Geant4 release 9.6+P02

ELECTROMAGNETC PHYSICS LOW ENERGY CATEGORY

October 10-11, 2013 – Bordeaux, France

Content

Context

- Physics processes & models
 - Livermore, including polarized photon models
 - Penelope models
 - Ion ICRU'73 model
 - Geant4-DNA processes and models
 - MuElec processes and models
 - Monash U. models
 - Atomic de-excitationprocess and models
- □ How to implement a Physics list ?
- Documentation





Purpose

- Extend the coverage of Geant4 electromagnetic interactions with matter
 - for photons, electrons, positrons and ions
 - down to very low energies (sub-keV scale)
- Possible domains of applications
 - Space science
 - Medical physics
 - Underground physics
 - Microdosimetry for radiobiology and microelectronics
- Choices of physics models include
 - □ Livermore : electrons and photons [250 eV 1 GeV]
 - Penelope : electrons, positrons and photons [100 eV 1 GeV]
 - Microdosimetry models
 - Geant4-DNA project: [eV ~ few 100 MeV]
 - MuElec for Silicon : [eV 1 GeV/u]

Software design

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- Identical to the software design proposed by the Standard EM working group
 - Applicable to all low energy electromagnetic software classes
 - Allows a coherent approach to the modelling of all electromagnetic interactions
- A physical interaction or process is described by a <u>PROCESS CLASS</u>
 - Naming scheme : « G4ProcessName »
 - Eg. : « G4ComptonScattering » for photon Compton scattering
- A physical process can be simulated according to several models, each model being described by a <u>MODEL CLASS</u>
 - Naming scheme : « G4ModelNameProcessNameModel »
 - **Eg.** : « G4LivermoreComptonModel » for the Livermore Compton model
 - Models can be alternative and/or complementary in certain energy ranges
- According to the selected model, model classes provide the computation of
 - the process total cross section & the stopping power
 - the process final state (kinematics, production of secondaries...)
- □ All required data files are located in the \$G4LEDATA directory



Livermore models

Livermore models

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- Full set of models for electrons and gammas
- Based on publicly available evaluated data tables from the Livermore data library
 - EADL : Evaluated Atomic Data Library
 - EEDL : Evaluated Electrons Data Library
 - EPDL97 : Evaluated Photons Data Library
 - Mixture of experiments and theories
 - Binding energies: Scofield
- Data tables are interpolated by Livermore model classes to compute
 - Total cross sections: photoelectric, Compton, Rayleigh, pair production, Bremsstrahlung
 - Shell integrated cross sections: photo-electric, ionization
 - Energy spectra: secondary e- processes
- Validity range (recommended) : 250 eV 100 GeV
 - Processes can be used down to 100 eV, with a reduced accuracy
 - In principle, down to ~10 eV
- Included elements from Z=1 to Z=100
 - Include atomic effects (fluorescence, Auger)
 - Atomic relaxation : Z > 5 (EADL transition data)
- Naming scheme: G4LivermoreXXXModel (eg. G4LivermoreComptonModel)

