

Highlights in EM physics in v10.00

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Outline

Geant4 EM physics status

• Where we are now?

Hightlight on selected developments

- Geant4 EM physics consolidation
- Multiple scattering
- EM physics Lists

New EM models

- Compton scattering
- Microdosimetry in Silicon
- Geant4-DNA models
- Built-in EM biasing options

Summary

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Geant4 series 9.X had been under development for more than 6 years

• The latest public version 9.6p03 was provided in Mar 2014

After Higgs discovery a long shutdown at LHC 2013-2015

Good time for significant modifications

Geant4 provided the version 10.00 with major revision of the toolkit (December, 2013):

- Multi-threading
- Removed obsolete code
- Introduced/modified some interfaces
- EM physics sub-packages are modified coherently with the rest of Geant4

Physics performance between 9.6p03 and 10.0 are similar

- Some CPU performance improvement is expected for 10.0 sequential
- CPU advantage for the MT mode



General cleanup of practically all classes

- Removed obsolete classes and interfaces
- Usage of G4Log, G4Exp, G4Pow fast math functions
- G4PhysicsVector and G4Physics2DVector are revised Improved sampling of e+e- pair production by muons and hadrons

Improved PAI models and Urban model for fluctuations Only one consolidated Urban model for multiple scattering

• All benchmarks show good results for this model

Significant update of DNA models for physics and chemistry

New example for radiation chemistry simulation
EM sub-packages become multi-threading (MT) capable

Stability of sampling calorimeter response versus Geant4 version



Stable results for EM physics in general are expected for 10.0 Some CPU performance improvements in sequential mode

Migration of EM to MT includes

- General cleanup of EM classes and classes for data handling
- Use only const interfaces

EM physics tables for cross sections, stopping powers and ranges take significant memory

• Sharing of tables between threads is one of the main requirements to EM



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HIGHTLIGHT ON SELECTED DEVELOPMENTS

Consolidation of EM physics

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Standard EM development was concentrated on HEP

• Important physics sub-package for LHC experiments

For many years EM low-energy sub-package was developed separately

• Focused on medical and space science requirements

The were many recommendations to extend Geant4 EM physics using the best features of both packages

 Previously there were technical limitations to use in one run both standard and low-energy models

First round of migration to common design for the low-energy package was done for Geant4 9.3 (December 2009) and reported at MC2010

- Common validation become possible
- Reuse the same components in different sub-packages
- New polarisation, DNA and adjoint sub-libraries following the same design

For Geant4 9.6 unification was completed

- Angular generators for sampling of final states
- De-excitation module
- Built-in biasing
- Using common validation suite it becomes possible to improve physics performance of both standard and low-energy models
 - Applicability range of models is better defined
 - New EM Physics List combining best models per particle type and energy range is provided

CPU performance and applicability ranges of gamma models

Many models available for each process

 Plus one full set of polarized models
Differ for energy range, precision and CPU speed

Final state generators Different mixtures available the Geant4 EM constructors

Model	E _{min}	$\mathrm{E}_{\mathrm{max}}$	CPU
G4LivermoreRayleighModel	100 eV	10 PeV	1.2
G4PenelopeRayleighModel	100 eV	10 GeV	0.9
G4KleinNishinaCompton	100 eV	10 TeV	1.4
G4KleinNishinaModel	100 eV	10 TeV	1.9
G4LivermoreComptonModel	100 eV	10 TeV	2.8
G4PenelopeComptonModel	10 keV	10 GeV	3.6
G4LowEPComptonModel	100 eV	20 MeV	3.9
G4BetheHeitlerModel	1.02 MeV	100 GeV	2.0
G4PairProductionRelModel	10 MeV	10 PeV	1.9
G4LivermoreGammaConversionModel	1.02 MeV	100 GeV	2.1
G4PenelopeGammaConversionModel	1.02 MeV	10 GeV	2.2
G4PEEFluoModel	1 keV	10 PeV	1
G4LivermorePhotoElectricModel	10 eV	10 PeV	1.1
G4PenelopePhotoElectricModel	10 eV	10 GeV	2.9

1 MeV gammas in Al

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Validation details at url: **Similar** situation for **e**[±]

https://geant4.cern.ch/collaboration/working_groups/electromagnetic/indexv.shtml

Bremsstrahlung validation J. Appl. Phys. 41 (1970) 2682-2692



Standard bremsstrahlung model had limitations in accuracy of energy spectra for 1 and 2.8 MeV benchmark data

Original FORTRAN Penelope and Geant4 Penelope models were in better agreement with the data

G4SeltzerBergerModel uses the best data for double differential cross section

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ELSHIELD 1-D Benchmark

J. Allison et al., "New Geant4 Model and Interface Developments for Improved Space Electron Transport Simulations: First results" Proc. of RADECS 2011, pp. 115-119, IEEE CFP11449-PRT.



