Geant4 release 10.4 + P02

LOW ENERGY ELECTROMAGNETIC PHYSICS

Mihaly Novak
Material from Sebastien Incerti (CNRS)

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Content

- Context
- Physics processes & models
  - Livermore, including polarized photon models
  - Penelope models
  - Ion ICRU'73 model
  - Geant4-DNA processes and models, beyond physics
  - MicroElec processes and models
  - Monash University models
  - Atomic de-excitation process and models
- How to implement a Physics list ?
- Documentation

Context

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 and nanodosimetry for radiobiology and microelectronics
  - …

- Main choices of physics models include
  - Livermore : electrons and photons [250 eV* – GeV]
  - Penelope : electrons, positrons and photons [100 eV* – 1 GeV]
  - Microdosimetry & nanodosimetry models
    - Geant4-DNA project: [eV – ~ few 100 MeV]
    - MicroElec for Silicon : [eV – 10 GeV/u]

Software design

- 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 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…)
- All required data files are located in the $G4LEDATA directory

Physics 1/7

Livermore models

Livermore models

- 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- – Alternative set by Bearden for fluoresence lines
  - EEDL : Evaluated Electrons Data Library
  - EPDL97 : Evaluated Photons Data Library
  - EPICS2014 for photoelectric effect
  - Mixture of experiments and theories
  - Binding energies: Scofield

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

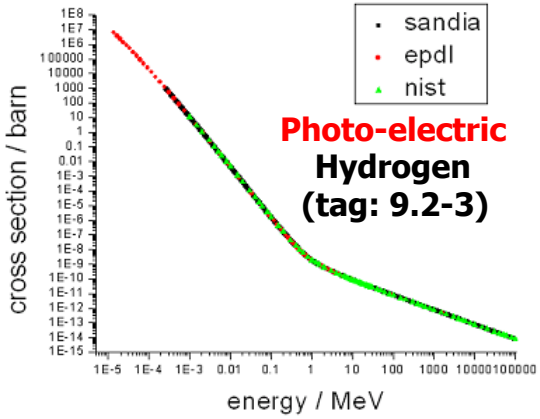
- Data tables are interpolated by Livermore model classes to compute
  - Total cross sections: photoelectric, Compton, Rayleigh, pair production, Bremsstrahlung
  - Shell integrated cross sections: photo-electric, ionization
  - Energy spectra: secondary e- processes
- Validity range (recommended) : 250 eV (recommended)
  - Processes can be used down to 100 eV, with a reduced accuracy
  - Technically, 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)

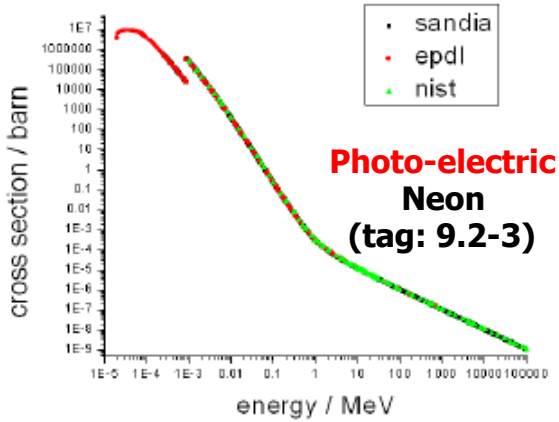
Available Livermore models

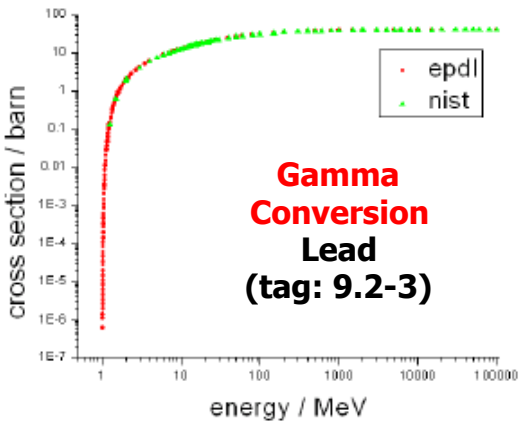
Physics Process	Process Class	Model Class	Low Energy Limit
Gammas			
Compton	G4ComptonScattering	G4LivermoreComptonModel	eV
Polarized Compton	G4ComptonScattering	G4LivermorePolarizedComptonModel	eV
Rayleigh	G4RayleighScattering	G4LivermoreRayleighModel	eV
Polarized Rayleigh	G4RayleighScattering	G4LivermorePolarizedRayleighModel	250 eV (kill)
Conversion	G4GammaConversion	G4LivermoreGammaConversionModel	1.022 MeV
Polarized Conversion	G4GammaConversion	G4LivermorePolarizedGammaConversionModel	1.022 MeV
Photo-electric	G4PhotoElectricEffect	G4LivermorePhotoElectricModel	eV
Polarized Photo-electric	G4PhotoElectricEffect	G4LivermorePolarizedPhotoElectricModel	eV
Electrons			
Ionization	G4eIonisation	G4LivermoreIonisationModel	eV
Bremsstrahlung	G4eBremsstrahlung	G4LivermoreBremsstrahlungModel	10 eV

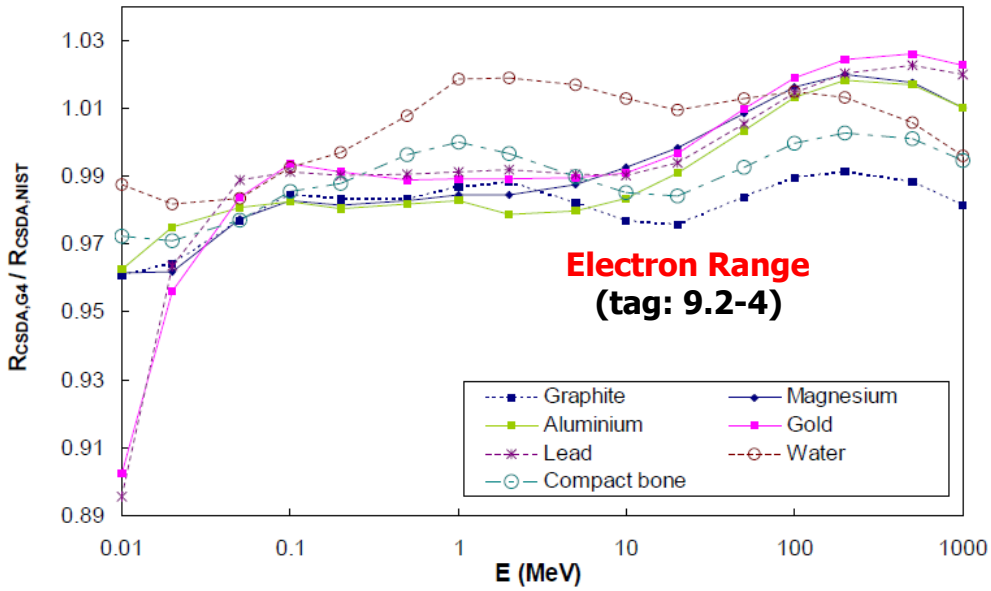
Eg. of verification of Livermore models

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









Polarized Livermore models

- 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)

Physics 2/7

Penelope models

Penelope physics

- 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 350 (2015) 41-48
  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
  - Recommended 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	eV	1 GeV
Rayleigh	G4RayleighScattering	G4PenelopeRayleighModel	eV	1 GeV
Conversion	G4GammaConversion	G4PenelopeGammaConversionModel	1.022 MeV	1 GeV
Photo-electric	G4PhotoElectricEffect	G4PenelopePhotoElectricModel	eV	1 GeV
Electrons/Positrons				
Ionization	G4eIonisation	G4PenelopeIonisationModel	eV	1 GeV
Bremsstrahlung	G4eBremsstrahlung	G4PenelopeBremsstrahlungModel	eV	1 GeV
Positrons				
Annihilation	G4eplusAnnihilation	G4PenelopeAnnihilationModel	eV	1 GeV

Physics 3/7

Ions

Ion energy loss model

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

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

Ion energy loss model

- Restricted stopping powers are calculated using 3 approaches
  - $T < T_{Low}$: Free electron gas model
  - $T_{Low} \leq T \leq T_{High}$: parameterization (ICRU'73) approach
  - $T > T_{High}$: 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
    - Targets : 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} = 1 GeV/nucleon
    - T_{Low} = 0.025 MeV/nucleon (lower boundary of ICRU'73 tables)

How to use the ion model ?

