Physical models for track structure simulations with emphasis on Geant4-DNA

GEANT4-DNA
A SIMULATION TOOLKIT

geant4-dna.org

Ioanna Kyriakou
Medical Physics Laboratory, Department of Medicine
University of Ioannina, Greece
ikyriak@uoi.gr

XI International Geant4 School
University of Pavia, Physics department
18 January 2024

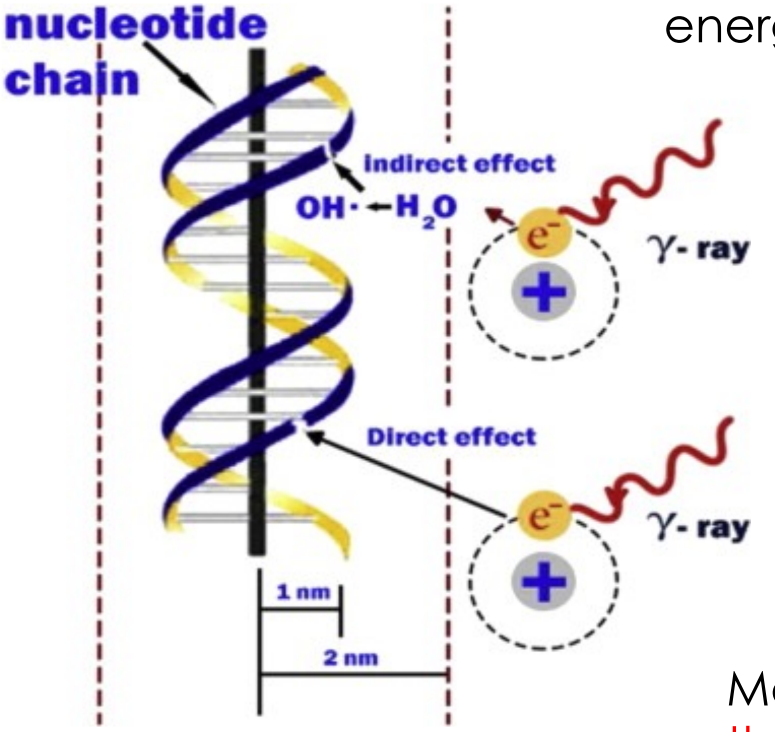
Contents of this talk

Contents of this talk

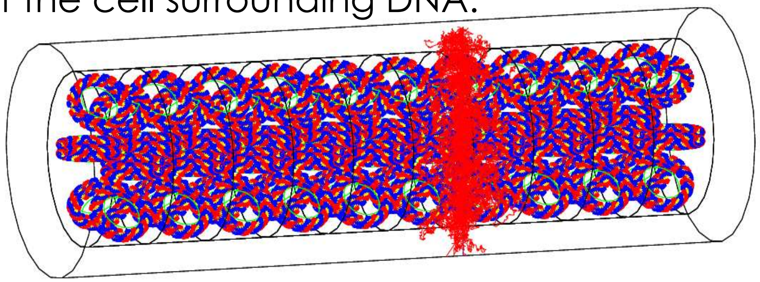
- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

Direct Action

- **Direct Action:** DNA damage type caused by energy transfer from radiation to DNA molecule.



Long DNA strands are folded and packed in cell. To simulate direct action, we need particle interaction models for (**condensed-phase) DNA** and **particle transport models for liquid water** medium which is the main part of the cell surrounding DNA.



DNA and track lets of 500keV He^+

Main technical challenge is that we deal with the reaction with/in microscopic geometry!

Why Geant4-DNA?
- Requirements for radiobiological simulations -

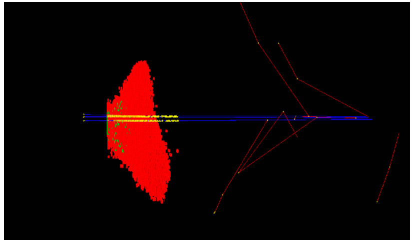
- **High spatial resolution (few µm, nm), low energy limit, reliable physics for sub-keV energies**

  Geant4:

  Fast / Low spatial resolution, E_{limit} ~ 250eV

  Geant4-DNA:

  Slow/ High spatial resolution, E_{limit} ~ 10eV



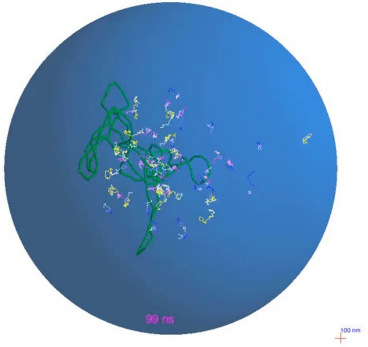
- **Interface for water radiolysis**

  Geant4:

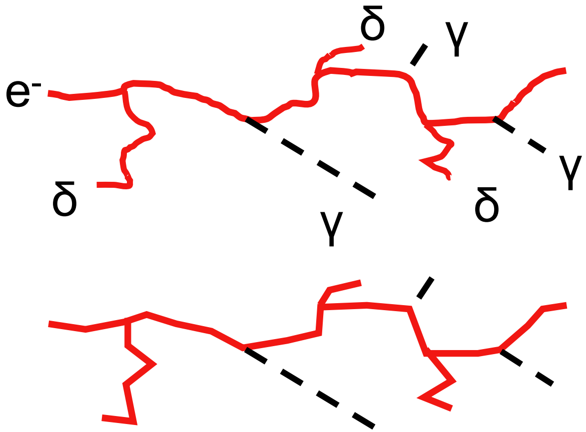
  No interface

  Geant4-DNA:

