

# Electromagnetic Physics II

## Low Energy Models

Geant4 Tutorial at Chalk River

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using slides of Sebastien Incerti (CNRS, Bordeaux)

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# Outline

- Context
- Physics Processes and 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 processes and models
- Implementing a physics list with low energy EM settings
- 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 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]

# 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 : « G4**ProcessName** »
  - Eg. : « G4**ComptonScattering** » for photon Compton scattering
- A physical process can be simulated according to **several models**, each model being described by a [MODEL CLASS](#)
  - Naming scheme : « G4**ModelNameProcessNameModel** »
  - Eg. : « G4**LivermoreComptonModel** » 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

- 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 fluorescence lines
  - **EEDL** : Evaluated **Electrons** Data Library
  - **EPDL97** : Evaluated **Photons** Data Library
  - **EPICS2014** for photoelectric effect
  - 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- and gamma
- 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)

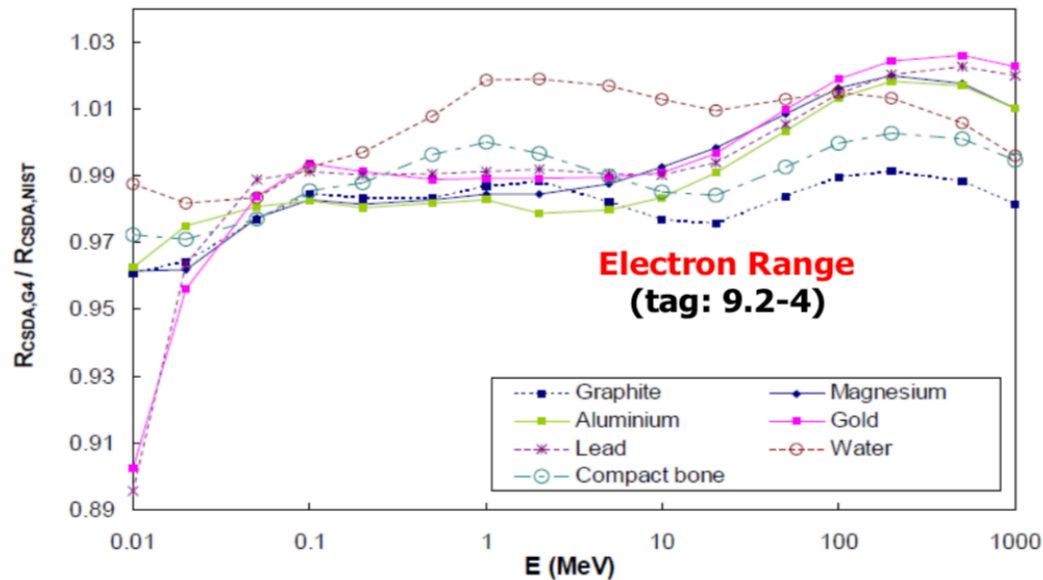
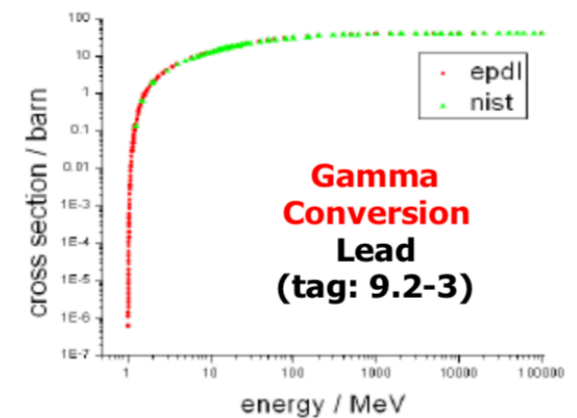
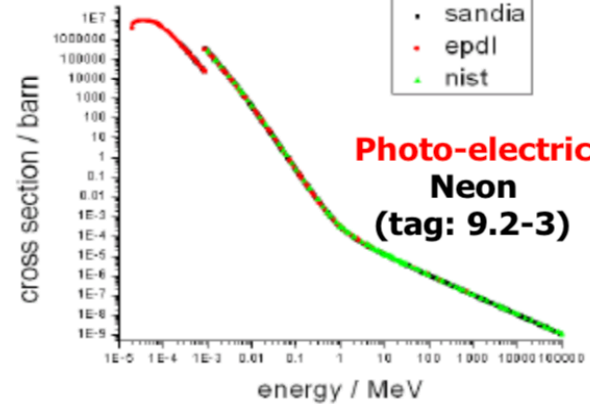
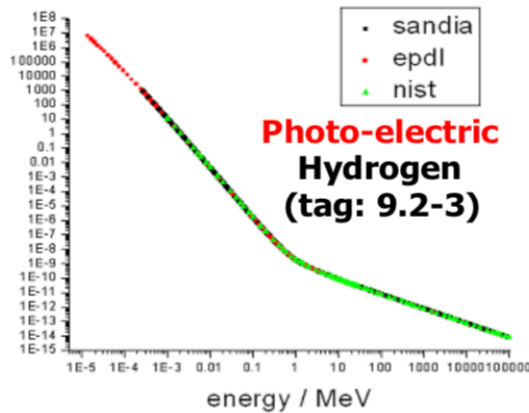
See <http://www-nds.iaea.org/epdl97>

