http://geant4.org

GEANT4 LOW ENERGY ELECTROMAGNETIC PHYSICS

On behalf of the Geant4 Standard and Low Energy EM Physics working groups
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Located in $G4INSTALL/sources/processes/electromagnetic

Geant4 EM packages

- Standard
  - gammas, e+- up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV
- Muons
  - up to 1 PeV
  - energy loss propagator
- X-rays
  - X-ray and optical photon production processes
- High-energy
  - processes at high energy (E>10GeV)
  - physics for exotic particles
- Polarisation
  - simulation of polarised beams
- Optical
  - optical photon interactions
- Low-energy
  - Livermore library g, e- from 250 eV up to 1 GeV
  - Livermore library based polarized processes
  - PENELOPE code rewrite, g, e- , e+ from 250 eV up to 1 GeV (version 2008 version as default)
  - hadrons and ions up to 1 GeV
  - microdosimetry models for radiobiology (Geant4-DNA project) from 4 eV to 10 MeV
  - atomic de-excitation (fluorescence + Auger + PIXE)
- Adjoint
  - New sub-library for reverse Monte Carlo simulation from the detector of interest back to source of radiation
- Utils : general EM interfaces

Content

- Context
- Physics models
  - Livermore, including polarized photon models
  - Penelope
  - Ion ICRU'73 model
  - Geant4-DNA
  - Atomic de-excitation
- How to implement a Physics list ?
- Documentation

CONTEXT

Purpose

- Extend the coverage of Geant4 electromagnetic interactions with matter
  - for photons, electrons, hadrons and ions
  - down to very low energies (sub-keV scale)

- Possible domains of applications
  - space science
  - medical physics
  - microdosimetry for radiobiology
  - …

- Choices of Physics models include
  - Livermore library: electrons and photons [250 eV – 1 GeV]
  - Penelope (Monte Carlo): electrons, positrons and photons [250 eV – 1 GeV]
  - Microdosimetry models (Geant4-DNA project): [eV – ~100 MeV]

Major software upgrade

- Identical to the one proposed by the Standard EM working group
  - Applicable to all low energy electromagnetic software classes
  - For the first time in Geant4 history, allows a coherent approach to the modelling of all electromagnetic interactions
  - No more artificial separation between the 2 EM categories
  - Several bugs & limitations accumulated over past years have been solved
  - Please use Geant4 9.4 release and above

- A physical interaction or process is described by a process class
  - 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 model class
  - 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…)

PHYSICS MODELS

1) Livermore models

Livermore models

- Full set of models for electrons and gammas
- Based on publicly available evaluated data tables from the Livemore 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
  - Sub-levels integrated cross sections: photo-electric, ionization
  - Energy spectra: secondary e- processes
- Validity range : 250 eV - 100 GeV
  - Processes can be used down to 100 eV, with a reduced accuracy
  - In principle, validity range 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)

Livermore models

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Gammas				
Compton	G4ComptonScattering	G4LivermoreComptonModel	250 eV	100 GeV
Polarized Compton	G4ComptonScattering	G4LivermorePolarizedComptonModel	250 eV	100 GeV
Rayleigh	G4RayleighScattering	G4LivermoreRayleighModel	250 eV	100 GeV
Polarized Rayleigh	G4RayleighScattering	G4LivermorePolarizedRayleighModel	250 eV	100 GeV
Conversion	G4GammaConversion	G4LivermoreGammaConversionModel	1.022 MeV	100 GeV
Polarized Conversion	G4GammaConversion	G4LivermorePolarizedGammaConversionModel	1.022 MeV	100 GeV
Photo-electric	G4PhotoElectricEffect	G4LivermorePhotoElectricModel	250 eV	100 GeV
Polarized Photo-electric	G4PhotoElectricEffect	G4LivermorePolarizedPhotoElectricModel	250 eV	100 GeV
Electrons				
Ionization	G4eIonisation	G4LivermoreIonisationModel	250 eV	100 GeV
Bremsstrahlung	G4eBremsstrahlung	G4LivermoreBremsstrahlungModel	250 eV	100 GeV

