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

geant4-dna.org

Ioanna KYRIAKOU

Medical Physics Laboratory, Department of Medicine
University of Ioannina, Greece

ikyriak@uoi.gr

Geant4-DNA tutorial
Pohang Accelerator Laboratory, Republic of Korea
07/02/2025

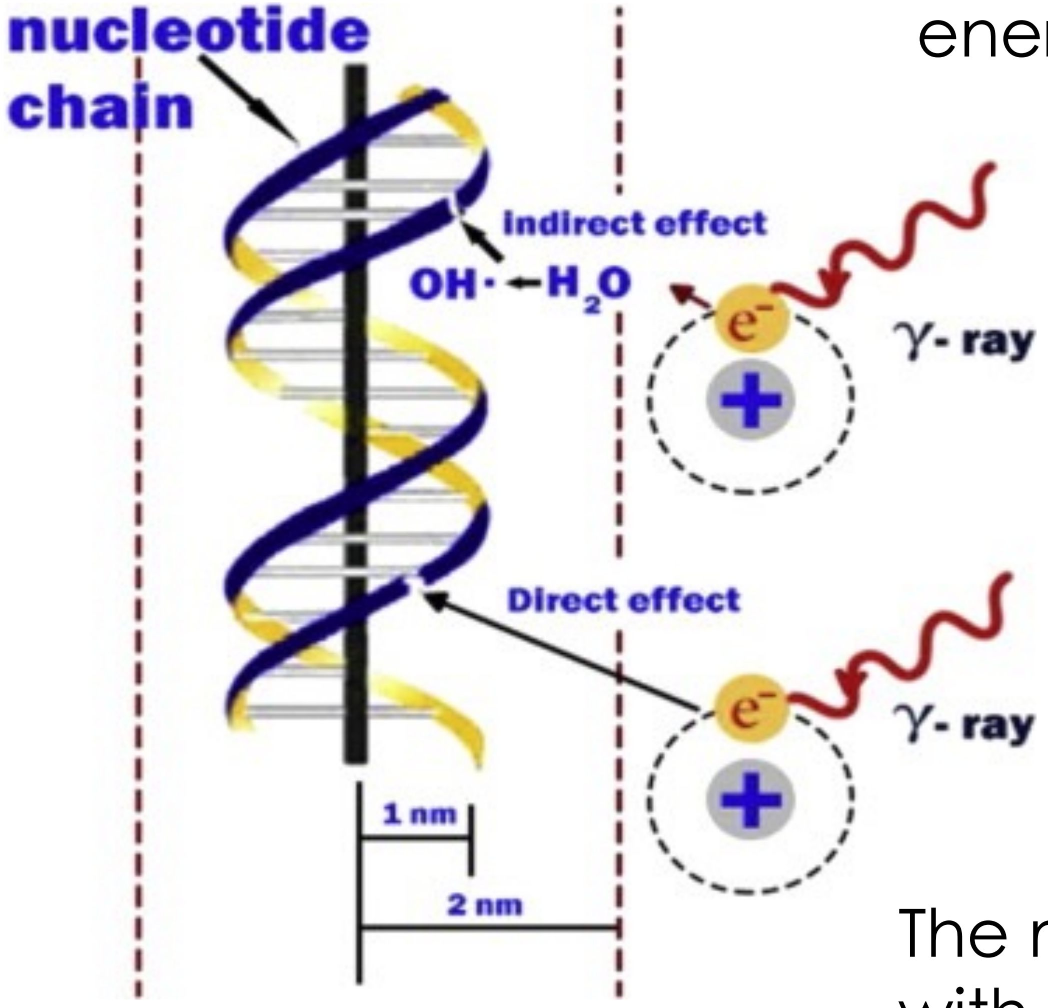
Contents of this talk

- 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

Contents of this talk

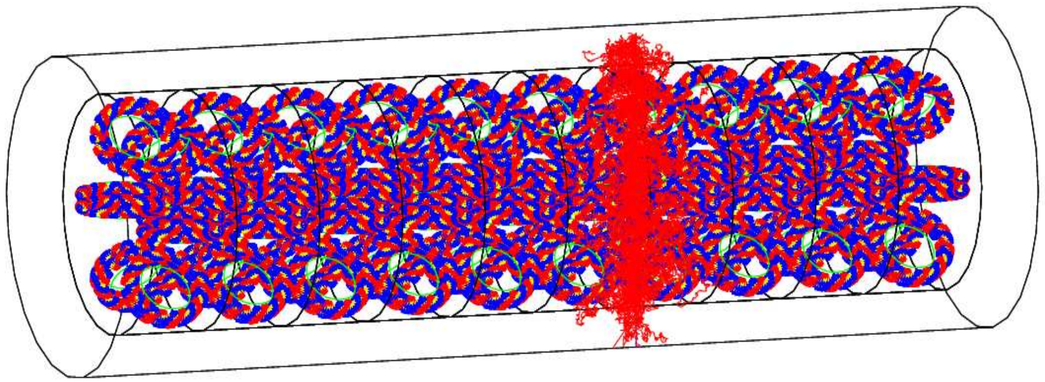
- Why Geant4-DNA
- Track-structure vs condensed history
- Geant4-DNA physics implementation and models
- Combination with standard EM and hadronic physics
- Physics for non-water materials
- Other developments
- Geant4 physics extended examples

Direct action



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

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



DNA and tracks of 500 keV He$^+$

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

Ref.: J. Rad. Res. App. Sci. 8, 247-254 (2015)

Why Geant4-DNA?
- Requirements for radiobiological simulations -

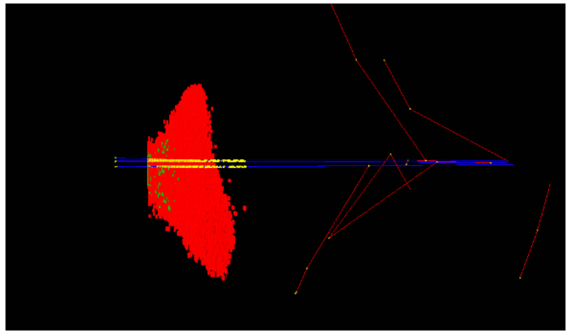
- **High spatial resolution (few µm, nm), low energy limit, reliable physics for sub-keV energies**

  Geant4:

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

  Geant4-DNA:

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



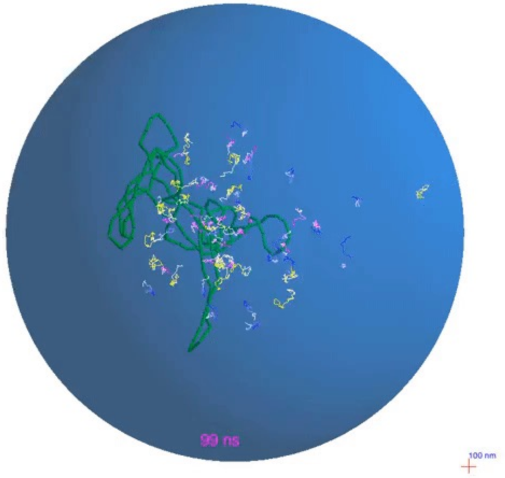
- **Interface for water radiolysis**

  Geant4:

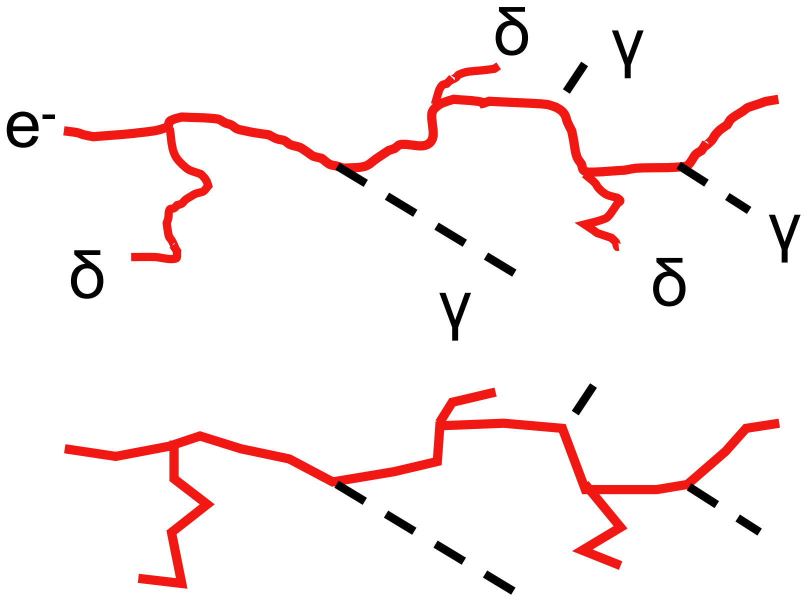
  No interface

  Geant4-DNA:

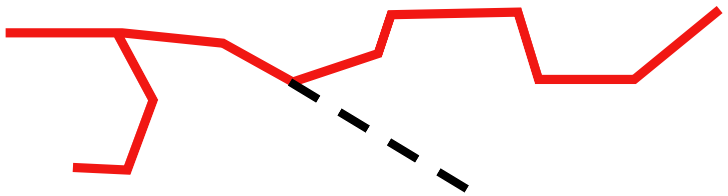
  Production/Diffusion of chemical molecules