- Model name: G4IonParametrisedLossModel
- Only applicable to ions with Z≥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: 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<3, we use G4BraggModel (p) or G4BragglonModel (alpha), and G4BetheBlochModel with the G4hIonisation and G4ionIonisation processes

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

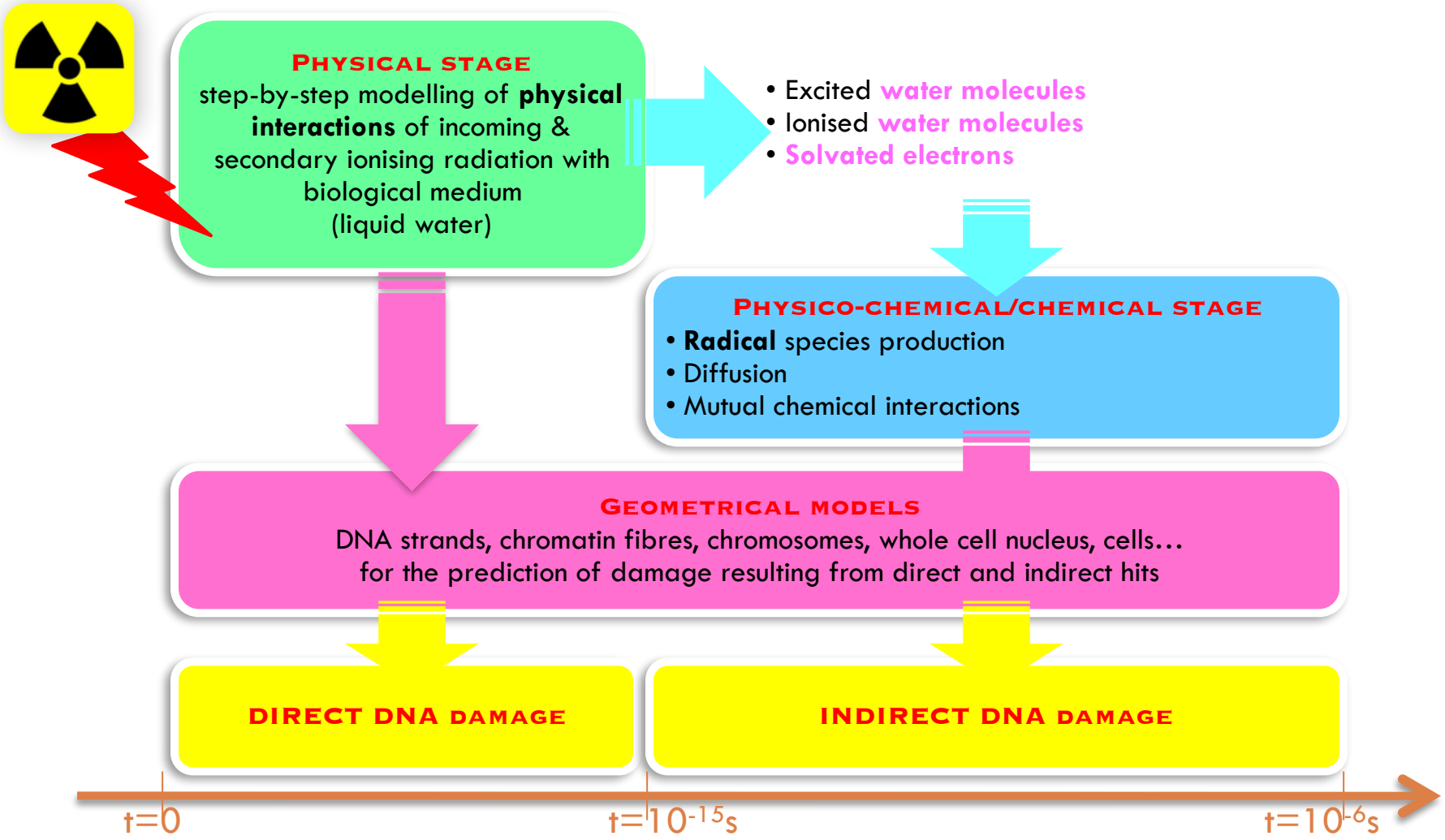
Physics 4/7

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 for radiobiology »)
  - Early direct and non-direct effects to DNA in cells
- A full multidisciplinary activity of the Geant4 Low Energy Electromagnetic Physics working group, involving physicists, chemists, 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

How can Geant4-DNA simulate early DNA damage ?



Geant4 for radiobiology

- Several models are available for the description of physical processes involving e^-, p, H, He, He^+, He^{2+}, Li, Be, B, C, N, O, Si, Fe
- Include elastic scattering, excitation (electronic + vibrations), ionisation, charge exchange and molecular attachment
- These models are valid for liquid water medium and a few biological materials
- 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
- Can be combined with other EM categories
  - Standard, LowE thanks to common software design
- Many extended examples in the extended/medical/dna category

Overview of physics models for liquid water

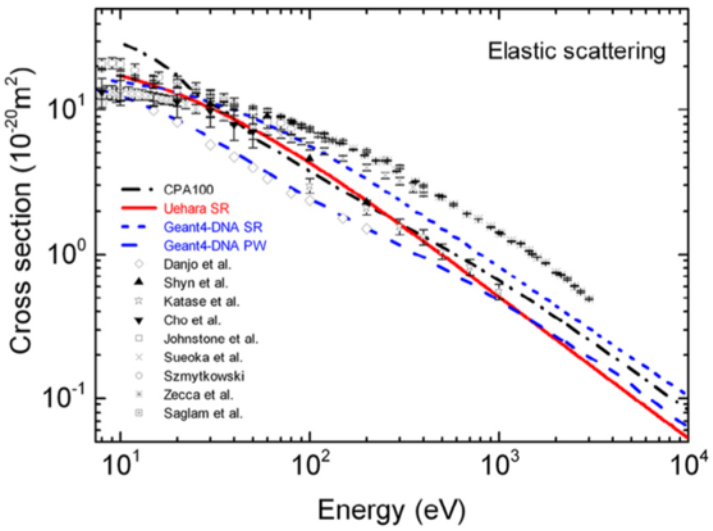
- Electrons
  - Elastic scattering
    - Screened Rutherford and Brenner-Zaider below 200 eV
    - Updated alternative version by Uehara
    - Independent Atom Method (IAM) by Mott et al. & data in ice from CPA100 code
    - Partial wave framework model by Champion et al.,
      3 contributions to the interaction potential
  - Ionisation
    - 5 levels for H2O
    - Dielectric formalism & FBA using Heller optical data up to 1 MeV, and low energy corrections, by Emfietzoglou et al.
    - Improved alternative version by Emfietzoglou and Kyriakou
    - Relativistic Binary Encounter Bethe (RBEB) by Terrissol from CPA100 code
  - Excitation (*)
    - 5 levels for H2O
    - Dielectric formalism & FBA using Heller optical data and semi-empirical low energy corrections, , derived from the work of Emfietzoglou et al.
    - Improved alternative version by Emfietzoglou and Kyriakou
    - Dielectric formalism by Dingfelder from CP100 code
  - Vibrational excitation (*)
    - Michaud et al. xs measurements in amorphous ice
    - Factor 2 to account for phase effect
  - Dissociative attachment (*)
    - Melton xs measurements