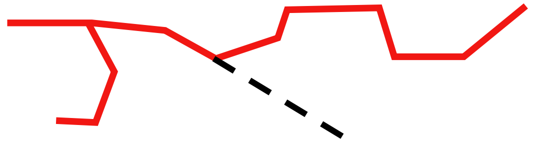
  Production/Diffusion of chemical molecules



Requirement for physics: High spatial resolution

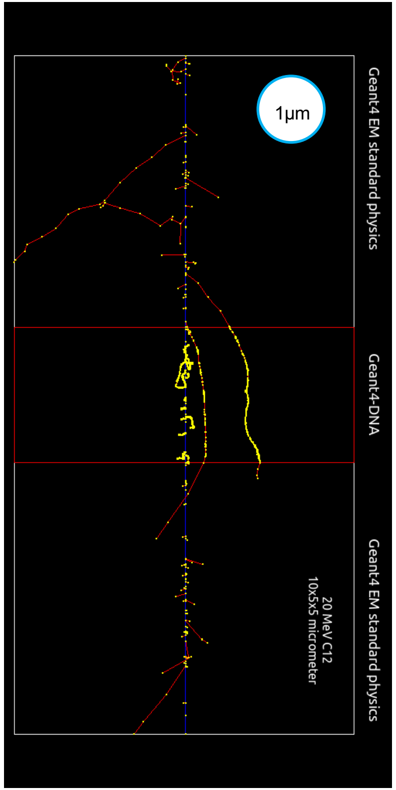


High accuracy/Slow computing



Low accuracy /**Fast computing**

Trajectory in real world



Track-Structure approach

- All physical interactions are simulated individually in a sequential manner
- Example: Geant4-DNA, PARTRAC, RITRACKS, NOREC, KURBUC…

Condensed-History approach

- Several discrete physical interactions are "condensed" into a single transport step
- Multiple-scattering approximation
- Example: Geant4, PHITS, EGS, FLUKA, PENELOPE, MCNP…

Contents of this talk

- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

Classification of Monte Carlo models

- Continuous Slowing Down (CSD)
  - ✓ The simplest transport model
  - ✓ Main input: Stopping power (SP)
- Condensed History (CH): Class I
  - ✓ Groups both elastic and inelastic collisions
  - ✓ Main input: Multiple scattering theories
- Condensed History (CH): Class II
  - ✓ Groups only soft collisions
  - ✓ Hard collisions (including δ-rays) simulated in a discrete manner
  - ✓ Main input: Restricted SP, knock-on cross sections, and more…
- Track Structure (TS): Class III
  - ✓ All collisions are simulated in a discrete manner
  - ✓ Full secondary electron cascade is included
  - ✓ Offers molecular resolution
  - ✓ Main input: single-collision cross sections (total, differential, etc.)

✓ Their main difference is on the treatment of elastic and inelastic collisions

The unique capabilities of TS codes

- Simulation of energy deposition in nm-µm volumes

  Microdosimetry (stochastic quantities)

  Nanodosimetry (ionization cluster-size distributions)

- Simulation of the chemical stage (⍰”indirect” damage)

  Radiolysis of water & radical diffusion

- Simulation of the molecular spectrum of DNA damage

  “complexity” of damage (low- vs. high-LET)

- Provide radiation “quality”