Requirement for physics: High spatial resolution



High accuracy/Slow computing



Low accuracy /**Fast computing**

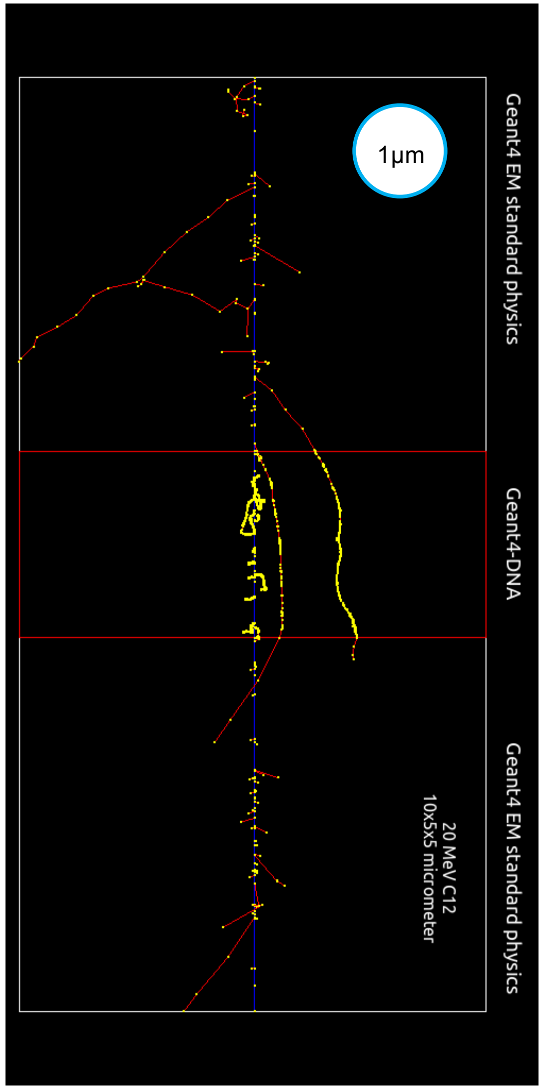
Trajectory in real world

Track-Structure approach

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

Condensed-History approach

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



Ref.: Nucl. Instrum. and Meth. B 273, 95-97 (2012), Prog. Nucl. Sci. Tec. 2, 898-903 (2011)

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.)

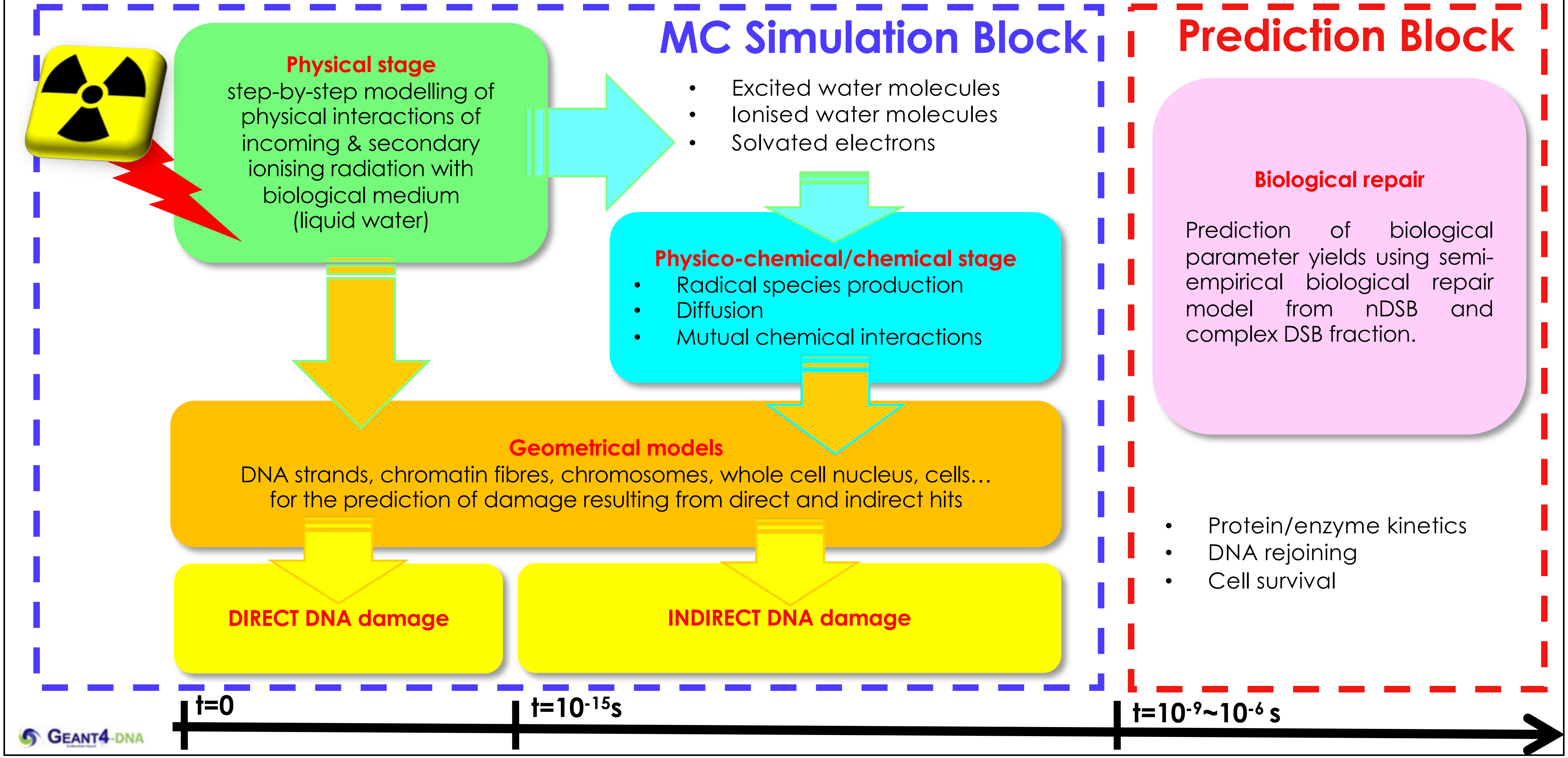
✓ Their main difference is on the treatment of elastic and inelastic collisions

The unique capabilities of TS codes

- Simulation of **energy deposition in nm-µm volumes**
  - Microdosimetry (stochastic quantities)
  - Nanodosimetry (ionisation cluster-size distributions)
- Simulation of the **chemical stage** ("**indirect**" action / 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

Geant4-DNA approach



MC Simulation Block

Physical stage

step-by-step modelling of physical interactions of incoming & secondary ionising radiation with biological medium (liquid water)

- Excited water molecules
- Ionised water molecules
- Solvated electrons

Physico-chemical/chemical stage

- Radical species production
- Diffusion
- Mutual chemical interactions

Geometrical models

DNA strands, chromatin fibres, chromosomes, whole cell nucleus, cells…
for the prediction of damage resulting from direct and indirect hits

DIRECT DNA damage

INDIRECT DNA damage

Prediction Block

Biological repair

Prediction of biological parameter yields using semi-empirical biological repair model from nDSB and complex DSB fraction.

- Protein/enzyme kinetics
- DNA rejoining
- Cell survival

t=0

$t=10^{-15}s$

$t=10^{-9}\sim10^{-6}$ s

GEANT4-DNA

Geant4-DNA physics

- **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
  - Generic 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
- Option4 and option6 can go up to 1 MeV (beyond the default limits, Born models are used)

Overview of Physics processes & models for liquid water

- **Electrons**
  - Ionisation
    - Dielectric optical data-model with low-energy corrections from the work of Emfietzoglou (**Option2**)
    - Improved alternative version by Emfietzoglou & Kyriakou (**Option4**)
    - Relativistic Binary Encounter Bethe (RBEB) by Terrissol from CPA100 (**Option6**)
    - 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 (**Option2**)
    - Improved alternative version by Emfietzoglou & Kyriakou (**Option4**)
    - Dielectric model by Dingfelder (**Option6**)
    - 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. CS measurements in amorphous ice
  - Dissociative attachment (*)
    - Melton CS measurements

