Geant4 Low Energy Electromagnetic Physics

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on behalf of both Geant4 Electromagnetic WG

2015 Geant4 Collaboration Meeting
Fermilab
Sept. 28 – Oct. 2

Contents

1. Low energy limit treatment of gamma models
2. Monash gamma models
   - Compton model G4LowEPComptonModel
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   - New set of fluorescence line data by Bearden et al.
   - Auger cascade simulation
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4. ICRU'73 ion models
5. Further verification & validation activities
   - Gamma models
   - Bremmsstrahlung
6. Geant4-DNA updates

What is included in LowE EM Physics ?

Low Energy Electromagnetic Processes

Livermore processes for gamma and electrons

Information on **Livermore processes** is available from this page.

Penelope processes for gamma, electrons and positrons

Information on **Penelope processes** is available from this page.

Ion processes

Information on the **ICRU'73 ion parameterized model** is available from this page.

Geant4-DNA processes

Information on **Geant4-DNA processes** is available from this page.

MicroElec processes

Information on **MicroElec processes** for microdosimetry in Silicon from this page.

Monash University processes

Information on **Monash University processes** for gammas from this page.

How to simulate atomic deexcitation?

Follow this page.

TwiKi page

https://twiki.cern.ch/twiki/bin/view/Geant4/LowEnergyElectromagneticPhysicsWorkingGroup

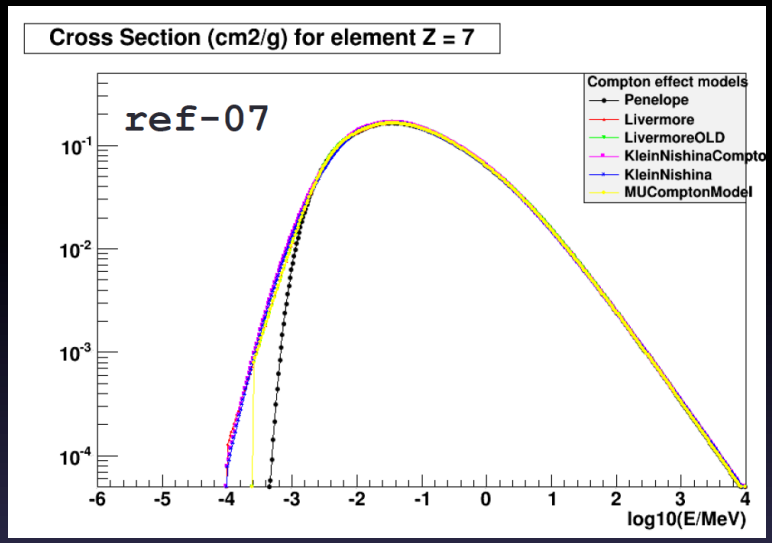
1) Handling of low energy limits

Apply uniform handling of low energy limits of models for gammas, after infinite loops where reported by CMS for very low energy gammas

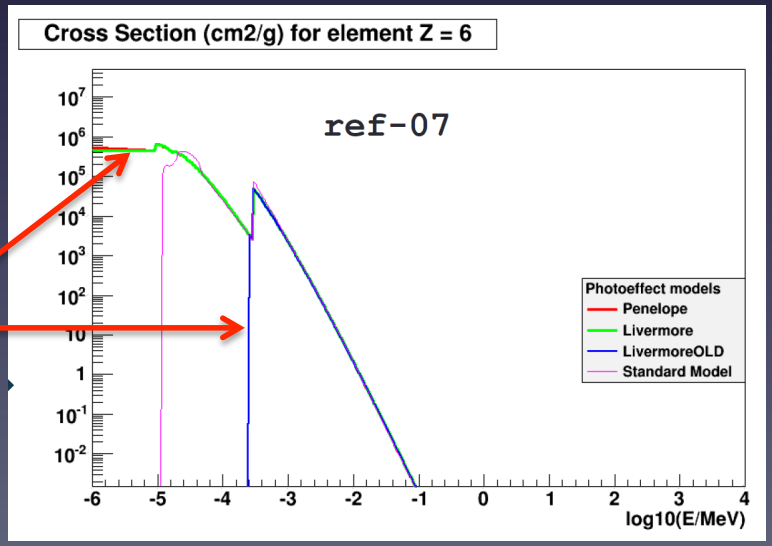
- Compton scattering
  - Cross section is set to zero below E_{min}, where E_{min} is the first data point of tabulated value: if $E<E_{min}$, $\sigma(E)=0$
- Photoelectric effect
  - Non-zero cross section below E_{min}: if $E<E_{min}$, $\sigma(E)=\sigma(E_{min})$

