Light version

Low Energy Electromagnetic Physics

Sébastien Incerti et al.

CNRS/IN2P3/Bordeaux U., France

on behalf of both EM Working Groups

G4 10.4 BETA
30 June 2017

Overview of physics models for liquid water

- **Electrons**
  - **Elastic scattering**
    - Screened Rutherford and Brenner-Zaider below 200 eV
    - Updated alternative version by Uehara
    - Independent Atom Method (IAM) by Mott et al. & VLE data in ice from CPA100 code
    - Partial wave framework model by Champion et al., 3 contributions to the interaction potential
  - **Ionisation**
    - 5 levels for H_2O
    - Dielectric formalism & FBA using Heller optical data up to 1 MeV, and low energy corrections, by Emfietzoglou et al.
    - Improved alternative version by Emfietzoglou and Kyriakou
    - Relativistic Binary Encounter Bethe (RBEB) by Terrissol from CPA100 code
  - **Excitation (*)**
    - 5 levels for H_2O
    - Dielectric formalism & FBA using Heller optical data and semi-empirical low energy corrections, , derived from the work of Emfietzoglou et al.
    - Improved alternative version by Emfietzoglou and Kyriakou
    - Dielectric formalism by Dingfelder from CP100 code
  - **Vibrational excitation (*)**
    - Michaud *et al.* xs measurements in amorphous ice
    - Factor 2 to account for phase effect
  - **Dissociative attachment (*)**
    - Melton xs measurements

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

PhD thesis of H. N. Tran (2012), Q. T. Pham (2014), J. Bordes (2017)

(*) only available in Geant4-DNA

- **Protons & H**
  - **Excitation (*)**
    - Miller & Green speed scaling of e^- excitation at low energies and Born and Bethe theories above 500 keV, from Dingfelder *et al.*
  - **Ionisation**
    - Rudd semi-empirical approach by Dingfelder *et al.* and Born and Bethe theories & dielectric formalism above 500 keV (relativistic + Fermi density)
  - **Charge change (*)**
    - Analytical parametrizations by Dingfelder *et al.*
  - **Nuclear scattering**
    - Classical approach by Everhart *et al.*
- **He^0, He^+, He^{2+}**
  - **Excitation (*) and ionisation**
    - Speed and effective charge scaling from protons by Dingfelder *et al.*
  - **Charge change (*)**
    - Semi-empirical models from Dingfelder *et al.*
  - **Nuclear scattering**
    - Classical approach by Everhart *et al.*
- **Li, Be, B, C, N, O, Si, Fe**
  - **Ionisation**
    - Speed scaling and global effective charge by Booth and Grant
- **Photons**

from EM « standard » and « low energy »

- Default: « Livermore » (EPDL97)

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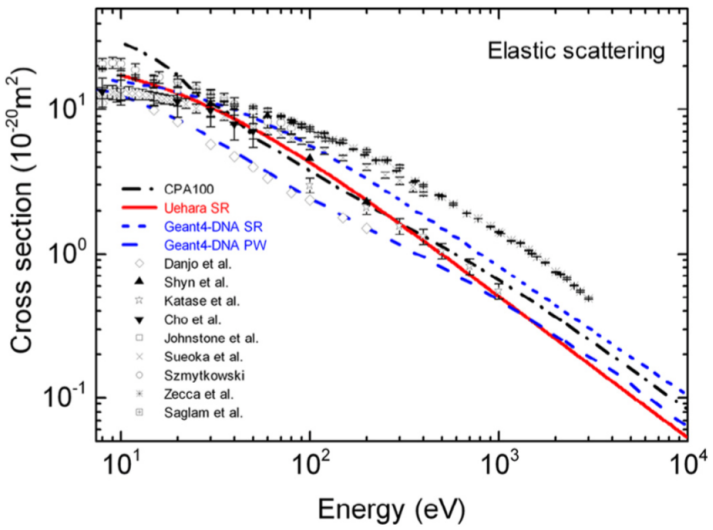
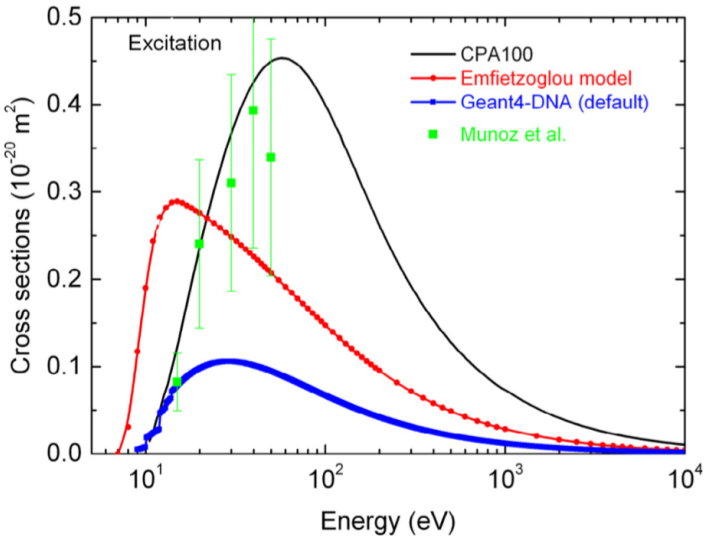
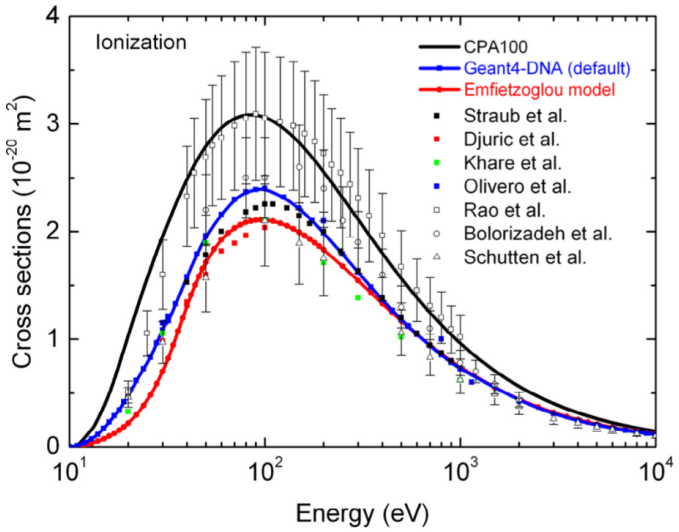
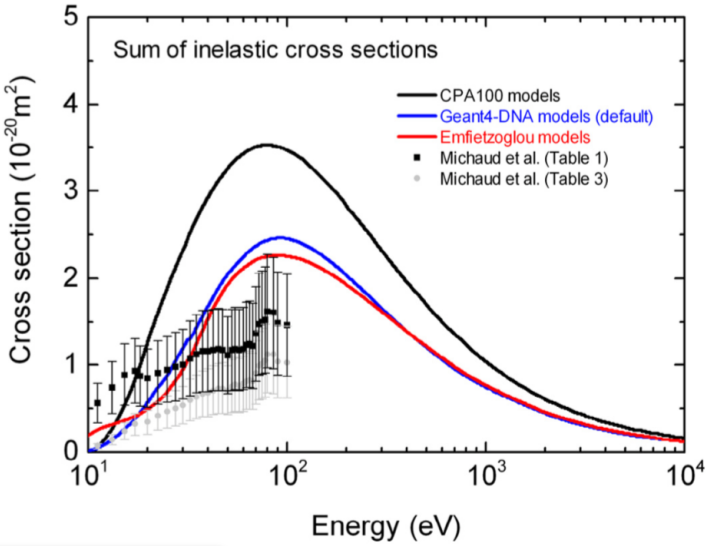
Cross section models for electrons









Phys. Med. 31 (2015) 861 (link)

Ioannina models (1)