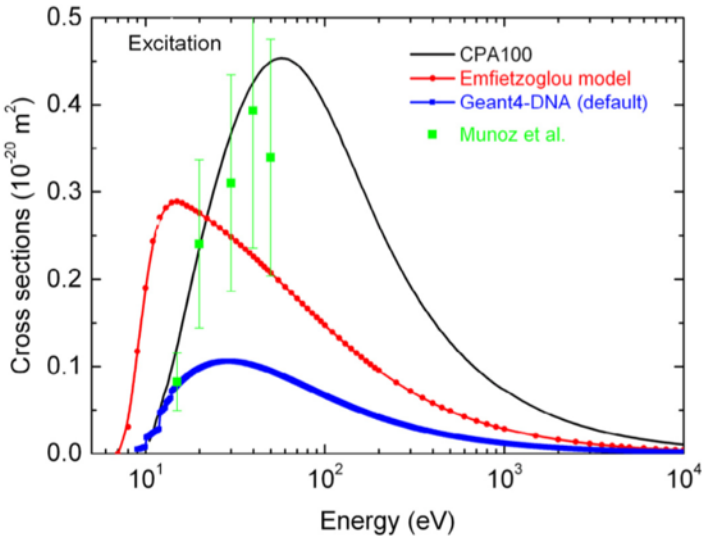
Med. Phys. 37 (2010) 4692
Appl. Radiat. Isot. 69 (2011) 220
Med. Phys. 42 (2015) 3870
Phys. Med. 31 (2015) 861
Nucl. Instrum. and Meth. B 343 (2015) 132
Phys. Med. 32 (2016) 1833

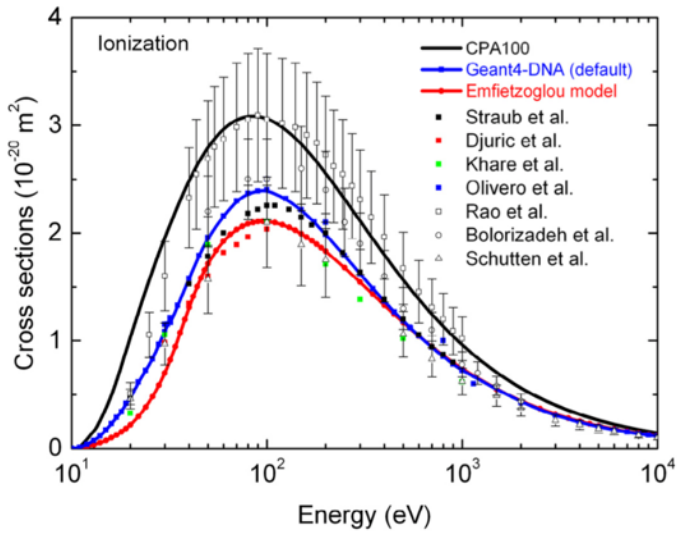
- Protons & H
  - Excitation (*)
    - Miller & Green speed scaling of e- excitation at low energies and Born and Bethe theories above 500 keV, from Dingfelder et al.
  - Ionisation
    - Rudd semi-empirical approach by Dingfelder et al. and Born and Bethe theories & dielectric formalism above 500 keV (relativistic + Fermi density)
  - Charge change (*)
    - Analytical parametrizations by Dingfelder et al.
  - Nuclear scattering
    - Classical approach by Everhart et al.
- He0, He+, He2+
  - Excitation (*) and ionisation
    - Speed and effective charge scaling from protons by Dingfelder et al.
  - Charge change (*)
    - Semi-empirical models from Dingfelder et al.
  - Nuclear scattering
    - Classical approach by Everhart et al.
- Li, Be, B, C, N, O, Si, Fe
  - Ionisation
    - Speed scaling and global effective charge by Booth and Grant
- Photons
  - from EM « standard » and « low energy »
    - Default: « Livermore » (EPDL97)

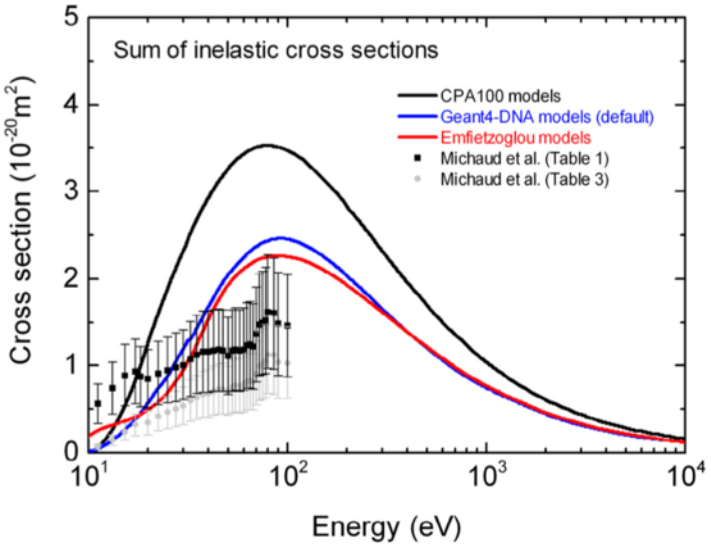
(*) only available in Geant4-DNA

Cross section models for electrons







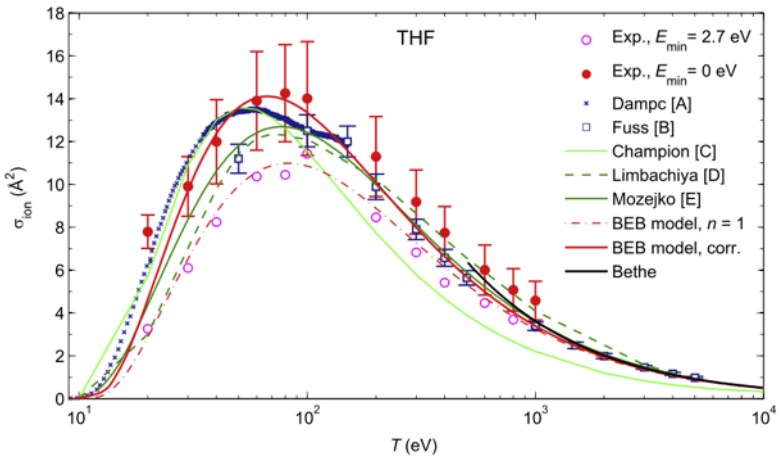


Phys. Med. 31 (2015) 861

Other materials

- Part of the effort to extend Geant4-DNA models to other materials than liquid water
- Cross sections for biological materials are proposed since Geant4 10.4 Beta, applicable to DNA constituents
  - tetrahydrofuran (THF), trimethylphosphate (TMP), pyrimidine (PY) and purine (PU)
  - serving as models for the deoxyribose and phosphate groups in the DNA backbone as well as for the pyrimidine nucleobases, respectively
- For the following incident particles
  - electrons (12 eV-1keV, el. + exci. + ioni.) : from measurements @ PTB, Germany
  - protons (70 keV-10 MeV, ioni.) from the HKS approach