Handling of low energy limits

Compton scattering



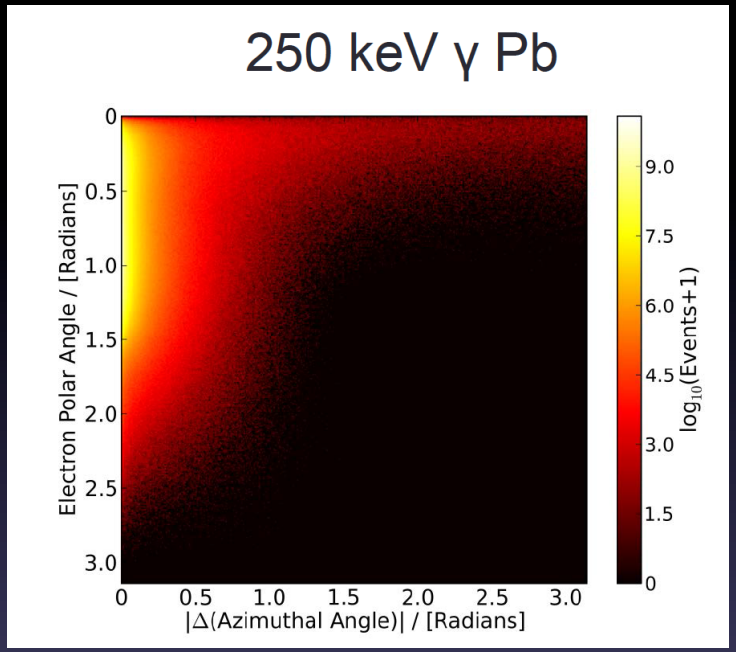
Photoelectric effect



Livermore
(current & old)

2) Monash Compton model

- G4LowEPComptonModel
  - Developped by J. M. C. Brown @ Monash U.
  - Two-body relativistic 3D framework
  - Relativisitc impulse approximation
  - Electron distibution is not uniform in ϕ wrt photon scattering plane
  - Bound atomic electrons
- CPU penalty of 10% compared to Penelope
- In G4EmStandardPhysics_option4 below 20 MeV



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journal homepage: www.elsevier.com/locate/nimb

A low energy bound atomic electron Compton scattering model for Geant4

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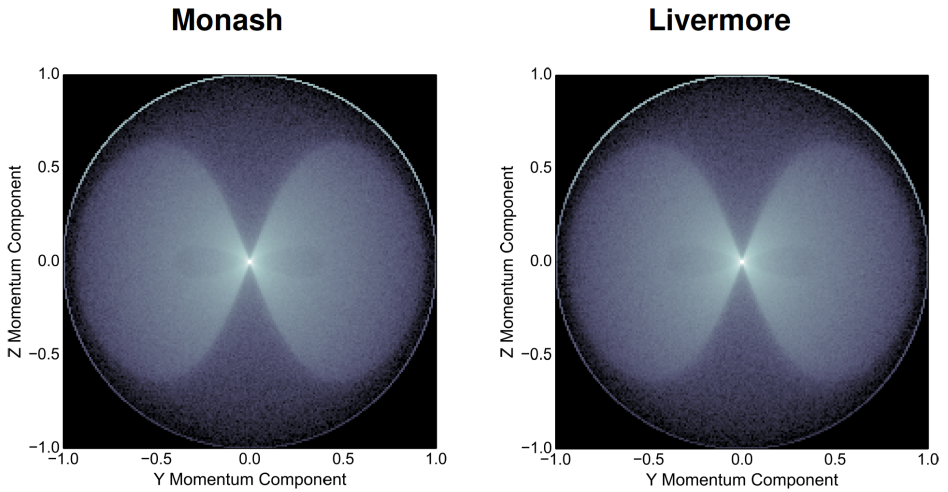
http://dx.doi.org/10.1016/j.nimb.2014.07.042