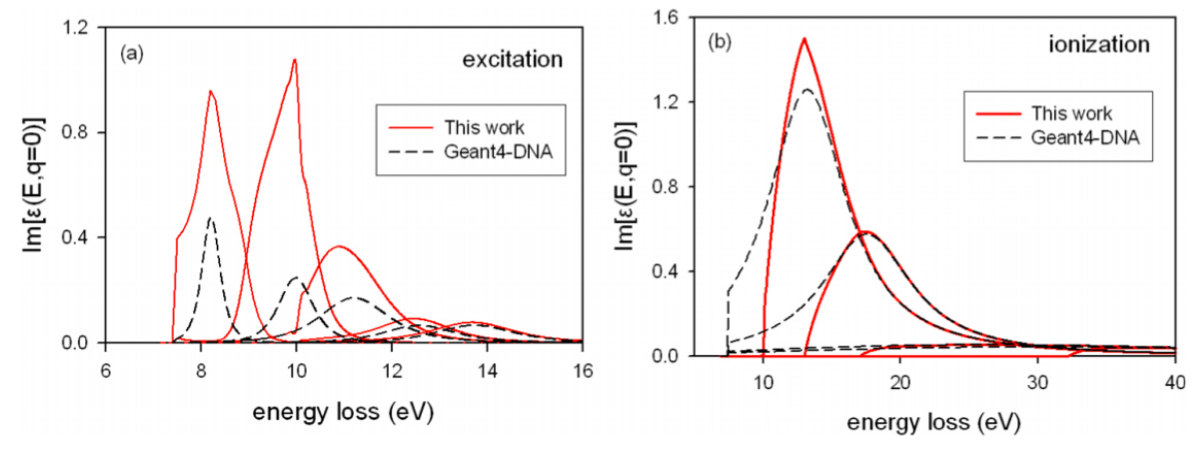
Med. Phys. 42 (2015) 3870 (link)

On behalf of
Ioanna Kyriakou
(Ioannina U., Greece)
SEE TALK session 5B

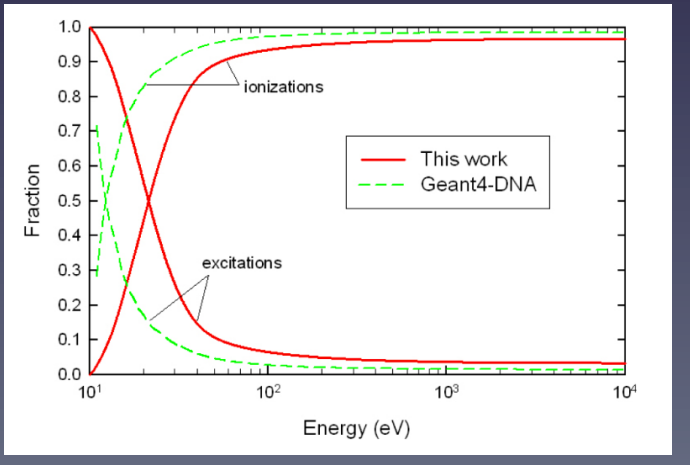
- A new set of alternative models improving the accuracy of electrons interactions, developped by I. Kyriakou and D. Emfietzoglou, Ioannina U., Greece
- Main improvements
  - truncation algorithm modifies imaginary part of the dielectric function model :
    - enhance the contribution of the excitation states [see (a)]

      while eliminating the contribution of each ionization state below the corresponding binding energy with a concomitant smoothing at the near-threshold region [see (b)]
  - low energy corrections for exchange and correlation in electron–electron interactions and corrections for the departure from the plane-wave 1rst-order perturbation theory
  - elastic sc.: screening factor proposed by Uehara from vapor experimental data, instead of Grosswendt-Waibel

Imaginary part of the dielectric function model



Contribution of ionizations and excitations to the total inelastic cross section

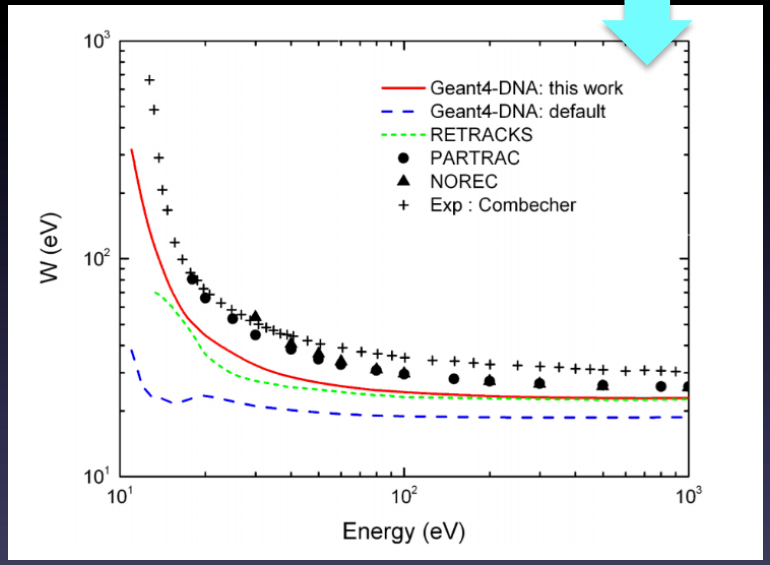


Ioannina models (2)

On behalf of
Ioanna Kyriakou
(Ioannina U., Greece)
SEE TALK session 5B

Exzample of verification & validation in liquid water

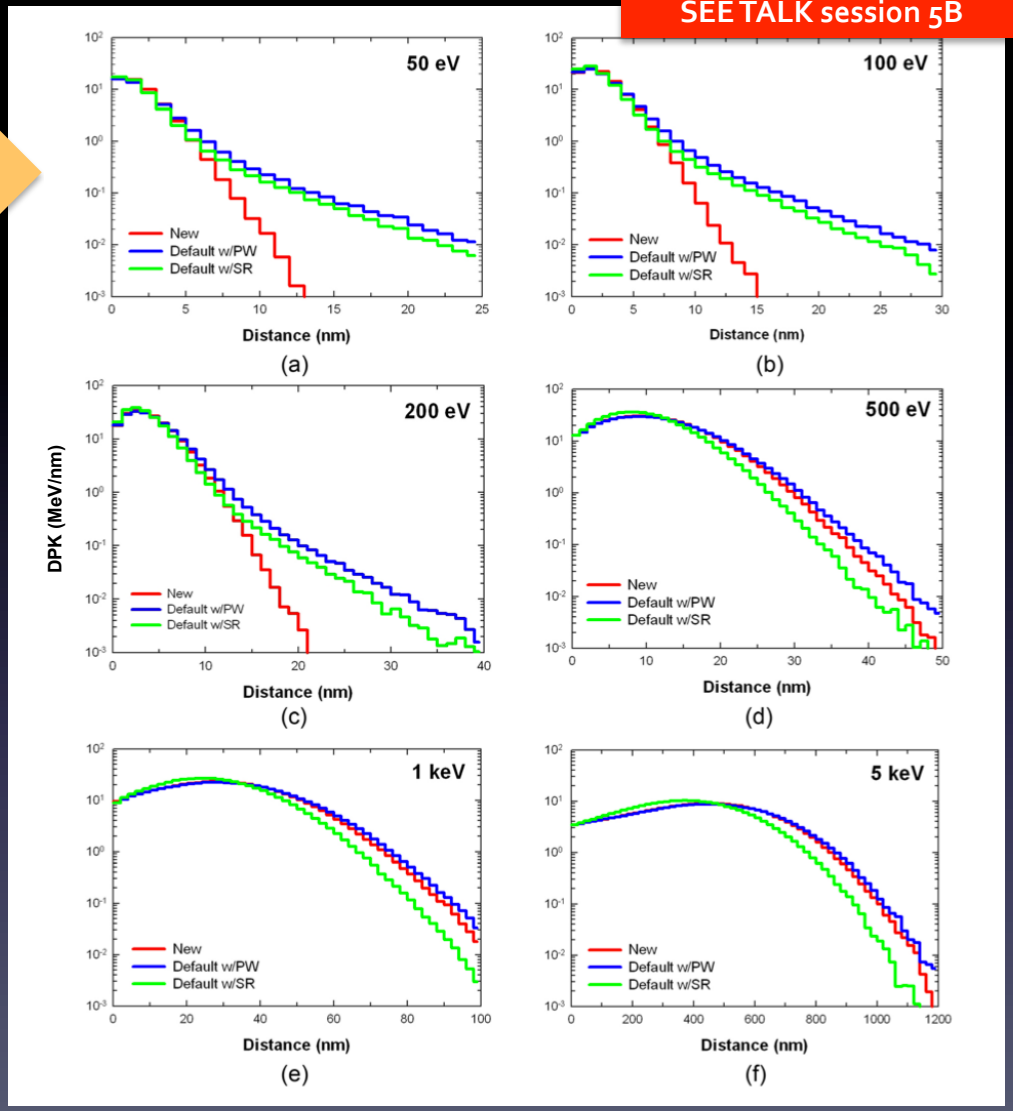
- Dose Point Kernels
- W-value (mean energy to create an ion pair)



The larger the excitation-to-ionization cross section ratio is, the higher the W-value since a smaller number of ion pairs will be formed (for the same electron energy dissipated)

Some difference with the experimental data for gaseous water is expected and confirms the well-established higher ionization yield of the liquid phase compared to the gas phase.

