4 workshops

New EM working group goals

- Provide the best support of LHC and other HEP experiments
  - Run-3 and Run-4 at LHC
  - FCC requirements
  - Other requirements
- Provide support and contribute to the Geant4 medical physics benchmarking group (G4MSBG)
  - consolidation of the Geant4 testing system for medical physics applications
- Provide support to ESA-ESTEC on space science application development of Geant4
- Continue developments for Livermore and Penelope low-energy models
- Continue developments and provide support for Optical physics
- Part of the EM working group members are active developers of the Geant4-DNA project for simulation of biological effects of radiation, which should continue even more actively due to this merge

Organization of the joint EM physics group

- Approved merge of the new joint group was done in the way preserving membership in SB
  - Coordinator – V.Ivanchenko
  - Deputy (low-energy) – L.Pandola
  - Deputy (optical processes) – D.Sawkey
  - Deputy (Geant4-DNA coordinator) – S.Incerti
- Cooperative groups:
  - Physics Validation Task Force – M.Novak
  - Geant4 Medical Physics Benchmarking Group – S.Guatelli
- Geant4 EM group pages were reviewed and updated: http://geant4.web.cern.ch/collaboration/working_groups/electromagnetic
  - Please visit and comment

Highlights of EM developments for Geant4 10.6

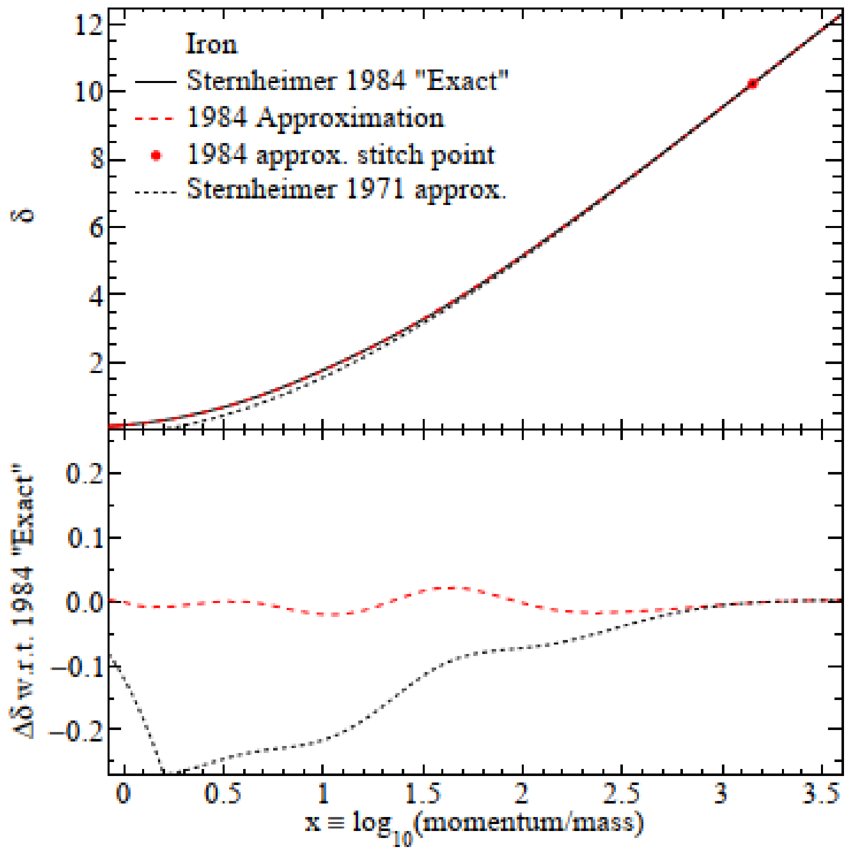
Attempt to speed-up of EM physics

- We continue EM model improvements according to HEP needs and requirements
- During 2019 significant efforts were focused on attempts to speed-up EM classes
  - M. Novak identify several places where existing code was not efficient
    - first of all many unnecessary calls to log
    - Not optimal G4PhysicsVector code for interpolation
    - Not effective EM element selectors due to repeated log calls
  - V. Ivanchenko introduced G4GeneralGammaProcess
  - L. Urban tried tuning Urban model parameters CPU/accuracy
  - V. Ivanchenko reduced memory used for bremsstrahlung data
- We have commited all important developments in Geant4 10.5ref08
  - Full test with EM testing suite and Geant-Val
  - CMSSW make special build using this version of Geant4
- It was possible due to git migration
  - Many cross sub-libraries modifications

Materials updates

- New static methods added – may be useful for HEP
  - G4Material::GetMaterial(Const G4String&, G4double density)
  - G4Material::GetMaterial(G4double Z, G4double A, G4double density)
  - G4Material::GetMaterial(size_t nComponents, G4double density)
  - These methods may help to reduce duplicate material definitions in HEP detector descriptions
- New class G4DensityEffectCalculator (Matthew Strait, University of Minnesota, USA)
  - Based on R.M. Sternheimer publications as our default but do not use parameterisation, instead resolving non-linear equation
  - By user request compute density effect correction on fly without any parameterisation
    - We plan to provide UI command(s) for 10.6
- For the default computation of the density correction for compounds the logic was changed
  - If a compound is not inside NIST materials DB but some element dominates in the mass fraction, then density correction is based on parameterisation for this element