Monash pol. Compton model

- New model model G4LowEPPolarizedComptonModel for polarized Compton scattering by J. M. C. Brown @ Monash U.
- Adapted from new MT version of G4LowEPComptonModel
- Polarisation algorithms implemented from G4LivermorePolarizedComptonModel
- Both scatter momentum distributions and polarisation distributions match with respect to G4LivermorePolarizedComptonModel
- Fixed additional FPE issue in Livermore that reset photon polarisation plane after scattering

Implementation Momentum Distributions

Scattered Photon Distributions: Si 250 keV (Log Intensity Scale)



Courtesy of J.M.C. Brown

3) Atomic deexcitation: UI commands

- Initialisation of fluorescence

```
/run/initialize
/process/em/deexcitation region true true true
/process/em/fluo true
/process/em/auger true
/process/em/pixe true
```

- Production cuts for cuts < 990 eV

```
/cuts/setLowEdge 250 eV
```

- Selection of shell ionisation cross section models for protons and electrons

```
/process/em/pixeXSmodel value (value is ECPSSR_Analytical or ECPSSR_FormFactor or Empirical)
/process/em/pixeElecXSmodel value (value is Livermore or Penelope)
```

- New flag to disable the use of production thresholds

```
/process/em/deexcitationIgnoreCut true
```

Atomic deexcitation: new set of fluorescence lines

- Transition energies are taken from the Evaluated Atomic Data Library (EADL)
- This library contains calculated data for isolated neutral atoms
- It is known that the simplifications used in this library for the calculation of transition probabilities and transition energies can lead to visible inconsistencies, as explained in the interesting review by Salvat and Fernandez-Varea (2009) : they suggest to correct transition energies during the simulation
  - Energy shifts can be observed when simulating lines with Geant4, compared to expected values
- The set of measured transition lines by Bearden et al. (1967) is used worldwide for material analysis (X-Ray Data Booklet)
- A new alternative set has been provided by S. Paltani (U. of Geneva)

  Default: `$G4LEDATA/fluor`

  New set: `$G4LEDATA/fluor_Bearden`
- To use this set, add in your Physics list:

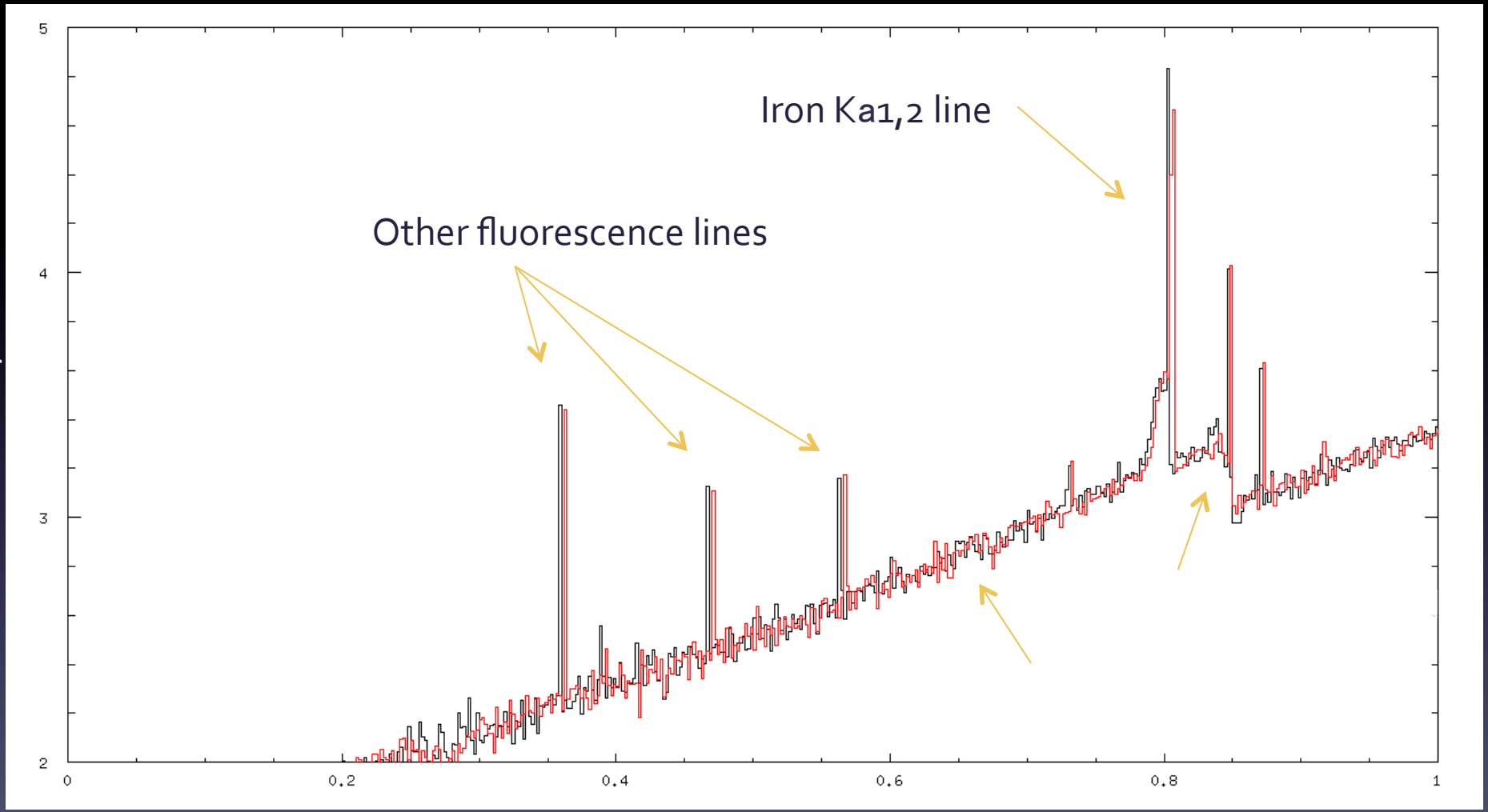
```
G4AtomicTransitionManager::Instance()->SetFluoDirectory("fluor_Bearden");
```

  or dedicated UI command

```
/process/em/fluoBearden true
```

- Principle of change
  - Replacement of fluorescence lines available in Bearden (1967) directly into Geant4 files
  - Lines not in Bearden (1967) left as they are (most of them are absent)
  - Some lines resolved in Geant4 are not resolved in Bearden (1967)
  - Astrophysical impact of lines not in Bearden (1967) (or unresolved) negligible