Med. Phys. 42 (2015) 3870 (link)
J. Appl. Phys. 32 (2016) 119, 194902 (link)



Much less diffusive DPKs with the new inelastic model. With the default model, small excitation cross sections (dominant at large distance and low energy) allow these very low energy electrons to diffuse much longer distances in the medium before their energy falls below the cut-off

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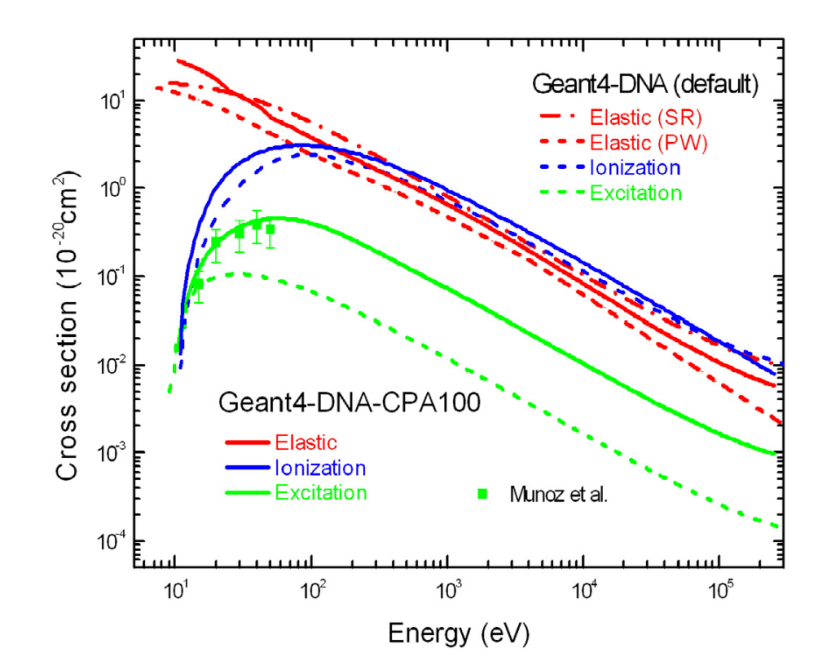
Phys. Med. 32 (2016) 1833 (link)

CPA100 models (1)

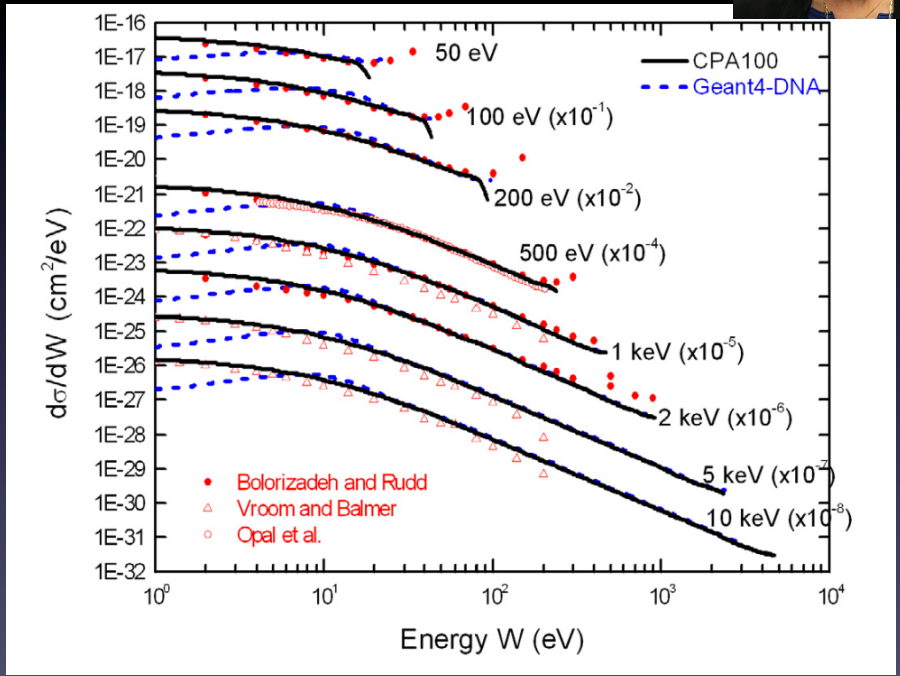
On behalf of
Marie-Claude Bordage
(CNRS, France)

An alternative set of models for electrons (10 eV – 255 keV)
from the original CPA10 Track Structure code
(M. Terrissol, M. C. Bordage, Toulouse U. , France)

Integral cross sections for electrons



Differential ionisation cross section



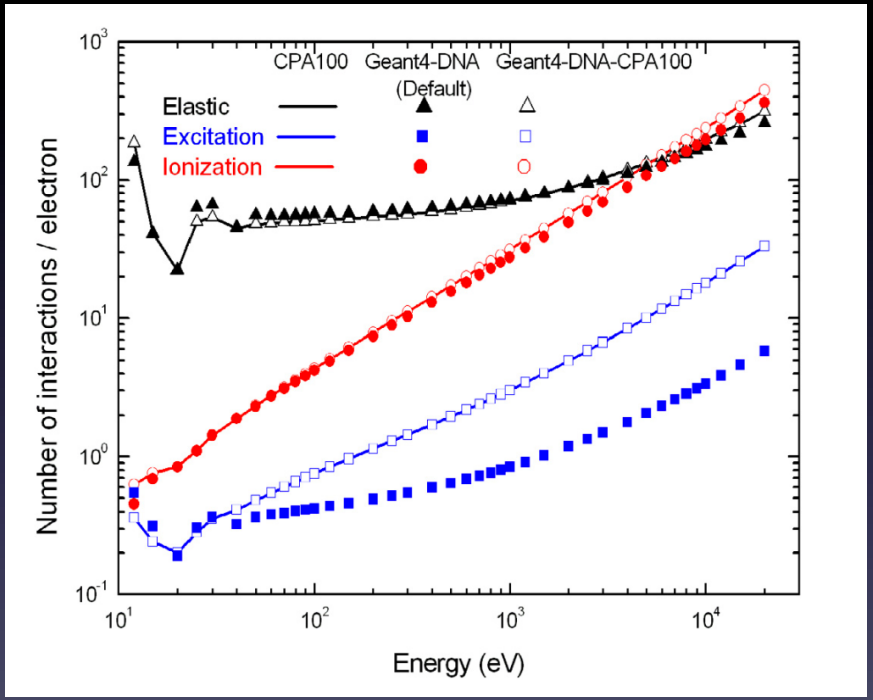
- CPA100 excitation model is in better agreement with the only experimental data in the gaseous water by Munoz et al.
- one order of magnitude, between the CPA100 model and the Geant4-DNA default model for each excitation state

- good agreement between data and CPA100 cross sections, especially at low ejected kinetic energies (where the differential cross section is the largest).
- main differences between Geant4-DNA default model and the experimental data are observed at ejected electron energy W lower than 10 eV.