Accuracy of the new approach for Iron (M. Strait)



- Pure iron: 1984 approximation is quite close to the exact solution
- Impure iron (say, steel): 1971 approximation, up to 1.3% off

- Patch already used by NOvA to obtain improved $\mathrm{d}E/\mathrm{d}x$ in steel by up to 1.3%
  - Important because this difference cannot be calibrated out in a neutrino experiment
  - Same will be true for DUNE at the level of 0.6%

Improving Geant4 performance by removing redundant G4Log calls (M.Novak)

- It turned out, that G4Log(E) is called many times at a step with the same argument in several EM and hadronic processes
- The first observation of Mihaly was in G4ElementSelector

- for EM models, the `G4VEmModel` base class provides the possibility to (automatically)build a collection of `G4EmElementSelector`-s for each material cuts couple
- this collection can be used at run-time, to sample the target atom for the given interaction (in case of multi-element materials)
- each individual (i.e. for a given *model* given *material* cuts couple) `G4EmElementSelector` of the collection stores a table of discrete probabilities of having the given interaction on a given element of the material (i.e. $P(Z_i) = \Sigma_{Z_i}/\Sigma$) over a discrete energy grid: equally spaced in log energy scale
- the implementation of the table is a vector of `G4PhysicsLogVector` (as many as elements in the given material)
- at run-time, the target atom is sampled according to this discrete probability distribution: the probabilities are interpolated for the given primary energy
- however, **the energy bin index was re-computed for each possible target element during the interpolation: because selectors are individual log-vectors** (was fixed in `10.05`)

How to call Log(E) only once?

To avoid redundant computations of G4Log(E_k), the proposed [1] solution was applied:

- to (1) store the logarithm of the kinetic energy whenever is already computed:

```
inline void G4DynamicParticle::SetKineticEnergy(G4double aEnergy)
{
  isLogEkinUpToDate = ( isLogEkinUpToDate && (theKineticEnergy == aEnergy) );
  theKineticEnergy = aEnergy;
}
```

```
inline G4double G4DynamicParticle::GetLogKineticEnergy() const
{
  if (!isLogEkinUpToDate) {
    theLogKineticEnergy = (theKineticEnergy > 0.) ?
                          G4Log(theKineticEnergy) : LOG_EKIN_MIN;
    isLogEkinUpToDate   = true;
  }
  return theLogKineticEnergy;
}
```

- and (2) propagate to the interpolation method i.e. introduce a new G4PhysicsVector::Value(G4double E_k, G4double LogE_k, size_t& ilast) method

```
G4double G4PhysicsVector::Value(G4double theEnergy, G4double theLogEnergy,
                                size_t& lastIdx) const
```

- Later we also removed logical variable from the G4DynamicParticle (with no effect on CPU but with simpler code)

Profiling of EM benchmark

10 [GeV] e^- in Simplified Sampling Calorimeter: 50 layers of 2.5 [mm] Pb and 5.7 [mm] liquid-Ar

Geant4-10.05-ref02:

Incl.	Self	Called	Function
9.48	0.67	40 680 456	G4PhysicsVector::Value(double, unsigned long&) const

Geant4-10.05-ref03: with the new Value(E_k, LogE_k, ilast) interface method

Incl.	Self	Called	Function
5.01	0.52	30 353 168	G4PhysicsVector::Value(double, double, unsigned long&) ...
2.45	0.18	10 327 288	G4PhysicsVector::Value(double, unsigned long&) const

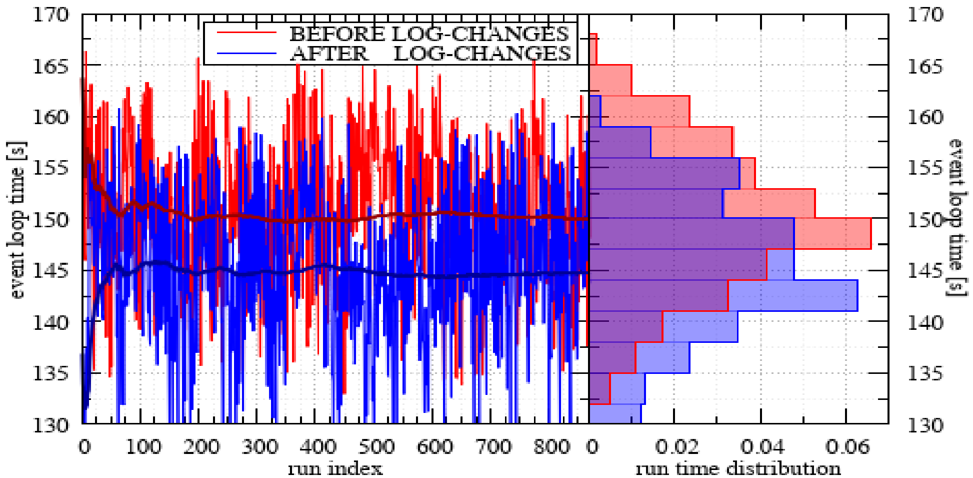
- Profiling of various EM benchmarks demonstrated, that number of calls to G4Log are really reduced
- However, no CPU improvements were reported by FNAL benchmarking team

M.Novak analysis of CPU benchmarks (1/2)