http://www-nds.iaea.org/epdl97

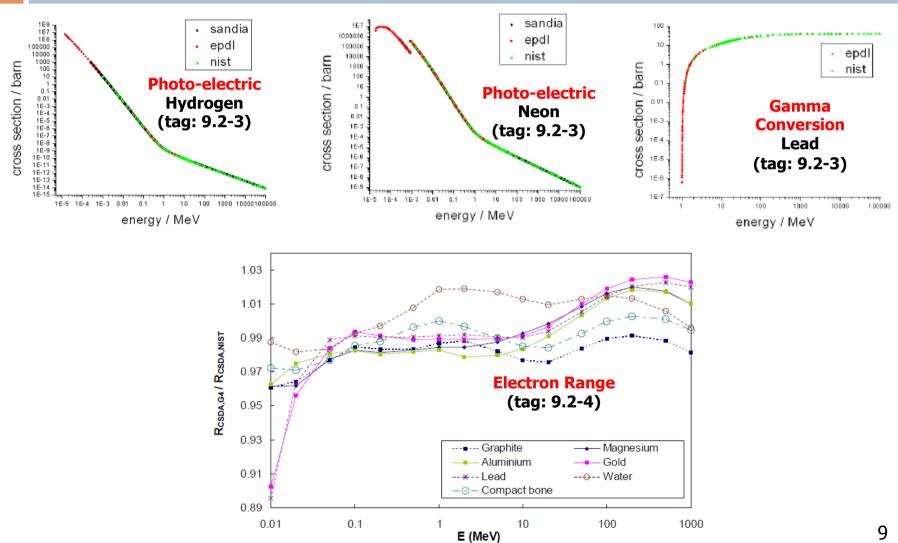
Available Livermore models

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Gammas				
Compton	G4ComptonScattering	G4LivermoreComptonModel	250 eV (kill)	100 GeV
Polarized Compton	G4ComptonScattering	G4LivermorePolarizedComptonModel	250 eV (kill)	100 GeV
Rayleigh	G4RayleighScattering	G4LivermoreRayleighModel	10 eV (kill)	100 GeV
Polarized Rayleigh	G4RayleighScattering	G4LivermorePolarizedRayleighModel	250 eV (kill)	100 GeV
Conversion	G4GammaConversion	G4LivermoreGammaConversionModel	1.022 MeV	100 GeV
Polarized Conversion	G4GammaConversion	G4LivermorePolarizedGammaConversionModel	1.022 MeV	100 GeV
Photo-electric	G4PhotoElectricEffect	G4LivermorePhotoElectricModel	\sim few eV	100 GeV
<mark>Polarized</mark> Photo-electric	G4PhotoElectricEffect	G4LivermorePolarizedPhotoElectricModel	10 eV	100 GeV
Electrons				
lonization	G4elonisation	G4LivermorelonisationModel	100 eV	100 GeV
Bremsstrahlung	G4eBremsstrahlung	G4LivermoreBremsstrahlungModel	10 eV	100 GeV

Eg. of verification of Livermore models

See Nucl. Instrum. and Meth. A 618 (2010) 315-322

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Polarized Livermore models

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- Describe in detail the kinematics of polarized photon interactions
- Based on the Livermore database
- Possible applications of such developments
 - design of space missions for the detection of polarized photons
- Naming scheme: G4LivermorePolarizedXXXModel
 - eg. G4LivermorePolarizedComptonModel
- More in the following publications

Nucl. Instrum. Meth. A 566 (2006) 590-597 (Photoelectric) Nucl. Instrum. Meth. A 512 (2003) 619-630 (Compton and Rayleigh) Nucl.Instrum. Meth. A 452 (2000) 298-305 (Pair production)



Penelope models

Penelope physics

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 Geant4 includes the low-energy models for electrons, positrons and photons from the Monte Carlo code PENELOPE (PENetration and Energy LOss of Positrons and Electrons) version 2008

Nucl. Instrum. Meth. B 207 (2003) 107-123

- Physics models
 - Specifically developped by the group of F. Salvat et al.
 - Great care dedicated to the low-energy description
 - Atomic effects, fluorescence, Doppler broadening...
- Mixed approach: analytical, parameterized & database-driven
 - Applicability energy range: 100 eV 1 GeV
- □ Also include positrons
 - Not described by Livemore models
- □ G4PenelopeXXXModel (e.g. G4PenelopeComptonModel)

Available Penelope models

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Gammas				
Compton	G4ComptonScattering	G4PenelopeComptonModel	100 eV	1 GeV
Rayleigh	G4RayleighScattering	G4PenelopeRayleighModel	100 eV	1 GeV
Conversion	G4GammaConversion	G4PenelopeGammaConversionModel	1.022 MeV	1 GeV
Photo-electric	G4PhotoElectricEffect	G4PenelopePhotoElectricModel	100 eV	1 GeV
Electrons/Positrons				
lonization	G4elonisation	G4PenelopelonisationModel	100 eV	1 GeV
Bremsstrahlung	G4eBremsstrahlung	G4PenelopeBremsstrahlungModel	100 eV	1 GeV
Positrons				
Annihilation	G4eplusAnnihilation	G4PenelopeAnnihilationModel	100 eV	1 GeV



lons

lon energy loss model

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- Describes the energy loss of ions heavier than Helium due to interactions with atomic shells of target atoms
- □ This model computes
 - Cross sections for the <u>discrete</u> production of <u>delta rays</u>
 - Delta rays are only produced <u>above the production threshold</u>, which inherently also governs the discrete energy loss of ions
 - Restricted electronic stopping powers, that is the <u>continuous</u> energy loss of ions as they slow down in an absorber
 - Below the production threshold
- Primarily of interest for medical and space applications

See more in Nucl. Instrum. Meth. B 268 (2010) 2343-2354

lon energy loss model

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- Restricted stopping powers are calculated from
 - $\Box \quad T < T_{Low}: Free electron gas model$
 - $\blacksquare \quad T_{Low} \leq T \leq T_{High}: parameterization (ICRU'73) approach$
 - \Box T > T_{High}: Bethe-Bloch formula (using an effective charge and higher order corrections)

