Geant4 11.4.3

Electromagnetic Physics II
Low Energy, DNA and Microelectronics Models

Dennis Wright

Geant4 Tutorial at Jefferson Lab

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based on slides of Sebastien Incerti (CNRS, Bordeaux)

Outline

- Purpose and Design
- Low Energy 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
- Implementing a physics list with low energy EM settings

Purpose

- Provide Geant4 electromagnetic interactions
  - for e^-, e^+, γ, $ions$
  - down to very low energies (sub-keV scale)

- Applications
  - space science
  - medical physics
  - underground physics (dark matter, neutrino experiments, …)
  - micro- and nano-dosimetry (radiobiology, micro-electronics)
  - …
- Physics model choices include
  - Livermore: e^-, γ (250 eV - ~GeV)
  - Penelope: e^-, e^+, γ (100 eV - 1 GeV)
  - Geant4-DNA (eV - few 100s MeV)
  - MicroElec for silicon (eV - 10 GeV)

Software Design

- Same as that used by Geant4 standard electromagnetic
  - applies to all low energy EM classes
  - allows coherent approach to the modeling of all EM interactions

- As in standard EM, process classes are named:
  - G4ProcessName
  - for example, G4ComptonScattering for photon Compton scattering

- Model class names include the process name
  - G4ModelNameProcessNameModel
  - e.g., G4LivermoreCompton Model for Livermore Compton model
  - within a process, can replace one model for another, or have more than one model

- Model classes provide
  - process total cross section and stopping power
  - process final state (kinematics, secondaries)

- All required data files located in $G4LEDATA directory

Livermore Models

Livermore Models (e^- and γ)

- Based on evaluated data tables from Livermore data library
  - EADL: Evaluated Atomic Data Library
  - EEDL: Evaluated Electron Data Library
  - EPDL97: Evaluated Photon Data Library
  - EPICS2014 for photoelectric effect
  - Mixture of experiments and theories
  - Scofield binding energies

- Data tables are interpolated to compute
  - total cross sections for processes
  - shell integrated cross sections (photelectric, ionization)
  - energy spectra

- Recommended validity range: 250 eV - 1 GeV
  - can be used down to 100 eV with reduced accuracy
  - 10 eV is technical lower limit

- For all elements Z = 1 to Z = 100 de-excitation classes provide
  - atomic effects (fluorescence, Auger) included
  - atomic relaxation for Z > 5 (EADL transition data)

Polarized Livermore Models

- Detailed kinematics of polarized photon interactions
- Based on Livermore database
- Applications
  - Design of space missions for detection of polarized photons
- Naming convention: G4LivermorePolarizedXXXModel
  - Example: G4LivermorePolarizedComptonModel
- See following publications
  - Photoelectric: Nucl. Instr. Meth. A 566 (2006) 590-597
  - Compton and Rayleigh: Nucl. Instr. Meth. A 512 (2003) 619-630
  - Pair production: Nucl. Instr. Meth. A 452 (2000) 298-305

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	G4LivermorePolarizedGammaConversion Model	1.022 MeV
Photo-electric	G4PhotoElectricEffect	G4LivermorePhotoElectricModel	eV
Polarized Photo-electric	G4PhotoElectricEffect	G4LivermorePolarizedPhotoElectricModel	eV
Electrons			
Ionization	G4elonisation	G4LivermoreIonisationModel	eV
Bremsstrahlung	G4eBremsstrahlung	G4LivermoreBremsstrahlungModel	10 eV

Penelope Models

Penelope Models (e^-, e^+ and γ)

- Geant4 includes low-energy models from the Penelope (PENetration and Energy LOss of Positrons and Electrons) Monte Carlo code
  - Nucl. Intr. Meth. B 350 (2015) 41-48
  - Nucl. Intr. Meth. B 207 (2003) 107-123

- Physics models
  - developed by F. Salvat et al.
  - special attention to low energy description of atomic effects, fluorescence, Doppler broadening

- Mixed approach: analytical, parameterized and database-driven

- Recommended energy range: 100 eV - 1 GeV

- Includes treatment of positrons (not handled by Livermore)

- 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

Ion Energy Loss Model

Energy Loss for Ions

- Model describes energy loss for ions due to interactions with atomic electrons of target atoms
  - Z > 2
- Model computes
  - cross sections for discrete production of δ rays
    - δ rays only produced above secondary production threshold → determines discrete energy loss of ions
  - restricted electronic stopping powers
    - that is, continuous energy loss as ions slow down
    - below production threshold
- Applications
  - medical
  - space
- See: Nucl. Instr. Meth. B 268 (2010) 2343-2354