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

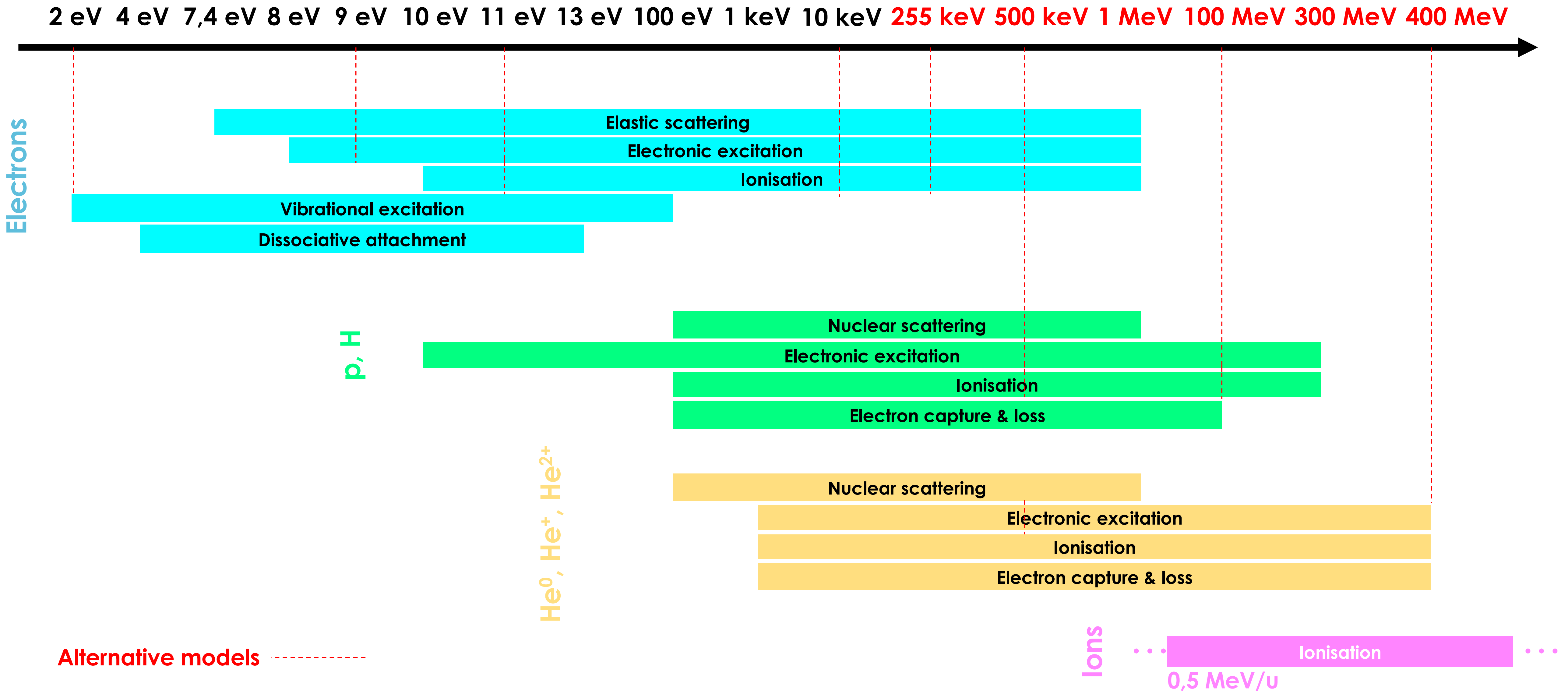
- **He0, He+, He2+**
  - Excitation, ionisation
    - Speed and effective charge scaling from protons by Dingfelder et al.
  - Charge change (*)
    - Analytical parametrizations by Dingfelder et al.
  - Nuclear scattering
    - Classical approach by Everhart et al.

- **Li, Be, B, C, N, O, Si, Fe and all other ions**
  - Ionisation
    - Speed scaling and global effective charge by Booth and Grant

- **Photons**
  - from EM physics: Livermore » (EPDL97), EPICS2017 (NEW)

NOTE
Software in: `$G4SRC/source/processes/electromagnetic/dna/processes`
See publications for more detail

Energy coverage of processes



2 eV 4 eV 7,4 eV 8 eV 9 eV 10 eV 11 eV 13 eV 100 eV 1 keV 10 keV 255 keV 500 keV 1 MeV 100 MeV 300 MeV 400 MeV

Electrons

- Elastic scattering
- Electronic excitation
- Ionisation
- Vibrational excitation
- Dissociative attachment

p, H

- Nuclear scattering
- Electronic excitation
- Ionisation
- Electron capture & loss

He^0, He^+, He^{2+}

- Nuclear scattering
- Electronic excitation
- Ionisation
- Electron capture & loss

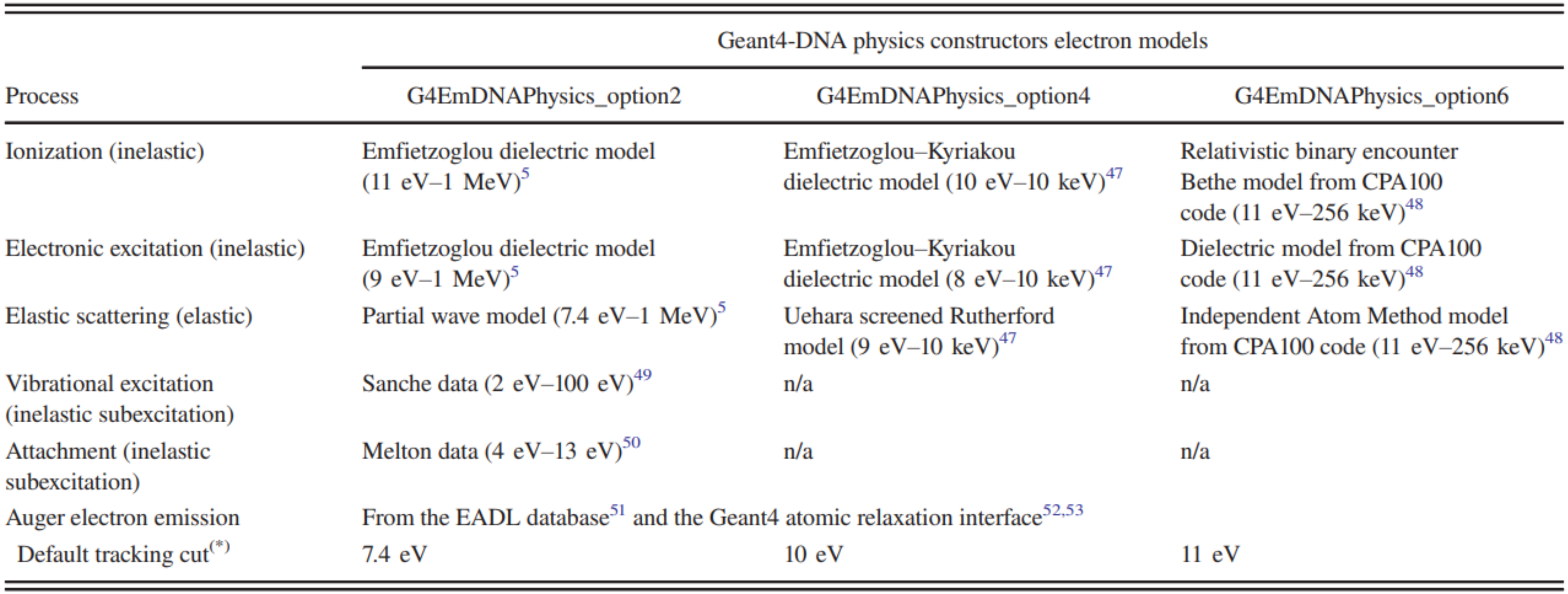
Ions

- Ionisation

0,5 MeV/u

Alternative models

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), and **positron** physics are activated

Ref.: Med. Phys. 45, 722-739 (2018)

Geant4-DNA inelastic models for electrons

Geant4-DNA Option 2 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 ionisation 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…)

- **Geant4-DNA Option 4 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

- **Geant4-DNA Option 6 inelastic models** (11 eV – 256 keV)
    - ionisations based on the **Binary-Encounter-Bethe** (BEB) **atomic model** of 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

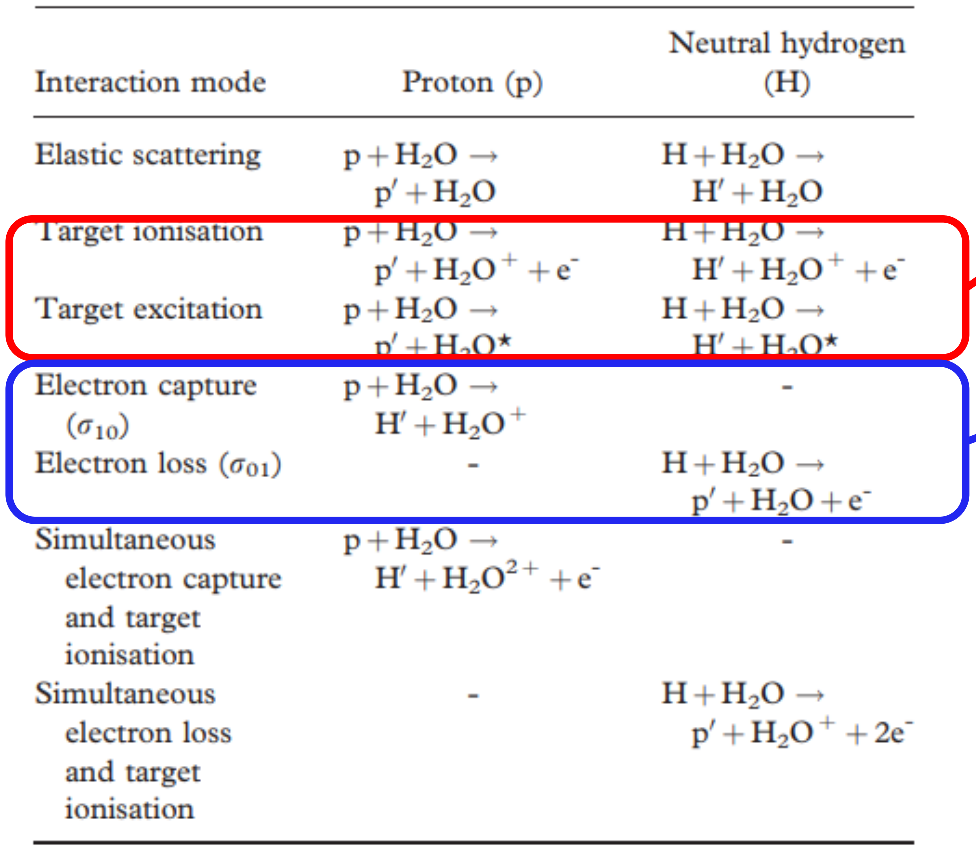
- Model **deficiencies**
  - They neglect spin-effects
  - They are non-relativistic (except for Option 4)
  - They neglect solid-state effects (or include ad hoc corrections)

- General observation
  - All models perform poorly at low energies & small-medium angles