# Available Livermore **models**

Physics Process	Process Class	Model Class	Low Energy Limit
<b>Gammas</b>			
Compton	G4ComptonScattering	G4LivermoreComptonModel	eV
<b>Polarized</b> Compton	G4ComptonScattering	G4LivermorePolarizedComptonModel	eV
Rayleigh	G4RayleighScattering	G4LivermoreRayleighModel	eV
<b>Polarized</b> Rayleigh	G4RayleighScattering	G4LivermorePolarizedRayleighModel	250 eV (kill)
Conversion	G4GammaConversion	G4LivermoreGammaConversionModel	1.022 MeV
<b>Polarized</b> Conversion	G4GammaConversion	G4LivermorePolarizedGammaConversionModel	1.022 MeV
Photo-electric	G4PhotoElectricEffect	G4LivermorePhotoElectricModel	eV
<b>Polarized</b> Photo-electric	G4PhotoElectricEffect	G4LivermorePolarizedPhotoElectricModel	eV
<b>Electrons</b>			
Ionization	G4elonisation	G4LivermorelonisationModel	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)

# 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 developed 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
<b>Gammas</b>				
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
<b>Electrons/Positrons</b>				
Ionization	G4elionisation	G4PenelopelionisationModel	eV	1 GeV
Bremsstrahlung	G4eBremsstrahlung	G4PenelopeBremsstrahlungModel	eV	1 GeV
<b>Positrons</b>				
Annihilation	G4eplusAnnihilation	G4PenelopeAnnihilationModel	eV	1 GeV

# 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

- ▣  $T < T_{\text{Low}}$ : Free electron gas model
- ▣  $T_{\text{Low}} \leq T \leq T_{\text{High}}$ : [parameterization \(ICRU'73\)](#) recommendation
- ▣  $T > T_{\text{High}}$ : [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
  - $T_{\text{High}} = 1 \text{ GeV/nucleon}$
  - $T_{\text{Low}} = 0.025 \text{ MeV/nucleon}$  (lower boundary of ICRU'73 tables)



# How to use the ion model ?

- Model name: `G4IonParametrisedLossModel`
- Only applicable to ions with  $Z \geq 3$
- Already included in Geant4 EM physics constructors
  - Low Energy EM: `G4EmLivermorePhysics`, `G4EmLivermorePolarizedPhysics`, `G4EmPenelopePhysics`, `G4EmLowEPPPhysics`
  - 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 `G4BraggIonModel` (alpha), and `G4BetheBlochModel` with the `G4hIonisation` and `G4IonIonisation` processes