Ion Energy Loss Model Details

- Different restricted stopping power calculations for each of three energy regions:
  - $T < T_{low}$: free electron gas model
  - $T_{low} \leq T \leq T_{high}$: ICRU73 parameterization
  - $T > T_{high}$: Bethe-Bloch formula (using effective charge and higher order corrections)

- ICRU73 parameterization
  - Energy limits
    - $T_{high} =$ 1 GeV/nucleon
    - $T_{low} =$ 0.025 MeV/nucleon
  - Large number of ion-material combinations
    - Li - Ar, Fe
    - 25 elemental materials, 31 compounds
  - stopping powers based on binary theory, effective charge approach for Fe
  - special case: water
    - revised ICRU73 tables by P. Sigmund
    - Mean ionization potential is 78 eV

Using the Model

- Model name: G4IonParametrisedLossModel
- Applicable only 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
- To be used with G4ionIonisation process (from standard EM)
  - not activated by default when using this process
  - invoke this model by using the SetEmModel method of the G4ionIonisation process
- Restricted to one Geant4 particle type: G4GenericIon
  - G4ionIonisation also applicable to α particles (G4Alpha) and ^3He ions (G4He3), but G4IonParametrisedLossModel must not be activated for these ions
  - For $Z < 3$ use G4BraggModel (protons) or G4 G4BraggIonModel (α) and G4BetheBlochModel with the G4hIonisation and G4ionIonisation processes

ICRU 73 Data Tables

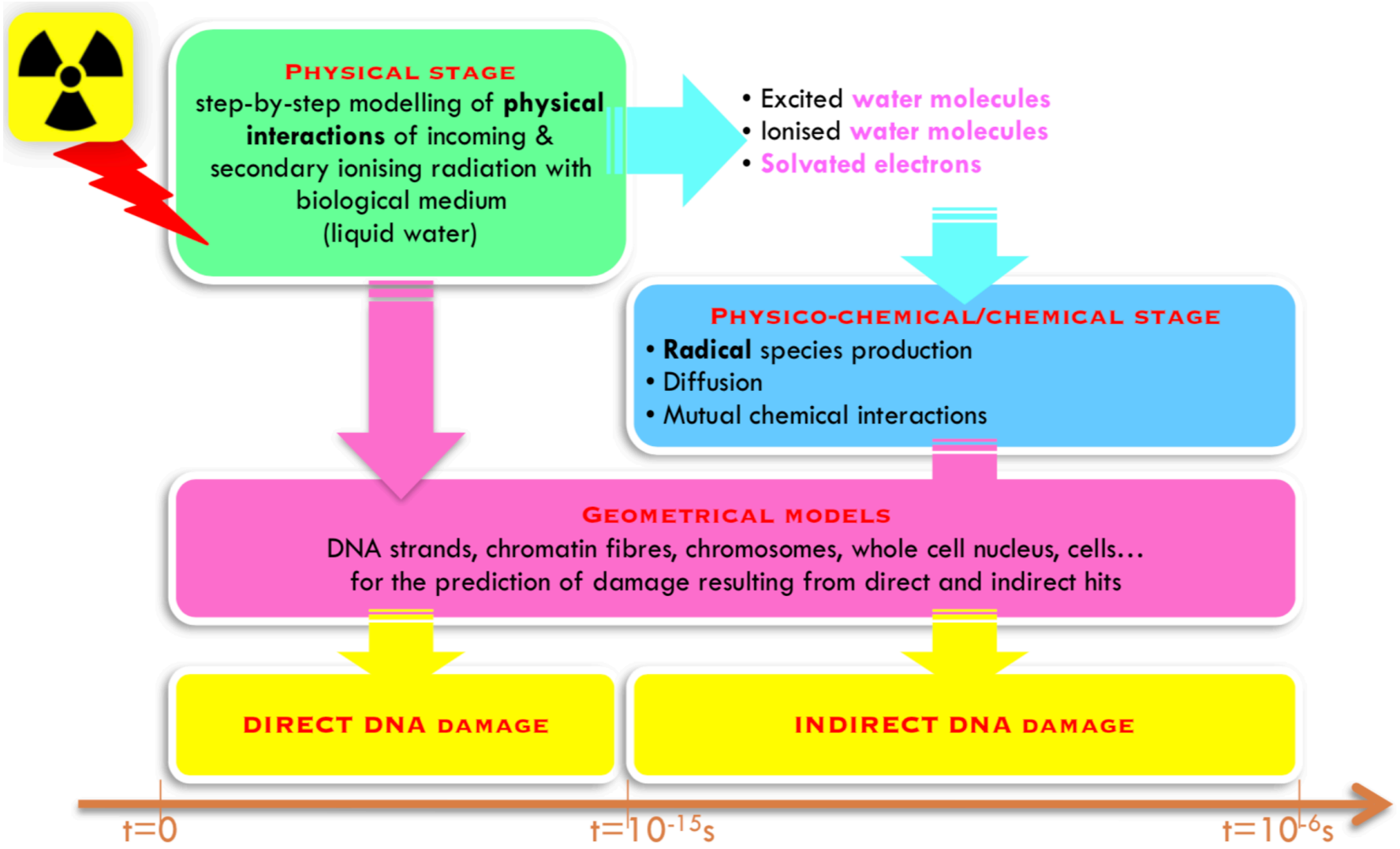
- Ion model uses
  - ICRU73 stopping powers if corresponding ion-material combinations are covered in the ICRU 73 report
  - otherwise a Bethe-Bloch formalism is applied
- Elemental materials are matched to the corresponding ICRU73 stopping powers by means of the atomic number of the material
  - material name may be arbitrary in this case
- For compounds, ICRU73 stopping powers used if material name coincides with the name of Geant4 NIST materials
  - G4_WATER, for example
- A list of applicable materials is given in the ICRU 73 report
- All required data files located in $G4LEDATA directory