NOTE: not easy to obtain stable time measurement i.e. with small σ (fullCMS on AMD): **INITIAL**

SHARED Geant4 + no-field: $\tilde{t} = 149.99, \tilde{\sigma} = 6.78$ v.s. $\tilde{t} = 144.8, \tilde{\sigma} = 7.24 \rightarrow -3.46$ %

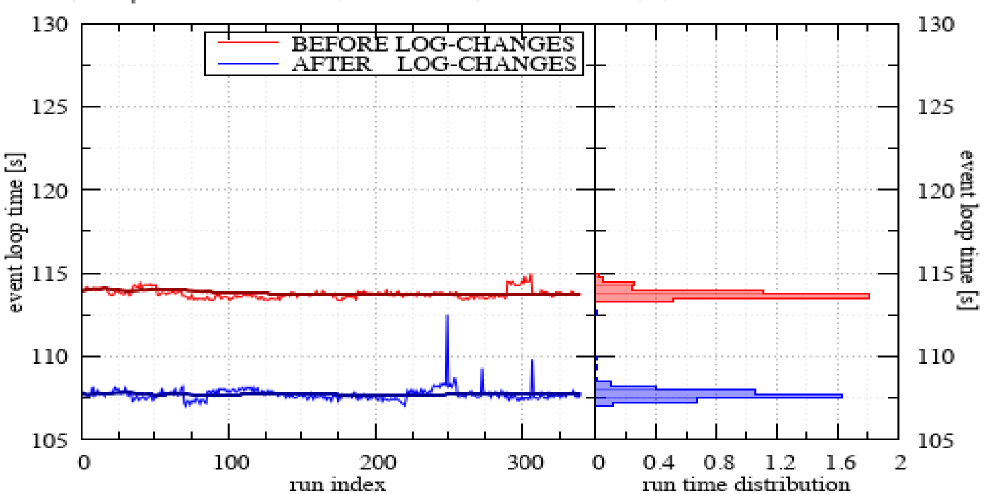
3 Run-s per Execution and all Run-s are used



NOTE: not easy to obtain stable time measurement i.e. with small σ (fullCMS on AMD): **FINAL**

STATIC Geant4 + no-field: $\tilde{t} = 113.75, \tilde{\sigma} = 0.26$ v.s. $\tilde{t} = 107.72, \tilde{\sigma} = 0.39 \rightarrow -5.3$ %

20 Run-s per Execution and the first 3 Run-s are excluded from each Execution



M.Novak analysis of CPU benchmarks (2/2)

The corresponding performance improvements:

`fullCMS` **(combined EM-Hadronic shower)**:

- ~**8** % on my **MacBook Pro** (MacOS 10.13.2), 2.8 GHz Intel Core i7 processor with 16 GB 1600 MHz DDR3 memory using Apple LLVM version 10.0.0 (clang-1000.10.44.4) (**all local**)
- ~**5.3** % on my **AMD Desktop** (SLC 6.10 Carbon), 3.5 GHz AMD PRO A10-9700 R7 processor with 8 GB DDR4-2400 SDRAM memory using gcc 8.2.0 sourced from /cvmfs/sft.cern.ch/lcg/... (i.e. **not all local**)

`HadCalCMS` **(pure EM-shower)**:

- ~**2.3-4.2** % on my **MacBook Pro** (MacOS 10.13.2), 2.8 GHz Intel Core i7 processor with 16 GB 1600 MHz DDR3 memory using Apple LLVM version 10.0.0 (clang-1000.10.44.4) (**all local**)
- ~**2.3** % on my **AMD Desktop** (SLC 6.10 Carbon), 3.5 GHz AMD PRO A10-9700 R7 processor with 8 GB DDR4-2400 SDRAM memory using gcc 8.2.0 sourced from /cvmfs/sft.cern.ch/lcg/... (i.e. **not all local**)

- Results are sensitive to hardware configuration and current state of hardware: temperature, I/O, pre-history

G4PhysicsVector cleaned-up by M.Novak

New Version: all at once, i.e. finding the bin index and interpolation with all the necessary checks