Eg. total electron ionisation cross sections in THF



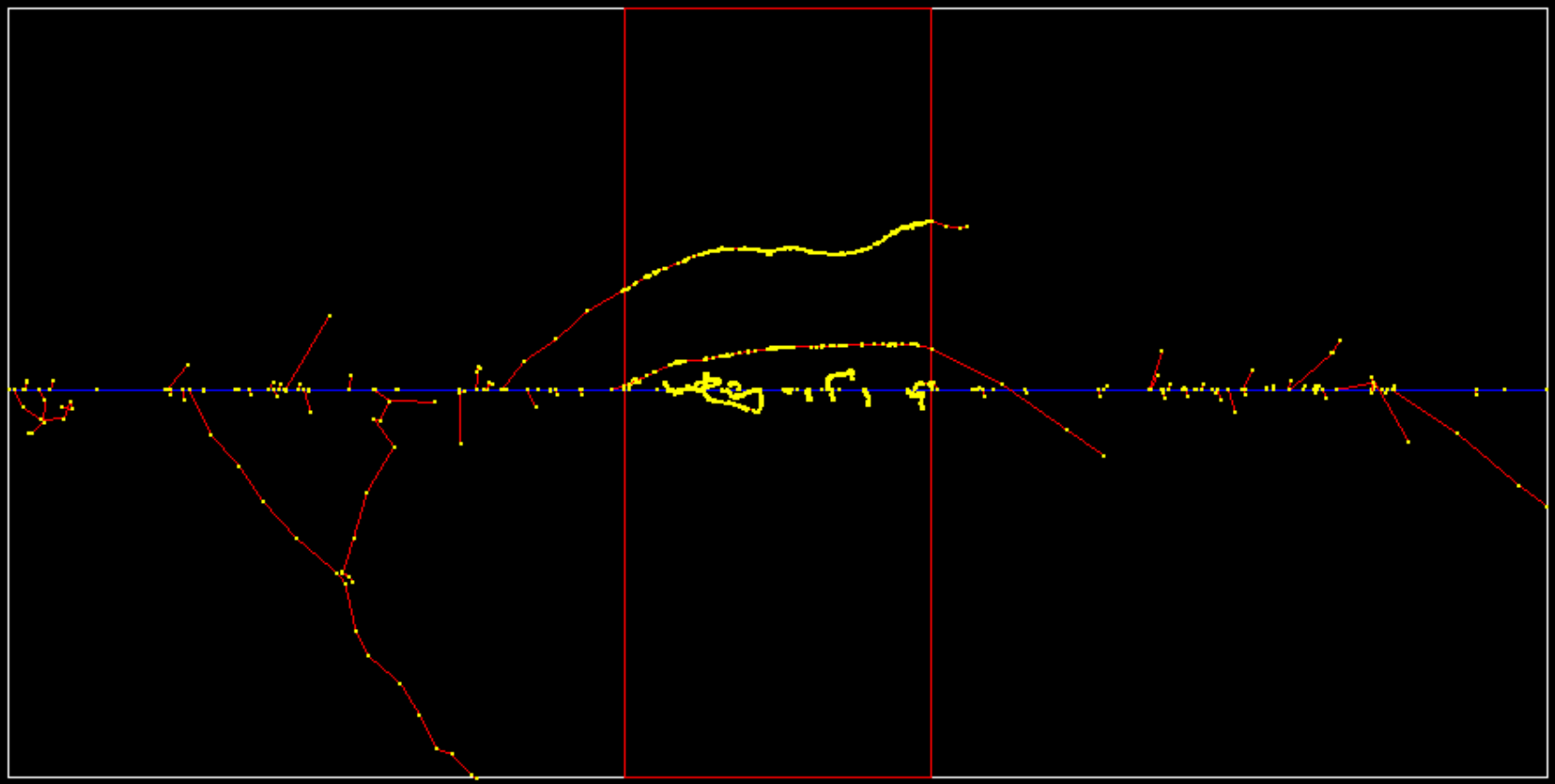
Rad. Phys. Chem. 130 (2017) 459–479

Multiscale combination of EM processes

Thanks to a unified software design, users can easily combine Geant4-DNA processes and models with existing Geant4 physics such as:

- Geant4 photon processes and models
  - Photoelectric effect, Compton sc., Rayleigh sc., pair production
  - Livermore (EPDL97) included by default
- Geant4 alternative electromagnetic processes and models for charged particles
  - Ionisation, bremsstrahlung, etc…
  - Electrons, positrons, ions, etc…
- Geant4 atomic deexcitation (fluorescence + Auger emission, including cascades)
  - EADL97, Bearden
- …and also Geant4 hadronic physics

Mixed physics lists in geometrical regions: the « microdosimetry » extended example

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Nucl. Instrum. and Meth. B 273 (2012) 95
Prog. Nucl. Sci. Tec. 2 (2011) 898

Geant4-DNA Physics constructors

3 recommended constructors

Constructor name	Content
G4EmDNAPhysics	Default models
G4EmDNAPhysics_option1 (beta)	Same as G4EmDNAPhysics but uses New multiple scattering model G4LowEWentzelVIModel
G4EmDNAPhysics_option2	Same as G4EmDNAPhysics but faster (usage of CDCS for ionisation processes)
G4EmDNAPhysics_option3	Same as G4EmDNAPhysics (historical)
G4EmDNAPhysics_option4	Electron ionisation and excitation models by Ioannina team
G4EmDNAPhysics_option5 (beta)	Same but faster (usage of CDCS)
G4EmDNAPhysics_option6	CPA100 models

All are located in

$G4INSTALL/source/physics_lists/constructors/electromagnetic

Overview of verification activities

Quantity	Incident particle	References
Cross sections	electron, proton, alpha particle	Phys. Med. 31, 861 (2015) Med. Phys. 37, 4692 (2010)
Dose Point Kernels	electron	Nuclear Inst. and Methods in Physics Research B 398, 13 (2017) Appl. Radiat. Isot. 83, 137 (2014)
Frequency of energy deposition	electron, proton, alpha particle	Nuclear Inst. and Methods in Physics Research B 306, 158 (2013)
Ionization cluster size	electron	Eur. Phys. J. D 60, 85 (2010)
Lineal energy	proton	Appl. Radiat. Isot. 69, 220 (2011)
Mean energy deposition	proton	Appl. Radiat. Isot. 69, 220 (2011)
Radial doses	proton, alpha particle, ions	Nuclear Inst. and Methods in Physics Research B 333, 92 (2014) Phys. Med. Biol. 59, 3657 (2014)
Range	electron, proton, alpha particle	Nuclear Inst. and Methods in Physics Research B 269, 2307 (2011)
S-values	electron	Nuclear Inst. and Methods in Physics Research B 319, 87 (2014) Med. Phys. 42, 3870 (2015)
Slowing down spectrum	electron	Nuclear Inst. and Methods in Physics Research B 397, 45 (2017) Phys. Med. Biol. 57, 1087 (2012)
Stopping power or stopping cross section	electron, proton, alpha particle, C, O, Si, Fe	Med. Phys. 37, 4692 (2010) Phys. Med. Biol. 57, 209 (2011) Nuclear Inst. and Methods in Physics Research B 269, 2307 (2011)
W-value	electron	Phys. Med. Biol. 57, 1087 (2012) Med. Phys. 42, 3870 (2015)