Proton interactions in Geant4-DNA

- **Ionisation**
  - For slow protons (energy < 500 keV): fit to exp. data of Rudd et al. (1985)
  - For fast protons (energy > 500 keV): 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 (< 500 keV): analytical expression of Miller & Green (1973)
  - The rest are the same as for ionisation
- **Charge transfer**
  - Analytic formula by Dingfelder et al. (2000) with parameters chosen by fit to exp. data of water vapor
- **Nuclear elastic**
  - This interaction is important for very low proton energies (at the keV energy scale)
  - See Tran et al. (2015) for details

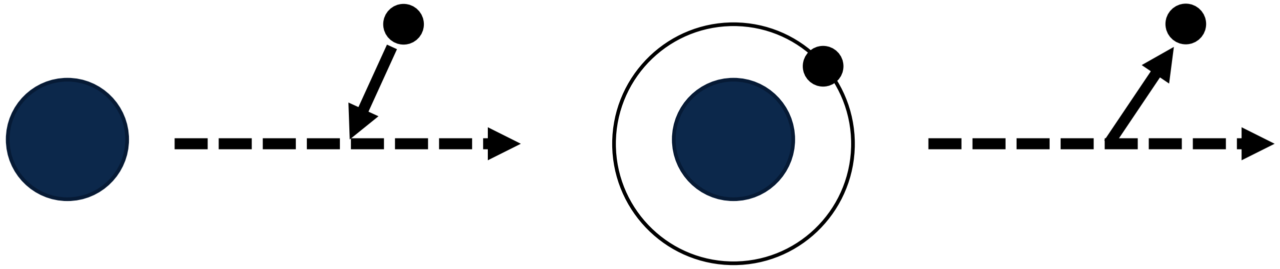
Interactions for protons and neutral H in Geant4-DNA



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 > 1 MeV

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



Ref. : Int. J. Radiat. Biol., 87(2), 141–160 (2010)

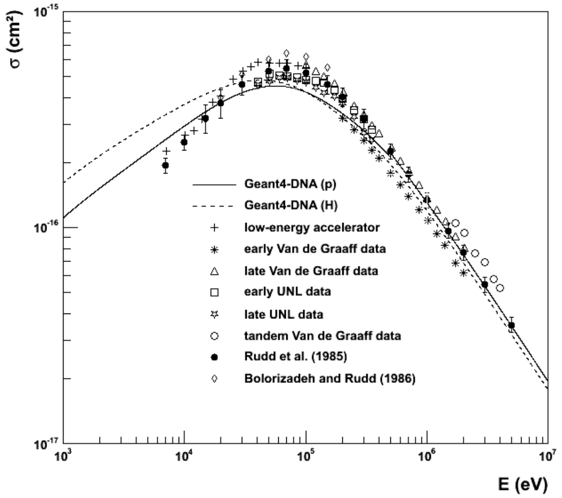
Helium and ion interactions in Geant4-DNA

- **Speed scaling** procedure using the corresponding proton cross sections

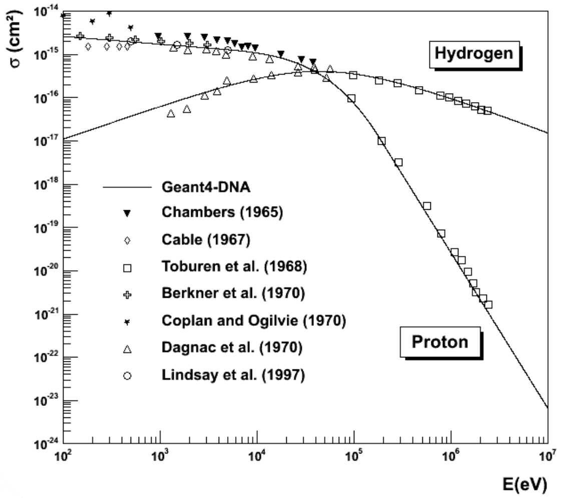
- Takes into account the **effective charge** of the incident projectile
  - Different effective charges used for He, He+, He++ projectiles
  - Charge transfer processes using the analytical fit by Dingfelder (2005)
  - For ions heavier than helium, only ionisation is taken into account using an effective charge formula by Booth and Grant (1965)

Validation and verification (for proton and helium)

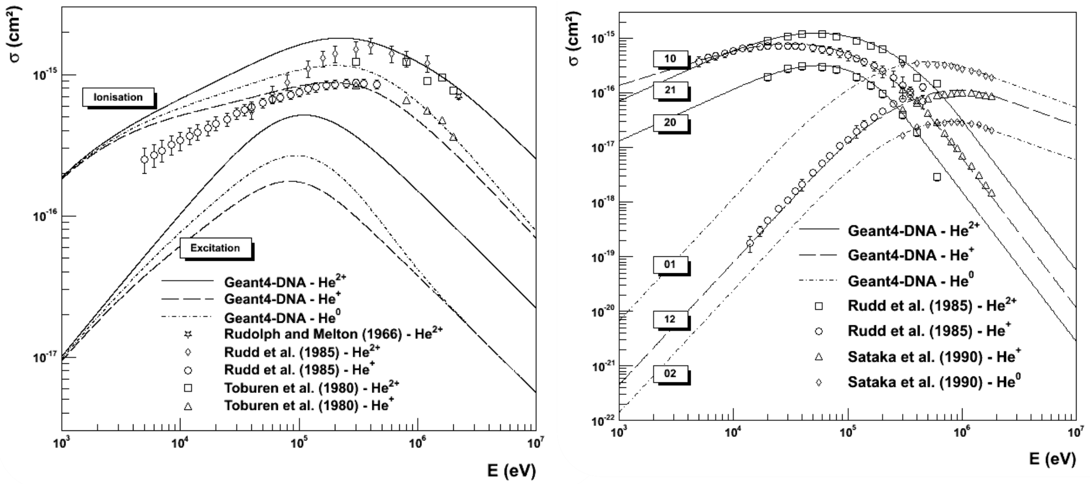
Proton CS: Ionisation



Proton CS: Charge exchange

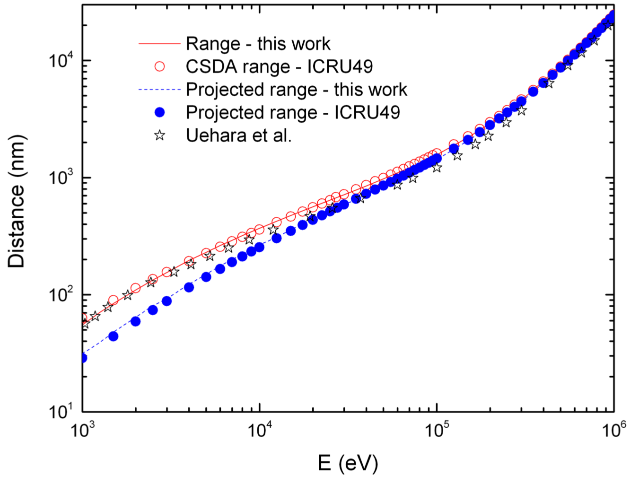


Helium CS: Ionisation & excitation, charge exchange

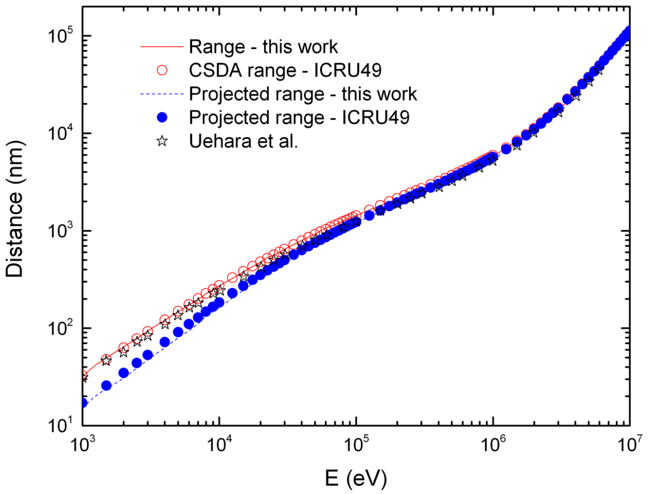


Ref.: Med. Phys. 37, 4692-4708 (2010)

Proton range



Helium range



Ref.: Nucl. Instrum. Meth. B 343, 132-137 (2015)

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

- Geant4-DNA is mainly dedicated to **(very) low energy charged particles**
  - Is it possible to simulate neutral particles such as photons?
  - 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
  - Geant4 **alternative EM** processes for charged particles
  - Geant4 **atomic de-excitation** (fluorescence + Auger emission, including cascades)
  - …and also Geant4 **hadronic physics**

Other processes: photons

- 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*`
      - Difference lies on the way they sample the final state
  - **Compton scattering**
    - Class: `G4LivermoreComptonModel`
  - **Photoelectric effect**
    - Class: `G4LivermorePhotoElectricModel`
  - **Rayleigh scattering**
    - Class: `G4LivermoreRighleighModel`
- 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 to Geant4-DNA
- There are different options that one can use to include bremsstrahlung interactions
  - Livermore, Penelope, Standard