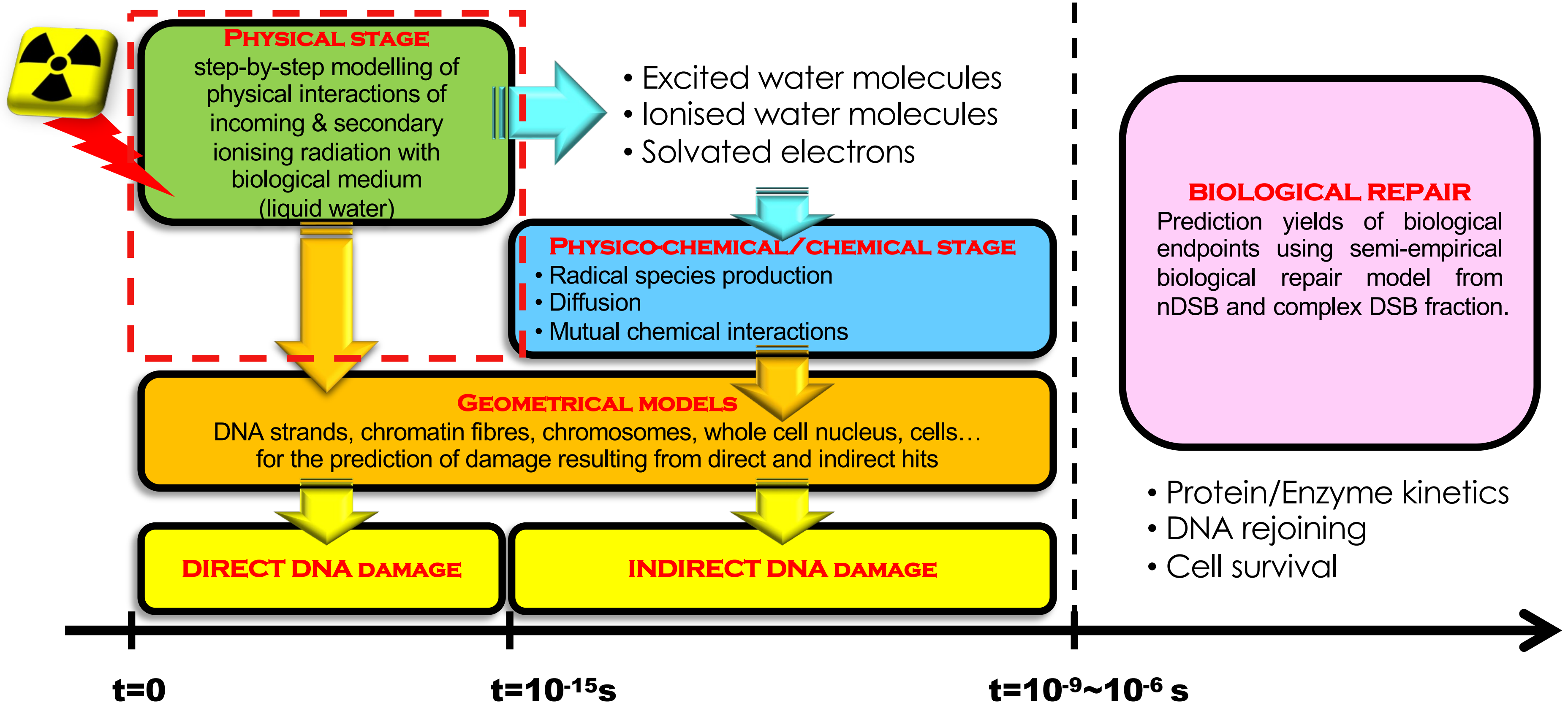
  Calculations of RBE at the DNA level

  Calculations of the Quality Factor based on the lineal energy (e.g., ICRU 40, TDRA)

Contents of this talk

- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

Geant4-DNA implementation



Geant4-DNA physics models

Geant4-DNA processes and models allows the transport in liquid water:

- **Electrons:** ionisation, excitation, elastic scattering, vibrational excitation, electron attachment
- **Protons, H $^{(0,+)}$:** ionisation, excitation, elastic, charge increase/decrease processes
- **Alpha, He$^{(0,+,2+)}$:** ionisation, excitation, elastic, charge increase/decrease processes
- **General ions:** ionisation

Geant4-DNA Physics constructors for simulations in liquid water:

- **G4EmDNAPhysics_option2 (since version 9.1)** : accelerated default constructor, simulating **electron interactions (elastic, inelastic, dissociative attachment, vibrational excitation) up to 1 MeV**, as well as other particle interactions
- **G4EmDNAPhysics_option4 (since version 10.2)** : contains **electron** elastic and inelastic models, **up to 10 keV-> extended up to 10 MeV (to be released)**
- **G4EmDNAPhysics_option6 (since version 10.4)**: contains CPA100 **electron** elastic and inelastic models, **up to 256 keV**

NOTE:

- protons can be tracked up to 300 MeV
- opt4,opt6 can go up to 1 MeV (beyond the default limits, Born models are used)

Overview of Physics models for liquid water

Electrons

- **Ionisation**
  - ✓ Dielectric optical data-model with low-energy corrections from the work of Emfietzoglou(Opt2)
  - ✓ Improved alternative version by Emfietzoglou & Kyriakou (Opt4)
  - ✓ Relativistic Binary Encounter Bethe (RBEB) by Terrissol from CPA100 (Opt6)
  - ✓ Relativistic (and improved) extension up to 10 MeV by Emfietzoglou & Kyriakou (NEW Opt4)
- **Excitations**
  - ✓ Dielectric optical-data model and low-energy corrections from the work of Emfietzoglou(Opt2)
  - ✓ Improved alternative version by Emfietzoglou & Kyriakou (Opt4)
  - ✓ Dielectric model by Dingfelder (Opt6)
  - ✓ Relativistic (and improved) extension up to 10 MeV by Emfietzoglou & Kyriakou (NEW Opt4)
- **Elastic scattering**
  - ✓ Screened Rutherford and Brenner-Zaider below 200 eV
  - ✓ Updated alternative version by Uehara
  - ✓ Independent Atom Method (IAM) & ice data from CPA100 code
  - ✓ Partial wave model by Champion et al.
  - ✓ ELSEPA based

Vibrational excitation (*)
Michaud et al. xs measurements in amorphous ice
Dissociative attachment (*)
Melton CS measurements

see: $G4SRC/source/processes/electromagnetic/dna/processes

Protons & H

- ✓ Excitation (*)
  - ✓ Miller & Green speed scaling of e- excitation up to 500keV and Born & Bethe above 500 keV, from Dingfelder et al.
  - ✓ Relativistic PWBA up to 300MeV
- ✓ Ionisation
  - ✓ Rudd semi-empirical by Dingfelder et al. and Born & Bethe theories & dielectric formalism above 500 keV
  - ✓ Relativistic PWBA up to 300MeV
- ✓ Charge change (*)
  - ✓ Analytical parametrizations by Dingfelder et al.
- ✓ Nuclear scattering
  - ✓Classical approach by Everhart et al.

He0, He+, He2+

- ✓ Speed and effective charge scaling from protons by Dingfelder 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 : Livermore » (EPDL97)
- ✓ EPICS2017 new

Geant4-DNA physics constructors

	Geant4-DNA physics constructors electron models		
Process	G4EmDNAPhysics_option2	G4EmDNAPhysics_option4	G4EmDNAPhysics_option6
Ionization (inelastic)	Emfietzoglou dielectric model (11 eV–1 MeV)[5]	Emfietzoglou–Kyriakou dielectric model (10 eV–10 keV)[47]	Relativistic binary encounter Bethe model from CPA100 code (11 eV–256 keV)[48]
Electronic excitation (inelastic)	Emfietzoglou dielectric model (9 eV–1 MeV)[5]	Emfietzoglou–Kyriakou dielectric model (8 eV–10 keV)[47]	Dielectric model from CPA100 code (11 eV–256 keV)[48]
Elastic scattering (elastic)	Partial wave model (7.4 eV–1 MeV)[5]	Uehara screened Rutherford model (9 eV–10 keV)[47]	Independent Atom Method model from CPA100 code (11 eV–256 keV)[48]
Vibrational excitation (inelastic subexcitation)	Sanche data (2 eV–100 eV)[49]	n/a	n/a
Attachment (inelastic subexcitation)	Melton data (4 eV–13 eV)[50]	n/a	n/a
Auger electron emission	From the EADL database[51] and the Geant4 atomic relaxation interface[52,53]		
Default tracking cut[(*)]	7.4 eV	10 eV	11 eV