Physico-chemical stage

- During this stage, water molecules
  - Dissociate if ionized
  - Relax or dissociate if excited

Electronic state	Dissociation channels	Fraction (%)
All single ionization states	$H_3O^+ + {}^\bullet OH$	100
Excitation state A1B1: (1b1) → (4a1/3s)	${}^\bullet OH + H^\bullet$ $H_2O + \Delta E$	65 35
Excitation state B1A1: (3a1) → (4a1/3s)	$H_3O^+ + {}^\bullet OH + e^-_{aq}$ (Al) ${}^\bullet OH + {}^\bullet OH + H_2$ $H_2O + \Delta E$	55 15 30
Excitation state: Rydberg, diffusion bands	$H_3O^+ + {}^\bullet OH + e^-_{aq}$ (Al) $H_2O + \Delta E$	50 50
Dissociative attachment	${}^\bullet OH + OH^- + H_2$	100

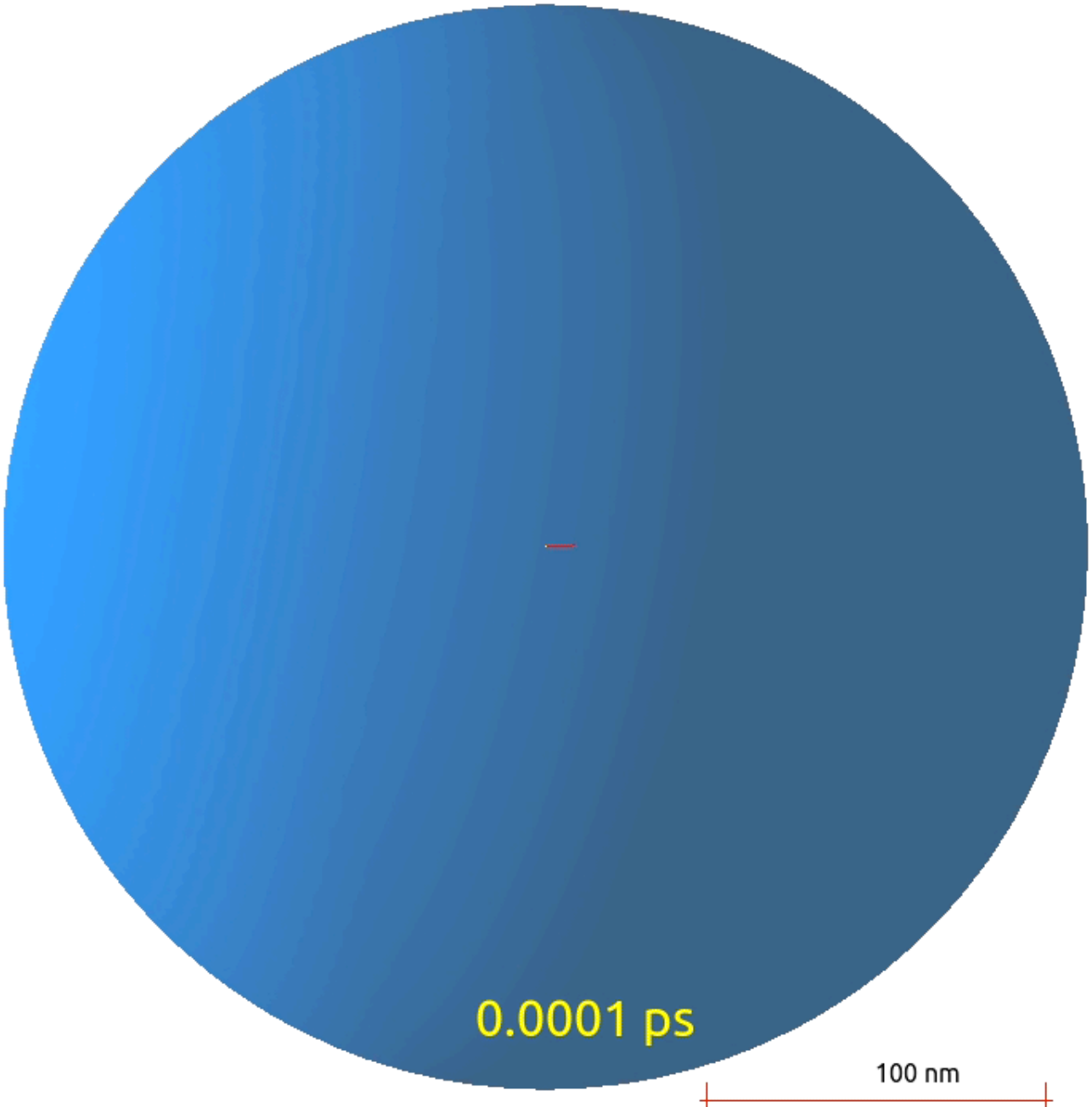
- Products thermalize down to their energy of diffusion at equilibrium

Chemical stage

Species	Diffusion coefficient D (10^{-9} m^2 s^{-1})
H_3O^+	9.0
H•	7.0
OH^-	5.0
e^-_{aq}	4.9
H_2	5.0
•OH	2.8
H_2O_2	1.4

We followed the set of parameters published by the authors of the PARTRAC software (Kreipl et al., REB 2009). However, these parameters can be modified by the user.

Reaction	Reaction rate (10^7 m^3 mol^{-1} s^{-1})
$H_3O^+ + OH^- \rightarrow 2\ H_2O$	14.3
$•OH + e^-_{aq} \rightarrow OH^-$	2.95
$H• + e^-_{aq} + H_2O \rightarrow OH^- + H_2$	2.65
$H_3O^+ + e^-_{aq} \rightarrow H• + H_2O$	2.11
$H• + •OH \rightarrow H_2O$	1.44
$H_2O_2 + e^-_{aq} \rightarrow OH^- + •OH$	1.41
$H• + H• \rightarrow H_2$	1.20
$e^-_{aq} + e^-_{aq} + 2\ H_2O \rightarrow 2\ OH^- + H_2$	0.50
$•OH + •OH \rightarrow H_2O_2$	0.44


0.0001 ps
100 nm

A new interface to describe geometries in Geant4-DNA

- PDB : Protein Data Bank
  http://www.rcsb.org/pdb/
  - 3D structure of molecules
  - Proteins
  - Nucleic acids
- Description of DNA molecules
  - 1FZX.pdb
    - Dodecamer
    - 12 DNA base pairs
    - (2,8 x 2,3 x 4,01 nm^3)
  - 1ZBB.pdb
    - Tetranucleosome
    - 2 nucleosomes : 347 pairs of bases
    - (9,5 x 15,0 x 25,1 nm^3)

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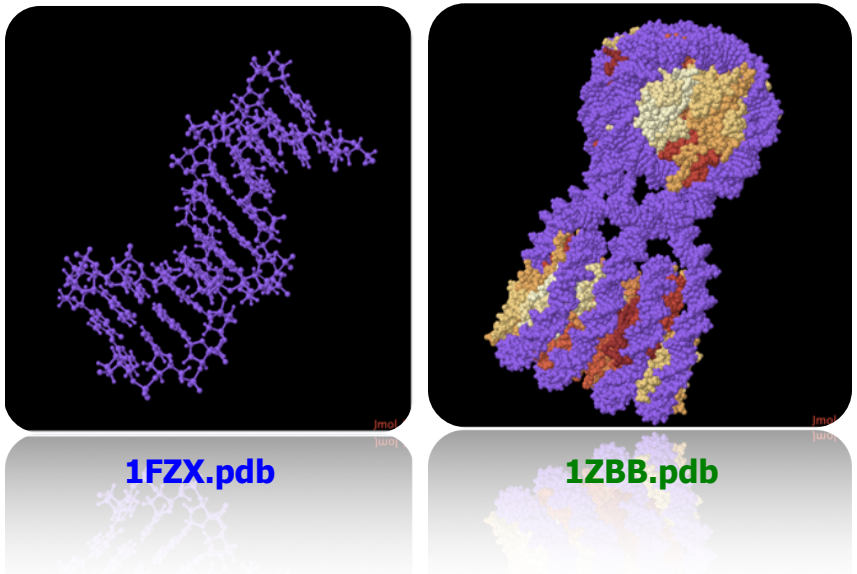