Dose deposition in 10 um Si layer by 2, 3, 5, 7 MeV electron beams and 2 mm Al shielding

Penelope predicts a bit lower peak position – difference in model of fluctuations In general all EM Physics Lists of 9.5 predicts the same dose 11

PIXE x-Ray radiation from complex sample: any EM Physics List



Stainless steel sample simulation compared to experimental values, taking into account Aluminum "funny filter" of 250 um and 0.26% hole-detector surface proportion.



One of the key component for EM simulation

Physics Tables moved from processes to models

- Urban and Wentzel models may work in the same Physics List for different energy ranges
- Sampling of scattering is performed AlongStep
 - Before ionisation samples energy loss

In all EM builders (except Opt3) Wentzel model is used for all charged particles

- Except e+- below 100MeV where Urban95 model is used
- Long Rutherford tail better simulated by the Wentzel model
- ATLAS and LHCb requirements to have the same model for high energy particles (p> 1 GeV/c)
- In standard Opt3 builder UrbanMsc95 model is used for all hadrons and ions

MSC and single scattering models

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Model	Particle type	Energy limit	Specifics and applicability
Urban (Urban 2006)	Any	-	Default model for electrons and positrons below 100 MeV, (Lewis 1950) approach, tuned to data, <u>used for LHC production</u> .
Screened Nuclear Recoil (Mendenhall and Weller 2005)	p, ions	< 100 MeV/A	Theory based process, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space app.
Goudsmit-Saunderson (Kadri 2009)	e⁺, e⁻	< 1 GeV	Theory based cross sections (Goudsmit and Saunderson 1950). EPSEPA code developed by Penelope group, final state using EGSnrc method (Kawrakov et al. 1998), precise electron transport
Coulomb scattering (2008)	any	-	Theory based (Wentzel 1927) single scattering model, uses nuclear form- factors (Butkevich et al. 2002), focused on muons and hadrons
WentzelVI (2009)	any	-	MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons.
Ion Coulomb scattering (2010) Electron Coulomb scattering (2012)	lons e⁺, e⁻	-	Model based on Wentzel formula + relativistic effects + screening effects for projectile & target. From the work of P. G. Rancoita, C. Consolandi and V. Ivantchenko.

MuScat benchmark Nucl. Instr. Meth. B 251 (2006) 41

172 MeV/c muon scattering - MuScat, Geant4 10.0beta X²/N $\chi^2/N= 2.11$ $\chi^2/N= 5.33$ Opt0(WVI) Urban95 $\chi^2/N = 6.94$ Urban93 V Urban96 $\chi^2/N = 4.94$ Ж SingleScat $\chi^2/N=1.62$ ሪን 10 AI Be1 Be2 C CH, Fe H,1 H₂2 Li1 Li2 Total

Single scattering and WentzelVI models are closer to the data than Urban models

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Energy profiles for Sandia data UrbanMsc95/UrbanMsc93



Agreement between different Geant4 multiple scattering models and Sandia data was improved in Geant4 9.6 versus 9.4

The most significant effect for Opt3

Stability of the Urban model results versus step size is significantly better for 9.6

Electron scattering benchmark Ross et al., Med. Phys. 35, (2008) 4121

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For Geant4 10.0 only one G4UrbanMscModel is kept

Geant4 10.00: EM Physics builders for HEP

List of particles: for which EM physics processes are defined

- γ , e[±], μ^{\pm} , π^{\pm} , K[±], p, Σ^{\pm} , Ξ^{-} , Ω^{-} , anti(Σ^{\pm} , Ξ^{-} , Ω^{-})
- τ^{\pm} , B^{\pm} , D^{\pm} , D_{s}^{\pm} , Λ_{c}^{+} , Σ_{c}^{+} , Σ_{c}^{++} , Ξ_{c}^{+} , $\underline{anti}(\Lambda_{c}^{+}, \Sigma_{c}^{+}, \Sigma_{c}^{++}, \Xi_{c}^{+})$
- d, t, He3, He4, Genericlon, anti(d, t, He3, He4)