Other processes: atomic de-excitation

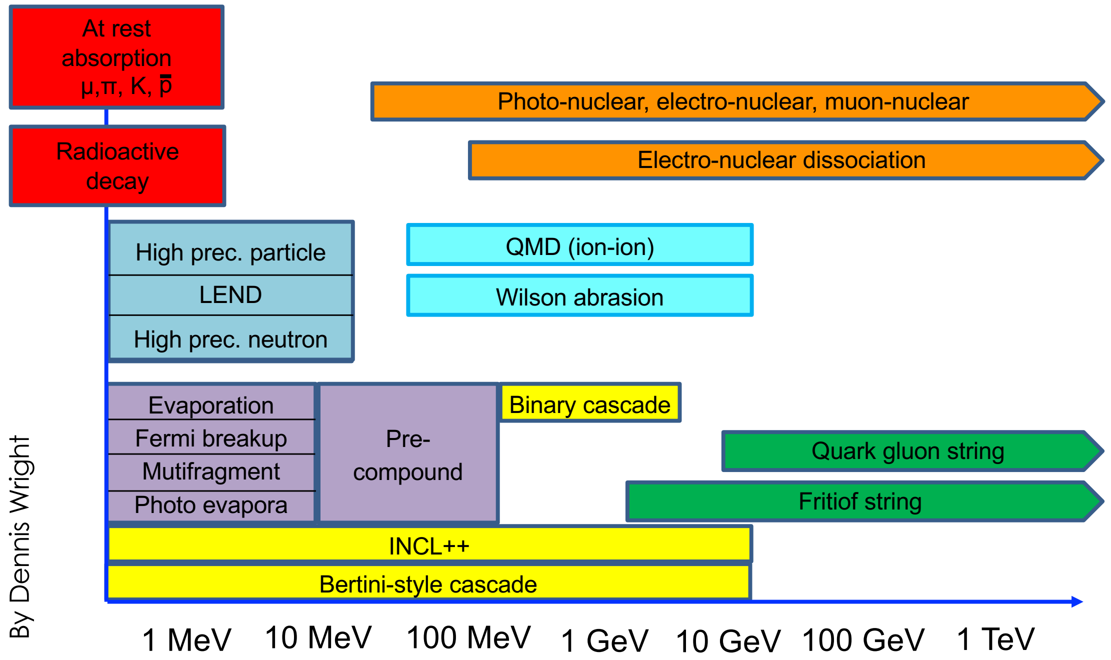
- Follows **vacancies created in atomic shells** to describe secondary effects after ionisation of an atom by the projectile
  - **Fluorescence emission**
  - **Auger cascades**
  - **PIXE (Particle Induced X-ray Emission)**

- Used for applications such as radiobiology, for material composition analysis, study of detector performance, optimization, etc.

- These simulations exist in the EM package of Geant4 and are not specific to Geant4-DNA

- Can be activated or deactivated with the use of **UI commands** in macro files

Other processes: hadronic processes



By Dennis Wright

High energy hadron models

FTF :Fritiof Parton String
QGS :Quark Gluon String

Low energy hadron models

BERT :Bertini-style cascade
BIC :Binary cascade
INCLXX :Liège intra-nuclear cascade (INCL)

Option for low energy hadron models

…P :Precompound model for nuclear de-excitation (for example, FTFP, QGSP, etc.)

Neutron model

HP :High Precision neutron **E < 20 MeV**

Recommendation for medical applications “QGSP_BIC”