X-ray reflection on a disk

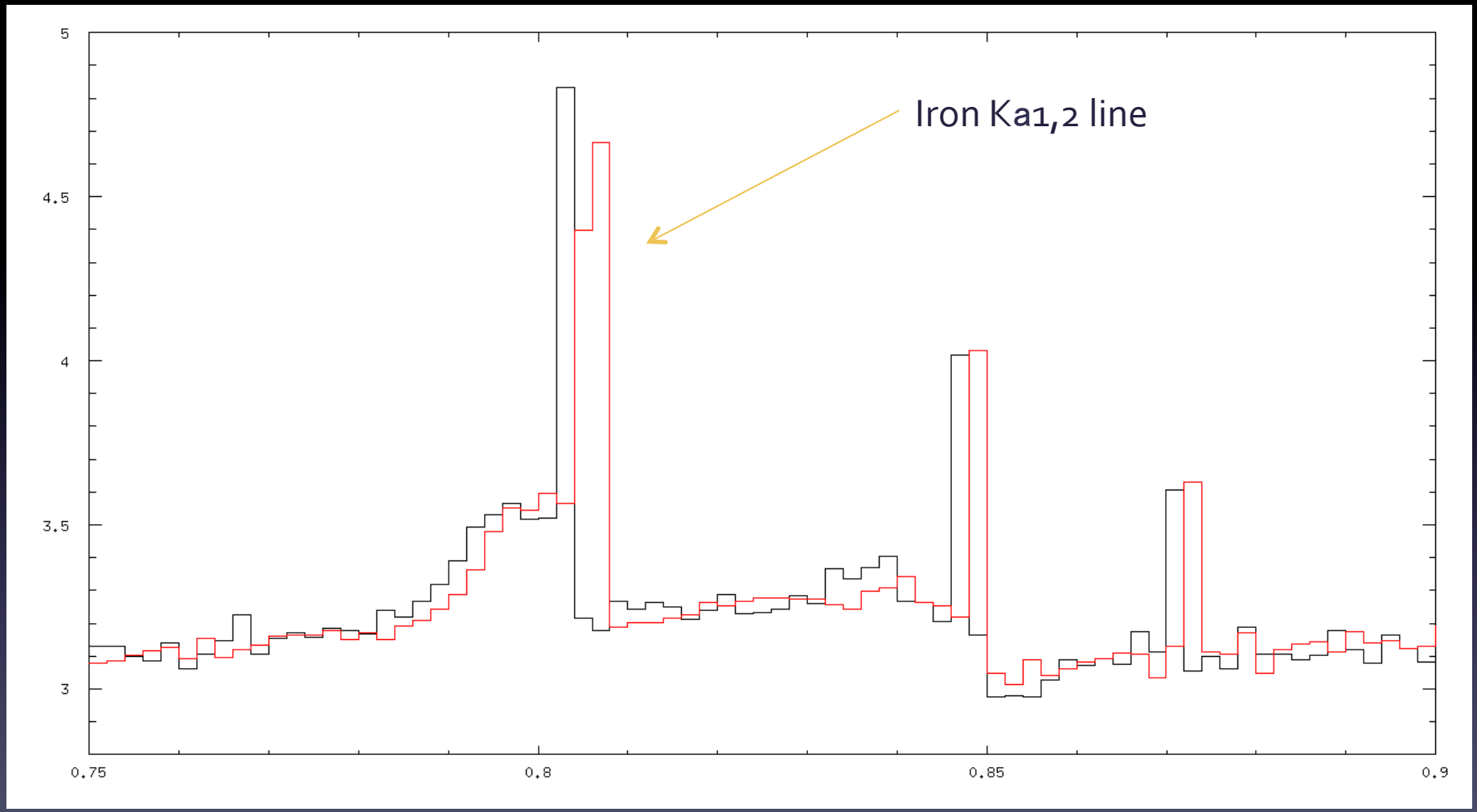


Geant4

Bearden (1967)

Courtesy of S. Paltani, Geneva U.