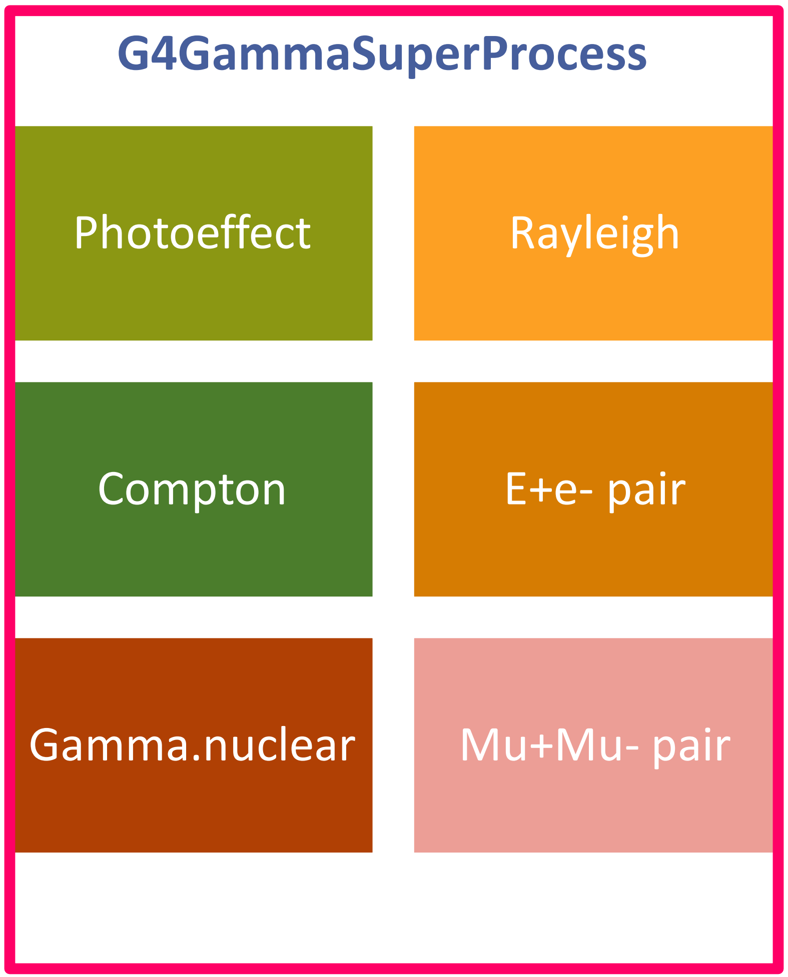
```
G4double G4PhysicsVector::LogVectorValue(const G4double theEnergy,
                                         const G4double theLogEnergy) const
{
  const G4double ek = std::max(binVector[0],
                               std::min(binVector[numberOfNodes-1], theEnergy))
  // compute the lowerindex of the bin (idx \in [0,N-2] will be guaranted)
  const size_t  idx = ComputeLogVectorBin(theLogEnergy);
```

Finding i: 2 lines only (instead of ~25) without any branching (4)

```
  const G4double x2 = binVector[idx+1];
  const G4double dl = x2-x1;
  const G4double  b = std::max(0., std::min(1., (ek - x1)/dl));
  if (useSpline) { // spline interpolation
    const G4double os = 0.166666666667; // 1./6.
    const G4double  a = 1.0 - b;
    const G4double c0 = (a*a*a-a)*secDerivative[idx];
    const G4double c1 = (b*b*b-b)*secDerivative[idx+1];
    return a*dataVector[idx] + b*dataVector[idx+1] + (c0+c1)*dl*dl*os;
  } else {          // linear interpolation
    const G4double y1 = dataVector[idx];
    const G4double y2 = dataVector[idx+1];
    return y1 + b*(y2-y1);
  }
```

- If we do not need re-compute G4Log we do not need many branches inside G4PhysicsVector methods
- These improvements affect both EM and hadronics but not change histories!

G4GammaGeneralProcess



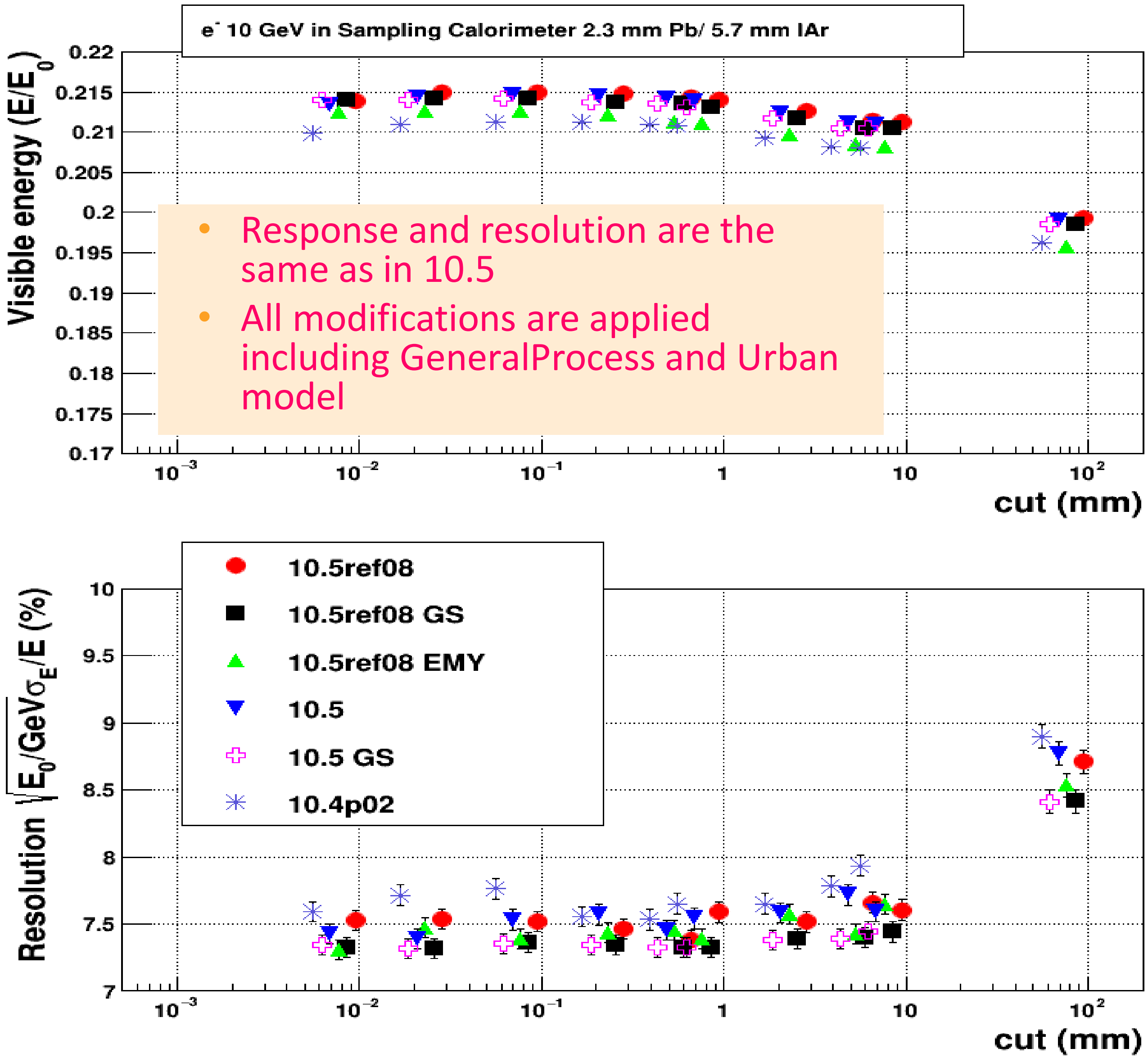
- SteppingManager see only 1 physics process
  - Only 1 mean free path
  - Plus transportation
- User see all processes as before
- Enabled via UI command
  - In 10.5ref08 is defaults for Opt0, Opt1, Opt4…
  - In 10.6 will be optional, UI command may be used to enable
- Reduced number of instructions
  - Advantage in CPU
  - Extra PhysicsTables shared between threads – a bit more memory
  - Final numbers for CPU/memory should be checked by users