In addition, Bremsstrahlung, Livermore photon physics(+ Rayleigh Scattering), positron physics, are activated

see: $G4SRC/source/physics_lists/constructors/electromagnetic/src/G4EmDNABuilder.cc

From Incerti et al., Med. Phys. 45, 722-739 (2018)

Geant4-DNA inelastic models for electrons

➢ DNA_Option2 inelastic models (9 eV-1 MeV)

- ✓ Projectile-target interaction based on the plane-wave Born approximation (PWBA) with relativistic corrections
- ✓ Target response based on the energy-loss-function (ELF) determined from Emfietzoglou's dielectric model of liquid water (2002)
  - Uses experimental optical data
  - Accounts for individual ionization and excitation channels
- ✓ Includes corrections to PWBA through Coulomb-Exchange terms
- ✓ Includes solid-state effects (via the ELF)

Geant4-DNA inelastic models for electrons (cont…)

- **DNA_Option4 inelastic models (10 eV – 10 keV)**
  - ✓ Projectile-target interaction based on the non-relativistic PWBA
  - ✓ Target response based on an improved version of the ELF of Option 2 using the Emfietzoglou-Kyriakou algorithm (2015)
  - ✓ Improved implementation of the Coulomb-Exchange corrections of Option 2
- **DNA_Option6 inelastic models (11 eV-256 keV)**
  - ✓ Ionizations based on the Binary-Encounter-Bethe (BEB) atomic model (Kim & Rudd, 1994)
  - ✓ Excitations based on the ELF model of Dingfelder (1998)
  - ✓ Solid-state effects included only in excitations (through ELF)

Geant4-DNA elastic models for electrons

- **Option 2**
  - ✓ Based on Schrodinger partial wave calculations
    - Neglects spin-effects
    - Non-relativistic calculations
    - Ad hoc corrections for solid-state effects
- **Option 4**
  - ✓ Based on Born approximation calculations (screened Rutherford)
    - Relativistic
    - Neglects spin-effects
    - Neglects solid-state effects
- **Option 6**
  - ✓ Based on Schrodinger partial wave calculations
    - Same problems w/default
    - Neglects solid state effects

- **Model deficiencies**
  - ✓ They neglect spin-effects
  - ✓ They are non-relativistic (except of Opt4)
  - ✓ They neglect solid-state effects (or include ad hoc corrections)
- **General observation**
  - ✓ All models perform poorly at low energies & small-medium angles

Proton interactions in Geant4-DNA

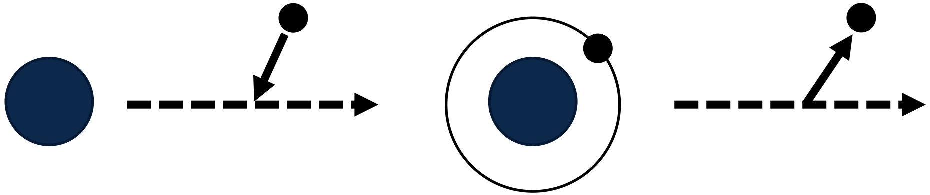
- **Ionization**
  - ✓ For slow protons (energy <500keV): fit to exp. data of Rudd et al. (1985)
  - ✓ For fast protons (energy >500keV): RPWBA calculations using the dielectric model of Dingfelder et al. (2000)
  - ✓ NEW extension 100 Mev - 300 MeV: RPWBA calculations using the dielectric model of Emfietzoglou et al. (2005) (implementation by Dominguez_Munoz et al., 2022)
- **Excitation**
  - ✓ For slow protons (<500keV): analytical expression of Miller & Green (1973)
  - ✓ The rest are the same as for ionization
- **Charge transfer**
  - ✓ Analytic formula by Dingfelder et al. (2000) with parameters chosen by fit to exp. data of water vapour
- **Nuclear elastic**
  - ✓ This interaction is important for very low proton energies (at the keV energy scale)
  - ✓ See Tran et al. (2015) for details

Interactions for protons and neutral H in Geant4-DNA

Interaction mode	Proton (p)	Neutral hydrogen (H)
Elastic scattering	$p + H_2O \rightarrow p' + H_2O$	$H + H_2O \rightarrow H' + H_2O$
Target ionisation	$p + H_2O \rightarrow p' + H_2O^+ + e^-$	$H + H_2O \rightarrow H' + H_2O^+ + e^-$
Target excitation	$p + H_2O \rightarrow p' + H_2O^\star$	$H + H_2O \rightarrow H' + H_2O^\star$
Electron capture (σ_{10})	$p + H_2O \rightarrow H' + H_2O^+$	-
Electron loss (σ_{01})	-	$H + H_2O \rightarrow p' + H_2O + e^-$
Simultaneous electron capture and target ionisation	$p + H_2O \rightarrow H' + H_2O^{2+} + e^-$	-
Simultaneous electron loss and target ionisation	-	$H + H_2O \rightarrow p' + H_2O^+ + 2e^-$

Main energy loss mechanism for energies > 1MeV

Charge-transfer processes contribute to the energy loss mechanism for energies ≤0.3MeV