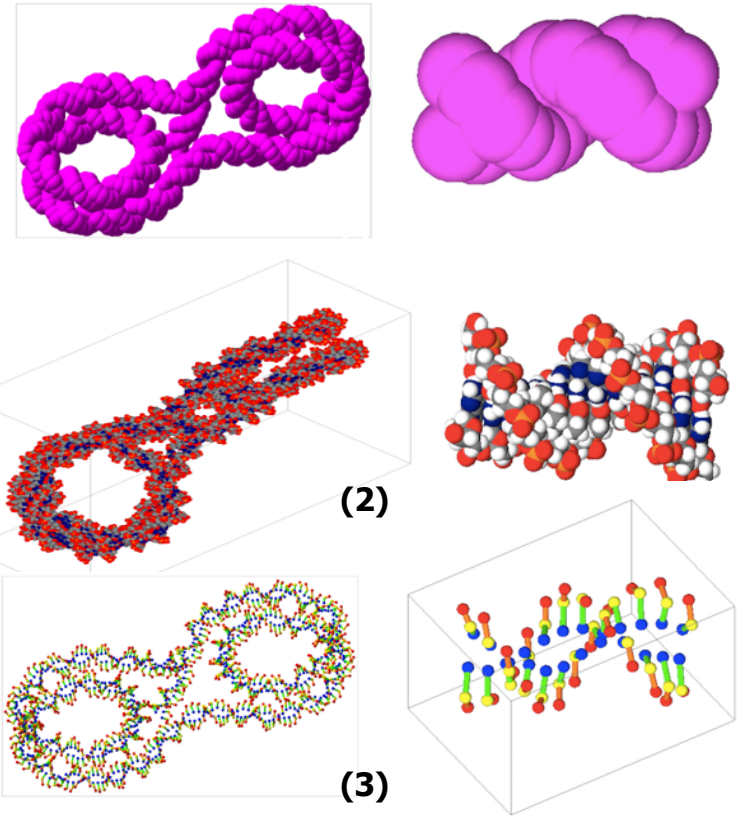
1FZX.pdb 1ZBB.pdb

RCSB PDB PROTEIN DATA BANK

http://pdb4dna.in2p3.fr
http://geant4-dna.org

« pdb4dna » extended example

- 1) A C++ library
  - Reading of PDB files
  - Build bounding boxes from atom coordinates
  - Search for closest atom from a given point
  - Geometry and visualization : 3 granularities
    - (1) Barycenter of nucleotides
    - (2) Atomistic
    - (3) Barycenter of nucleotide components
- 2) A Geant4-DNA example
  - Water box surrounding the molecule
  - The output results consists in a ROOT file, containing for each event:
    - energy deposit in bounding boxes
    - number of single strand breaks (SSB)
    - number of double strand breaks (DSB)



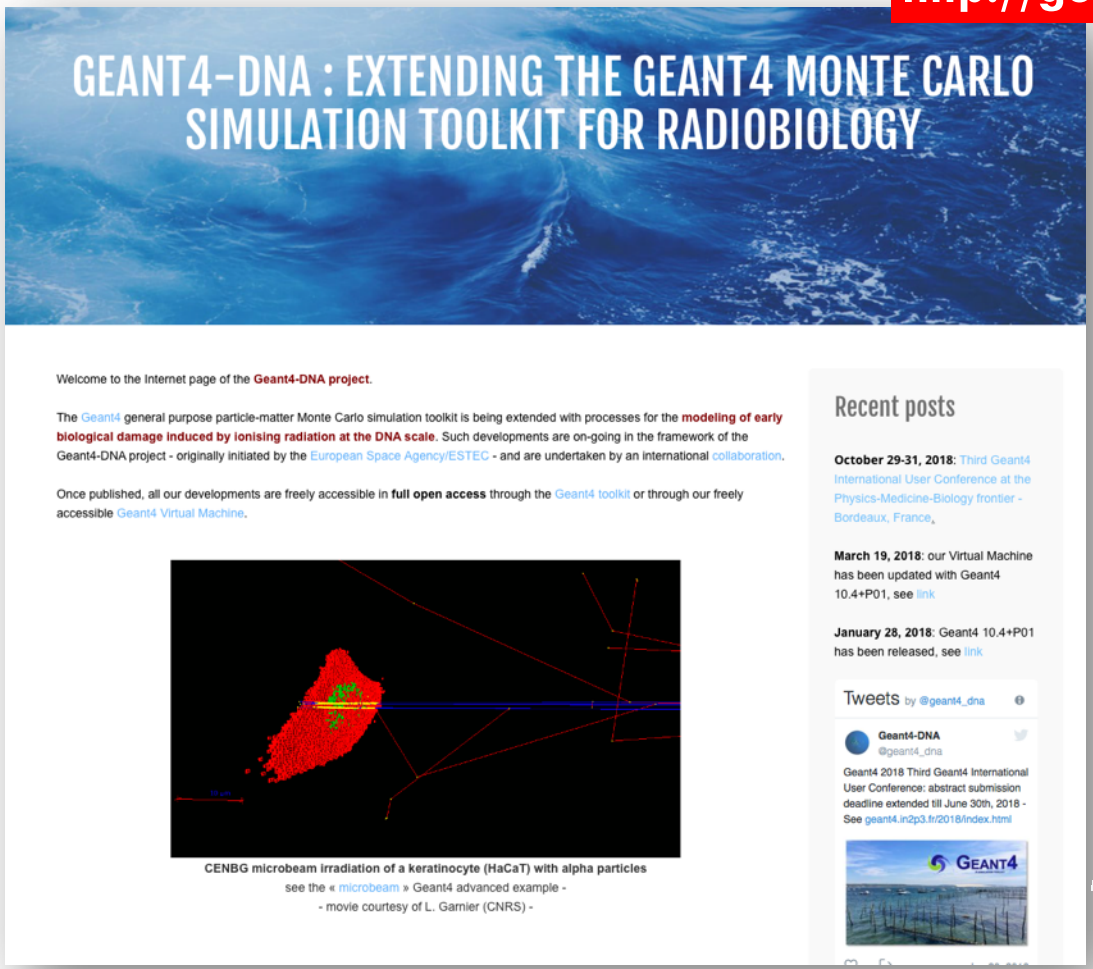
Comput. Phys. Comm. 192 (2015) 282

Geant4-DNA examples included in Geant4

Example code name	Purpose	Location
dnaphysics	• Usage of Geant4-DNA Physics processes • variable density	$G4INSTALL/examples/extended/medical/dna
microdosimetry	Combination of Standard EM or Low Energy EM processes with Geant4-DNA Physics processes	$G4INSTALL/examples/extended/medical/dna
range	Range simulation with Geant4-DNA	$G4INSTALL/examples/extended/medical/dna
slowing	Calculation of electron slowing down spectra	$G4INSTALL/examples/extended/medical/dna
spower	Calculation of stopping power	$G4INSTALL/examples/extended/medical/dna
svalue	Usage of Geant4-DNA Physics processes in spheres	$G4INSTALL/examples/extended/medical/dna
wvalue	Calculation of W values	$G4INSTALL/examples/extended/medical/dna
clustering	Clustering code	$G4INSTALL/examples/extended/medical/dna
icsd	Usage of alternative materials	$G4INSTALL/examples/extended/medical/dna
chem1, chem2, chem3, chem4	Usage of Geant4-DNA chemistry	$G4INSTALL/examples/extended/medical/dna
wholeNuclearDNA	Cell nucleus	$G4INSTALL/examples/extended/medical/dna
pdb4dna	Interface to PDB database	$G4INSTALL/examples/extended/medical/dna
microbeam	3D cellular phantom	$G4INSTALL/examples/advanced
neuron	3D neural network	$G4INSTALL/examples/extended/medical/dna
TestEm12	DPK	$G4INSTALL/examples/extended
TestEm14	Extraction of cross sections	$G4INSTALL/examples/extended