Eg. of validation of Livermore models

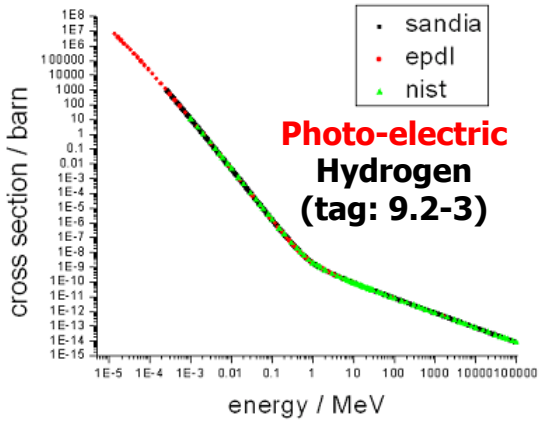


Photo-electric
Hydrogen
(tag: 9.2-3)

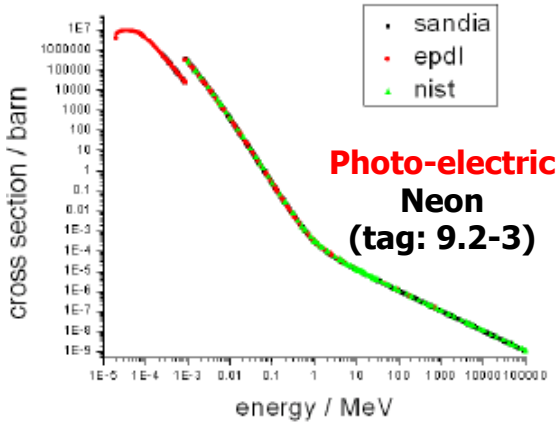
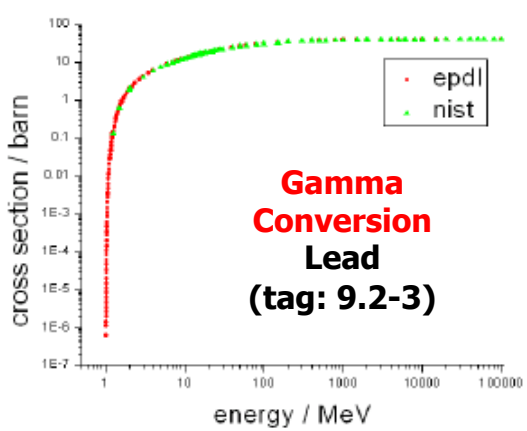
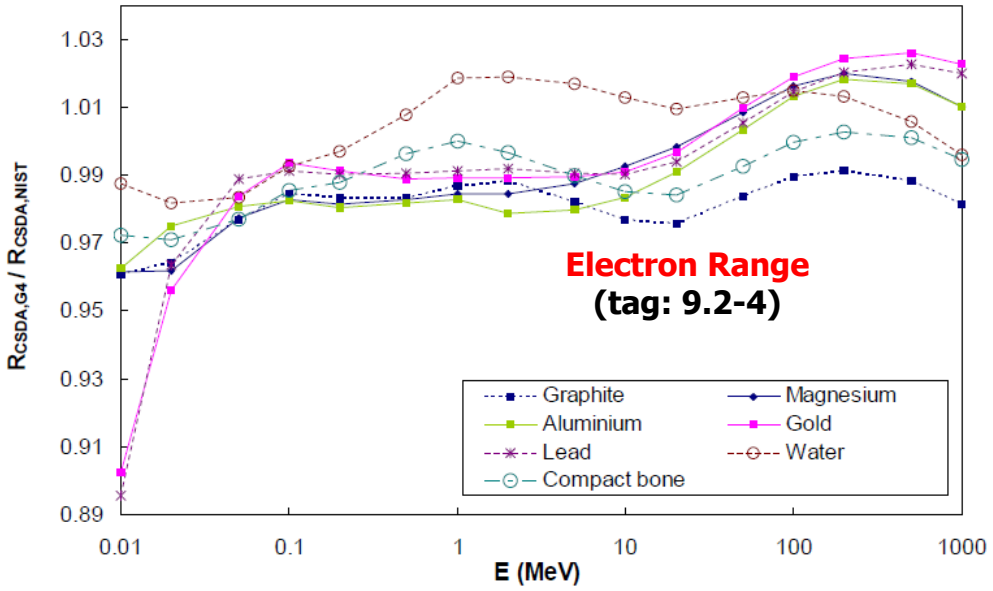