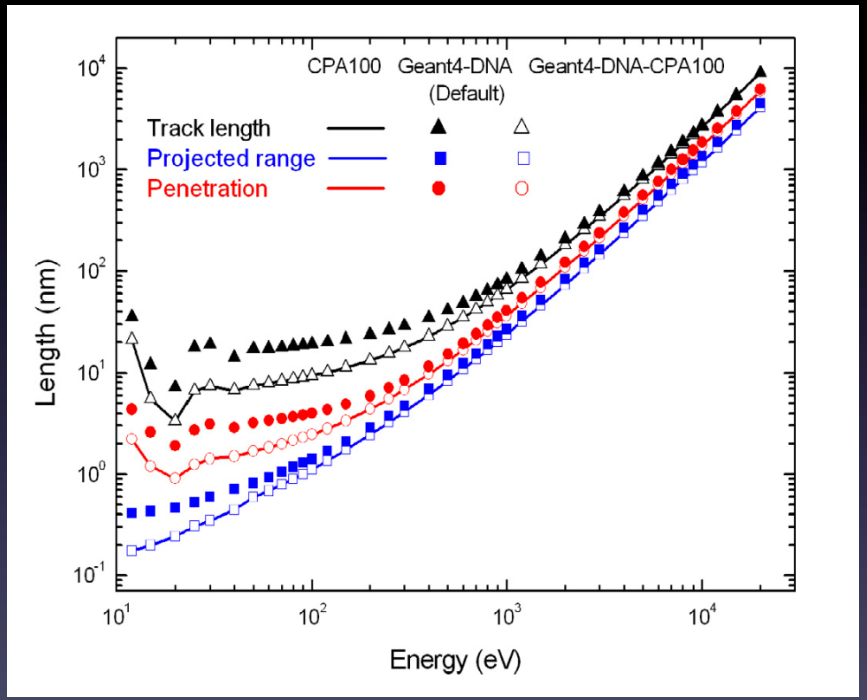
Phys. Med. 32 (2016) 1833 (link)

CPA100 models (2)

Numbers of interactions



Track length, penetration & projection range



The main differences appear in the number of excitations from 20 keV down to 20 eV, originating from the difference of magnitude between CPA100 and Geant4-DNA default excitation cross sections

- differences between the models are larger when considering track length, rather than the number of collisions, especially at low energies (<1 keV) (eg. 50% at 50 eV)
- electrons lose less energy and consequently travel larger distances in liquid water when simulated using Geant4-DNA default models compared to CPA100 (CPA100 inelastic cross sections are larger)

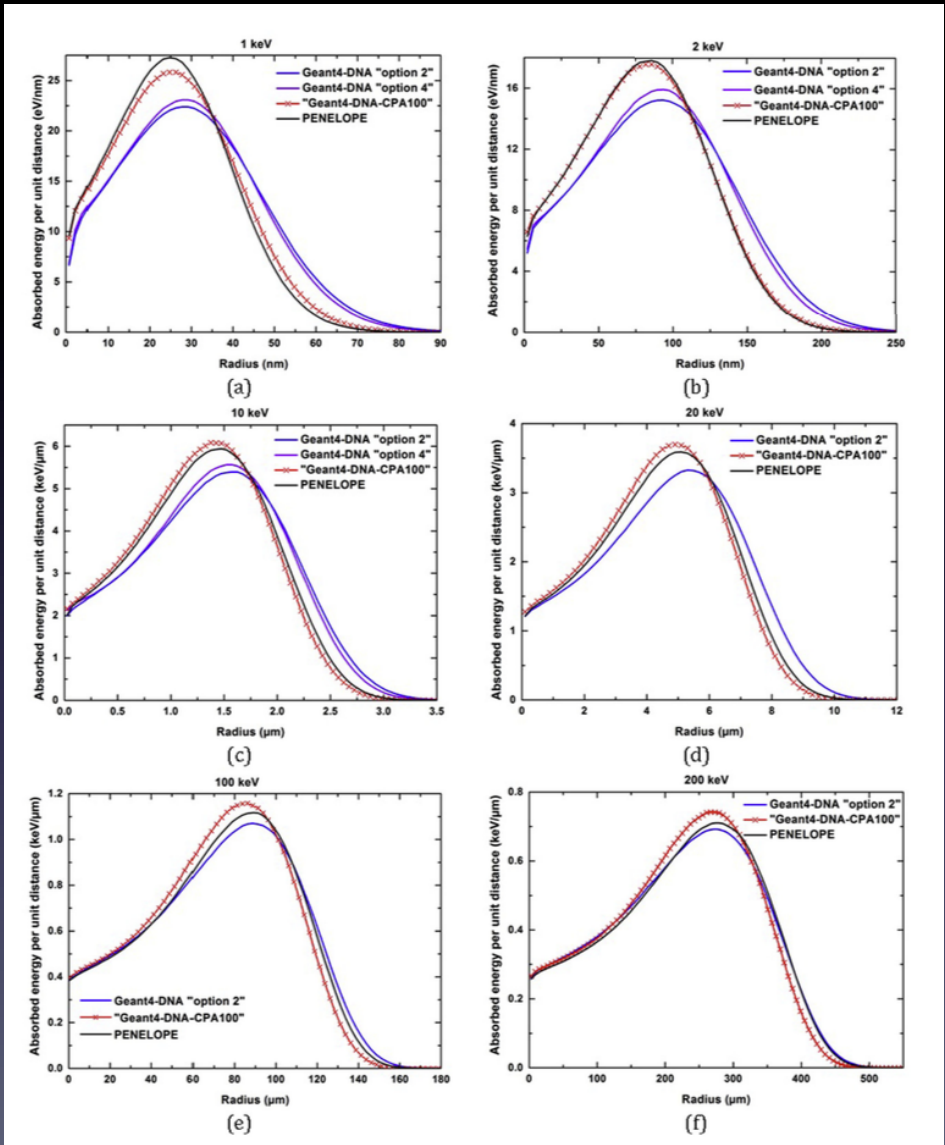
CPA100 models (3)

Example of Dose Point Kernel comparison in liquid water between

- Geant4-DNA option 2 (default)
- Geant4-DNA option 4 (Ioannina)
- Geant4-DNA CPA100 models
- PENELOPE 2011

The comparison with the reference Monte Carlo code PENELOPE, set to perform step-by-step simulation, showed good agreement < 20 keV.

For all tested energies, the maximum relative difference between simulated DPK, which occurs for 1 keV electrons, is less than 10 %.



Nucl. Instrum. and Meth. B 398 (2017) 13 (link)

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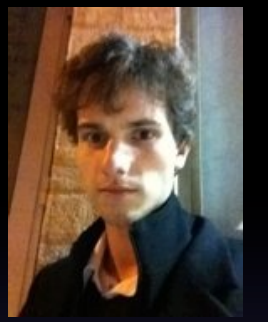
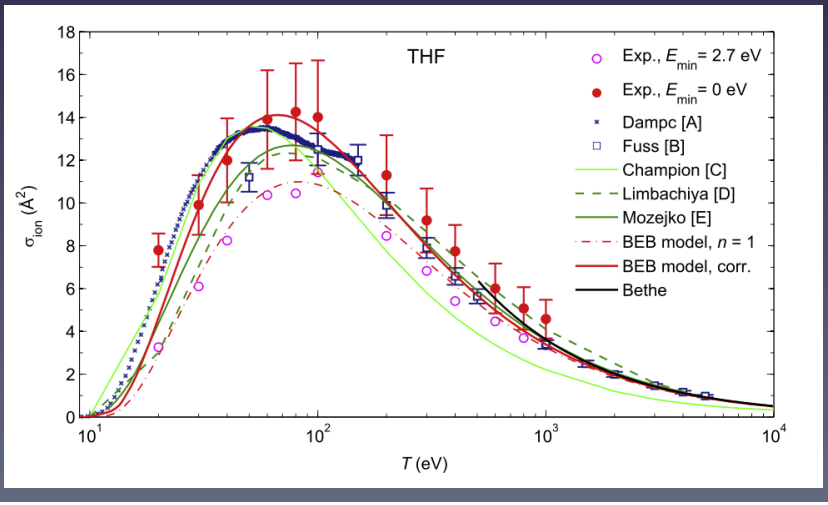
Other bio-materials (1)



- 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, by C. Villagrasa & S. Meylan (IRSN, France)
  - 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 bases
- For the following incident particles
  - electrons (12 eV-1keV, elastic + excitation + ionisation) : from measurements @ PTB, Germany
  - protons (70 keV-10 MeV, ionisation) from the HKS approach