Geant4-DNA website

http://geant4-dna.org



Twitter
@Geant4-DNA

Facebook
Geant4-DNA

Physics 5/7

MicroElec processes & models

New processes and models for microelectronics

- Purpose
  - extend Geant4 with processes and models for the simulation of particle-matter 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 « MicroElec » for microelectronics

New processes and models for microelectronics

- Processes and models

Physics Process	Process Class	Model Class	Low Energy Limit	High Energy Limit
Electrons				
Elastic scattering	G4MicroElecElastic	G4MicroElecElasticModel	5 eV (kill < 16.7 eV)	100 MeV
Ionization	G4MicroElecInelastic	G4MicroElecInelasticModel	16.7 eV	100 MeV
Protons and heavy ions				
Ionization	G4MicroElecInelastic	G4MicroElecInelasticModel	50 keV/u	10 GeV/u

- A dedicated advanced user example is available (« microelectronics »)
- 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

Physics 6/7

Monash U. models

Improved Compton model

- Monash U. (J. M. C. Brown) recently proposed to improve the accuracy of Livermore gamma models
  - Unpolarized Compton scattering off atomic bound electrons in the relativistic impulse approximation, derived from Livermore Compton model
  - Polarized version is also available
  - 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

Nucl. Instrum. Meth B 338 (2014) 77 – 88

Improved Compton model

Nucl. Instrum. Meth A 835 (2016) 186 – 225

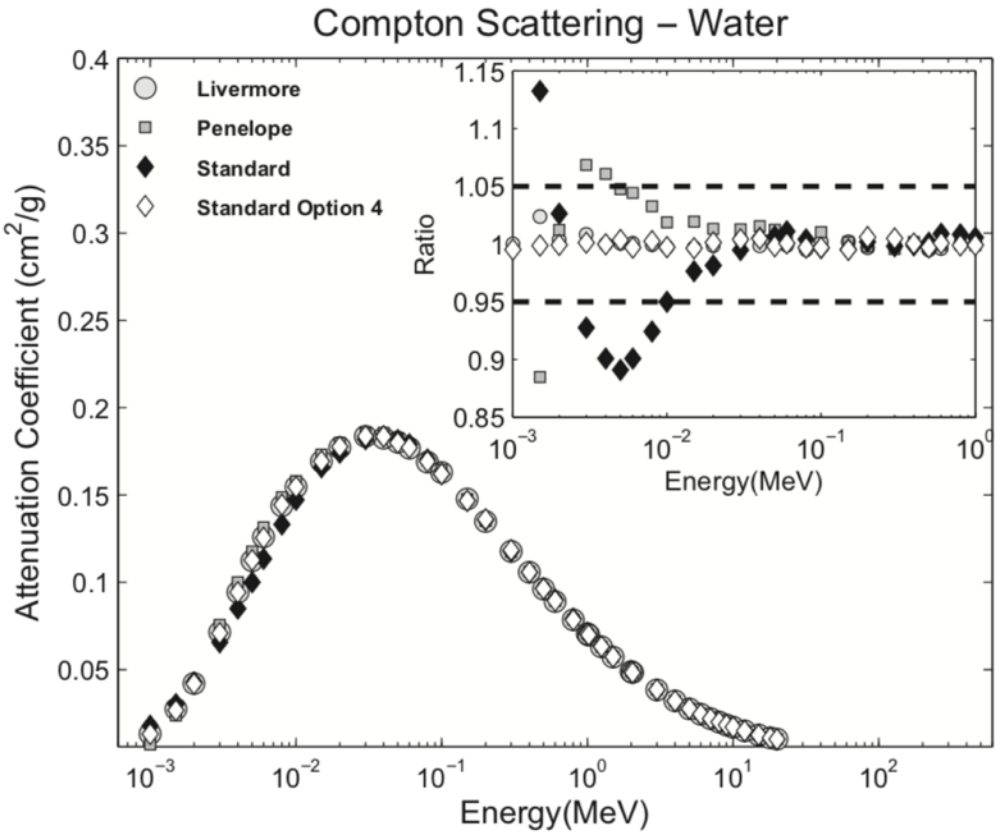


Fig. 11. Compton scattering attenuation coefficient, calculated for different GEANT4 models. `G4LowEPComptonModel` is used in the Option4 EM physics configuration. The inset shows the ratio of the coefficient calculated using each alternative GEANT4 electromagnetic physics list to the value from NIST XCOM [49]. The dashed lines correspond to a $\pm 5\%$ difference.

Improved Compton model

- Model class is G4LowEPComptonModel
  (or G4LowEPPolarizedComptonModel for the polarized version)

- You can register it easily to your Physics list

```
G4ComptonScattering* cs = new G4ComptonScattering;
cs->SetEmModel(new G4KleinNishinaModel(),1);
G4VEmModel* theLowEPComptonModel = new G4LowEPComptonModel();
theLowEPComptonModel->SetHighEnergyLimit(20*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

Physics 7/7

Atomic de-excitation

Atomic de-excitation effects

- 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
- Alternative set for fluorescence lines by Bearden et al. (1967)
  - X-Ray Data Booklet
- Thanks to a common interface (G4UAtomicDeexcitation), atomic de-excitation is compatible with both Standard & Low Energy Electromagnetic physics categories
  - See more in

NIMB 372 (2016) 91-101
X-Ray Spec. 40 (2011) 135-140

Including atomic effects

- Activation of atomic effects can be easily done directly via UI commands

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

- Boolean parameters in the "/process/em/" deexcitation commands correspond to activation of fluorescence, Auger, Auger cascade, and PIXE respectively

- 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

- To select Bearden et al. (1967) fluorescence lines instead of EADL, use (before /run/initialize):