L.Urban optimization of the G4UrbanMscModel

- L.Urban investigated possibility to speed-up EM simulation
  - For 10.5ref08 he proposed modifications for step limit parameters:
    - Lambdalimit from 1 mm to 0.4 mm
    - FactorSafety from 0.6 to 0.67
    - Laszlo expected few % speed-up for calorimeter applications
- Validation was performed using full EM testing suite and all Geant-Val tests
  - Majority of test results are not changed
  - Some change of showers were observed the new high granular W/Si calorimeter for EM shower shape and in SimplifiedCalorimer W/Sci for hadronic response
- Proposed solution:
  - Make these parameters available to users via G4EmParameters class and UI commands
  - Use as the default 10.5 values

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

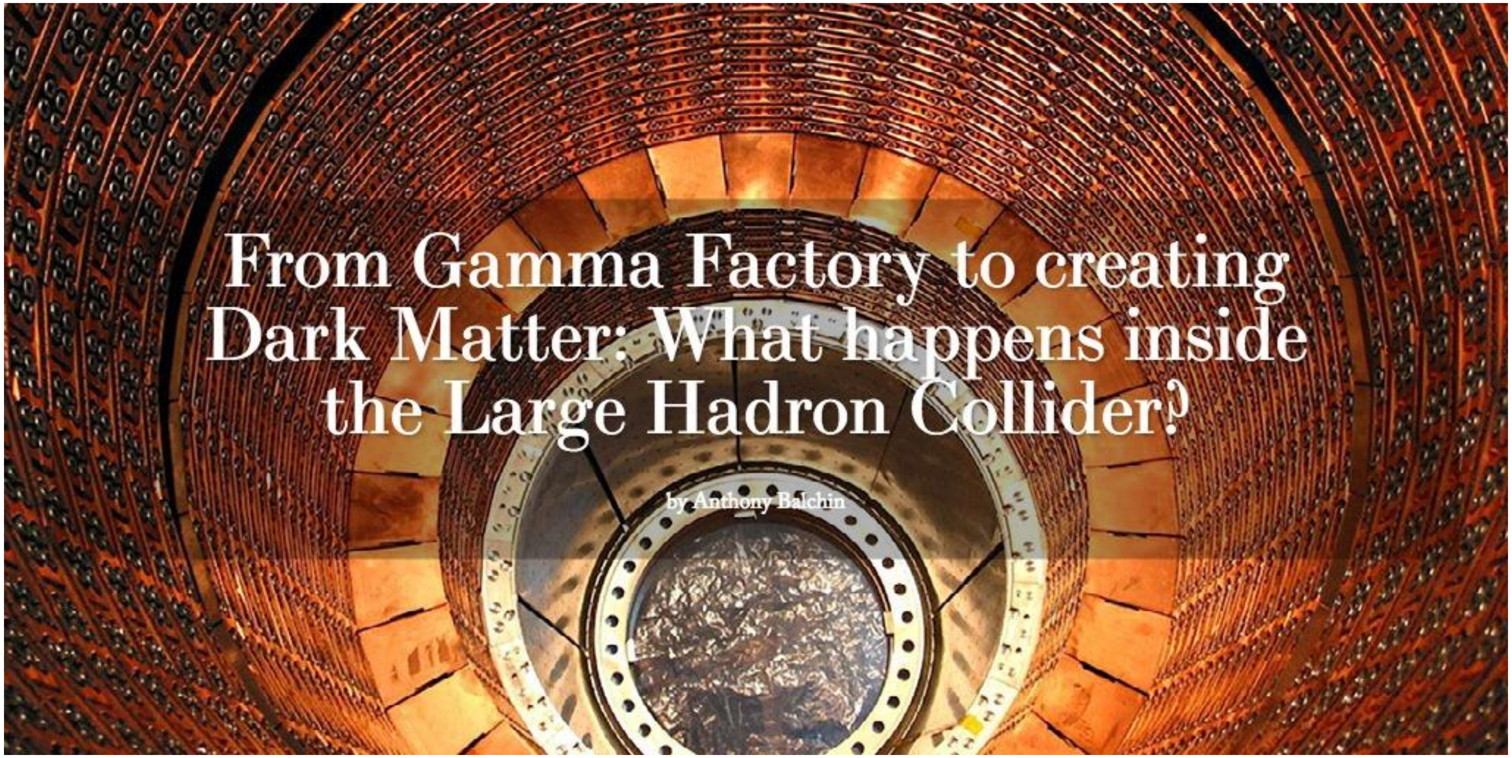


Other EM physics model updates

- G4SeltzerBergerModel – at initialization download tables only for elements used in geometry
  - In utit tests where no geometry is defined lazy initialization may be used
  - The initialization of the model allows usage outside Geant4
- G4PairProductionRelModel – M.Novak extended applicability down to threshold
  - G4BetheHeitler5DModel now inherit of it and by product have LPM effect implemented
- G4ScreeningMottCrossSection revised in order reducing memory and recover corrections for energies below 1 MeV
- Directional bremsstrahlung splitting – D.Sawkey at Parallel 4A
- Optical processes, builders, and examples updates – D.Sawkey at Parallel 8B

Geant4-DNA developments

- **Physics (LowE + Geant4-DNA)**
  1. Atomic deexcitation & radioactive decay benchmarks – Samer Bakr et al. (parallel 8B)
  2. New models for electrons in gold (version 1 and 2) – Ioanna Kyriakou (parallel 4A) & Dousatsu Sakata
  3. Checking and validation of sub-excitation electron thermalization models – Wook Geun Shin et al. (parallel 8B)
  4. New models for electrons in DNA material – Marie Claude Bordage (parallel 4A)
  5. Evaluation of proximity functions (extended example « microprox ») – Sebastien Incerti et al.- parallel 3B