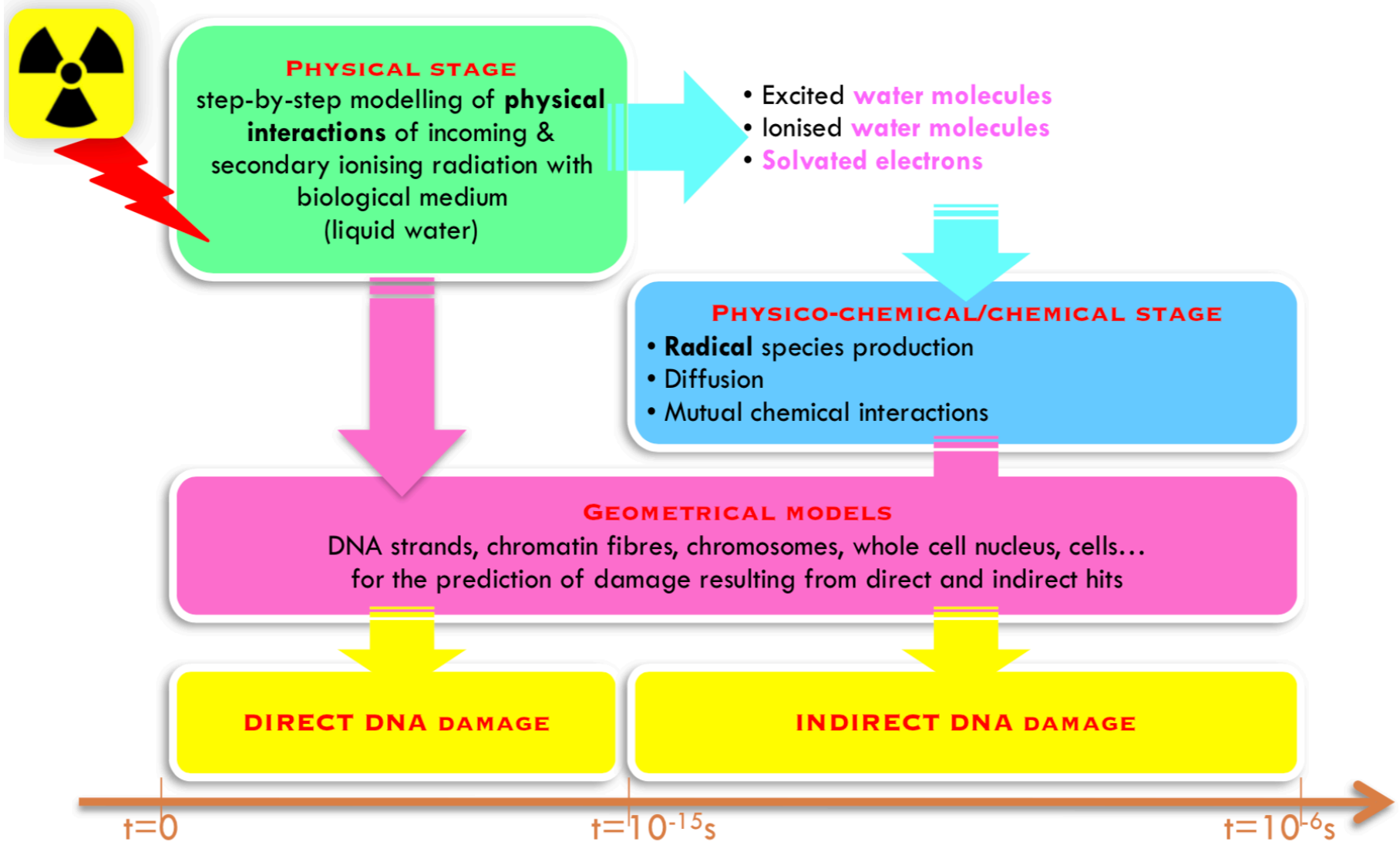
# ICRU 73 data tables

- The ion model
  - uses ICRU'73 stopping powers, if the 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

# 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 radiation effects to DNA in cells
- A fully 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 ?