```
/process/em/fluoBearden true
```

(or G4AtomicTransitionManager::Instance()->SetFluoDirectory("fluor_Bearden"); in your Physics list)

- As an example, look into $G4INSTALL/examples/extended/electromagnetic/TestEm5 and macro pixe.mac

Note on production thresholds

- 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 addition, independently, one can also fully deactivate production cuts for the simulation of all atomic deexcitation products
  /process/em/deexcitationIgnoreCut true

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

  /run/initialize

Changing shell cross section models

- The user has the possibility to select alternative ionisation shell cross section models for PIXE simulation

NIMB 358 (2015) 210-222
NIMB 316 (2013) 1-5
X-Ray Spec. 42 (2013) 177-182
X-Ray Spec. 40 (2011) 127-134
X-Ray Spec. 40 (2011) 135-140
NIMB 267 (2009) 37-44

- The following UI command is available for **ions**:

  /process/em/pixeXSmodel value

  where value is equal to Empirical or ECPSSR_FormFactor or ECPSSR_Analytical.

- 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, M shells in the range 0.1-100 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

- These UI commands should be put before the UI command:

  /run/initialize

How to implement a Physics list ?

Physics lists

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

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/examples/extended/electromagnetic/TestEm14

2. Much more safe: use the available low energy EM physics constructors, these are named as
   - G4EmLivermorePhysics
   - G4EmLivermorePolarizedPhysics
   - G4EmPenelopePhysics
   - G4EmDNAPhysics, G4EmDNAPhysics_optionX (X=1 to 6)
   - G4EmLowEPPhysics

How to use the already available physics constructors ?

- 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_lists/constructors/electromagnetic
- An implementation example of physics list that uses EM physics constructors is available in
  - $G4INSTALL/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/examples/extended/electromagnetic/TestEm7
- These constructors are added to the Geant4 reference physics lists (FTFP_BERT, …) via the method RegisterPhysics (G4VPhysicsConstructor*)
  - see $G4SRC/source/physics_list/lists subdirectory

Recent EM UI commands

- Transport of electrons
  - /process/em/lowestElectronEnergy X eV

    In all ionization processes which simulate energy loss along step, a lowest energy limit is introduced, which forces full energy deposition at a step independently on material. Its value may be changed via a new UI commands or through the interface class G4EmParameters.

    The default value is 100 eV, for Opt3, Opt4, Livermore, Penelope and LowEEP physics constructors for e+- (see source code)

- Configuration per G4Region for PAI, MicroElec, or Geant4-DNA models
  - Done on top of any EM physics constructor
  - Number of G4Regions is not limited
  - See example for PAI models configuration in TestEm8
  - UI commands
    - /process/em/AddPAIRegion proton MYREGION pai
    - /process/em/AddMicroElecRegion MYREGION
    - /process/em/AddDNARegion MYREGION opt0

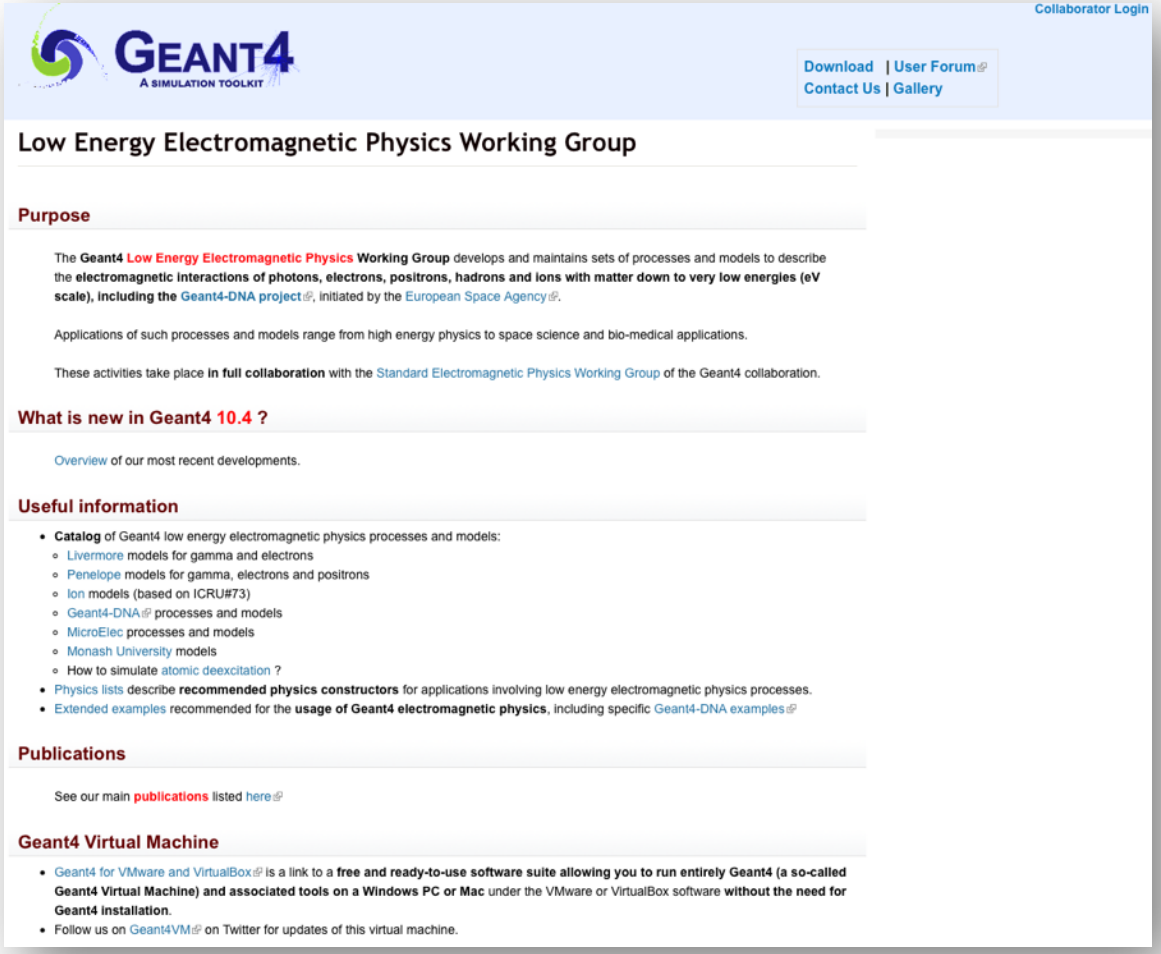
Documentation

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

Low Energy EM WG TWiki

Geant4 → Collaboration → Low Energy Electromagnetic Physics



Collaborator Login

GEANT4
A SIMULATION TOOLKIT

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Low Energy Electromagnetic Physics Working Group

Purpose

The **Geant4 Low Energy Electromagnetic Physics Working Group** develops and maintains sets of processes and models to describe the **electromagnetic interactions of photons, electrons, positrons, hadrons and ions with matter down to very low energies (eV scale), including the Geant4-DNA project**, initiated by the European Space Agency.

Applications of such processes and models range from high energy physics to space science and bio-medical applications.

These activities take place **in full collaboration** with the Standard Electromagnetic Physics Working Group of the Geant4 collaboration.

What is new in Geant4 10.4 ?

Overview of our most recent developments.

Useful information

- **Catalog** of Geant4 low energy electromagnetic physics processes and models:
  - Livermore models for gamma and electrons
  - Penelope models for gamma, electrons and positrons
  - Ion models (based on ICRU#73)
  - Geant4-DNA processes and models
  - MicroElec processes and models
  - Monash University models
  - How to simulate atomic deexcitation ?
- Physics lists describe **recommended physics constructors** for applications involving low energy electromagnetic physics processes.
- Extended examples recommended for the **usage of Geant4 electromagnetic physics**, including specific Geant4-DNA examples

Publications

See our main **publications** listed here

Geant4 Virtual Machine

- Geant4 for VMware and VirtualBox is a link to a **free and ready-to-use software suite allowing you to run entirely Geant4 (a so-called Geant4 Virtual Machine) and associated tools on a Windows PC or Mac** under the VMware or VirtualBox software **without the need for Geant4 installation**.
- Follow us on Geant4VM on Twitter for updates of this virtual machine.

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)
  - are interested in specific low energy applications (Geant4-DNA, MicroElec)

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