Microdosimetry in Radiobiology

Geant4-DNA

- Initiated in 2001 by Petteri Nieminen (European Space Agency/ ESTEC)
- To adapt general purpose Geant4 toolkit for the simulation of the interaction of radiation with biological systems at the cellular level
  - early direct and non-direct radiation effects on DNA in cells
- Cross-disciplinary effort of physicists, chemists and biophysicists
- Applications
  - radiobiology, radiotherapy, hadron therapy
    - early prediction of DNA strand breaks due to ionizing radiation
  - radio-protection for human space exploration

How Can Geant4-DNA Simulate Early DNA Damage?



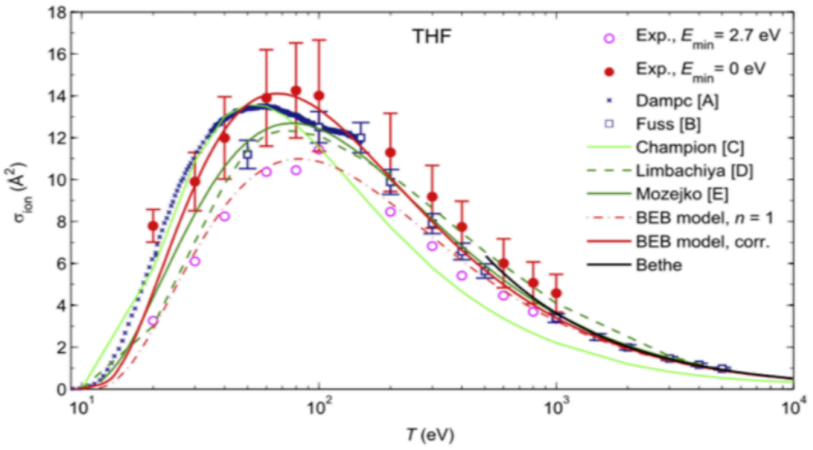
Geant4 for Radiobiology

- Models available for description of physical processes involving $e^-, p, H, He, He^+, He^{2+}, Li, Be, B, C, N, O, Si, Fe$
- Processes included: elastic scattering, excitation(electronic + vibrations), ionization, charge exchange, molecular attachment
- These models valid for liquid water medium and a few biological materials
- Models available in Geant4-DNA
  - published in literature
  - may be purely analytical or use interpolated cross section data
- They are all discrete processes
- Can be combined with standard and low energy EM
- Many extended examples in examples/extended/medical/dna