Constructor	Components	Comments
G4EmStandardPhysics	Default (QGSP_BERT, FTFP_BERT)	ATLAS, and other HEP productions, other applications
G4EmStandardPhysics_optio n1	Fast due to simple step limitation, cuts used by photon processes (FTFP_BERT_EMV)	Similar to one used by CMS, good for crystals, not good for sampling calorimeters
G4EmStandardPhysics_optio n2	Experimental: updated photon models and bremsstrahlung on top of Opt1	Similar to one used by LHCb

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Combined EM Physics List constructors



Focus on accuracy instead of maximum simulation speed Ion stopping model based on the ICRU'73 data

• Step limitation for multiple scattering using distance to boundary Strong step limitation by the ionisation process defined per particle type

Recommended for hadron/ion therapy, **Space applications**

Constructor	Components	Comments
G4EmStandardPhysics_option3	Urban MSC model for all particles	Proton/ion therapy
G4EmStandardPhysics_option4	The best combination of models per particle type and energy range	Goal to have the most accurate EM physics
G4EmLivermorePhysics	Livermore models for γ, e ⁻ below 1 GeV, Standard models above 1 GeV	Livermore low- energy electron and gamma transport
G4EmPenelopePhysics	Penelope models for γ , e [±] below 1 GeV, Standard models above 1 GeV	Penelope low- energy e [±] and gamma transport
G4EmLowEPPhysics	Monash model for Compton, Livermore for e, γ. WentzelVI, Use G4NuclearStopping for ions	Experimental for low-energy models



In reference PhysicsLists we do not provide single scattering mode In examples it is available in many places,

 examples/extended/electromagnetic/TestEm5, Em7...
if single scattering is applied everywhere simulation may be extremly slow (1000 or more times)

However, there is a possibility to enable single scattering via UI Command

• "/process/msc/ThetaLimit 0.0"

This command will enable single scattering for muons in all physics Lists except Opt3; will enable single scattering for pions, kaons, protons, anti-protons at all enegries, for e+- above 100 MeV in Opt0, Opt1, Opt2.

NEW EM MODELS

New *G4LowEPComptonModel* Monarsh University

Geant4 Penelope



Using a two-body fully relativistic three-dimensional scattering framework in the Relativistic Impulse Approximation for bound atomic electrons

J.M.C. Brown et al, IEEE NSS/MIC 2011, pp. 1385-1389 (2011); NIM A in progress

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New micro-dosimetry model for ionisation in Silicon (MuElec) based on dielectric functions computation

Extend Geant4 with models for the simulation of **particle-matter** interactions in **highly integrated microelectronic components** For electrons, protons, heavy ions in Silicon Electrons: **16.7 eV** – 100 MeV, Ions: 50 keV/u – 1 GeV/u

Discrete simulation \rightarrow all interactions simulated (no condensed)



- Named as MicroElec for microelectronics
 - Based on dielectric function computation
- Applicable to the G4_Si NIST material
- Dedicated advanced example microelectronics released with Geant4 10.0

Nucl. Inst.. Meth B 288 (2012) 66 Nucl. Inst. Meth B 287 (2012) 124 IEEE Trans. Nucl. Sci. 59 (2012) 2697

Specialized models per G4Region: example of Geant4-DNA physics

Standard EM physics constructor as a base

G4EmConfigurator is used to add Geant4-DNA models Geant4-DNA models are enabled only in the small G4Region for energy below 10 MeV

CPU performance optimisation



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Adding MuElec through EmCofiguratore examples/advanced/microelectronics/src/PhysicsList.cc

G4EmConfigurator* em_config = G4LossTableManager::Instance()->EmConfigurator();

G4VEmModel* mod;

// ---> MicroElec processes activated mod = new G4MicroElecElasticModel(); em_config->SetExtraEmModel("e-","e-_G4MicroElecElastic",mod,"Target",0.0,100*MeV);

mod = new G4MicroElecInelasticModel(); em_config->SetExtraEmModel("e-","e-_G4MicroElecInelastic",mod,"Target",16.7*eV,100*MeV);

mod = new G4MicroElecInelasticModel(); em_config->SetExtraEmModel("proton","p_G4MicroElecInelastic",mod,"Target",50*keV,10*GeV);

mod = new G4MicroElecInelasticModel();

em_config->SetExtraEmModel("GenericIon","ion_G4MicroElecInelastic",mod,"Target",50*keV, 10*GeV);