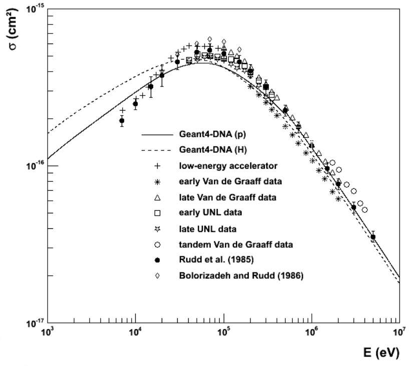
Liamsuwan et al., IJRB (2011) 141-160

Helium and Ion interactions in Geant4-DNA

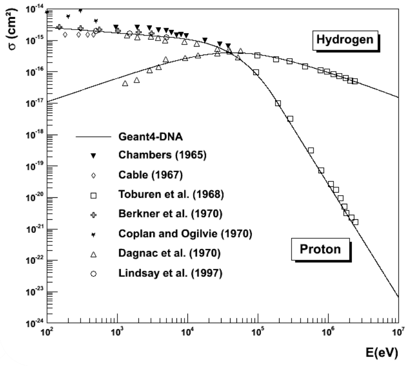
- Speed scaling procedure using the corresponding proton cross sections
- Takes into account the effective charge of the incident projectile
  - ✓ Different effective charges used for He, He+, He++ projectiles
  - ✓ Charge transfer processes using the analytical fit by Dingfelder (2005)
  - ✓ For ions heavier than helium, only ionization is taken into account using an effective charge formula by Booth and Grant (1965)

Validation and Verification (For proton and Helium)

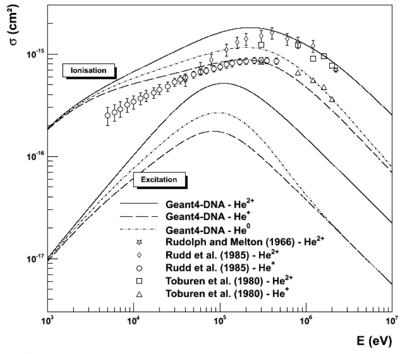
Proton CS: Ionisation*

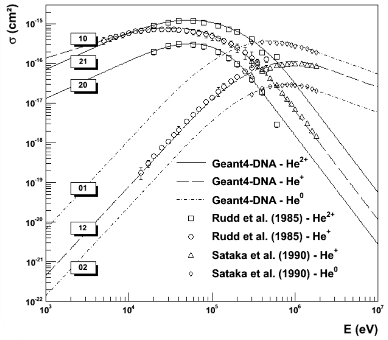


Charge exchange*

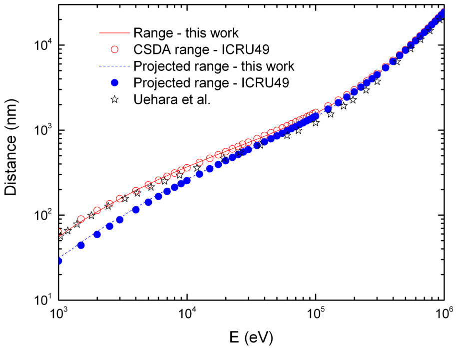


Helium CS: Ionisation & Excitation* Charge exchange*



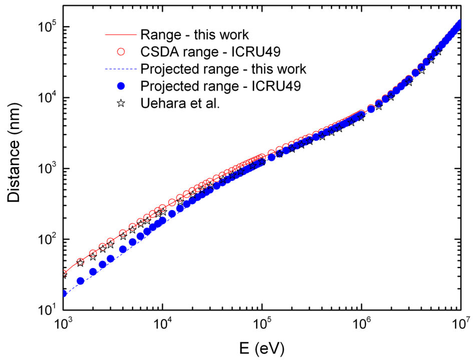


Range: Proton*



* Incerti et al., Med. Phys. 37 (2010) 4692-4708

Range: Helium*



* Tran et al., NIMB 343(2015) 132-137

Contents of this talk

- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

Multi scale combination of physics processes

No worries!

- Geant4-DNA is mainly for low energy charged particles
  - Is it possible to simulate, neutral particle such as photon?
  - Can we include the physics processes for high energy particles?

- Any Geant4-DNA process can be combined with other Geant4 process such as:
  - Geant4 **photon** processes and models
  - Geant4 alternative EM processes and models for charged particles
  - Geant4 **atomic de-excitation** (fluorescence + Auger emission, **including cascades**)
  - …and also Geant4 **hadronic physics**

Other processes: Geant4 Photon models

- Cross sections for photons were recently updated (since version 11.0)
- Based on the database **EPICS2017** (major update of the existing **Livermore** database EPDL97)
- Four photon processes:
  - Gamma conversion (Classes: G4LivermoreGammaConversionModel and G4LivermoreGammaConversion5DModel*)
  - Compton (Class: G4LivermoreComptonModel)
  - Photoelectric (Class: G4LivermorePhotoElectricModel)
  - Rayleigh scattering (Class: G4LivermoreRighleighModel)

  * Difference lies on the way they sample the final state
- **Other (older) choices for photons: Livermore (EPDL97, EPICS2014 for photoelectric and PENELOPE)**