Other Materials

- Geant4-DNA can handle a few materials other than water
- Cross sections for biological materials which apply to Geant4-DNA:
  - Tetrahydrofuran (THF), trimethylphosphate (TMP), pyrimidine (PY) and purine (PU)
  - serve as proxies for deoxyribose and phosphate groups in DNA backbone and pyrimidine nucleobases, respectively
- For the following incident particles
  - Electrons (12 eV - 1 keV)
  - Protons (70 keV - 10 MeV)

Eg. total electron ionisation cross sections in THF



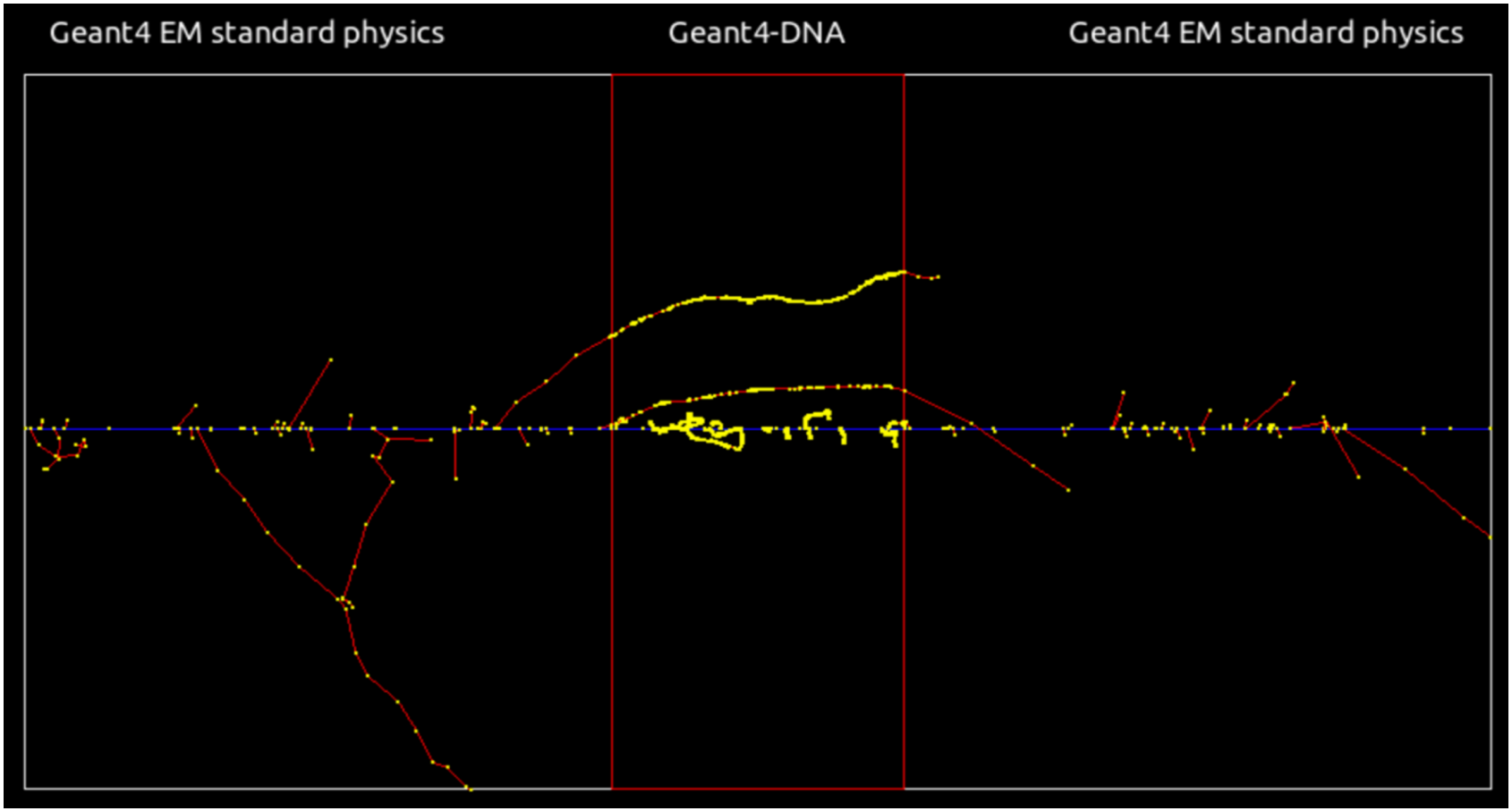
Rad. Phys. Chem. 130 (2017) 459–479

Multi-scale Combination of EM Processes

- Unified software design of EM code allows combination of Geant4-DNA processes and models with other Geant4 EM physics, such as
  - Photon processes and models
    - Photoelectric, Compton, Rayleigh, pair production
    - Livermore (EPDL 97)
  - Geant4 alternative EM processes and models for charged particles
    - ionization, bremsstrahlung, etc.
    - e^-, e^+, ions, etc.
  - Geant4 atomic de-excitation (fluorescence, Auger emission), including cascades
    - EADL97, Bearden
  - Also Geant4 hadronic physics