Eg. total electron ionisation cross sections in THF



More details in
Rad. Phys. Chem. 130 (2017) 459–479

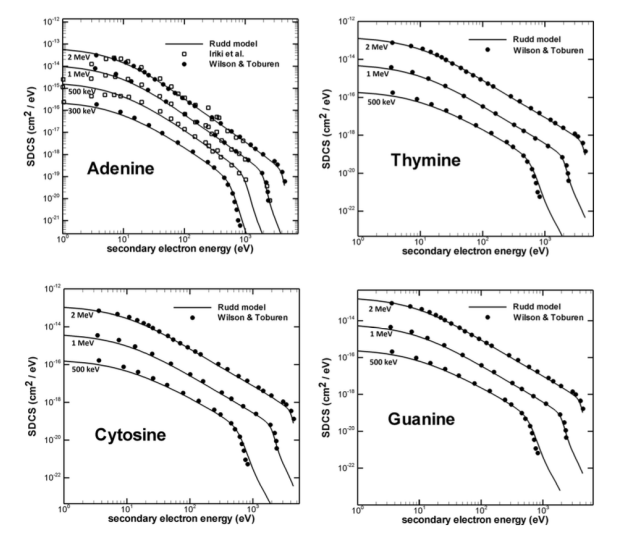
2018-2019

J. Appl. Phys. 122 (2017) 014701 (link)

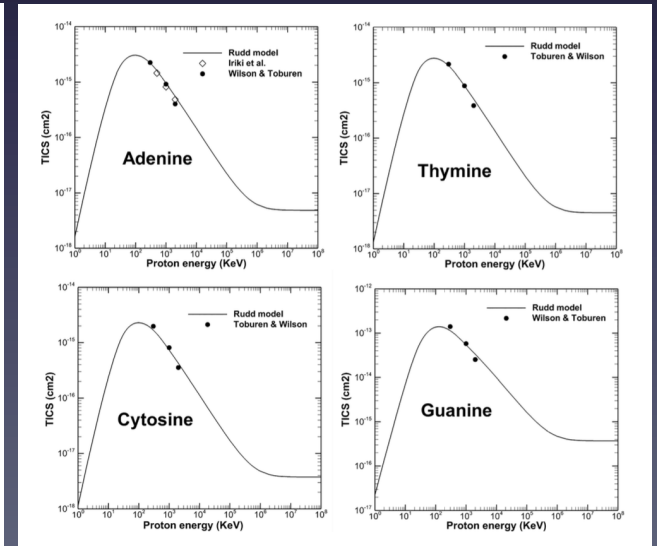
Other bio-materials (2)

- New model describing ionisation of the four bases of DNA (adenine, thymine, cytosine and guanine) by incident protons, by Z. Francis (St Joseph U., Lebanon)
- 1 keV – 10^8 keV
- based on the relativistic analytical Rudd approach, fitted to experimental data
- will be publicly released in the near future

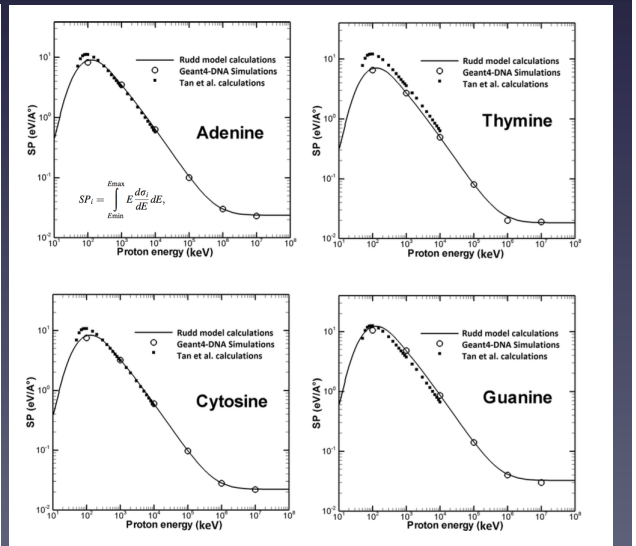
Single differential cross section



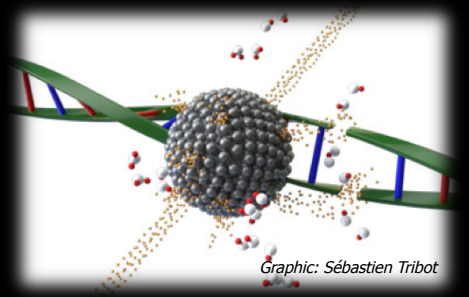
Total cross section



Stopping power

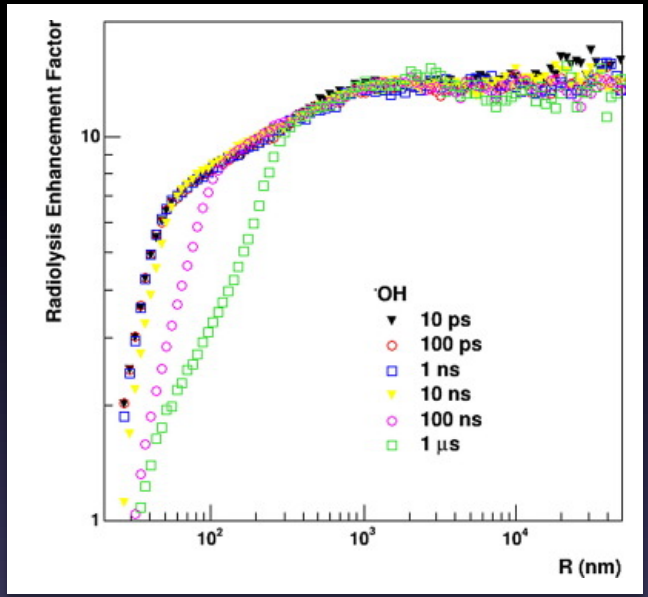


Investigation of radiotherapy sensitization using high-Z nanoparticles



- "Hot" topic: high-Z NP internalized in cells could boost energy deposition and increase the efficacy of radiotherapy

- Well established for photon beams (photoelectric effect), not so clear for proton beams…



- Still a challenge to perform mechanistic simulations
  - We initiated a specific Geant4-DNA activity on the subject in 2015
  - Simulation of physics + physico-chemistry + chemistry around NP (using Livermore for Gold)
  - Eg. Radiolysis Enhancement Factor as a function of distance from GNP compared to WNP
  - Underlined the necessity to extend Geant4-DNA models to high-Z metals

Nucl. Instrum. Meth. B 373 (2016) 126 (link)

on-going

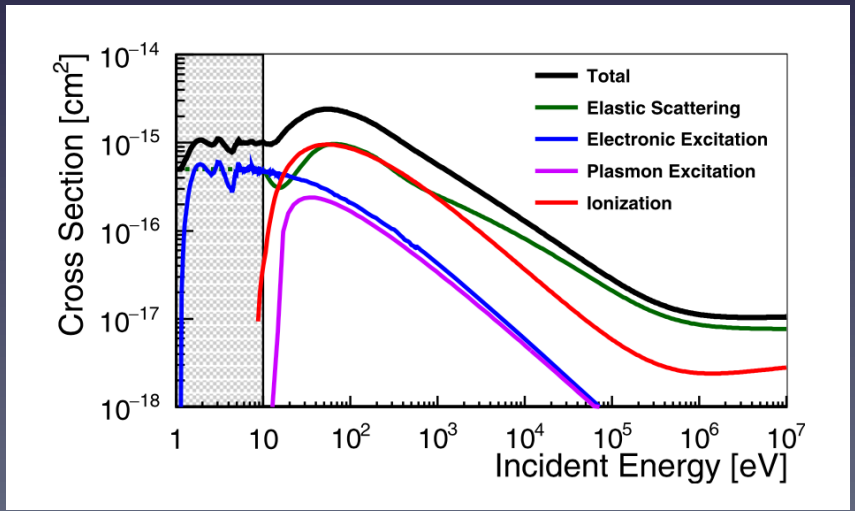
J. Appl. Phys. 120 (2016) 244901 (link)