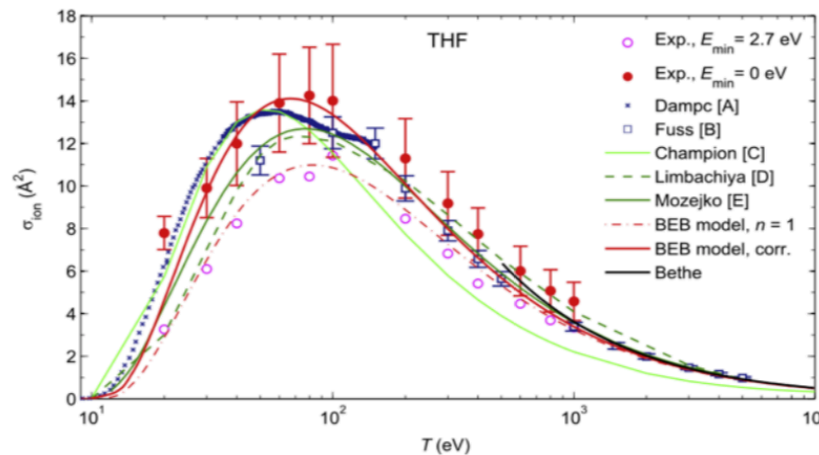
# Geant4 for radiobiology

- 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

# 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**



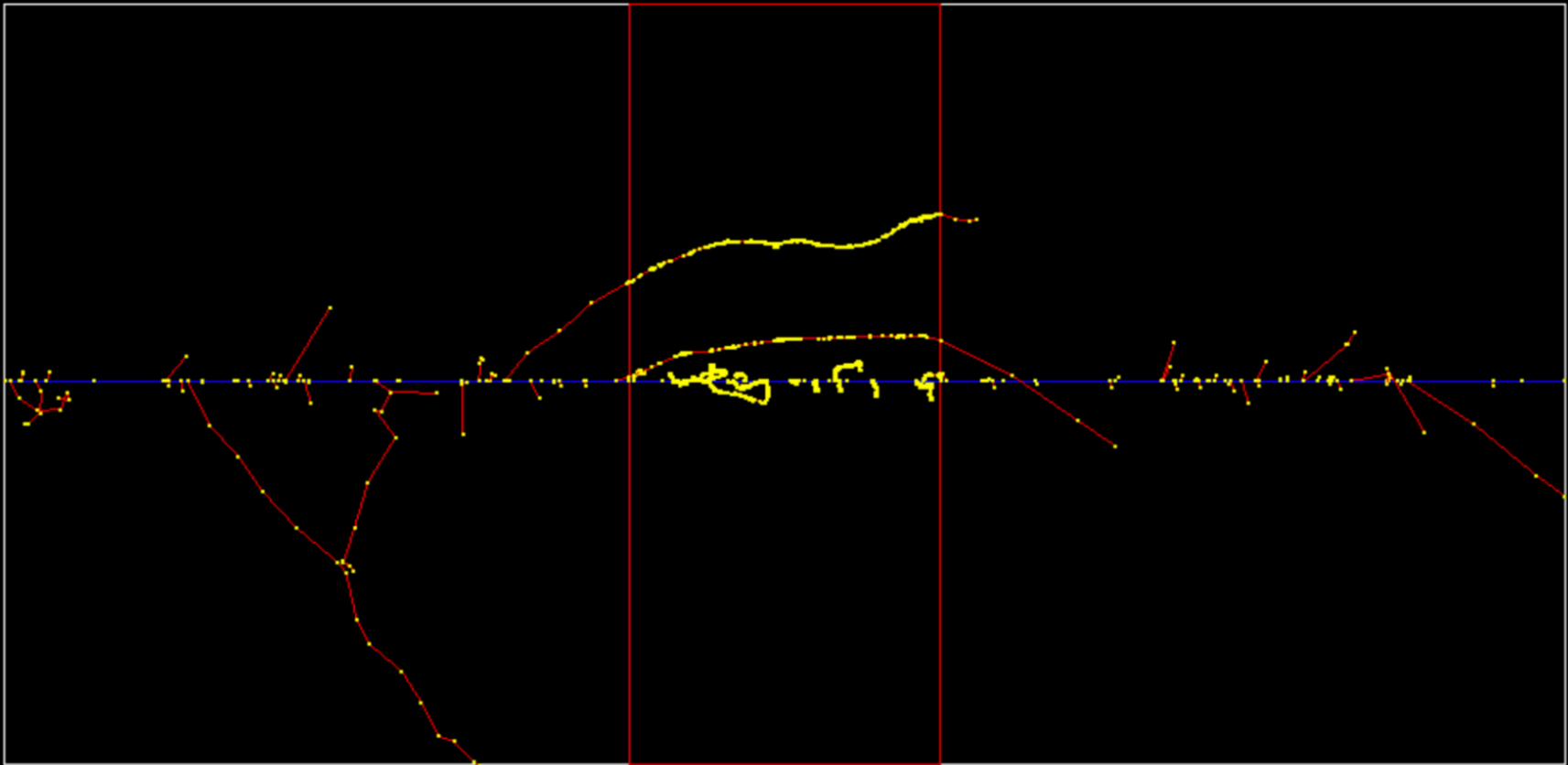
G4 10.2

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

Geant4 EM standard physics

Geant4-DNA

Geant4 EM standard physics






```
/gps/particle ion  
/gps/ion 6 12 6  
/gps/energy 20 MeV
```