Photo-electric
Neon
(tag: 9.2-3)



Gamma Conversion
Lead
(tag: 9.2-3)



Electron Range
(tag: 9.2-4)

Polarized Livermore processes

- 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
- Documentation
  - Nucl. Instrum.Meth. **A566**: 590-597, 2006 (Photoelectric)
  - Nucl. Instrum.Meth. **A512**: 619-630, 2003 (Compton and Rayleigh)
  - Nucl.Instrum.Meth. **A452**:298-305,2000 (Pair production)
- Naming scheme: G4LivermorePolarizedXXXModel
  - eg. G4LivermorePolarizedComptonModel

PHYSICS MODELS

2) Penelope models

Penelope physics

- Geant4 includes the low-energy models for $e^{\pm}$ and gamma−rays from the Monte Carlo code PENELOPE (PENetration and Energy LOss of Positrons and Electrons) version 2001 (and 2008 as beta)
  - Nucl. Instrum. Meth. **B 207** (2003) 107
- Physics models
  - Specifically developed by the Barcelona group (F. Salvat *et al.*)
  - Great care was dedicated to the low-energy description
    - atomic effects, fluorescence, Doppler broadening, etc.
- Mixed approach: analytical, parametrized & database-driven
  - applicability energy range: 250 eV - 1 GeV
- Includes also positrons (not described by Livermore models)
- G4PenelopeXXXModel (e.g. G4PenelopeComptonModel)

Penelope models

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Gammas				
Compton	G4ComptonScattering	G4PenelopeComptonModel	250 eV	1 GeV
Rayleigh	G4RayleighScattering	G4PenelopeRayleighModel	250 eV	1 GeV
Conversion	G4GammaConversion	G4PenelopeGammaConversionModel	1.022 MeV	1 GeV
Photo-electric	G4PhotoElectricEffect	G4PenelopePhotoElectricModel	250 eV	1 GeV
Electrons/Positrons				
Ionization	G4elonisation	G4PenelopelonisationModel	250 eV	1 GeV
Bremsstrahlung	G4eBremsstrahlung	G4PenelopeBremsstrahlungModel	250 eV	1 GeV
Positrons				
Annihilation	G4eplusAnnihilation	G4PenelopeAnnihilationModel	250 eV	1 GeV

PHYSICS MODELS

3) Ions

Ion energy loss model

- Describes the energy loss of ions heavier than Helium

  due to interaction with the atomic shells of target atoms

- The model computes
  - Restricted stopping powers: continuous energy loss of ions as they slow down in an absorber
  - Cross sections for the production of δ-rays
    - δ-rays are only produced above a given threshold, which inherently also governs

      the discrete energy loss of ions

- Primarily of interest for
  - Medical applications
  - Space applications

Ion stopping powers (1/2)

- Electronic stopping powers are an important ingredient to determine the mean energy loss of ions along simulation steps
  - For eg. impacts the ion range

- Restricted stopping powers: account for the fact that the continuous energy loss description is restricted to energies below T_{cut}
  (where T_{cut} denotes the lower production threshold of δ -rays)

- Restricted stopping powers are calculated according to
  (T = kinetic energy per nucleon)
  - $T < T_{Low}$: Free electron gas model
  - $T_L \leq T \leq T_{High}$: Interpolation of tables or parameterization approach
  - $T > T_H$: Bethe formula (using an effect. charge) + high order corr.

Ion stopping powers (2/2)

- Parameterization approach
  - Model incorporates ICRU 73 stopping powers into Geant4

- ICRU73 model
  - Covers a large range of ion-material combinations: Li to Ar, and Fe
  - Stopping powers: based on binary theory
  - Special case: water
    - Revised ICRU 73 tables of P. Sigmund are used (since Geant4 9.3.b01)
    - Mean ionization potential of water of 78 eV
  - Current model parameters (Geant4 9.3.b01):
    - T_{High} = 10 MeV/nucleon (except Fe ions: T_H = 1 GeV/nucleon)
    - T_{Low} = 0.025 MeV/nucleon (lower boundary of ICRU 73 tables)
  - For ions heavier than Ar
    - Scaling of Fe ions based on effective charge approach