High-Z materials : gold

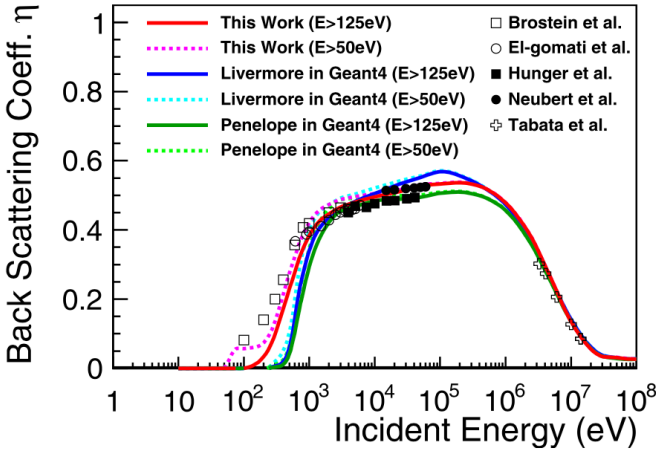
Dousatsu Sakata (Bordeaux U., France)
See Dousatsu's talk 5B session

- Extension of Geant4-DNA for the modelling of radiosensitization from gold nanoparticles
- Activity initiated in 2016 by D. Sakata (Bordeaux U., France)
- Discrete processes for electrons: elastic (ELSEPA), ionization (modified RBEBV), electronic (4 channels) and bulk plasmon (Quinn's) excitation
- Models will be delivered in the near future (probably 2018)

Integral cross sections for electrons



Eg. of validation (5 cm gold plate)



Message #1

This is the first time ever that
open source Track Stucture models
in water & biomaterials & metals
are made available
freely to the community !

Atomic deexcitation: shell ionisation cross section models

- Two main activities to improve PIXE models
  - Extended shell ionisation cross section models ("ECPSSR_FormFactor") from ECPSSR theory by M. Reis, A. Taborda, S. Incerti

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    - M shells revised, L shells corrected
    - 0.1 MeV up to 100 MeV (i/o 10 MeV), up to Z=92
    - protons and alphas
    - $G4LEDATA/pixe/ecpssr in G4EMLOW 7.1 (> 6.53)
  - New alternative ECPSSR set based on s.o.a recommendation by Cohen, Crawford and Siegele (ANSTO Australia) for K, L, M shells and protons and alphas up to a few MeV; models being implemented by S. Bakr, S. Guatelli et al.

coming soon

    - 0.2-5.2 MeV for protons, 0.2-40.2 (M: 10.2) MeV for alphas
    - will be released in 10.4 for protons and alphas

By Samer Bakr
UOW
see talk
3A session

Livermore/EPICs 2014

- A new set of photoelectric cross section data has been introduced in Geant4, based on EPICS 2014 data (recent revision of "Livermore")
- Livermore photoelectric model has been upgraded
  - Photoelectron angular distribution sampling has been improved. Observed speedup between 4% and 10%.
  - A new fit (two steps) of updated cross-sections data has been performed
    - threshold from 600KeV to 5KeV
    - speedup between 17% and 21%.
- In G4EMLOW 7.1

See Marilena Bandieramonte (CERN) talk, 3A session

Multiscale combination of EM processes

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

- Geant4 **photon** processes and models
  - Photoelectric effect, Compton sc., Rayleigh sc., pair production
  - Livermore (EPDL97) included by default in all Geant4-DNA constructors
- 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 by default, Bearden
  - now all activated by default in all Geant4-DNA constructors

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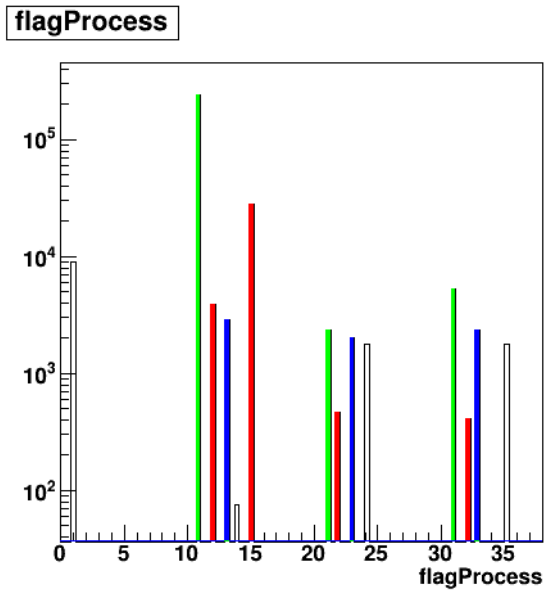
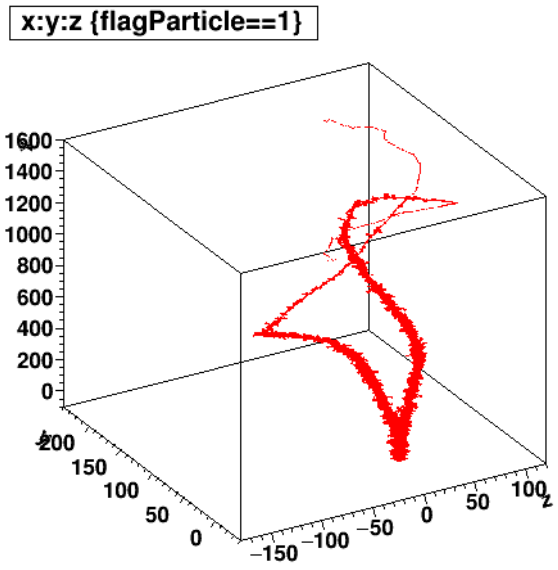
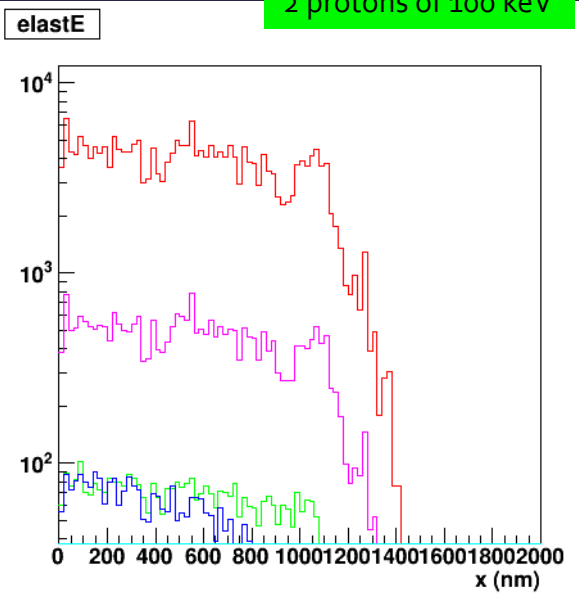
"Automatic" combination

- It is now possible to apply an automatic combination of Geant4-DNA with Geant4 standard EM Physics
  - G4EmDNAPhysicsActivator in your PhysicsList
    - `RegisterPhysics(new G4EmDNAPhysicsActivator());`
  - can be controlled directly with UI command, specifying Region name !
    - `/process/em/AddDNARegion World DNA_Opt0`
- Combination per particle type
  - Electrons: Geant4-DNA < 1 MeV, STD EM above (G4UrbanMscModel or G4eCoulombScatteringModel, G4MollerBhabbaModel)
  - Protons: Geant4-DNA < 100 MeV, STD EM above (G4WentzelVIModel, G4eCoulombScatteringModel, G4BraggModel, G4BetheBlochModel), Hydrogen: up to 100 MeV (Geant4-DNA only)
  - He^{q+}: Geant4-DNA < 400 MeV, STD EM above (for He^{2+}, He^{+} only: G4UrbanMscModel or G4IonCoulombScatteringModel, G4BraggIonModel, G4BetheBlochModel)
  - GenericIons: Geant4-DNA < 1 TeV; STD EM above (G4UrbanMasModel or G4IonCoulombScatteringModel, G4BraggIonModel, G4BetheBlochModel)
- Please try extended/medical/dna/dnaphysics example

2 protons of 100 keV







Phys. Med. 31 (2015) 861 (link)