Mixed Physics Lists in Geometrical Regions

- Microdosimetry extended example: 20 MeV fully ionized C in water



Geant4-DNA Physics Constructors

- Three 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 constructors located in $G4INSTALL/source/physics_lists/constructors/electromagnetic

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 (10^{-12} to 10^{-6} s)

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

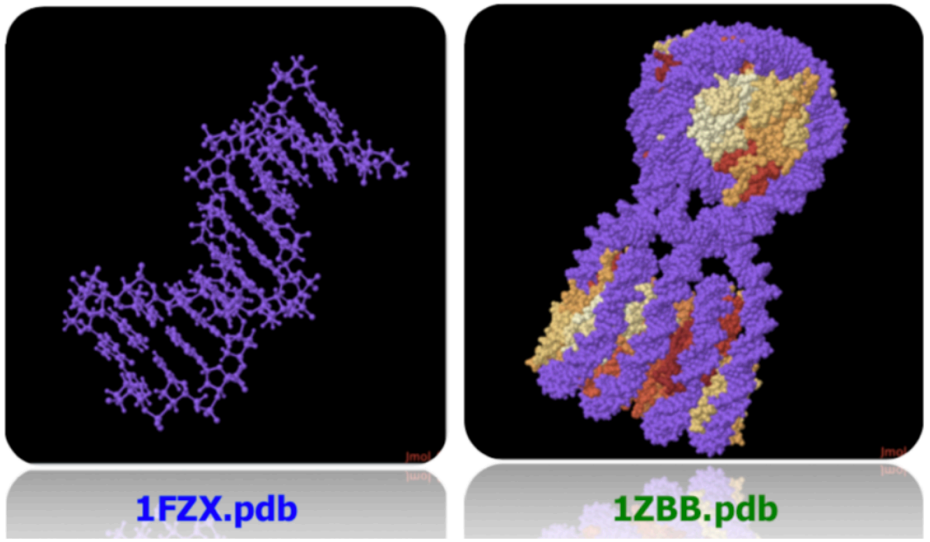
We followed the set of parameters published by the authors of the PARTRAC software (Kreipl et al., REB 2009). However, these parameters can be modified by the user.