Other processes: Bremsstrahlung

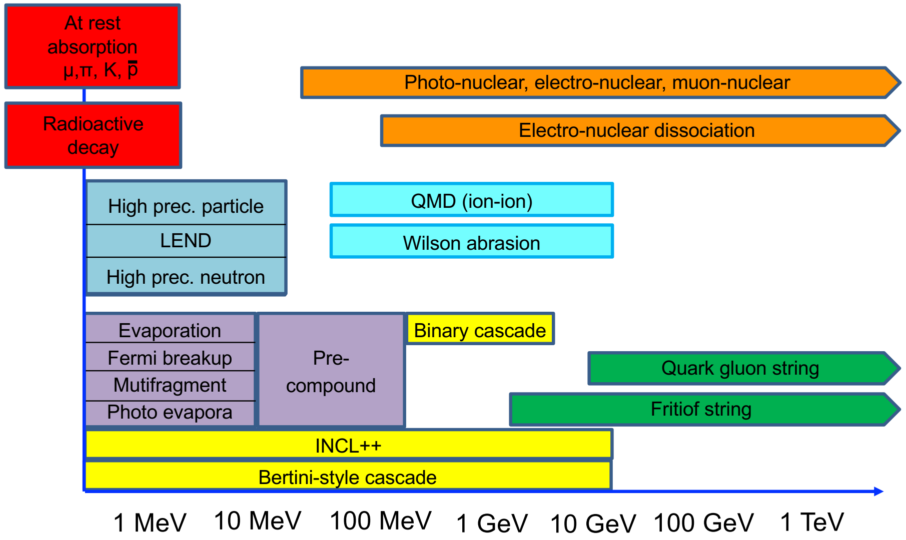
- Significant only for light charged particles (i.e. e-, e+) and for high Z materials
- For water it becomes important above ~10 MeV
- These simulations exist in the EM packages of Geant4 and are not specific of Geant4-DNA
- There are different options that one can use to include bremsstrahlung interactions (Livermore, Penelope, Standard)

Other processes: Atomic de-excitation package

- **Follows vacancies created in atomic shells to describe secondary effects following ionization of an atom by the projectile**
  - ✓ Fluorescence emission
  - ✓ Auger cascades
  - ✓ PIXE (Particle Induced X-ray Emission)
- **Used for applications such as in radiobiology, experimental material composition, detector performance and optimization etc.**
- **These simulations exist in the EM packages of Geant4 and are not specific of Geant4-DNA**
- **Can be activated or deactivated with the use of UI commands in the macro**

Other processes: Hadronic model

** some particles are not supported in Geant4-DNA



Recommendation for Medical application
QGSP_BIC

High Energy Hadron model

FTF : Fritiof Parton String model:

QGS : Quark Gluon String model:

Low Energy Hadron model

BERT : Bertini-style Cascade:

BIC : Binary Cascade:

INCLXX : Liege intra-nuclear cascade model (INCL)

Option for Low Energy Hadron model

---P : Precompund model for nuclear de-excitation (for example, FTFP, QGSP,etc)

Neutron model

HP : High Precision neutron model E<20MeV

How to activate?
please add following lines in your application

```
#include "QGSP_BIC.hh"

int main( int argc,char** argv ) {
    …
    G4RunManager * runManager = new G4RunManager{};
    runManager->SetUserInitialization( new QGSP_BIC{} );
    …
}
```

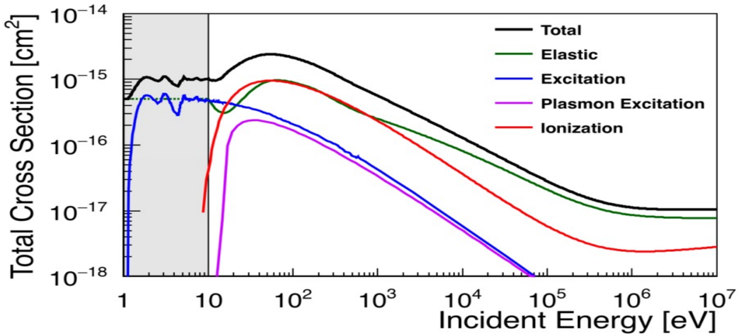
Contents of this talk

- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

GEANT4-DNA

2016 Electron Physics models for GOLD

- Extension of Geant4-DNA to model radiosensitization from GNPs
- Discrete physics models for electrons (10eV-1GeV)
- Available since version 11
- An approach based on the ELF for gold material was developed and will be available in one of the next releases of Geant4



Physics	Model
Elastic	Partial Wave Analysis (ELSEPA)
Ionization	M. Relativistic Binary-Encounter Bethe Vriens
Excitation	Experiment + Dirac B-Spline R Matrix
Plasmon Excitation	Quinn Model
Bremsstrahlung	Seltzer and Berger Model

J. Appl. Phys. 120, 244901 (2016)
Phys. Med. 63, 98-104 (2019)

see examples/extended/medical/dna/AuNP

GEANT4-DNA

PTB biomaterial cross sections

- Cross section data serving as models for different DNA constituents based on gas phase experiments from PTB lab (Germany)
- For electrons 12 eV-1keV (ionization, excitation, elastic)
- Available since version 10.4beta
- They serve as models for phosphate groups in the DNA backbone, DNA bases and deoxyribose
  - ✓ Tetrahydrofuran (THF) → deoxyribose
  - ✓ Trimethylphosphate (TMP) → phosphates
  - ✓ Pyrimidine (PY) → thymine, cytosine
  - ✓ Purine (PU) → adenine, guanine
- For protons based on the HKS approach for energies 70keV-10MeV (ionization)

Radiat. Phys. Chem. 130, 459-479 (2017)

see examples/extended/medical/dna/icsd

Contents of this talk

- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

GEANT4-DNA

Other recent developments in the physics of Geant4-DNA

- Extension of DNA-Option 4 up to 10 MeV for electron (in progress)
- Proton cross sections based on the improved DNA-Option 4 model (in progress)
- Extension of DNA-Option 6 to other biological targets in order to (available):
  - ✓ Simulate more reliably direct and indirect DNA damage
- Cross sections for N_2, O_2 molecules for atmospheric simulations (in progress)
- Cross sections for propane (C_3H_8) for gas detectors (in progress)
- Alternative inelastic cross sections for protons above 100 MeV up to 300 MeV based on the Relativistic PWBA (available)
- Electron cross sections for gold up to 1 MeV using the ELF approach (2018 model, in progress)