Overview of verification activities for VLE EM physics

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

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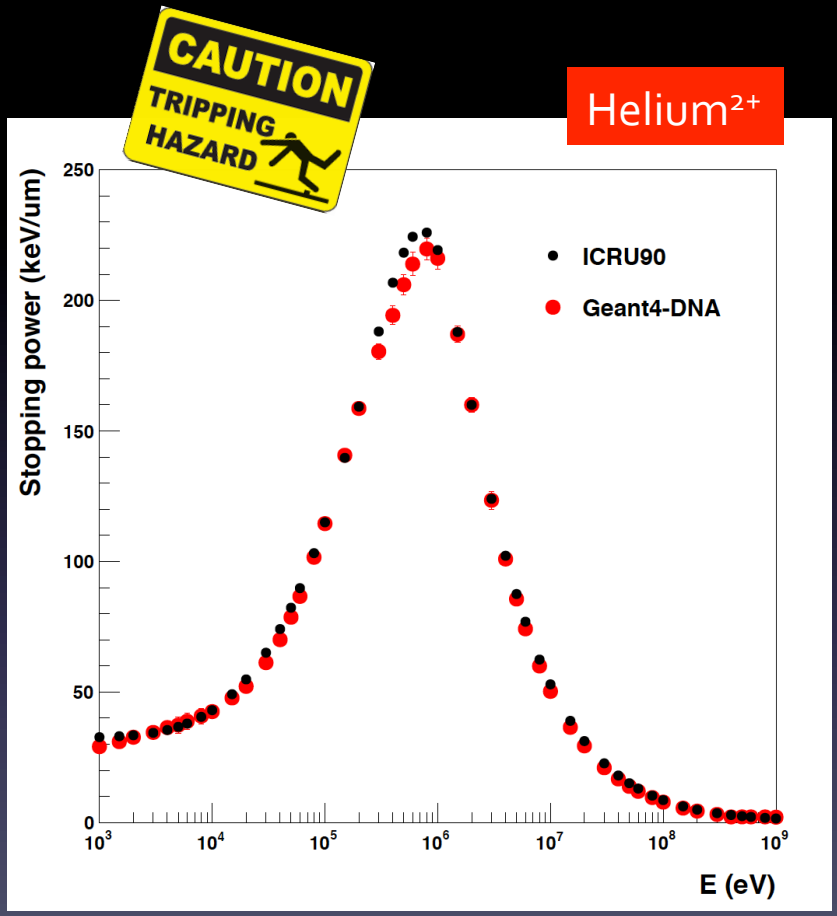
Verification: stopping power

- a reliable test to evaluate the accuracy of the code
- Geant4-DNA does not use SP tables
- users usually try to simulate SP by dividing energy loss over step length but forget to select stationnary regime
  - (alternative analytical calculation is always possible from differential ionisation cross sections)
- we provide specific stationary Geant4-DNA physics constructors for liquid water which activate stationary regime in all inelastic models



Nucl. Instrum. Meth. B 397 (2017) 45 (link)

See extended/medical/dna/spower example

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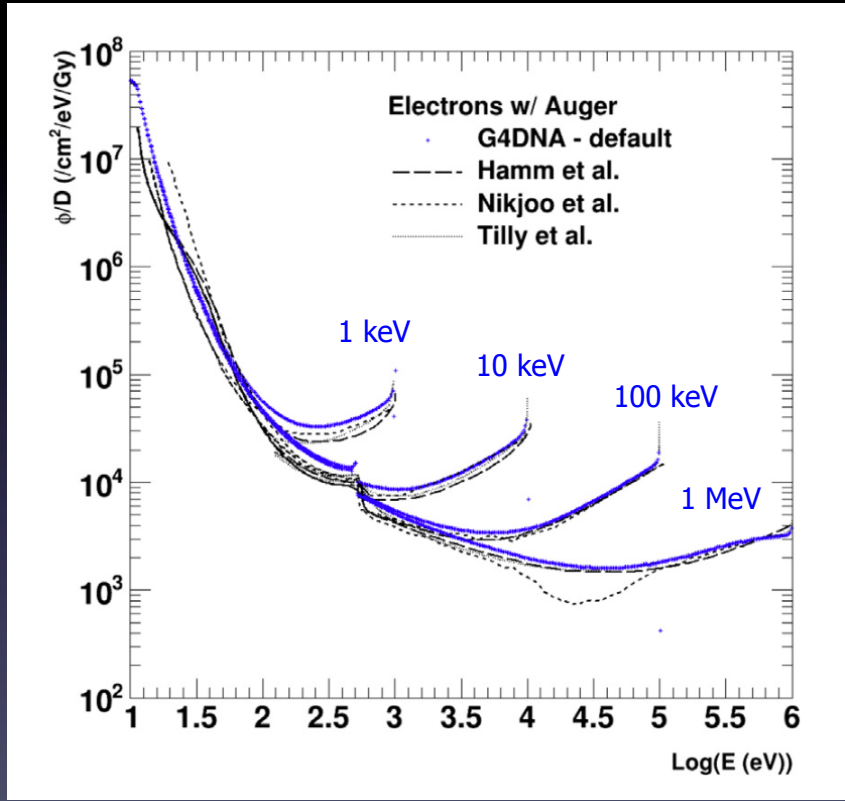
Verification: electron slowing down spectra

- a reliable test to evaluate the performance of track structure codes
- represent the fluence distribution (differential in energy) of both the primary and all subsequent generations of secondary electrons generated through the full slowing-down process
- ∅(E)dE is the total distance travelled by electrons while their energy is in the interval E, E+dE (Vassiliev, 2012)
- method: we record for each simulation step the kinetic energy of each electron undergoing a Geant4-DNA inelastic process in a log-binned histogram, setting for each record a statistical weight equal to the size of the step.
- small influence of sub-excitation processes at low energy; Auger electron production from O should be considered.



Nucl. Instrum. Meth. B 397 (2017) 45 (link)

See extended/medical/dna/slowing example

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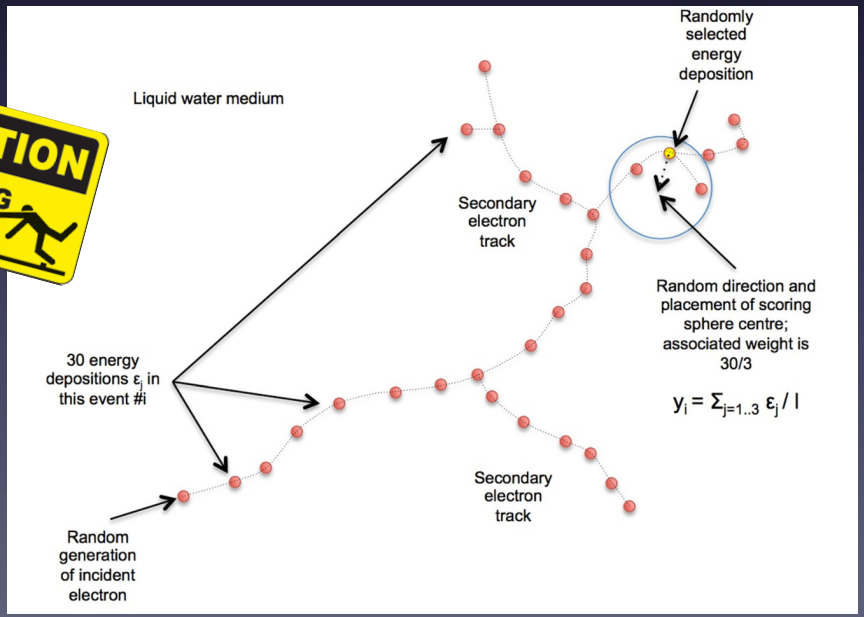
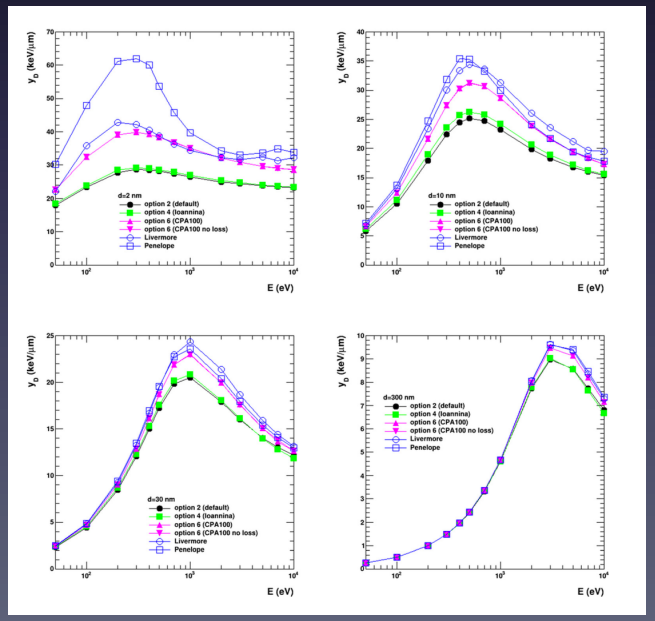
J. Appl. Phys. 122 (2017) 024303 (link)