How to activate?
please add following lines in your application

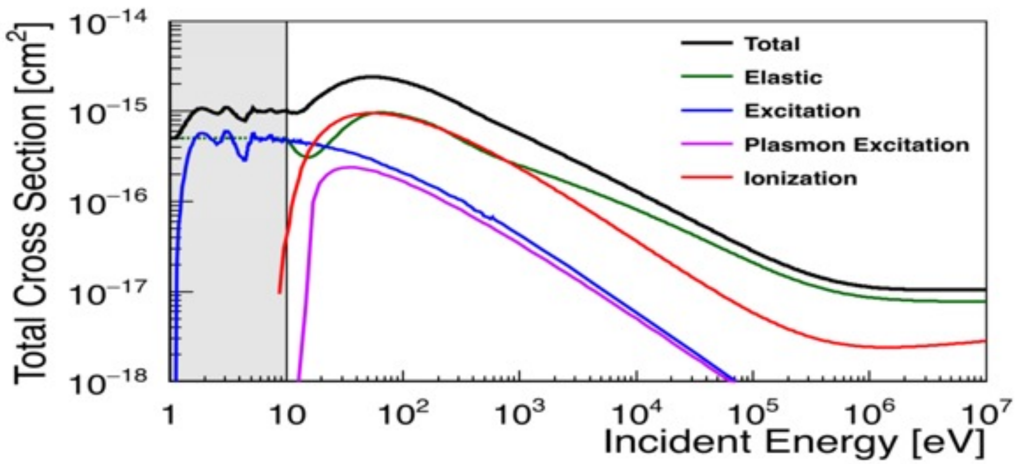
```
#include "QGSP_BIC.hh"

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

(some particles are not supported in Geant4-DNA)

Contents of this talk

Electron physics models for GOLD

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



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

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

See `examples/extended/medical/dna/AuNP`

Cross sections for DNA material

- **For DNA bases (A, T, G, C), sugar, phosphate**
  - Applicable to **electrons** in the 11 eV – 1 MeV range, derived from the CPA100 MCTS code
  - Processes
    - Elastic (IAM & ELSEPA, with Gaussian09 for molecular geometries)
    - Excitation (same scaling as for ionisation between liquid water and DNA components, as in CPA100)
    - Ionisation (Relativistic Binary Encounter Bethe Vriens)
  - Fully available in the option 6 Geant4-DNA physics constructor
    - Can be used **in any example** that uses option 6

Ref.: Nucl. Instrum. Meth. B 542, 51-60 (2023)
Ref.: Nucl. Instrum. Meth. B 488, 70-82 (2021)

- **For precursors of DNA material**
  - Based on gas-phase measurements from PTB lab. (Germany)
  - For 12 eV – 1 keV electrons (ionisation, excitation, elastic)
  - For 70 keV – 10 MeV protons (ionisation based on the HKS approach)
  - They serve as models for phosphate groups in the DNA backbone, DNA bases and deoxyribose
    - **Tetrahydrofuran** (THF) for deoxyribose
    - **Trimethylphosphate** (TMP) for phosphate
    - **Pyrimidine** (PY) for thymine, cytosine
    - **Purine** (PU) for adenine, guanine
    - (Nitrogen is also available)

Ref.: 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

Other recent developments in the physics of Geant4-DNA

- Extension of DNA-**Option 4 up to 10 MeV for electrons** (in progress)
- **Proton cross sections** based on the improved DNA-**Option 4** model (in progress)
- Extension of DNA-Option 6 to other biological targets is now available
  - Simulate **more reliably direct and indirect DNA damage**
- Cross sections for **N2, O2, CO2 molecules** for atmospheric simulations (in progress)
- Cross sections for **propane (C3H8)** for gas detectors (in progress)
- 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)

The 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)

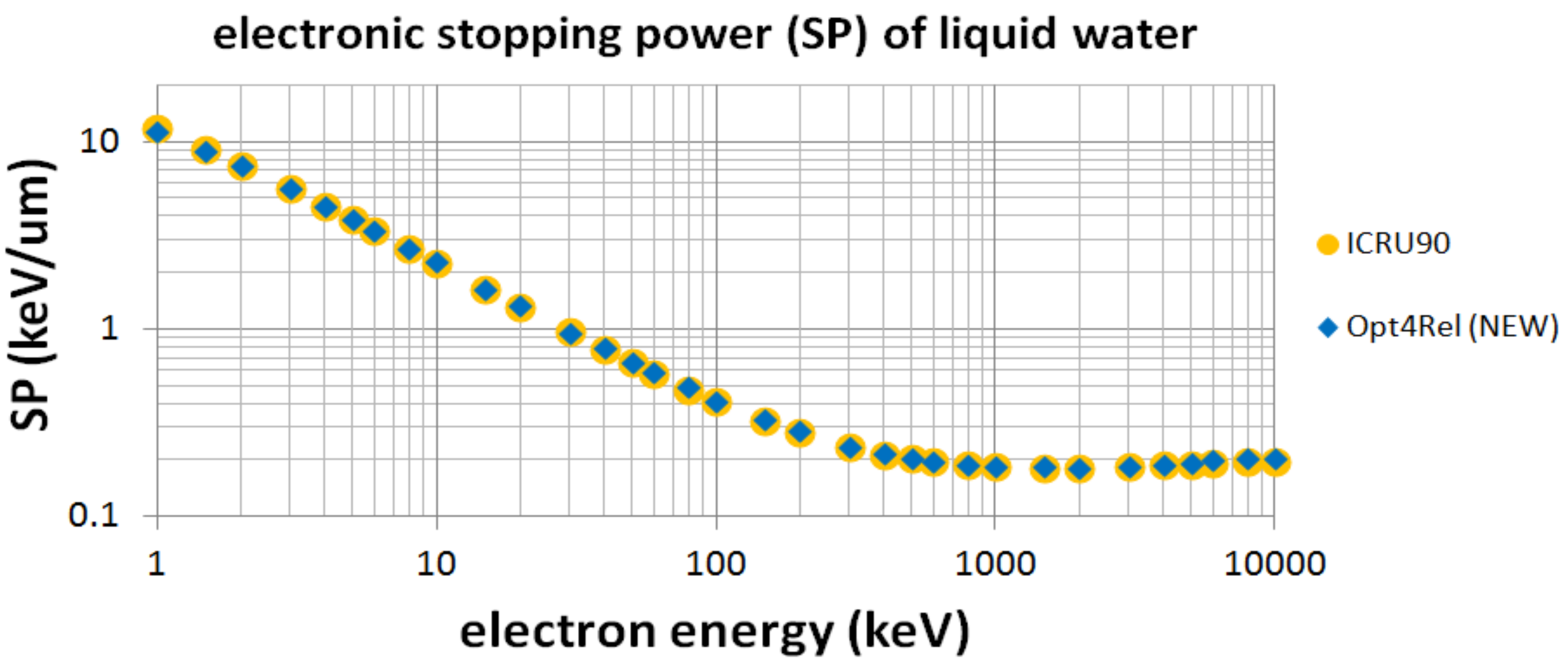
Alternative for elastic

Ref.: [Comput. Phys. Commun. 165, 157 (2005)]

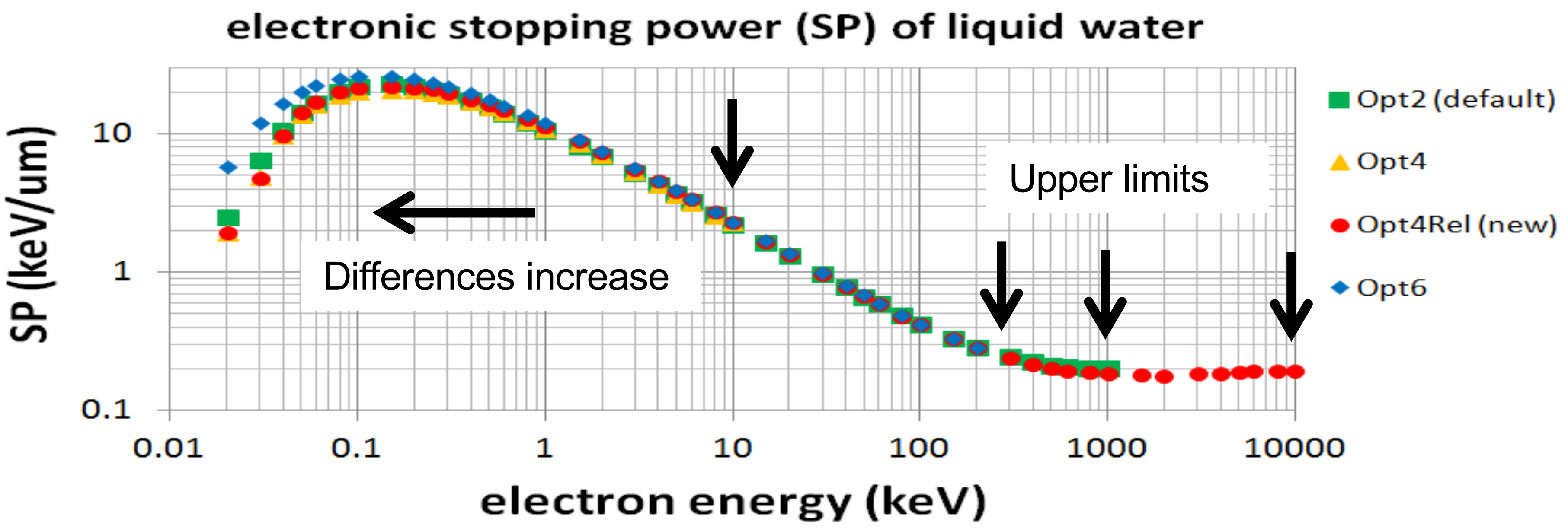
Extension of DNA_Option4 to relativistic energies

- On-going, will be released soon
- 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



Differences increase

Upper limits