ICRU'73 parameterization

- Large range of ion-materials combination:
 - Incident ions : Li to Ar, and Fe
 - 25 elemental materials, 31 compounds
- Stopping powers based on the binary theory, effective charge approach for Fe
- Special case: water
 - Revised ICRU'73 tables by P. Sigmund
 - Mean ionization potential is 78 eV
- Energy limits
 - $T_{High} = 10 \text{ MeV/nucleon}$ (except Fe ions: $T_{H} = 1 \text{ GeV/nucleon}$)
 - T_{1 ow} = 0.025 MeV/nucleon (lower boundary of ICRU'73 tables)

How to use the ion model ?

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- Model name: G4IonParametrisedLossModel
- \Box Only applicable to ions with Z \geq 3
- Already included in Geant4 EM physics constructors
 - Low energy EM: G4EmLivermorePhysics, G4EmLivermorePolarizedPhysics, G4EmPenelopePhysics, G4EmLowEPPhysics
 - Standard EM: G4EmStandard_option3, G4EmStandard_option4
- Designed to be used with the G4ionIonisation() process (from the Standard EM category)
 - Not activated by default when using G4ionIonisation
 - Users can employ this model by using the SetEmModel method of the G4ionIonisation process
- Restricted to one Geant4 particle type: G4Genericlon
 - The process G4ionIonisation is also applicable to alpha particles (G4Alpha) and He3 ions (G4He3), however the G4IonParametrisedLossModel model must not be activated for these light ions
 - Below Z<3, we use G4BraggModel (p) or G4BraggIonModel (alpha), and G4BetheBlochModel with the G4hlonisation and G4ionIonisation processes</p>

ICRU 73 data tables

- □ The ion model
 - uses ICRU'73 stopping powers, if corresponding ion-material combinations are covered by the ICRU'73 report
 - otherwise applies a Bethe-Bloch based formalism
- Elemental materials are matched to the corresponding ICRU 73 stopping powers by means of the atomic number of the material. The material name may be arbitrary in this case.
- For compounds, ICRU 73 stopping powers are used if the material name coincides with the name of Geant4 NIST materials
 - e.g. "G4_WATER"
- For a list of applicable materials, refer to the ICRU 73 report
- All needed data files are in the G4LEDATA set of data

http://geant4-dna.org

Physics 4/

Geant4-DNA

The Geant4-DNA project

Extending the Geant4 Monte Carlo simulation toolkit for radiobiology

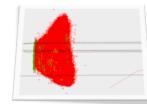
Geant4-DNA Software Physics Chemistry Examples & tutorials Publications Collaboration Funding

Welcome to the Internet page of the Geant4-DNA project.

The <u>Geant4</u> Monte Carlo simulation toolkit is being extended with processes for the **modeling of early biological** damages induced by ionising radiation at the DNA scale. Such developments are on-going in the framework of the Geant4-DNA project, initiated in 2000 by the <u>European Space Agency/ESTEC</u>.

On-going developments include

- Physics processes in liquid water and other biological materials
- Physico-chemistry and chemistry processes for water radiolysis
- Molecular geometries
- Quantification of damages (such as single-strand, doublestrand breaks, ...)



Recent posts The last Geant4 release (9.6+P01) is available for download, see our Software

section.

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Geant4 for microdosimetry in radiobiology

□ History

- initiated in 2001 by Petteri Nieminen (European Space Agency / ESTEC) in the framework of the « Geant4-DNA » project
- Objective : adapt the general purpose Geant4 Monte Carlo toolkit for the simulation of interactions of radiation with biological systems at the cellular and DNA level (« microdosimetry for radiobiology »)
- A full multidisciplinary activity of the Geant4 low energy electromagnetic Physics working group, involving physicists, theoreticians, biophysicists...
- □ Applications :
 - Radiobiology, radiotherapy and hadrontherapy
 - eg. early prediction of direct & non-direct DNA strand breaks from ionising radiation
 - Radioprotection for human exploration of Solar system
- Dedicated web site & publications : <u>http://geant4-dna.org</u>