Note: All constructors can be used up to 1 MeV for electrons (Born inelastic model)

ELSEPA code
Elastic Scattering of Electrons and Positrons by Atoms

- **Developed by Fransesc Salvat and co-workers at U. Barcelona**
  - ✓ Implemented in the PENELOPE code
  - ✓ Used in the NIST elastic scattering cross section database (SRD 64)
  - ✓ Used in ICRU Report 77 (2007) recommendations
- **Important features**
- ➢ Based on Dirac partial wave calculations

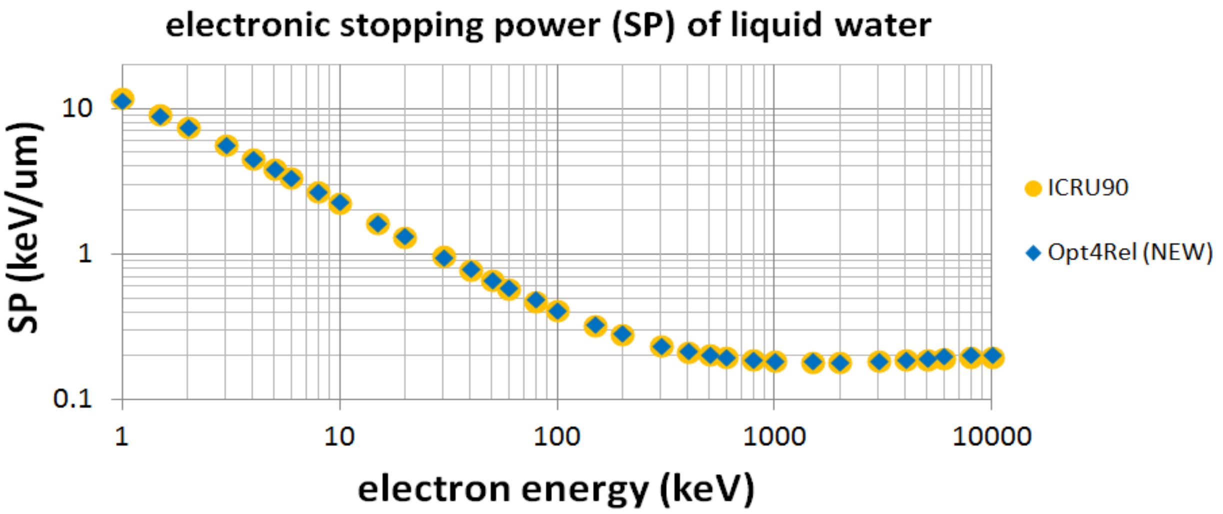
  Includes:
  - ✓ Spin effects
  - ✓ Relativistic effects
  - ✓ Low-energy corrections (exchange & correlation-polarization)
  - ✓ Solid-state corrections (Muffin-tin model)

Alternative for elastic

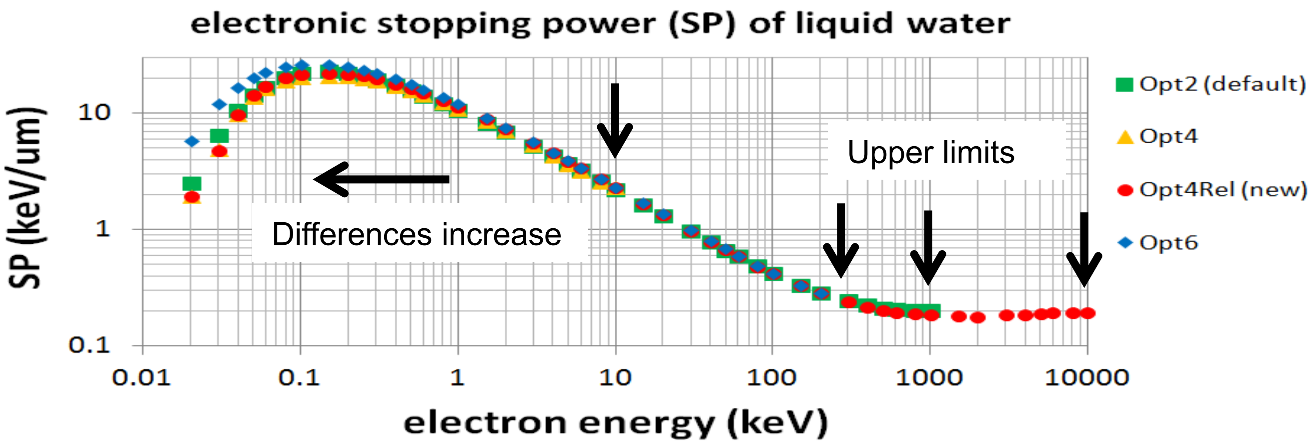
Extension of DNA_Option4 to relativistic energies

- ✓ Cover most of Medical Physics applications (including radiotherapy).
- ✓ Replace fully DNA_Option 2 to have a model for liquid water up to 10 MeV.
- ✓ Extend the code’s TS capabilities.
- ✓ Make some improvements to the existing DNA_Option4 model.