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 <a href="#">G4LowEWentzelVIModel</a>
 <b>G4EmDNAPhysics_option2</b>	Same as G4EmDNAPhysics but <b>faster</b> (usage of CDCS for ionisation processes)
G4EmDNAPhysics_option3	Same as G4EmDNAPhysics (historical)
 <b>G4EmDNAPhysics_option4</b>	<a href="#">Electron ionisation and excitation models</a> by Ioannina team
G4EmDNAPhysics_option5 (beta)	Same but <b>faster</b> (usage of CDCS)
 <b>G4EmDNAPhysics_option6</b>	<a href="#">CPA100</a> models

All are located in

[\\$G4INSTALL/source/physics\\_lists/constructors/electromagnetic](#)

$t = 10^{-15} \text{s}$

$t = 10^{-12} \text{s}$

# Physico-chemical stage

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

Electronic state	Dissociation channels	Fraction (%)
All <b>single ionization</b> states	$\text{H}_3\text{O}^+ + \cdot\text{OH}$	100
<b>Excitation</b> state A1B1: (1b1) $\rightarrow$ (4a1/3s)	$\cdot\text{OH} + \text{H}^\bullet$	65
	$\text{H}_2\text{O} + \Delta\text{E}$	35
<b>Excitation</b> state B1A1: (3a1) $\rightarrow$ (4a1/3s)	$\text{H}_3\text{O}^+ + \cdot\text{OH} + e^-_{\text{aq}} (\text{A1})$	55
	$\cdot\text{OH} + \cdot\text{OH} + \text{H}_2$	15
	$\text{H}_2\text{O} + \Delta\text{E}$	30
<b>Excitation</b> state: Rydberg, diffusion bands	$\text{H}_3\text{O}^+ + \cdot\text{OH} + e^-_{\text{aq}} (\text{A1})$	50
	$\text{H}_2\text{O} + \Delta\text{E}$	50
Dissociative attachment	$\cdot\text{OH} + \text{OH}^- + \text{H}_2$	100

- Products thermalize down to their energy of diffusion at equilibrium

$t=10^{-15}\text{s}$  $t=10^{-12}\text{s}$  $t=10^{-6}\text{s}$ 

# Chemical stage

Species	Diffusion coefficient D ( $10^{-9}\text{ m}^2\text{ s}^{-1}$ )
$\text{H}_3\text{O}^+$	9.0
$\text{H}\cdot$	7.0
$\text{OH}\cdot$	5.0
$e^-_{\text{aq}}$	4.9
$\text{H}_2$	5.0
$\cdot\text{OH}$	2.8
$\text{H}_2\text{O}_2$	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.](#)