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 extended 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 shows how to simulate track structures in liquid water using the Geant4-DNA physics processes and models, assembled in Geant4-DNA physics constructors. It also explains how to extract physical information at the step and track levels, 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 « **jetcounter** » **extended/medical/dna** example explains how to simulate a **gas dosimeter**.

See http://geant4-dna.org → Examples

Geant4-DNA Physics extended examples (cont.)

- The « **microdosimetry** » **extended/medical/dna** example shows how to use Geant4 and Geant4-DNA physics models in **different regions** of the geometrical setup, using the `G4EmDNAPhysicsActivator` class.
- 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 (y, z, …)**.
- The « **range** » **extended/medical/dna** example explains how to simulate **ranges**.
- The « **slowing** » **extended/medical/dna** example explains how to simulate **slowing down spectra**.

See http://geant4-dna.org → Examples

Geant4-DNA Physics extended examples (cont.)

- The « **splitting** » **extended/medical/dna** example explains how to accelerate simulation through **splitting in ionisation**.
- The « **spower** » **extended/medical/dna** example explains how to simulate **stopping powers**.
- The « **svalue** » **extended/medical/dna** example explains how to simulate "**S-values**" in spherical targets of liquid water.
- The « **wvalue** » **extended/medical/dna** example explains how to simulate "**W-values**" in liquid water.
- The « **AuNP** » **extended/medical/dna** example explains how to simulate track structures of electrons in a microscopic **gold volume** immersed in liquid water.

Ref.: Med. Phys. 45, e722-e739 (2018)
Ref.: Cancers 14, 35 (2022)

See http://geant4-dna.org → Examples

Geant4-DNA example: dnaphysics

Number of physical processes

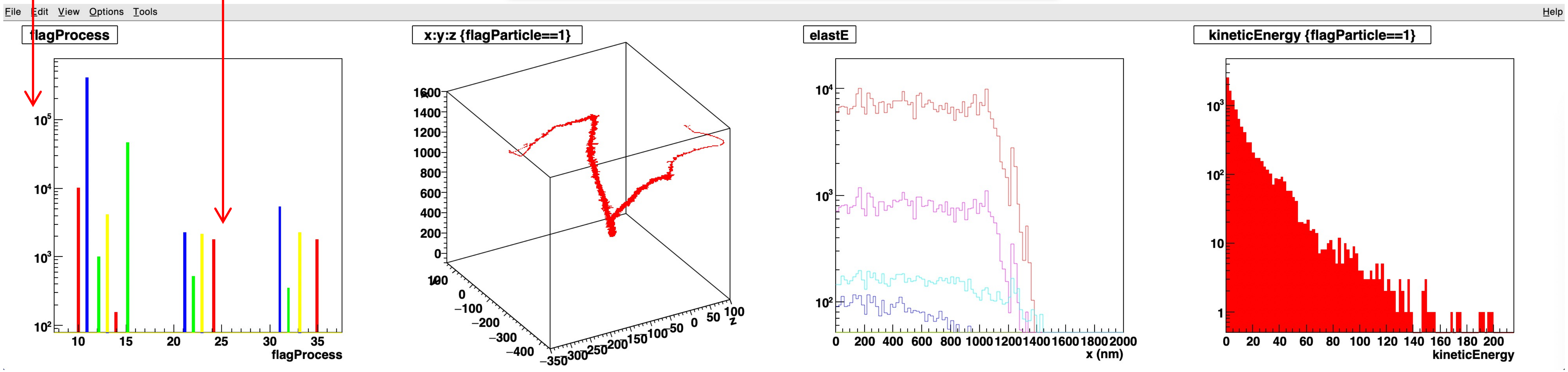
3D visualization of proton tracks

Longitudinal distributions

Secondary e- energy distribution

Type of physical processes (see README)

proton_G4DNAElastic	21
proton_G4DNAExcitation	22
proton_G4DNAIonisation	23
proton_G4DNAChargeDecrease	24



Thank you for your attention!

Any
questions?

ikyriak@uoi.gr

More slides…

Interaction types

- Inelastic collisions with **atomic electrons**
  - The dominant contribution to energy loss (and absorbed dose)
  - Leads to electronic excitations or ionisations
    - Hard collisions
      - **Eloss >> binding energy** → target electrons assumed quasi-free
    - Soft interactions
      - **Eloss ~ binding energy** → electronic structure must be considered
- Inelastic collisions with the **atomic nucleus** (Bremsstrahlung)
  - Important only at high energies (for electrons above ~1 MeV)
- Elastic collisions with the **atomic nucleus**
  - Mainly responsible for angular deflections
  - Energy loss is negligible

How to build a Geant4-DNA physics list?

Electron physics
mainly option2, 4, 6 is available

Proton physics

Ion physics

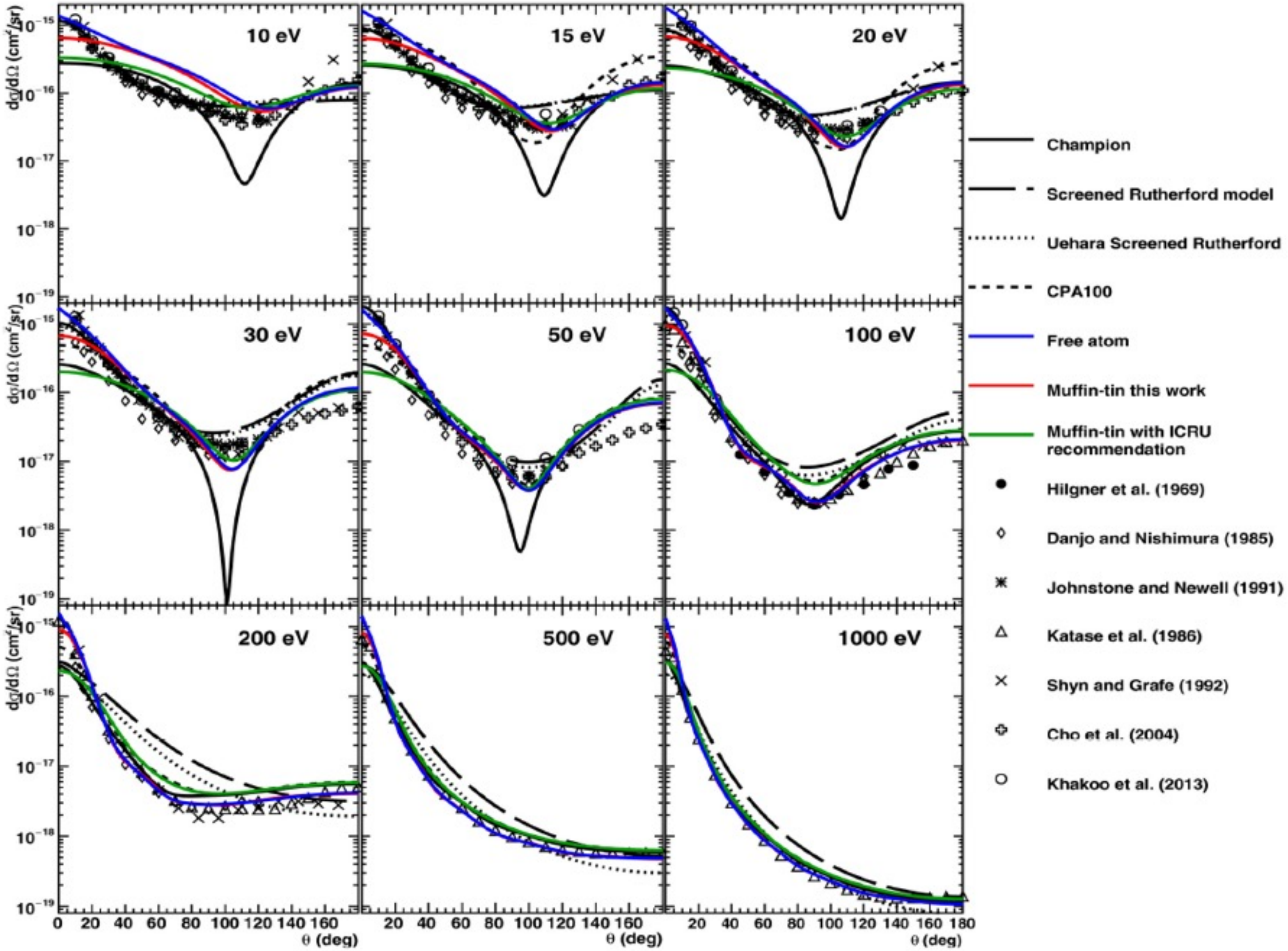
Alpha physics