Verification: microdosimetry

- For the first time, we provide an extended example capable of simulating microdosimetry spectra: lineal energy (y), specific energy (z), frequency-mean lineal energy, dose-mean lineal energy, frequency-mean specific energy, dose-mean specific energy
- energy scored in spheres of selected radius
- particular care for weighting of energy scoring…

$\overline{y}_F$ $\overline{y}_D$ $\overline{z}_F$ $\overline{z}_D$





See extended/medical/dna/microyz example

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Phys. Med. Biol. 62 (2017) 5908-5925 (link)

Accelerating simulations: variance reduction

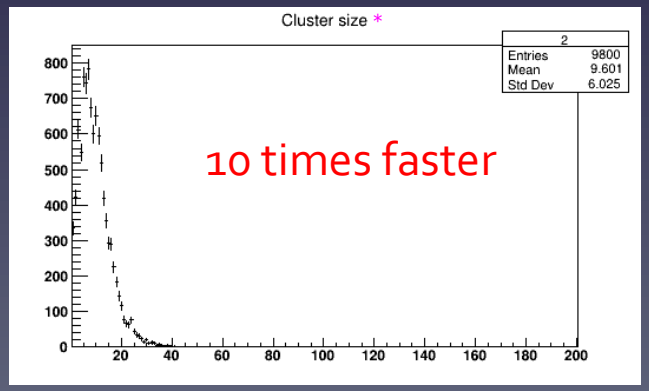
- An new extended example, "splitting", provided by J. Ramos-Mendes (UCSF) is provided to illustrate variance reduction technique in the Geant4-DNA ionisation process
- Method:
  - ionisation events are scored in a nanoscaled cylinder (6 nm x 10 nm).
  - ionised electrons generated by the first generation of secondary electrons are split (via G4WrappedProcess), i.e. new "clone electrons" are generated, labeled and propagated. The label is used to classify those new particles as if they were produced by independent histories to avoid overlapping of tracks at final analysis.
  - the splitting is performed only if the ionization event occurred in the cylinder.
- The user can define the split number using a UI command:

  `/vrt/numberOfSplit 10` (default is 1, no split)

See Jose's talk 3A session

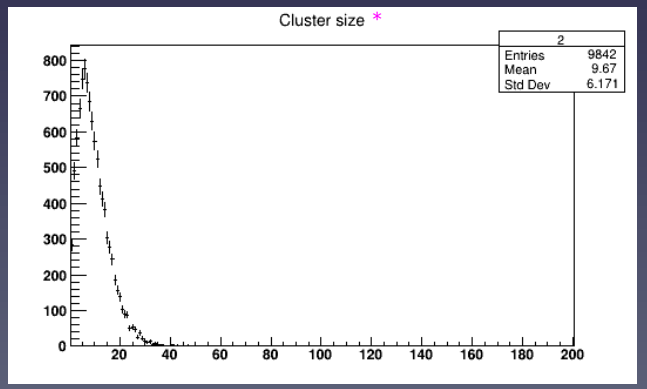
Example of He^{2+} of 4 MeV

100 primaries & numberOfSplit = 10



*number of ionisations produced within the scoring volume produced by a single history

1000 primaries & numberOfSplit = 1



See extended/medical/dna/splitting example

Message #2

This is the first time ever
that open source
Track Stucture applications
in water & biomaterials & metals
are made available
freely to the community !

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How to use Geant4-DNA for radiation chemistry ?

- Four examples are available in Geant4 in the

  « extended examples/medical/dna » category of Geant4 examples

  - CHEM1: activating chemistry
  - CHEM2: how to set minimum time step limits
  - CHEM3: user interactivity and visualization
  - CHEM4: extraction of radiochemical yields (G) in a range of deposited energy

- Note
  - Examples can be run in MultiThreading mode
  - Chemistry works in with G4_WATER material

Definition of radiochemical yield *G*

Number of molecules of a given species

for 100 eV of deposited energy

Time-dependent radiochemical yield

$$G(t) = \frac{N(t)}{E_{dep}}$$

Number of molecules at time *t*

Deposited energy scaling to 100 eV

An observable quantity commonly used to evaluate chemistry modeling accuracy…

Precautions for comparisons between codes

- scoring volume
- deposited energy
- species, reaction rates, diffusion constants
- compare all yields, not only one species…

Simulation of G-values


P. Piersimoni

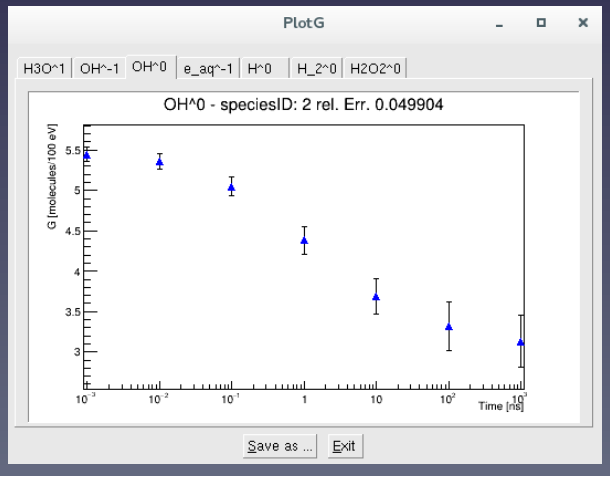
- A new extended example is provided: "chem4", my P. Piersimoni and M. Karamitros
- Hypotheses
  - infinite volume: the energy lost by the primary equals the deposited energy since all secondary particles slow down to thermal energy
  - two thresholds
    - The primary is killed once it has deposited more energy than a selectable minimum threshold, T1
    - When the primary particle looses more energy in few interaction steps than a maximum allowed threshold, T2, the event is aborted
    - this allows to calculate G-values on the deposited energy range [T1,T2]
    - can be set using UI commands :

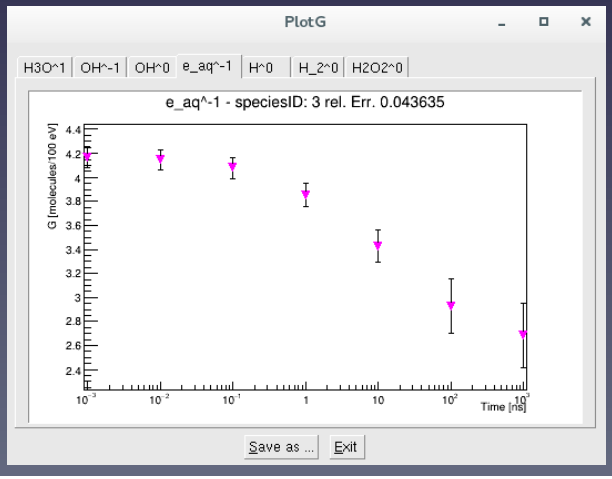
      /primaryKiller/eLossMin 1 keV # primary is killed if deposited E is greater than this value

      /primaryKiller/eLossMax 2 keV # event is aborted if deposited E is greated than this value


M. Karamitros

- Can run in MT mode
- Results are stored in ROOT format and can me vizualised using a dedicated interface (plotG)





Eg. : species by 10 incident electrons of 100 keV (beam.in)

Thank you