PHYSICS MODELS

4) Geant4-DNA

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 »)
- A full multidisciplinary activity of the Geant4 low energy electromagnetic Physics working group, involving physicists, theoreticians, biophysicsts…
- 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
  - Not limited to biological materials (ex. DNA bases)
- See next talk

PHYSICS MODELS

5) Atomic de-excitation

Atomic effects

- Atomic de-excitation initiated by other EM processes
  - Example: photo-electric effect, ionisation by e- and ions (eg. PIXE)
  - 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

- Atomic de-excitation simulation is now compatible with both Standard & Low Energy EM categories
  - Livermore, Penelope, Standard electromagnetic, and Geant4-DNA processes
  - photoelectric effect, ionization and Compton scattering

Including atomic effects

- When using Geant4 reference physics lists or physics builders, activation can be easily controlled UI commands for the whole geometry:

```
/run/initialize
/process/em/fluo true
/process/em/auger true
/process/em/pixe true
```

  or alternatively for a specific G4Region:

```
/run/initialize
/process/em/deexcitation region true true true
```

  where Boolean parameters corresponds to activation of "fluo", "auger", and "pixe" respectively

- Fluorescence is activated by default in Livermore and Penelope physics builders while Auger production and PIXE are not.
- The activation of atomic deexcitation in a user physics list can be done 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)
```

- See more details at our atomic deexcitation web-page:
  - https://twiki.cern.ch/twiki/bin/view/Geant4/LoweAtomicDeexcitation
- Examples to start from
  - see **$G4INSTALL/examples/extended/electromagnetic/TestEm**5 or 18

HOW TO IMPLEMENT A PHYSICS LIST ?

Physics lists

- A user can