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

PDB: An Interface to Describe Geometries in Geant4-DNA

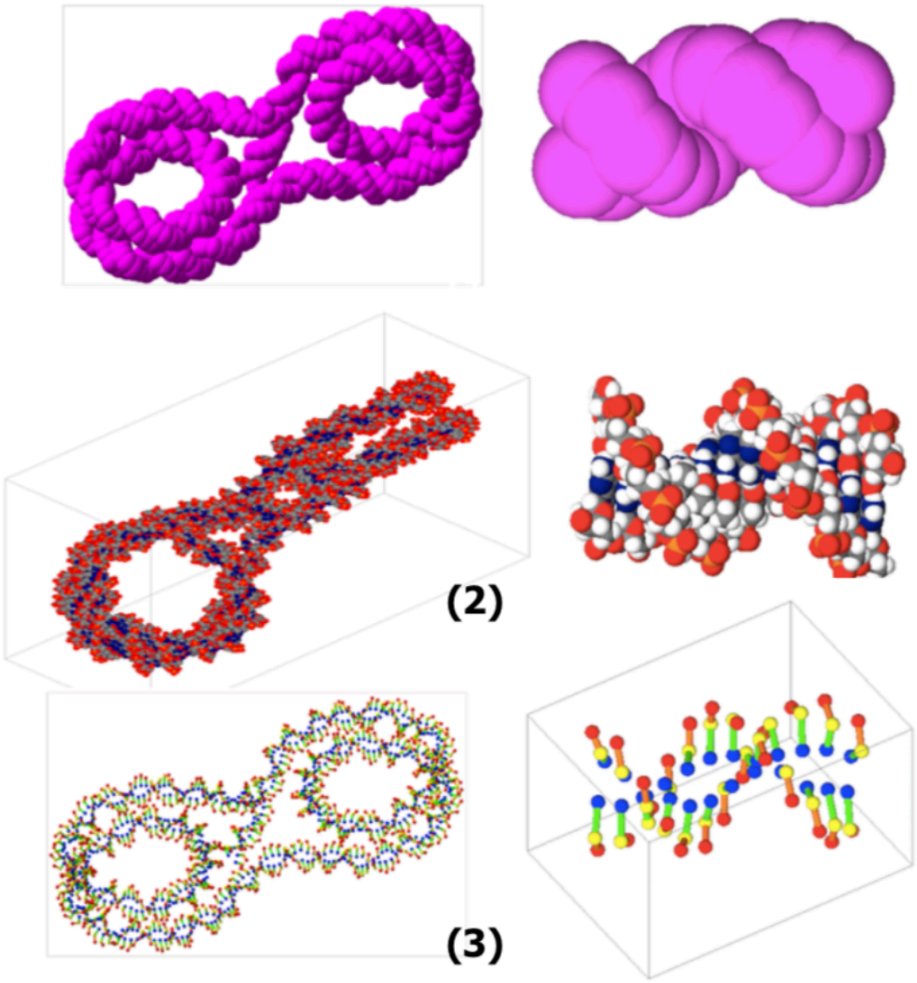
- PDB: Protein Data Bank (http://www.rcsb.org/pdb)
  - 3-D structure of molecules, proteins, nucleic acids
- Description of DNA molecules
  - 1FZX.pdb
    - dodecamer
    - 12 DNA base pairs
    - 2.8 x 2.3 x 4.01 nm^3
  - 1ZBB.pdb
    - tetranucleosome
    - two nucleosomes: 347 pairs of bases
    - 9.5 x 15.0 x 25.1 nm^3

```
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
```



pdb4dna Extended Example

- C++ library
  - read PDB files
  - build bounding boxes from atom coordinates
  - search for closest atom to given point
  - geometry and visualization
    - barycenter of of nucleotides
    - atomistic
    - barycenter of nucleotide components
- Geant4 DNA example
  - water box surrounding the molecule
  - output results in a ROOT file, containing for each event:
    - energy deposit in bounding boxes
    - number of single strand breaks
    - number of double strand breaks



Geant-DNA Extended Examples

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

Microelectronics

Processes and Models for Microelectronics

- Purpose:
  - Extend Geant4 to particle-matter interactions in highly integrated microelectronic components
  - For electrons, protons, heavy ions in silicon
- Same step-by-step approach as Geant4-DNA
  - Similarly based on complex dielectric function theory
- Applicable to many NIST materials (G4_Si, G4_Ge, G4_Ni, …)
- Names
  - Processes: MicroElecProcessName
  - Models: MicroElecProcessNameModel

Processes and Models for Microelectronics

Process	Class	Model Class	Low Energy Limit	High Energy Limit
Elastic scattering	G4MicroElecElastic	G4MicroElecElasticModel	5 eV	100 MeV
Ionization	G4MicroElecInelastic	G4MicroElecInelastic Model	16.7 eV	100 MeV
Ionization protons and ions	G4MicroElecInelastic	G4MicroElecInelastic Model	50 keV	10 GeV
"Electron capture"	G4MicroElecCapture	None	0	
Surface Crossing	G4MicroElecSurface	None	0	