Geant4 for microdosimetry in radiobiology

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- Several models are available for the description of physical processes involving e⁻, p, H, He, He⁺, He²⁺, C⁶⁺, N⁷⁺, O⁸⁺, Fe²⁶⁺
- Include elastic scattering, excitation (electronic + vibrations), ionisation and charge exchange
- □ For now, these models are valid for liquid water medium only
- Models available in Geant4-DNA
 - are published in the literature
 - may be purely analytical or use interpolated cross section data
- □ They are all discrete processes
 - See \$G4INSTALL/share/Geant4-9.6.2/examples/advanced/dnaphysics
- Can be combined with other EM categories (Standard, LowE common software design)
 - See \$G4INSTALL/share/Geant4-9.6.2/examples/advanced/microdosimetry

Geant4-DNA physics processes and models

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 1 keV – 400 MeV	-
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		Effective charge scaling 0.5 MeV/u - 10 ⁶ MeV/u
Vibrational excitation	2 – 100 eV Michaud et al.				
Attachment	4 – 13 eV Melton				

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MuElec processes & models

New processes and models for microelectronics

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- Purpose
 - extend Geant4 with processes and models for the simulation of particlematter interactions in highly integrated microelectronic components
 - for electrons, protons, heavy ions in Silicon
- They use the same step-by-step approach as Geant4-DNA processes and models
 - Similarly based on the complex dielectric function theory
- Applicable to the « G4_Si » NIST material
- Named as « MuElec » for microelectronics

New processes and models for microelectronics

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Processes and models

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Electrons				
Elastic scattering	G4MuElecElastic	G4MuElecElasticModel	<mark>16.7 eV</mark> (kill < 16.7 eV)	100 MeV
lonization	G4MuElecInelastic	G4MuElecInelasticModel	16.7 eV	100 MeV
Protons and heavy ions				
lonization	G4MuElecInelastic	G4MuElecInelasticModel	50 keV/u	1 GeV/u

- □ A dedicated Physics List and a user example will be delivered in G4 10
- Validation range
 - Electrons: 50 eV 50 keV
 - Protons: 50 keV/u 23 MeV/u

Nucl. Instrum. Meth B 288 (2012) 66 – 73 Nucl. Instrum. Meth B 287 (2012) 124 – 129 IEEE Trans. Nucl. Sci. 59 (2012) 2697 – 2703



Monash U. models

Improved Compton model

- Monash U. (J. Brown et al.) recently proposed to improve Livermore gamma models
 - Unpolarized Compton scattering off atomic bound electrons in the relativistic impulse approximation, derived from Livermore Compton model
 - As an alternative to Compton scattering models (Livermore and Penelope) developped from Ribberfor's Compton scattering framework
 - More accurate Compton electron ejection direction algorithms below 5 MeV
 - Special relativistic formalism + energy & momentum conservation, in order to compute
 - Energy and angular distribution of Compton scattered photons off non-stationary atomic bound electrons
 - Energy and ejected angular distributions of Compton electrons

Improved Compton model

Model class is G4LowEPComptonModel

You can register it easily to your Physics list

G4ComptonScattering* cs = new G4ComptonScattering; cs->SetEmModel(new G4KleinNishinaModel(),1); G4VEmModel* theLowEPComptonModel = new G4LowEPComptonModel(); theLowEPComptonModel->SetHighEnergyLimit(2*MeV); cs->AddEmModel(0, theLowEPComptonModel); ph->RegisterProcess(cs, particle);

- □ You can also use two Physics constructors
 - G4EmLowEPPhysics identical to G4EmLivermorePhysics except for Compton
 - G4EmStandard_option4 « best » of Geant4 EM



Atomic de-excitation

Atomic de-excitation effects

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- □ Atomic de-excitation is initiated by other EM processes
 - **E.g.** : photo-electric effect, Compton, ionisation by e- and ions
 - Leave the atom in an excited state
- EADL data contain transition probabilities
 - radiative: fluorescence
 - non-radiative:
 - Auger e-: inital and final vacancies in different sub-shells
 - Coster-Kronig e-: identical sub-shells
- Thanks to a common interface (G4UAtomicDeexcitation), atomic deexcitation is compatible with both Standard & Low Energy electromagnetic physics categories

See more in X-Ray Spec. 40 (2011) 135-140

Including atomic effects

The activation of atomic deexcitation in a user physics list can be done
 (' by hand)) using the G4EmProcessOptions class

G4EmProcessOptions emOptions;

emOptions.SetFluo(true); // To activate deexcitation processes and fluorescence emOptions.SetAuger(true); // To activate Auger effect if deexcitation is activated emOptions.SetPIXE(true); // To activate Particle Induced X-Ray Emission (PIXE)