In this case, MuElec model is only activated in target region However the code is a little fragile, look carefully the original code before applying to your codes. SLAC

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Geant4-DNA physics **models** are applicable to **liquid water**, the main component of biological matter

- Same interface as all other EM models (\rightarrow can be coupled),
- Improve CPU performance by setting a threshold "standard" vs. DNA models
- Physics builder provided with Geant4, microdosimetry advanced example.
- They can reach the very low energy domain down to electron thermalization
 - Compatible with molecular description of interactions
- Purely discrete
 - Simulate all elementary interactions on an event-by-event basis, no condensed history approximation

Models able to handle e⁻, p, H, He⁰, He⁺, He²⁺, C, N, O, Fe

- Elastic scattering, ionization, excitation, charge exchange, excitation, vibrational excitation, dissociative attachment
- Follow also the **physico-chemical** and **chemical** steps

 Conversion, thermalization, dissociation (H₃O⁺, OH⁻), molecular reactions Extensions provided for realistic DNA components (nucleotides)

DNA physics models following the same EM interfaces

Process	Geant4 process class	Geant4 model class	E _{min}	E _{max}		
		Electrons				
Electic conttoring	G4DNAElastic	G4DNAScreenedRutherfordElasticModel	9 eV(*)	1 MeV		
Elastic scattering		G4DNAChampionElasticModel	7.4 eV(*)	1 MeV		
Excitation	G4DNAExcitation	G4DNABornExcitationModel	9 eV	1 MeV		
Ionisation	G4DNAIonisation	G4DNABornIonisationModel	11 eV	1 MeV		
Vibrational excitation	G4DNAVibExcitation	G4DNASancheExcitationModel	2 eV	100 eV		
Attachment	G4DNAAttachment	G4DNAMeltonAttachmentModel	4 eV	13 eV		
	1	Protons	•	•		
Eit-ti		G4DNAMillerGreenExcitationModel	10 eV	500 keV		
Excitation	G4DNAExcitation	G4DNABornExcitationModel	500 keV	100 MeV		
T ' '		G4DNARuddIonisationModel	100 eV(*)	500 keV		
Ionisation	G4DINAIonisation	G4DNABornIonisationModel	500 keV	100 Me V		
Charge decrease	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	100 eV	100 MeV		
	. –	Hydrogen				
Excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	10 eV	500 keV		
Ionisation	G4DNAIonisation	G4DNARuddIonisationModel	100 eV(*)	100 MeV		
Charge increase	G4DNAChargeIncrease	G4DNADingfelderChargeIncreaseModel	100 eV	100 MeV		
	Neutral helium ionised twice					
Excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	1 keV	400 MeV		
Ionisation	G4DNAIonisation	G4DNARuddIonisationModel	1 keV(*)	400 MeV		
Charge decrease	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	1 keV	400 MeV		
Neutral helium ionised once						
Excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	1 keV	400 MeV		
Ionisation	G4DNAIonisation	G4DNARuddIonisationModel	1 keV(*)	400 MeV		
Charge decrease	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	1 keV	400 MeV		
Charge increase	G4DNAChargeIncrease	G4DNADingfelderChargeIncreaseModel	1 keV	400 MeV		
Neutral helium						
Excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	1 keV	400 MeV		
Ionisation	G4DNAIonisation	G4DNARuddIonisationModel	1 keV(*)	400 MeV		
Charge increase	G4DNAChargeIncrease	G4DNADingfelderChargeIncreaseModel	1 keV	400 MeV		
C, N, O, Fe ions						
Ionisation	G4DNAIonisation	G4DNARuddIonisationExtendedModel	1 keV(*)	400 MeV		

Speed-up option is now available (cumulat ed diff. cross sections)

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Geant4-DNA: study on direct effects SSB & DSB induction



Possibility to combine Geant4-DNA physics with nanometer scale geometries

- Nucleus of a human cell : 6x10⁹ base pairs of DNA
- Comparison to PARTRAC & experimental measurements

Published in NIMB 306 (2013) 158-164

Radiation chemistry in liquid water M. Karamitros et al., Progress in Nuclear Science and SLAC Technology, 2, 503-508 (2011)



An example to demonstrate radiation chemistry is released with 10.0

Bremsstrahlung Splitting for medical linac (D. Sawkey, Varian Medical Systems)



Brem splitting for medical linac (D. Sawkey, Varian Medical Systems)

Number of splitted gamma N=1000



Speedup depends on cuts and geometry Energy spectrum is reproduced with high accuracy

Summary



Recent achievements with Geant4 EM confirm that design choices of about 10 years ago were correct

- EM now easily extendable with new models
- LHC experiment support back port of new models to the old production releases is transparent
- Migration of EM to MT mode is done in a reasonable time scale Geant4 9.6 is a consolidated version accumulating developments carried out for many years
- New Geant4 10.0 keeps best models but offer new software capabilities
 - You may benefit from migration to version 10.0 even if you using only laptops

Next to follow – more paralisation, vectorization, and...