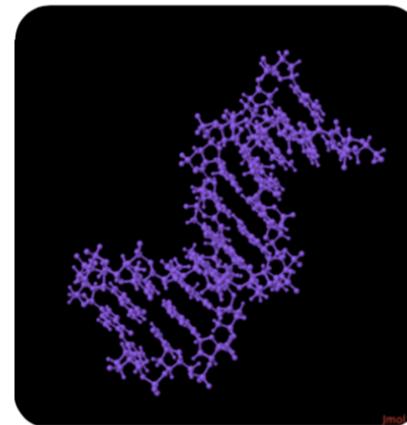
Reaction	Reaction rate ( $10^7\text{ m}^3\text{ mol}^{-1}\text{ s}^{-1}$ )
$\text{H}_3\text{O}^+ + \text{OH}\cdot \rightarrow 2\text{H}_2\text{O}$	14.3
$\cdot\text{OH} + e^-_{\text{aq}} \rightarrow \text{OH}\cdot$	2.95
$\text{H}\cdot + e^-_{\text{aq}} + \text{H}_2\text{O} \rightarrow \text{OH}\cdot + \text{H}_2$	2.65
$\text{H}_3\text{O}^+ + e^-_{\text{aq}} \rightarrow \text{H}\cdot + \text{H}_2\text{O}$	2.11
$\text{H}\cdot + \cdot\text{OH} \rightarrow \text{H}_2\text{O}$	1.44
$\text{H}_2\text{O}_2 + e^-_{\text{aq}} \rightarrow \text{OH}\cdot + \cdot\text{OH}$	1.41
$\text{H}\cdot + \text{H}\cdot \rightarrow \text{H}_2$	1.20
$e^-_{\text{aq}} + e^-_{\text{aq}} + 2\text{H}_2\text{O} \rightarrow 2\text{OH}\cdot + \text{H}_2$	0.50
$\cdot\text{OH} + \cdot\text{OH} \rightarrow \text{H}_2\text{O}_2$	0.44

# A new interface to describe geometries in Geant4-DNA

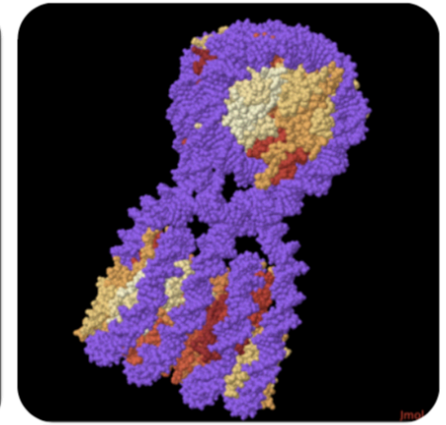
- **PDB : Protein Data Bank**  
<http://www.rcsb.org/pdb/>
  - ▣ 3D structure of molecules
  - ▣ Proteins
  - ▣ Nucleic acids
- Description of DNA molecules
  - ▣ **1FZX.pdb**
    - Dodecamer
    - 12 DNA base pairs
    - (2,8 x 2,3 x 4,01 nm<sup>3</sup>)
  - ▣ **1ZBB.pdb**
    - Tetranucleosome
   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

```

HEADER   STRUCTURAL PROTEIN/DNA           08-APR-05  1ZBB
TITLE    STRUCTURE OF THE 4_601_167 TETRANUCLEOSOME
...
ATOM     1  O5'  DA I  1    70.094  16.969 123.433  0.50238.00  O
ATOM     2  C5'  DA I  1    70.682  18.216 123.054  0.50238.00  C
ATOM     3  C4'  DA I  1    69.655  19.289 122.776  0.50238.00  C
...
TER      14223    DT J 347
...
HELIX    1  1 GLY A  44 SER A  57  1                14
HELIX    2  2 ARG A  63 ASP A  77  1                15
...
SHEET    1  A 2 ARG A  83 PHE A  84  0
SHEET    2  A 2 THR B  80 VAL B  81  1 O VAL B  81  N ARG A  83
  