- **Chemistry (Geant4-DNA)**
  1. Influence of phyiscs models and chemistry parameters on the simulation of radiochemical yields Wook Geun Shin et al. (parallel 8B)
  2. Porting of TOPASnBio IRT & alternative versions to Geant4 is on-going in coll. with José, Bruce et al.
- **Geometries & damage (Geant4-DNA)**
  1. Evaluation of DNA damage in a fractal nucleus geometry – Dousatsu Sakata et al. (parallel 7A)
  2. Dnadamage1 example by Hoang Tran et al. (parallel 3B)
- **MPEXS-DNA** : see Shogo Okada's talk at parallel 4A



Special topics for HEP: Gamma conversion to muon pair

Gamma Factory Workshop
CERN - March 25-28, 2019

Geant4 gamma conversion to muon pair process

- G4GammaConversionToMuonPair was implemented by H.Burkhardt in collaboration with R.Kokoulin and S.Kelner
- This class is a part of G4EmExtraPhysics constructor
  - Included in all reference Physics List
  - By default is disabled
  - May be enabled by UI command or C++ method
- The primary goal of the implementation of this process was to provide simulation of muon background in the interaction region of future linear collider
  - This is an ultra relativistic use case
  - The implementation is based on parameterization of asymptotic expressions

Requirements for EM physics by new dark matter search experiments

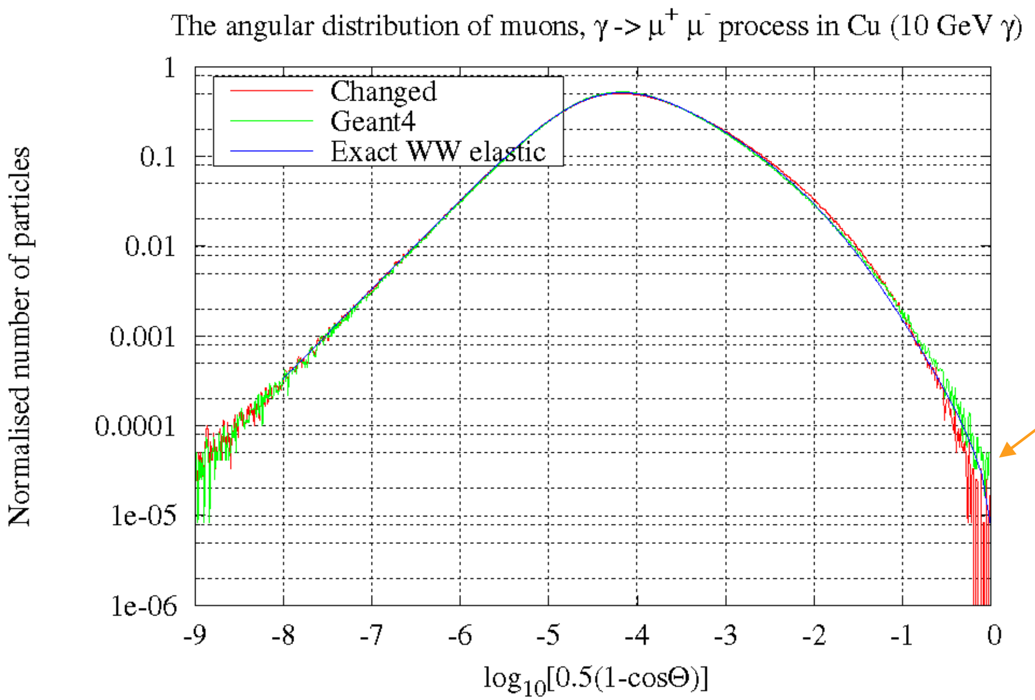
- After Higgs discovery there are intensive discussion on possible experiments for dark matter search
- Currently, several fix target experiments are under consideration or are already started
  - The most advanced is the new experiment at CERN SPS SHIP
  - Dark matter searches are performed by ATLAS and CMS
- EM physics is an important component
  - Diagrams for production and interaction of light dark matter particles are similar to normal EM diagrams
  - EM processes are responsible for background in these searches
- We started review of EM models
  - Addition necessary next to leading order corrections to existing processes
  - Addition of rare processes
  - Extension of validity areas