PIXE simulation for Copper target (NIM B 316 (2013) 1-5) SLAC



Geant4 muons versus L3 data Z->µ⁺µ⁻ (~45 GeV)



Endpoint Displacement of μ^{-} in the r ϕ Plane

geant4-09-05-ref-09, All MSC models, ARealisticRun, Gaussian fits

WentzelVI model is closer to the data than Urban models

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1 MeV gamma energy in a cavity

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9.4

Fano cavity test case

Ratio between simulated and theorical dose deposited by a 1.25 MeV photon beam crossing an ionization chamber

Geant4 release : 09-04-ref-02

Basic test (no fluct, no msc):

standard_opt0 : 0.9983 +/- 0.0002 for dRoverRange = 0.004 standard_opt3 : 1.0007 +/- 0.0002 for dRoverRange = 0.004

Full test (fluct & msc):



Fano cavity test case

Ratio between simulated and theorical dose deposited by a 1.25 MeV photon beam crossing an ionization chamber

9.6

Geant4 release : 09-06-ref-01

Basic test (no fluct, no msc):

standard_opt0 : 0.9976 +/- 0.0002 for dRoverRange = 0.004 standard_opt3 : 1.0006 +/- 0.0002 for dRoverRange = 0.004

Full test (fluct & msc):



dRoverRange

Proton Bragg peak in water Y. Kumazaki et al., Radiation Measurements 42 (2007) 1683 SLAC



Energy deposition in ALICE TPC Geant4 9.6ref09 (A.Bagulya, V.Grichine) Nucl. Instr. Meth. A, 565, 551-560 (2006) Int. J. Mod. Phys. *E*, 16, 2457-2462 (2007)



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Extension of MuElec model for higher energies – 10 GeV/u

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Geant4-DNA

Task: model the radiation-induced biological damage withGeant4http://geant4-dna.org

Strong limitations prevent its usage for the modelling of biological effects of ionizing radiation at the sub-cellular & DNA scale

 No step-by-step transport on small distances, a key requirement for micro/nano-dosimetry [detailed simulation required]

Low-energy limit applicability of EM physics models is limited to ~100 eV

- No description of target molecular properties
 - Liquid water, DNA nucleotides

Only physical particle-matter interactions

• Physical interactions are *not* the dominant processes for DNA damage

<u>Geant4-DNA project</u>: extension of Geant4 for the simulation of interactions of radiation with biological systems at the cellular and DNA level in order to predict early DNA damages → initiated by ESA, highly inter-disciplinary

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Models able to handle e⁻, p, H, He⁰, He⁺, He²⁺, C, N, O, Fe

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Geant4-DNA model inventory

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Particles	e-	р	н	He ⁺⁺ , He ⁺ , He ⁰	C, N, O, Fe,
Elastic scattering	> 9 eV - 1 MeV Screened Rutherford >7.4 eV - 1 MeV Champion	-	-	-	-
Excitation	9 eV – 1 MeV Born	10 eV – 500 keV Miller Green 500 keV – 100 MeV Born	10 eV – 500 keV Miller Green	Effective charge scaling from same models as for proton	-
Charge Change	-	100 eV - 100 MeV Dingfelder	100 eV - 100 MeV Dingfelder		
Ionisation	11 eV – 1 MeV Born	100 eV – 500 keV Rudd 500 keV – 100 MeV Born	100 eV – 100 MeV Rudd	1 keV – 400 MeV	Effective charge scaling 0.5 MeV/u – 10 ⁶ MeV/u
Vibrational excitation	2 – 100 eV Michaud et al.				
Attachment	4 – 13 eV Melton		-		



Radiochemical yield vs. time



- Effect of the two alternative electron elastic scattering models
- Results are obtained in 30 minutes on a cluster of 80 CPUs

Completely new functionality for a general-purpose Monte Carlo

How can Geant4-DNA model radiation biology ?



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