It is possible to specify the region in which de-excitation is needed
 emOptions.SetDeexcitationActiveRegion (const G4String&, G4bool, G4bool, G4bool);

- If no Region command is used, by default atomic de-excitation is applied everywhere
- If any Region is defined, then de-excitation should be applied to the World volume

Including atomic effects

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Alternativeley, we recommend the usage of physics constructors and Geant4 physics lists, where activation can be easily done directly via UI commands

/run/initialize /process/em/deexcitation region true false false /process/em/deexcitation region true true true /process/em/fluo true

/process/em/auger true

/process/em/pixe true

- Boolean parameters in the "/process/em/deexcitation" command correspond to activation of fluorescence, Auger, and PIXE respectively
- region is the name of the G4Region in which de-excitation should be activated
 - use the string World if the G4Region is the World volume
- Note that fluorescence is activated by default in the G4EmDNAPhysics, G4EmLivermorePhysics, G4EmLivermorePolarizedPhysics, G4EmLowEPPhysics., G4EmPenelopePhysics, G4EmStandard_option3 and G4EmStandard_option4 physics constructors while Auger production and PIXE are not
- As an example, look into \$G4INSTALL/share/Geant4-9.6.2/examples/extended/electromagnetic/TestEm5 and macro pixe.mac

Note on production thresholds

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- Remember that production cuts for secondaries are specified as range cuts. These are converted at initialisation time into energy thresholds for secondary gamma, electron, positron and proton production.
- A range cut value is set by default to 0.7 mm in Geant4 reference physics lists. This value can be specified in the optional SetCuts() method of the user physics list or via UI commands :
 - for eg. to set a range cut of 10 micrometers, one can use /run/setCut 0.01 mm
 - or, for a given particle type (for e.g. electron) /run/setCutForAGivenParticle e- 0.01 mm
- If a range cut equivalent to an energy lower than 990 eV is specified, then the energy cut is still set to 990 eV. In order to decrease this value (for eg. down to 250 eV, to see low energy emission lines of the fluorescence spectrum), one can use the UI command:

/cuts/setLowEdge 250 eV

or alternatively directly in the user physics list, in the optional SetCuts() method, using:

G4ProductionCutsTable::GetProductionCutsTable()->SetEnergyRange(250*eV, 1*GeV);

□ In your macro, these UI commands should be put before the UI command

/run/initialize

Changing shell cross section models

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The user has the possibility to select different ionisation cross section models for PIXE. Again, it is possible to use methods of the G4EmProcessOptions class in the user Physics list:

G4EmProcessOptions::SetPIXECrossSectionModel(const G4String&);

where the string can be "Empirical" or "ECPSSR_FormFactor" or "ECPSSR_Analytical"

Alternatively, when using the Geant4 reference physics lists (and "physics constructors"), the following UI command is available:

/process/em/pixeXSmodel value

where value is equal to Empirical or ECPSSR_FormFactor or ECPSSR_Analytical.

This UI command should be put after the UI command:

/run/initialize

- □ Shell cross sections models are available for K, L and selected M shells:
 - the Empirical models are from Paul "reference values" (for protons and alphas for K-Shell) and Orlic empirical model for L shells (only for protons and ions with Z>2);
 - the ECPSSR_FormFactor models derive from A. Taborda et al. calculations of ECPSSR values directly form Form Factors and it covers K, L shells in the range 0.1-100 MeV and M shells in the range 0.1-10 MeV;
 - the ECPSSR_Analytical models derive from an in-house analytical calculation of the ECPSSR theory.
- The Empirical models are the models used by default. Out of the energy boundaries of these models, the "ECPSSR_Analytical" models are used. We recommend to use default settings if not sure what to use.
- Note that shell cross section selection is also available for electrons via the following UI command:
 - /process/em/pixeElecXSmodel Livermore
 - /process/em/pixeElecXSmodel Penelope

X-Ray Spec. 40 (2011) 127-134 X-Ray Spec. 40 (2011) 135-140

How to implement a Physics list ?

Physics lists

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- A user can
 - use reference physics lists provided with Geant4 (QBBC,)
 - build his/her own physics list in his/her application
 - or use <u>already available</u> EM physics constructors
- 1. If you choose to build your own Physics list
 - refer to the Geant4 Low Energy EM working group website, Processes section
 - also you may refer to Geant4 examples
 - \$G4INSTALL/share/Geant4-9.6.2/examples/extended/electromagnetic/TestEm14
- 2. <u>Much more safe</u>: use the available physics constructors, these are named as
 - □ G4EmLivermorePhysics
 - G4EmLivermorePolarizedPhysics
 - G4EmPenelopePhysics
 - **G4EmDNAPhysics**
 - G4EmLowEPPhysics

How to use the already available physics constructors ?