Low-energy extension of muon pair production

- We started from detailed review of existing process G4GammaConversionToMuonPair
- In order to understand inaccuracy of approximations used process authors our summer student A.Sokolov performed special study in 2017
  - He integrated the Williams-Weizsacker differential cross section numerically in Wolphram Mathematica 11.0 for three different target materials: hydrogen, copper and lead
  - Studied effects of screening and nuclear form-factors

Validation of process $\gamma \rightarrow \mu^+\mu^-$

CERN summer student project (A.Sokolov)



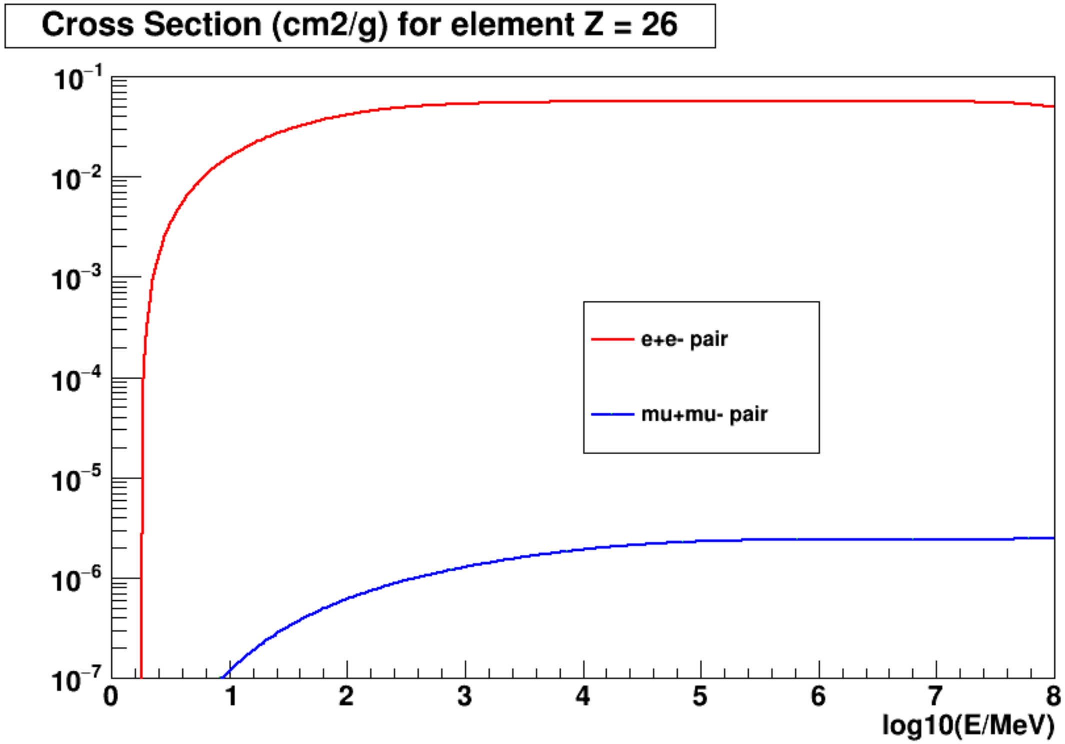
Large angle muons may be a background matter particles

important for Ship experiment design

- Total cross section were verified using numerical integration and accuracy was confirmed within 3%
- Improved expression for the elastic form-factor was introduced
  - There are no differences at high energies ~100 GeV
  - Some differences at ~10 GeV

Muon part production near the threshold

- In order to extend current model down to the threshold just recently an update of the G4GammaConversionToMuonPair was done
  - Previous low limit was at $4m_{\mu}$
- Approximation used in Geant4 Bethe-Heiltler model for e+e- pair production is applied to the muon pair production down to the threshold