  - use reference Physics lists provided with Geant4 (QBBC, ….)
  - build his/her own Physics list in his/her application
  - or use already available EM physics constructors

1. If you choose to build your own Low Energy EM Physics list
   - Refer to the Geant4 Low Energy EM working group website, look at the Processes and Physics lists sections
   - Also you may refer to Geant4 examples
     - $G4INSTALL/examples/extended/electromagnetic/TestEm14

2. More safe: if you prefer to use the available constructors, these are named as:
   - G4EmLivermorePhysics
   - G4EmLivermorePolarizedPhysics
   - G4EmPenelopePhysics
   - G4EmDNAPhysics

How to use the already available Physics constructors ?

- These classes derive from the G4VPhysicsConstructor abstract base class
- A good implementation example of Physics list that uses EM physics constructors is available in:
  $G4INSTALL/examples/extended/electromagnetic/TestEm2
- If some hadronic physics is needed additionally to EM Physics:
  $G4INSTALL/examples/extended/electromagnetic/TestEm7
- The source code for Physics list constructors is available in the following directory: $G4INSTALL/source/physics_list/builders
- The physics lists constructors are added to the Geant4 reference Physics lists via the method RegisterPhysics (G4VPhysicsConstructor*)
  - see $G4INSTALL/source/physics_lists/lists subdirectory

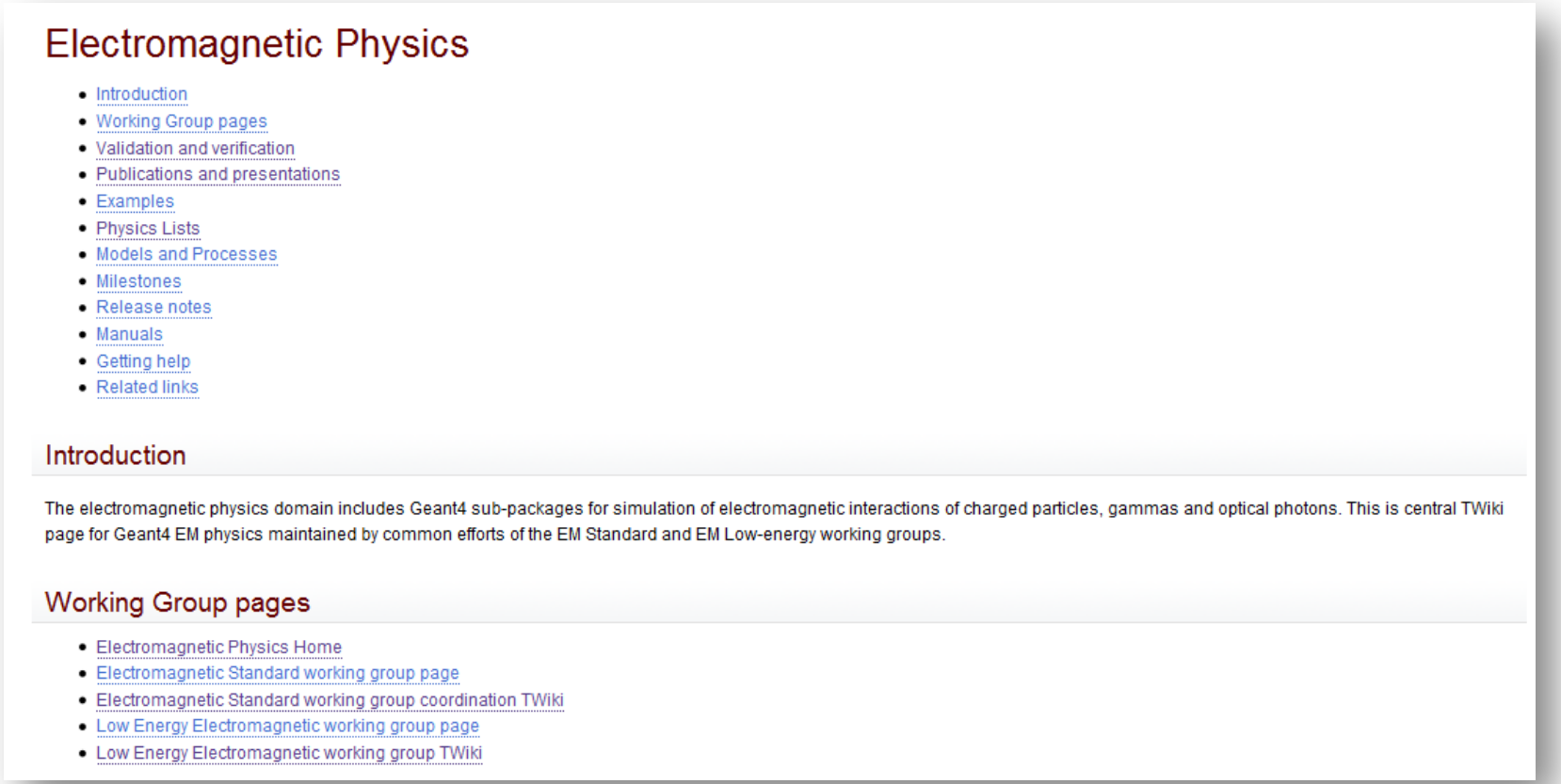
DOCUMENTATION

Web sites

- A unique reference web page on Geant4 EM Physics
  - http://geant4.cern.ch/collaboration/EMindex.shtml
- From there, links to :
  - Geant4 Standard Electromagnetic Physics working group pages
  - Geant4 Low Energy Electromagnetic Physics working group pages
- Also from Geant4 web site:
  - http://geant4.org
    - Who we are
      - Standard Electromagnetic Physics
      - Low energy Electromagnetic Physics

EM Physics TWiki