```
// DNA physics
G4EmDNABuilder::ConstructDNAElectronPhysics(emaxDNA, 4, fast, st);
G4EmDNABuilder::ConstructDNAProtonPhysics(eminBorn, emaxIonDNA, 4, fast, st);
G4EmDNABuilder::ConstructDNAIonPhysics(emaxIonDNA, st);

G4ParticleDefinition* part = genericIonsManager->GetIon("hydrogen");
G4EmDNABuilder::ConstructDNALightIonPhysics(part, 0, 4, emaxIonDNA, fast, st);

part = G4Alpha::Alpha();
G4EmDNABuilder::ConstructDNALightIonPhysics(part, 2, 4, emaxIonDNA, fast, st);

part = genericIonsManager->GetIon("alpha+");
G4EmDNABuilder::ConstructDNALightIonPhysics(part, 1, 4, emaxIonDNA, fast, st);

part = genericIonsManager->GetIon("helium");
G4EmDNABuilder::ConstructDNALightIonPhysics(part, 0, 4, emaxIonDNA, fast, st);
```

see:
`$G4SRC/source/physics_lists/constructors/electromagnetic/src/G4EmDNAPhysics_option4.cc`

Improvement of electron elastic scattering: ELSEPA-based

- A new cross section data set has been developed using the ELSEPA approach.
- Parameters have been qualitatively optimized.
- The new model offers **significant improvement at < 1keV energies and at small-medium angles**.
- Available since version 10.6, it is expected to become the new default elastic model.



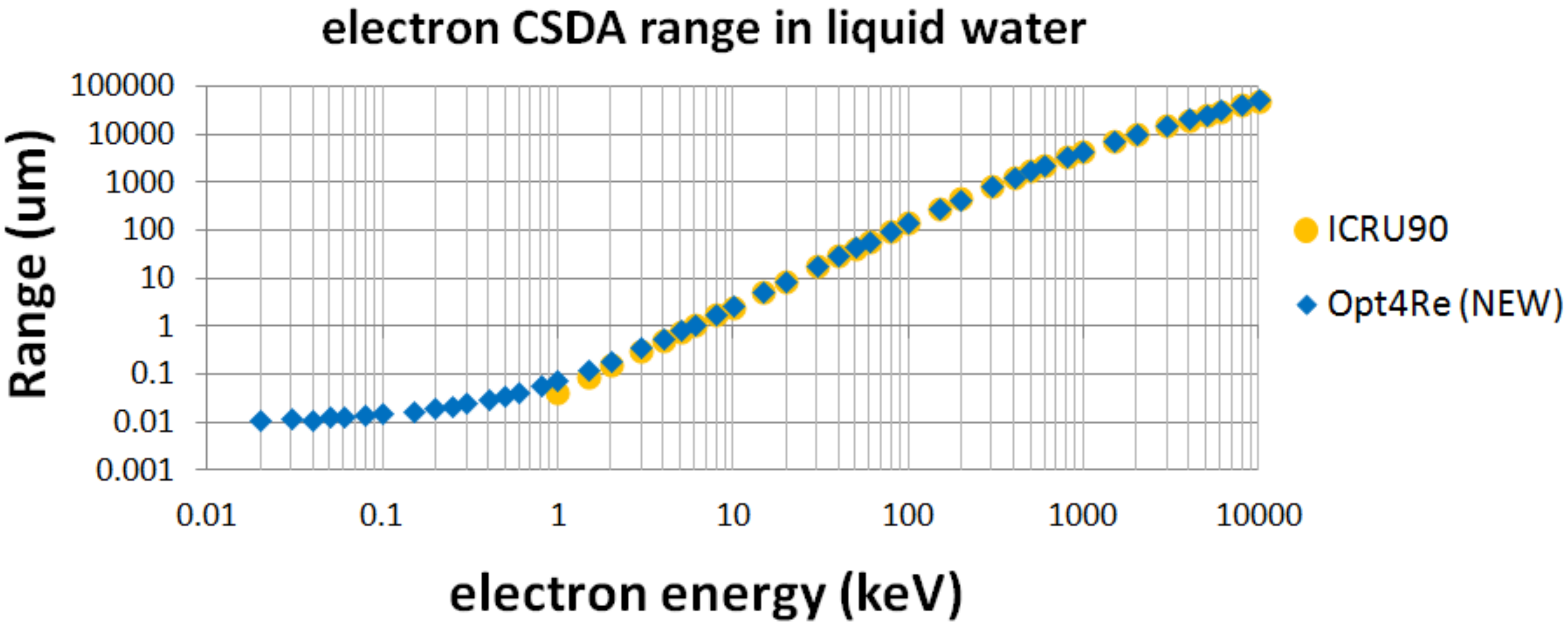
New features in relativistic DNA_Option 4

- Implementation of a new Energy-Loss-Function (ELF) using the algorithm developed at the Univ. of Ioannina with **improved features**
  - sum-rules,
  - parametrization of exp. data,
  - high energy asymptotic trend

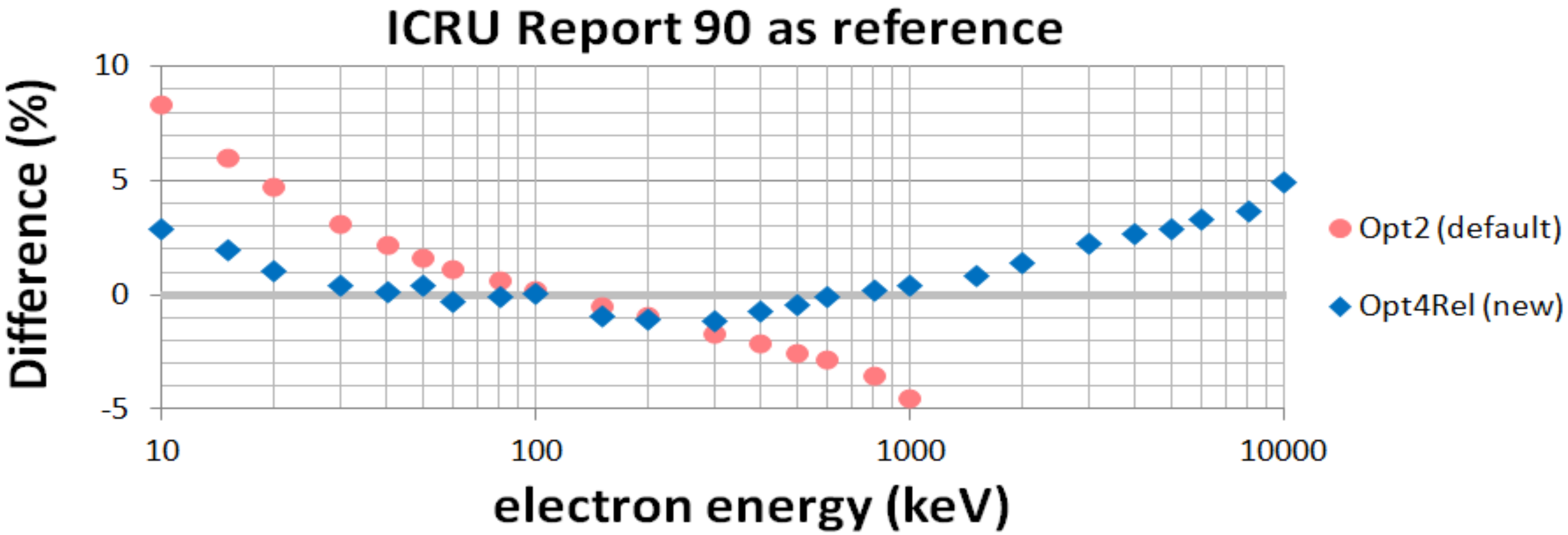
- More consistent implementation of **low-energy Born corrections**.

- Implementation of the **Fermi density correction** to the DCS (differential cross section).

New model within 5% from ICRU



Default model within 8% from ICRU



Basic magnitudes for the simulation of inelastic scattering with the use of a Monte Carlo code

- **Differential cross section** (DCS) over energy transfer (E):

$$\mathrm{DCS} \equiv \frac{\mathrm{d}\sigma}{\mathrm{d}E}$$

→ **TS codes**

- **Total cross section** (TCS) for inelastic scattering:

$$\mathrm{TCS} \equiv \sigma \equiv \int \frac{\mathrm{d}\sigma}{\mathrm{d}E}\, dE$$

→ **TS codes**

- **Stopping power** (SP) by electronic excitations:

$$\mathrm{SP} \equiv \int E\, \frac{\mathrm{d}\sigma}{\mathrm{d}E}\, dE$$

→ **CH codes**

Models based on the ELF

- Models based on the ELF

$$\boxed{\mathrm{DDCS} \equiv \frac{d^2\sigma(T)}{dEdq}}$$

  - T is the **kinetic energy** of the primary particle
  - E is the **energy-transfer** in the inelastic collision
  - q is the **momentum-transfer** in the inelastic collision
    - q is **equivalent to the scattering angle θ of the primary particle**

$$q = \sqrt{2m}[2T - W - 2\sqrt{T(T-W)}\cos\theta]^{1/2}$$

$(W \sim E)$

The central role of the Born approximation

The DDCS is calculated based on the plane-wave Born approximation (PWBA) or simply the **1st Born approximation**

Why ?

The advantage of the Born approximation

- The DDCS is factorized into a particle-dependent term and a **material-dependent** term
- The particle term is trivial
    - only the charge and velocity are needed
- The **material** term can be measured by many spectroscopic techniques

$$\boxed{\mathrm{DDCS}_{\mathrm{Born}} = \underbrace{(\text{particle term})}_{\text{trivial}} \text{ x } \underbrace{(\text{material term})}_{\text{measurable}}}$$

What is the material term?

$$\mathrm{DDCS}_{\mathrm{Born}} = \underbrace{(\text{particle term})}_{\text{trivial}} \times \underbrace{(\text{material term})}_{\text{measurable}}$$

For condensed media, the material term is the energy-loss-function (ELF)

For gases, the material term is the generalised-oscillator-strength (GOS)

ELF and GOS

- Both are functions of **energy-transfer** (E) and **momentum-transfer** (q)
- Both give the **probability of excitation of a target atom** for a given pair of values (E, q)
- Both are **properties of the medium** and do NOT depend on the particle, i.e. they are the same for electrons, protons, etc.

The 3-dimensional plot of ELF or GOS versus E and q is given a special name: the Bethe surface

Cross sections

$$\mathrm{DDCS_{Born}} = (\text{particle term}) \times \mathrm{ELF}(\mathrm{E},\mathrm{q})$$

$$\mathrm{DCS_{Born}} = (\text{particle term}) \times \int_{\mathrm{q_{min}}}^{\mathrm{q_{max}}} \mathrm{ELF}(\mathrm{E},\mathrm{q})\,dq$$

$$\mathrm{TCS_{Born}} = (\text{particle term}) \times \int_{\mathrm{E_{min}}}^{\mathrm{E_{min}}} dE \int_{\mathrm{q_{min}}}^{\mathrm{q_{max}}} \mathrm{ELF}(\mathrm{E},\mathrm{q})\,dq$$

$$\mathrm{SP_{Born}} = (\text{particle term}) \times \int_{\mathrm{E_{min}}}^{\mathrm{E_{min}}} E\,dE \int_{\mathrm{q_{min}}}^{\mathrm{q_{max}}} \mathrm{ELF}(\mathrm{E},\mathrm{q})\,dq$$

If the medium is a gas simply replace ELF by GOS

Methods to compute the ELF

- **Ab initio methods**
  - They are based on (complicated) theory
  - Computationally intensive
  - **Limited energy range** (~< 50 eV)

- **Homogeneous electron gas theory**
  - They are based on well-established theory
  - **Limited material range** (only simple metals, e.g. aluminum)

- **Optical-data models**
  - Semi-empirical
  - Depend on the availability of **experimental** optical data
  - Applicable to **many materials** and **wide energy range**

Constructing optical data models for ELF

- **Step 1**: Assume excitation (k) and ionisation (n) channels and the corresponding threshold energies
- **Step 2**: Decompose the ELF as following:

$$\mathrm{Im}\left[-\frac{1}{\varepsilon(E,q)}\right]=\sum_{n/k}\frac{\mathrm{Im}[\varepsilon_{n/k}(E,q)]}{|\varepsilon(E,q)|^2}$$

- **Step 3**: Obtain Im[ε(E,q=0)] from fit to experimental data
- **Step 4**: Perform *f-sum-rule* test for Im[ε(E,q=0)]
- **Step 5**: Calculate Re[ε(E,0)] via Kramers-Kronig
- **Step 6**: Calculate ELF(E,0) and perform *f-sum-rule* test for ELF
- **Step 7**: Extend ELF to q > 0 by dispersion relations

ELF and dielectric function

The **ELF** is defined through the **dielectric-response-function (DRF)** of the medium

$$\text{ELF}\left\{\mathrm{Im}\left[\frac{-1}{\underbrace{\varepsilon(E,q)}_{\text{DRF}}}\right]\right. = \frac{\varepsilon_2(E,q)}{\varepsilon_1^2(E,q)+\varepsilon_2^2(E,q)}$$

The DRF is a complex function and accounts for the screening and absorption properties of the medium

$$\varepsilon(E,q)=\underbrace{\varepsilon_1(E,q)}_{\text{screening}}+i\underbrace{\varepsilon_2(E,q)}_{\text{absorption}}$$

The **ELF** includes the different absorption channels of the medium as modified by the screening properties of the medium

$$\mathrm{Im}\left[\frac{-1}{\varepsilon(E,q)}\right]=\sum_{n}^{\text{all}}\frac{\varepsilon_2^{(n)}(E,q)}{|\varepsilon(E,q)|^2},$$

→ **Absorption channels**

→ **Screening**

Summary about ELF models

- **Main advantages:**
  - Self-consistency tests are available
  - Condensed-phase effects are in-built through the dielectric function
  - Experimental data of ELF available for many materials
  - Reliable over a wide energy range (Born approximation)

- **Main disadvantages:**
  - Limited experimental data for the ELF at q>0
  - Cross sections specific to the different ionisation shells and excitation levels are not well known

Analytic models

- **Several analytic models** for the ionisation cross section are available:
  - Moller
  - Weizsacker-Williams (WW)
  - Gryzinski
  - Vriens (BEA)
  - Seltzer (WW+BEA)
  - Miller-Wilson-Manson (MWM)
  - Kim-Rudd (BED, BEB)

The general idea

They try to predict the correct “mixing” of soft and hard collisions in the DCS

Moller, Gryzinski, Vriens (BEA) ignore the soft term:
apply <u>only</u> to hard collisions

Seltzer, MWM, BED, BEB consider <u>both</u>
the soft & hard terms

$$\frac{d\sigma_i}{dE} = f_{\mathrm{soft}} \frac{d\sigma_i}{dE}\bigg|_{\mathrm{soft}} + f_{\mathrm{hard}} \frac{d\sigma_i}{dE}\bigg|_{\mathrm{hard}}$$

They differ on how they determine these weighting functions

$$\frac{d\sigma_i}{dE} = \cancel{f_{\mathrm{soft}} \frac{d\sigma_i}{dE}\bigg|_{\mathrm{soft}}} + f_{\mathrm{hard}} \frac{d\sigma_i}{dE}\bigg|_{\mathrm{hard}}$$

$$\frac{d\sigma_i}{dE} = f_{\mathrm{soft}} \frac{d\sigma_i}{dE}\bigg|_{\mathrm{soft}} + f_{\mathrm{hard}} \frac{d\sigma_i}{dE}\bigg|_{\mathrm{hard}}$$

Use approx. GOS(q=0) for soft term

Use BEA for hard term

Most used analytic models

- **Seltzer's model**
  - Soft term based on photoelectric cross section (through the WW)
  - Hard term based on BEA-with-exchange (BEAX) model
  - $f_{soft} = f_{hard} = 1$
  - Used in KURBUC (vapor version), RETRACKS, Livermore (EEDL)

- **Kim-Rudd models (BED, BEB)**
  - Soft term based on the OOS (BED) or simple analytic approx (BEB)
  - Hard term based on the BEA-with-exchange (BEAX) model
  - f_{soft} and f_{hard} are adjusted to give the Bethe approximation
  - BEB is used in CPA100

Summary of analytic models

- **Main advantages:**
  - Simple to use with only few material parameters
  - Provide analytic expressions for the cross section
  - Cross sections specific to the different ionisation shells are available
  - Reliable over a wide energy range (Born approximation)

- **Main disadvantages:**
  - Self-consistency tests are NOT available
  - Apply ONLY to ionisations (excitations are NOT included)
  - For condensed media they are **NOT reliable below ~1 keV**