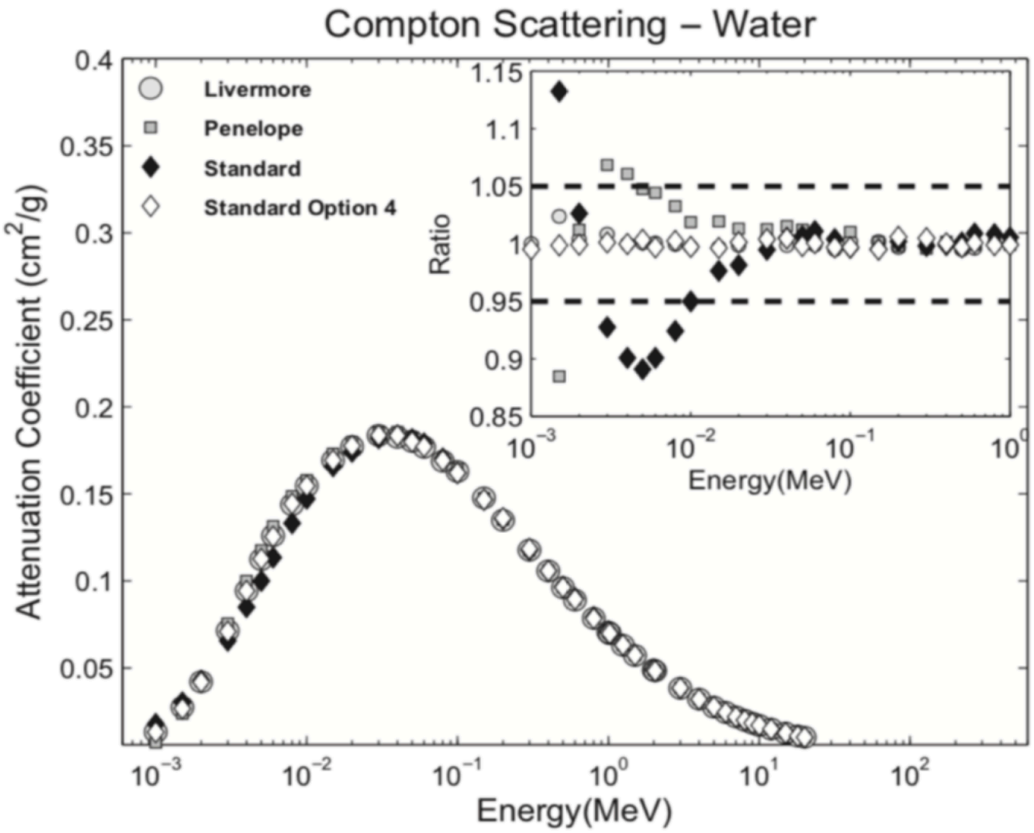
- Advanced user example: microelectronics

Improved Compton Model

Monash University Compton Model

- Improves the accuracy of the Livermore gamma models
  - Unpolarized Compton scattering from bound atomic electrons using relativistic impulse approximation
  - Polarized version also available
  - An alternative to the Livermore and Penelope Compton models
    - More accurate electron ejection direction below 5 MeV
    - Special relativistic formalism + energy-momentum conservation in order to compute
      - energy and angular distribution of Compton scattered photons from non-stationary bound atomic electrons
      - energy and ejected angular distributions of Compton electrons

Improved Compton Model Comparison



- Option4 EM physics list uses improved Compton model
- Inset: ratio of attenuation coefficient from four physics lists to data

Using the Improved Compton Model

- Model classes:
  - G4LowEPComptonModel
  - G4LowEPPolarizedComptonModel

- Register to 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);

- Or use one of two physics constructors
  - G4EmLowEPPhysics - identical G4EmLivermorePhysics except for Compton
  - G4EmStandard_option4 - best of Geant4 EM

Production Thresholds at Low Energy

- Recall that production thresholds specify range cuts for secondary γ, e^-, e^+ and p
- Geant4 default 0.7 mm, but can be changed with SetCuts() method in physics lists or with UI commands:
  - /run/setCut 0.01 mm sets range to 10 μm for all secondaries
  - /run/setCutForAGivenParticle e- 0.01 mm set only for e^-
- If range cut is equivalent to an energy lower than 990 eV, energy is still set to 990 eV
  - To decrease this, use UI command /cuts/setLowEdge 250 eV (for example)
  - Or, in SetCuts() method in physics list G4ProductionCutsTable::GetProductionCutsTable()->SetEnergyRange(250*eV, 1*GeV);
- Can also, independently, fully deactivate production cuts for simulation of all atomic de-excitation products
  - /process/em/deexcitationIgnoreCut true
- In your macro, these UI commands should be put before the UI command /run/initialize

Low Energy EM Summary

- Use low energy models (Livermore, Penelope) as alternative to standard Geant4 models when you
  - need precise treatment of electromagnetic showers and interactions at low energy (~keV and below)
  - are interested in atomic effects, such as fluorescence X-rays, Doppler broadening, etc.
  - can afford a more CPU-intensive simulation
  - cross-check another simulation (different physics list)
  - are interested in specific low energy applications (Geant4-DNA, MicroElec)

- Do not use for EM physics above ~MeV
  - Same results as standard EM
  - Big performance penalty