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



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

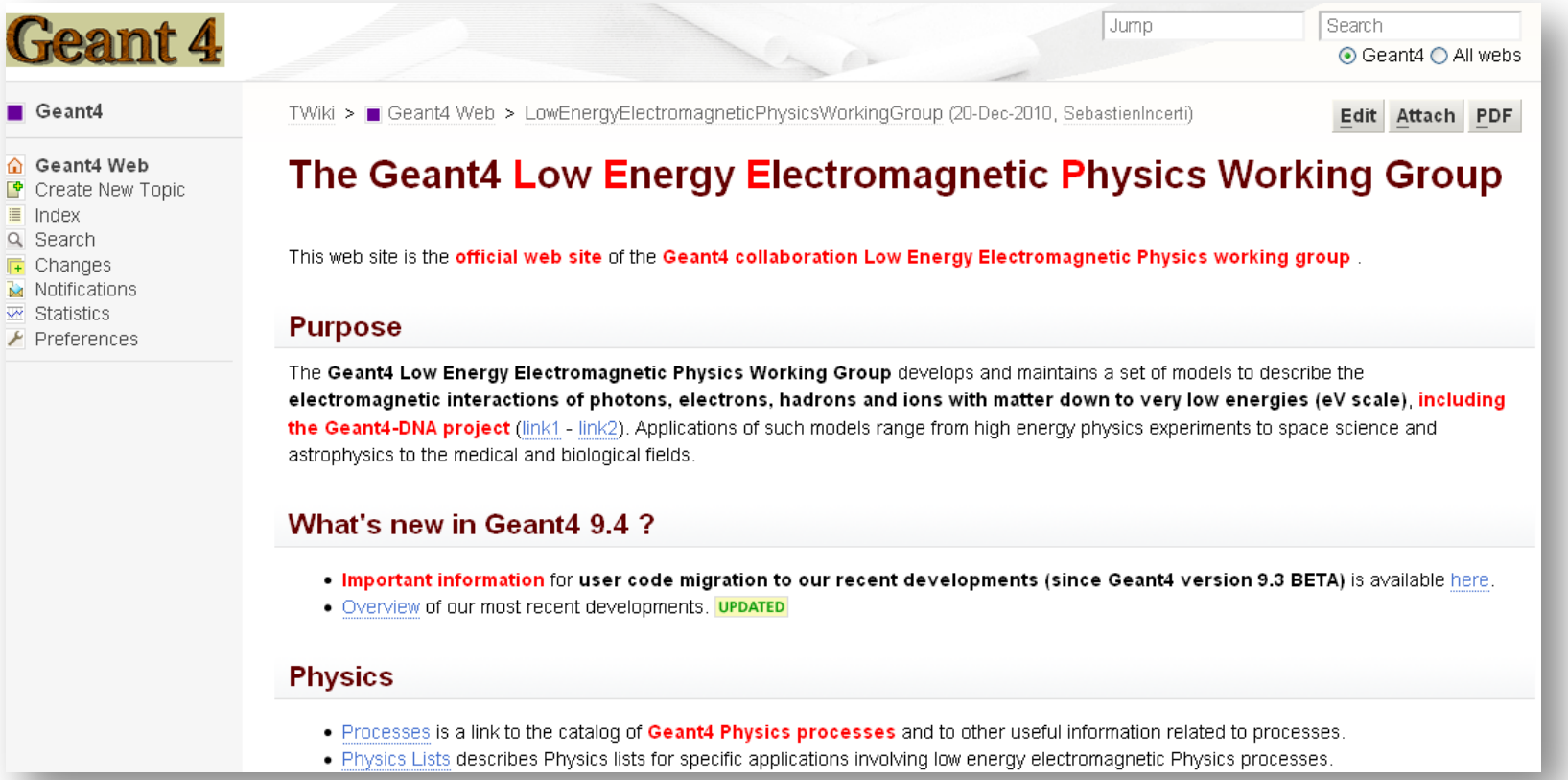
The electromagnetic physics domain includes Geant4 sub-packages for simulation of electromagnetic interactions of charged particles, gammas and optical photons. This is central TWiki page for Geant4 EM physics maintained by common efforts of the EM Standard and EM Low-energy working groups.

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 WG TWiki

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



Summary: when/why to use Low Energy 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)
  - are interested in atomic effects, as fluorescence x-rays, Doppler broadening, etc.
  - Geant4-DNA extension
  - can afford a more CPU-intensive simulation
  - want to cross-check another simulation (e.g. with a different model)

- Do not use when you are interested in EM physics > MeV
  - same results as Standard EM models, strong performance penalty

THANK YOU

How to use the new model ?

- Model name: G4IonParametrisedLossModel
- Applicable from Z>2
- Already included in G4EmStandardPhysics_option3, G4EmLivermorePhysics and G4EmPenelopePhysics physics builders
- Designed to be used with the G4ionIonisation process
  (in 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: G4GenericIon
  - 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<2, we use G4BraggModel, G4BragglonModel, and G4BetheBlochModel with the G4ionIonisation process

Using 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
- For compounds, ICRU 73 stopping powers are used if the material name coincides with the name of Geant4 NIST materials
  - e.g. G4_WATER
- 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 a list of applicable materials, the user is referred to the ICRU 73 report.
- All data files are in the G4LEDATA set of data.