```



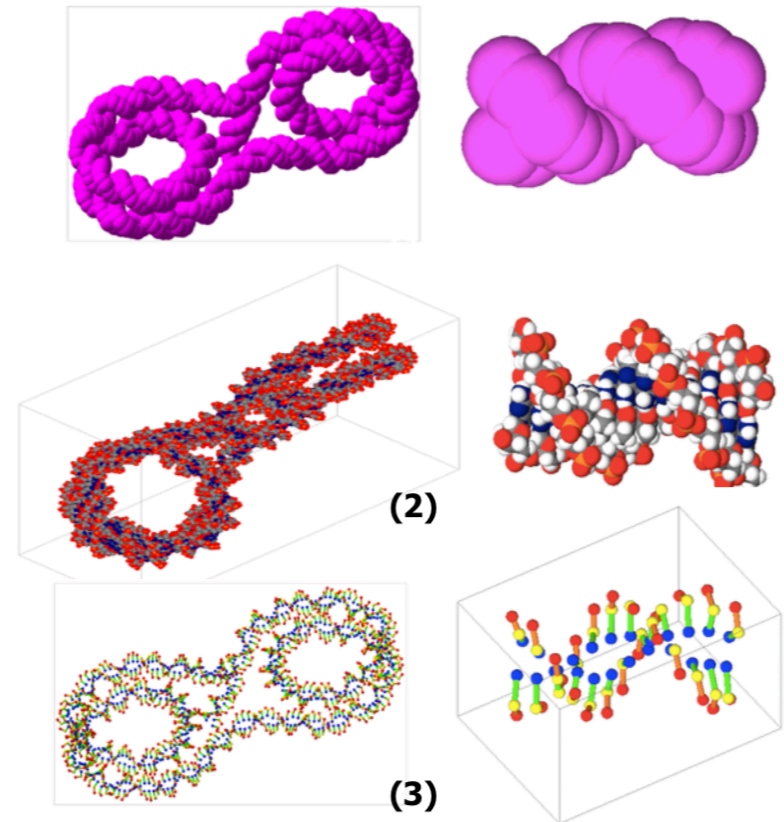
**1FZX.pdb**



**1ZBB.pdb**

# « **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)



# Geant4-DNA **examples included** in Geant4

Example code name	Purpose	Location
dnaphysics	<ul style="list-style-type: none"> <li>Usage of Geant4-DNA Physics processes</li> <li>variable density</li> </ul>	\$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
power	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

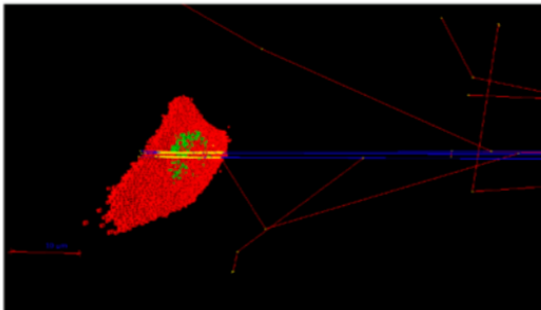
<http://geant4-dna.org>

## GEANT4-DNA : EXTENDING THE GEANT4 MONTE CARLO SIMULATION TOOLKIT FOR RADIOBIOLOGY

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

The **Geant4** general purpose particle-matter Monte Carlo simulation toolkit is being extended with processes for the **modeling of early biological damage induced by ionising radiation at the DNA scale**. Such developments are on-going in the framework of the Geant4-DNA project - originally initiated by the **European Space Agency/ESTEC** - and are undertaken by an international **collaboration**.

Once published, all our developments are freely accessible in **full open access** through the **Geant4 toolkit** or through our freely accessible **Geant4 Virtual Machine**.



CENBG microbeam irradiation of a keratinocyte (HaCaT) with alpha particles  
see the « [microbeam](#) » Geant4 advanced example -  
- movie courtesy of L. Garnier (CNRS) -

### Recent posts

**October 29-31, 2018:** [Third Geant4 International User Conference at the Physics-Medicine-Biology frontier - Bordeaux, France,](#)

**March 19, 2018:** our Virtual Machine has been updated with Geant4 10.4+P01, see [link](#)

**January 28, 2018:** Geant4 10.4+P01 has been released, see [link](#)

### Tweets by @geant4\_dna

**Geant4-DNA** @geant4\_dna  
Geant4 2018 Third Geant4 International User Conference: abstract submission deadline extended till June 30th, 2018 - See [geant4.in2p3.fr/2018/index.html](#)



**Twitter**  
**@Geant4-DNA**

**Facebook**  
**Geant4-DNA**



# 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
<b>Electrons</b>				
Elastic scattering	G4MicroElecElastic	G4MicroElecElasticModel	5 eV (kill < 16.7 eV)	100 MeV
Ionization	G4MicroElecInelastic	G4MicroElecInelasticModel	16.7 eV	100 MeV
<b>Protons and heavy ions</b>				
Ionization	G4MicroElecInelastic	G4MicroElecInelasticModel	50 keV	10 GeV