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- □ These classes derive from the G4VPhysicsConstructor abstract base class
- The source code for physics list constructors is available in the following directory
 \$G4SRC/source/physics list/builders
- An implementation example of physics list that uses EM physics constructors is available in
 - \$G4INSTALL/share/Geant4-9.6.2/examples/extended/electromagnetic/TestEm2
 - easy
 - in the header file of your physics list, declare : G4VPhysicsConstructor* emPhysicsList;
 - in the implementation file of your physics list : emPhysicsList = new G4EmDNAPhysics();
 - then, in the ConstructParticle() method of your physics list, call the ConstructParticle() method of emPhysicsList
 - and in the ConstructProcess() method of your physics list, call the ConstructProcess() method of emPhysicsList
- □ If some hadronic physics is needed additionally to EM Physics
 - \$G4INSTALL/share/Geant4-9.6.2/examples/extended/electromagnetic/TestEm7
- These constructors are added to the Geant4 reference physics lists via the method RegisterPhysics (G4VPhysicsConstructor*)
 - see \$G4SRC/source/physics_list/lists subdirectory

Documentation

Web sites

□ A unique reference web page on Geant4 EM Physics

<u>http://geant4.cern.ch/collaboration/EMindex.shtml</u>

□ From there, links to

- Geant4 Standard Electromagnetic Physics working group pages
- Geant4 Low Energy Electromagnetic Physics working group pages

□ Also from Geant4 web site

- <u>http://geant4.org</u>
 - Who we are
 - Standard Electromagnetic Physics
 - Low Energy Electromagnetic Physics

EM Physics TWiki

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https://twiki.cern.ch/twiki/bin/view/Geant4/ElectromagneticPhysics

Edit Attach PDF

TWiki > Geant4 Web > ElectromagneticPhysics (06-Jan-2011, IvantchenkoV)

Electromagnetic Physics

- Introduction
- Working Group pages
- Validation and verification
- Publications and presentations
- Examples
- Physics Lists
- Models and Processes
- Milestones
- Release notes
- Manuals
- Getting help
- Related links

Introduction

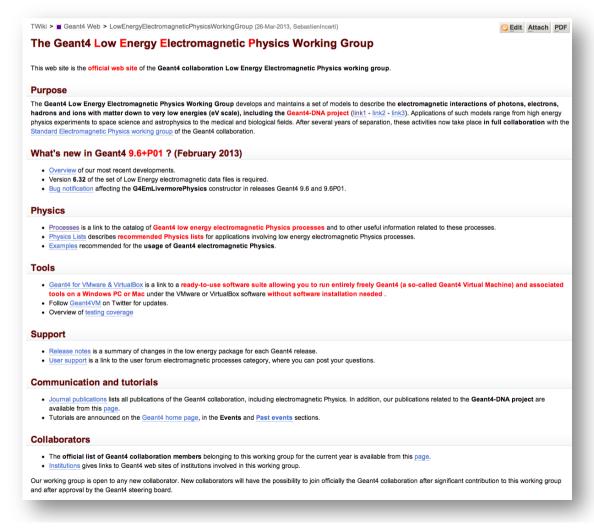
The electromagnetic physics domain includes Geant4 sub-packages for simulation of electromagnetic interactions of charged particles, gammas and optical photons. This is central TWiki page for Geant4 EM physics maintained by common efforts of the EM Standard and EM Low-energy working groups.

Working Group pages

- Electromagnetic Physics Home
- Electromagnetic Standard working group page
- Electromagnetic Standard working group coordination TWiki
- Low Energy Electromagnetic working group page
- Low Energy Electromagnetic working group TWiki

Low Energy EM WG TWiki

https://twiki.cern.ch/twiki/bin/view/Geant4/LowEnergyElectromagneticPhysicsWorkingGroup



Summary:

when/why to use the "Low Energy" EM models

- Use Low-Energy models (Livermore or Penelope), as an alternative to Standard models, when you:
 - need precise treatment of EM showers and interactions at low-energy (keV scale or below)
 - are interested in atomic effects, as fluorescence x-rays, Doppler broadening, etc.
 - can afford a more CPU-intensive simulation
 - want to cross-check another simulation (e.g. with a different Physics List)
- □ Do not use when you are interested in EM physics > MeV
 - same results as Standard EM models
 - strong performance penalty