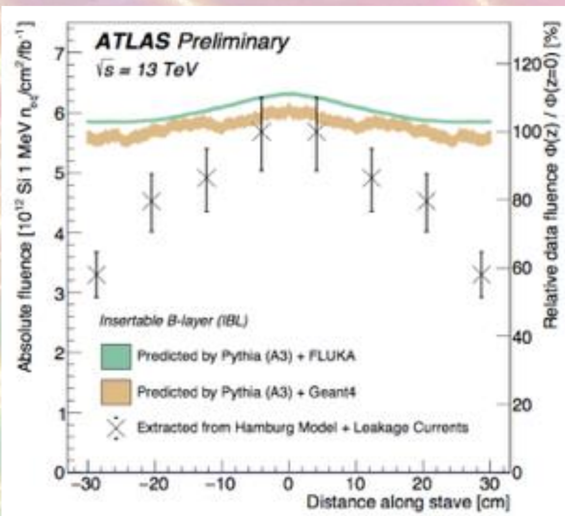


Special topics for HEP:

Radiation background simulation for LHC

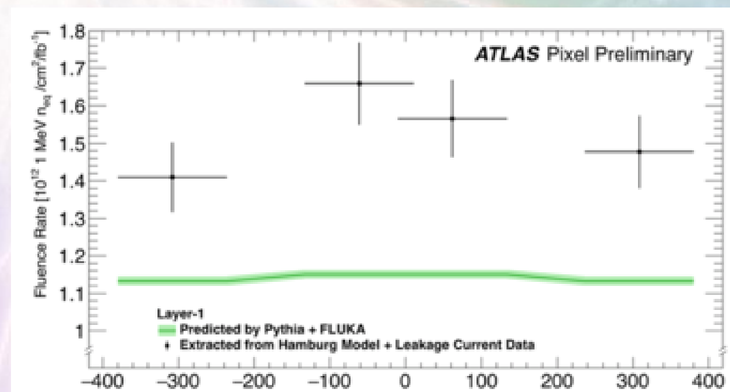
Post Run-2 Workshop on Radiation effects
for LHC Detectors
CERN - February 11-12, 2019

April 2018: ATLAS pixels



- Unexpected z dependence in IBL leakage currents
- **To investigate further** using other observables

- Outer pixel barrel measurements uncomfortably higher than FLUKA predictions
- **To investigate further**



Workshop summary on simulation results

- Common point of view: NIEL is responsible for Si damage
- ATLAS results for Geant4 and FLUKA are similar
- Full understanding of radiation effects requires
  - full simulation with pile-up
    - Nobody shown such results
  - Accounting effects from high energy projectiles
    - Does only NIEL responsible for the damage ?
- These problems are essential for Run-3 and SLHC
  - Silicon detectors in
    - Tracker & HGCal of CMS
  - Crystals, scintillators
  - Muon systems – there is a positive ATLAS & CMS experience for neutron background simulation with pileup

NIEL Calculator

- 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

RECENT UPDATES OF INFRASTRUCTURE

Configuration of EM physics

- 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
  - 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
- 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
  - EM physics configuration and PAI ionization model may be defined for or more G4Region(s)
    - This feature is used by ALICE and CMS

Important developments for EM configuration

- G4EmParameters class is splitted into 3 classes:
  - main, EmExtra, EmLow
  - Printout at initialisation is more compact
  - Extended list of parameters
  - Improved and fixed messeger classes
  - User interface unchanged
  - DNA parameters are printed if DNA physics instantiated
- SetMaxEnergy() has now internal low-limit 9.99 MeV
  - User cannot reduce it below anymore
- GATE developers provided extended ICRU90 data
  - These data will be integrated into G4EMLOW dataset
  - Will be used if user will enable ICRU90 flag

PROSPECTS AND PLANS

Prospects for 2020

- In 2019 we commit significant efforts of key developers to achieve maximum CPU speedup for EM physics
  - Several types of technical improvements makes 10.6 faster
    - Value is ~3-5% in ordinary applications
    - Not very high number but we had nothing in 10.5
  - Further speed-up may be achieved with
    - Kernel development on specialized tracking for gamma, e+-
    - Some extra EM code cleaning and optimization
    - New R&D for GPU, FPGA, …
- There are several physics problems to be addressed
  - Theory based model of fluctuations
  - Enable linear gamma polarization in all Physics Lists
  - Full implementation of triplet models
  - Improved ion transport
- We will follow HEP users requirements
  - LHC for Run-3 and Run-4
  - FCC high energy extensions
  - Other requirements

Low-energy and Geant4-DNA plans

- **Low Energy**
  - **EPICS2017 models**
    - New PhD student: Zhuxin Li @ CENBG, Oct. 2019 – Sep. 2022, in coll. with CERN group
  - **ANSTO PIXE models**
    - Paper published : Nucl. Instrum. Meth. B 436 (2018) 285-291 - PhD thesis of S. Baker @ Wollongong U.
    - Models will be committed
  - **Compton model by Jeremy @TUDelft**
    - Complete recalculation of atomic electron momentum PDFs and Compton profiles for elements Z=1 to Z=100
- **Geant4-DNA**
  - **Physics**
    - Gas models for nanodosimetry to finalize @ IRSN, France
    - GNP models (2 versions) to commit @ Wollongong U., Ioannina U., CENBG
    - Elastic model for electrons in liquid water down to 10 eV to commit @ CENBG
    - CPA100 models for biological targets to finalize @ Toulouse U.
  - **Chemistry**
    - TOPAS IRT being imported into Geant4-DNA and alternative approaches to finalize
  - **Geometries**
    - Library of multi-scale geometries
    - Combination of geometries with IRT
  - **DNA damage**
    - Oher example(s) following dnadamage1

THANK YOU