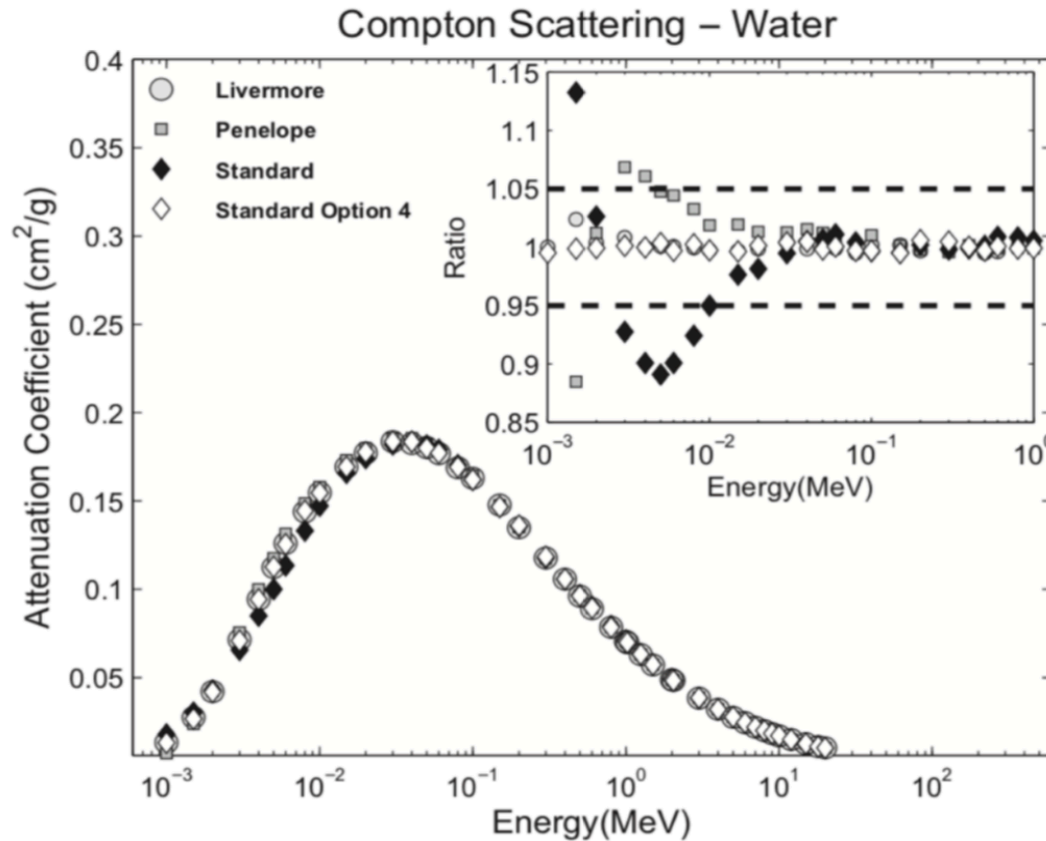
- A dedicated advanced user example is available (« **microelectronics** »)
- Validation range
  - ▣ Electrons: 50 eV – 50 keV
  - ▣ Protons: 50 keV – 23 MeV

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

# 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) developed from Ribberfor's Compton scattering framework
  - More accurate 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



**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`

# 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-: initial 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 1.0 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`





# 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 `/example/extended/electromagnetic/TestEm8`

### □ UI commands

- `/process/em/AddPAIRegion proton MYREGION pai`

- `/process/em/AddMicroElecRegion MYREGION`

- `/process/em/AddDNARegion MYREGION opt0`



# 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

Geant4 → Collaboration → Low Energy Electromagnetic Physics



The screenshot shows the TWiki page for the Geant4 Low Energy Electromagnetic Physics Working Group. The page has a light blue header with the Geant4 logo (a stylized 'G' with a blue and green swirl) and the text 'GEANT4 A SIMULATION TOOLKIT'. To the right of the logo are links for 'Download', 'User Forum', 'Contact Us', and 'Gallery'. In the top right corner, there is a 'Collaborator Login' link. The main content area is titled 'Low Energy Electromagnetic Physics Working Group' and is divided into several sections: 'Purpose', 'What is new in Geant4 10.4?', 'Useful information', 'Publications', and 'Geant4 Virtual Machine'. Each section contains descriptive text and links to related resources.

**GEANT4**  
A SIMULATION TOOLKIT

Collaborator Login

[Download](#) | [User Forum](#)  
[Contact Us](#) | [Gallery](#)

## 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