New model within 5% from ICRU



Default model within 10% from ICRU



Contents of this talk

- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

Geant4-DNA Physics examples

✓ Calculation of several physics related magnitudes…

Located in $G4EXAMPLES/extended

- The « clustering » **extended/medical/dna** example illustrates how to **identify ionisation clusters.**

- The « dnaphysics » **extended/medical/dna** example illustrates how to combine **Geant4-DNA physics processes and models** with Geant4 electromagnetic physics processes and models in specified regions of the geometrical setup using the **G4EmDNAPhysicsActivator** class. Alternatively, it shows how to use the **Geant4-DNA physics constructors.** It also explains how to extract physical information at the step level, such as process type, position, energy deposited, scattering angle... and how to use the **variable density material** feature for liquid water.

- The « icsd » **extended/medical/dna** example illustrates how to use cross section models for **DNA-related materials.**

- The « svalue » **extended/medical/dna** example explains how to simulate "**S-values**" in spherical targets of liquid water.

Geant4-DNA Physics examples (cont.)

- The « wvalue » **extended/medical/dna** example explains how to simulate "**W-values**" in liquid water.

- The « microdosimetry » **extended/medical/dna** example shows how to combine « by hand » Geant4 standard electromagnetic physics processes and models with Geant4-DNA physics processes and models in two regions filled with liquid water, illustrating the **combination of condensed history and discrete processes at different scales**.

- The « mfp » **extended/medical/dna** example explains how to extract **mean free paths**.

- The « microprox » **extended/medical/dna** example explains how to simulate **microdosimetry proximity functions**.

- The « microyz » **extended/medical/dna** example explains how to simulate **microdosimetry quantities (lineal energy, specific energy)**.

- The « range » **extended/medical/dna** example explains how to simulate **ranges**.

- The « spower » **extended/medical/dna** example explains how to simulate **stopping powers**.

Geant4-DNA Physics examples (cont.)

- The « **slowing** » **extended/medical/dna** example explains how to simulate **slowing down spectra**.
- The « **splitting** » **extended/medical/dna** example explains how to accelerate simulation through **splitting in ionisation**.
- The « **AuNP** » **extended/medical/dna** example explains how to simulate track structures of electrons in a microscopic **gold volume** immersed in liquid water.
- The « **TestEm5** » **extended/electromagnetic** example explains how to extract **atomic deexcitation information (**using the **dna.mac** macro file).
- The « **TestEm12** » **extended/electromagnetic** example explains how to extract **radial dose distributions** in spherical shells of liquid water (such as dose point kernels, using the **dna.mac** macro file).
- The « **jetcounter** » **extended/medical/dna** example explains how to simulate a **gas dosimeter**.

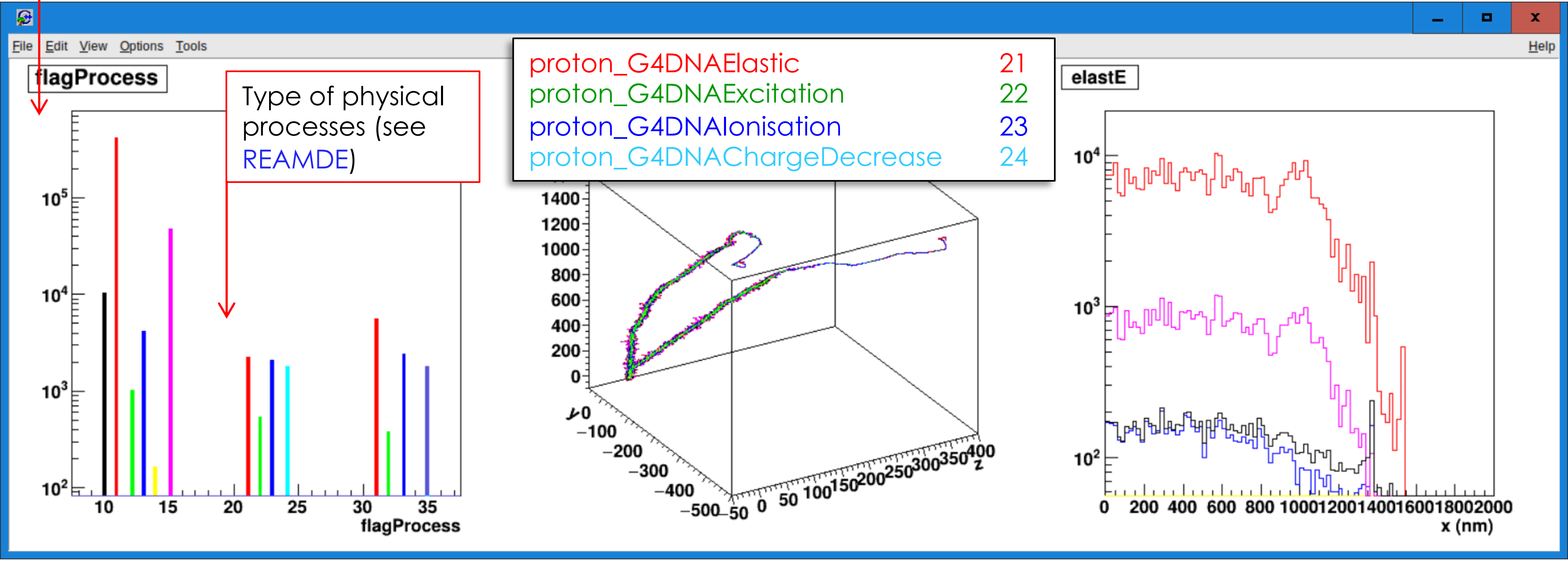
More info on medical/dna examples in Incerti et al., Med. Phys. (2018), Kyriakou et al., Cancers (2022) and dedicated publications…

Geant4-DNA example: dnaphysics

Number of physical processes

3D visualization of proton tracks

Radial distributions



Thank you for your attention!

Any
questions?

ikyriak@uoi.gr