X-ray reflection on a disk

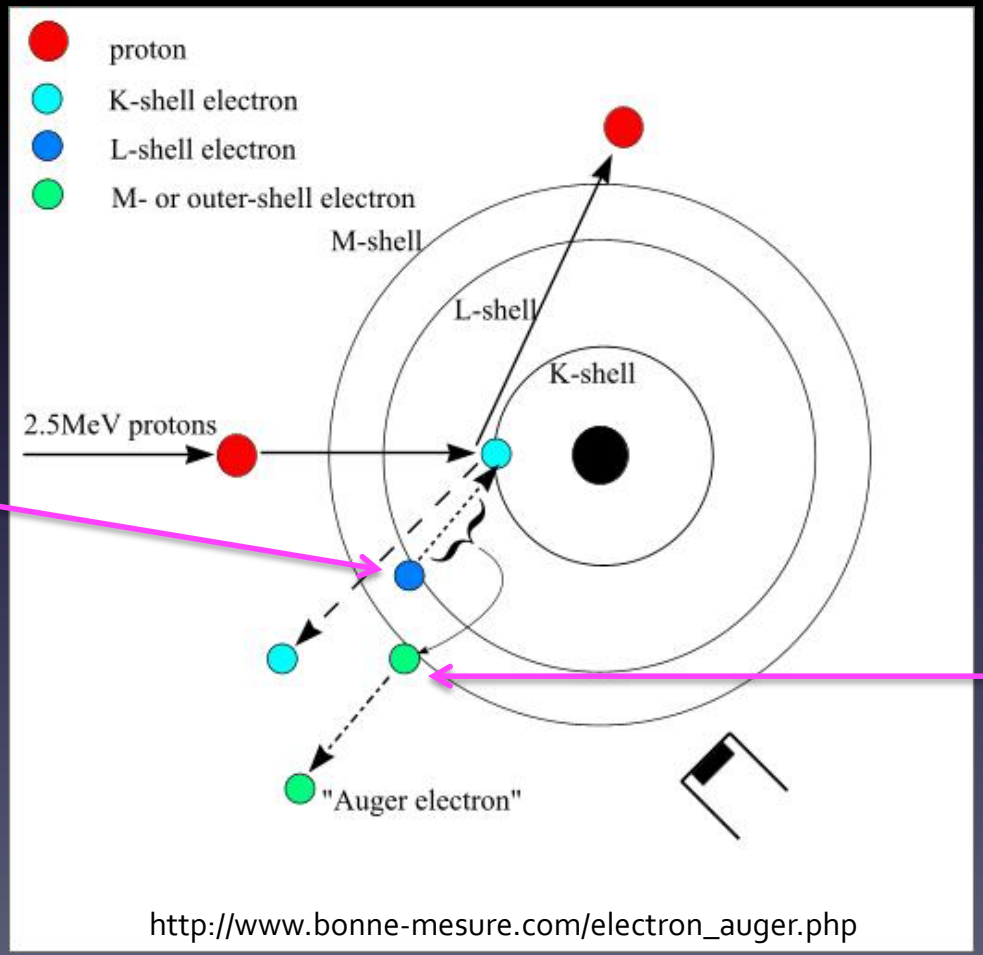


Geant4

Bearden (1967)

Courtesy of S. Paltani, Geneva U.

Atomic deexcitation: Auger cascade simulation



http://www.bonne-mesure.com/electron_auger.php

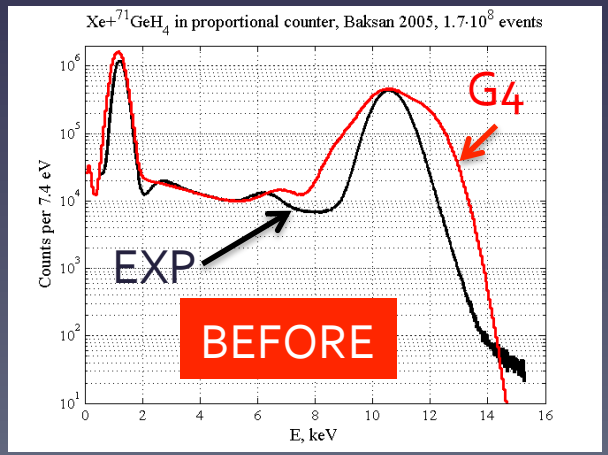
This vacancy is tracked

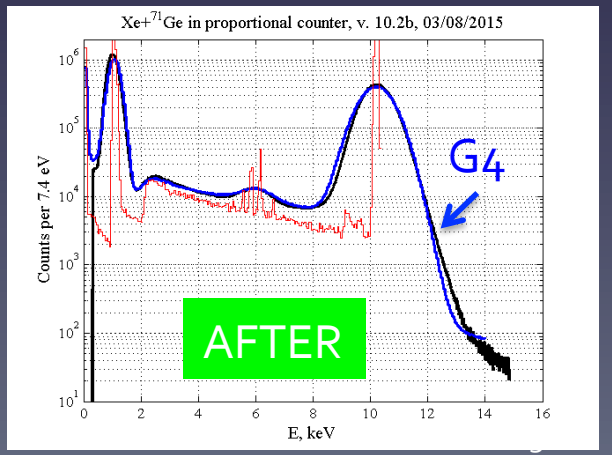
This vacancy is NOT tracked

Atomic deexcitation: Auger cascade simulation

- Added the possibility to simulate Auger cascades and the series of occuring vacancies, leading to multiple emission of Auger electrons
  - Bugzilla report #1727 by B. Suerfu
  - Provided a prototype extension
  - Confirmed by Y. Malyshkin
- We added specific UI command to explicitely simulate (or not) the Auger cascade (active only when Auger production is active)
  - `/process/em/augerCascade true` or `false`
  - `/process/em/deexcitationIgnoreCut true`
  - To be put just after `/run/initialize`

Note: combination with RadioactiveDecay will be ready for 10.2 G4ECDecay & G4ICDecay

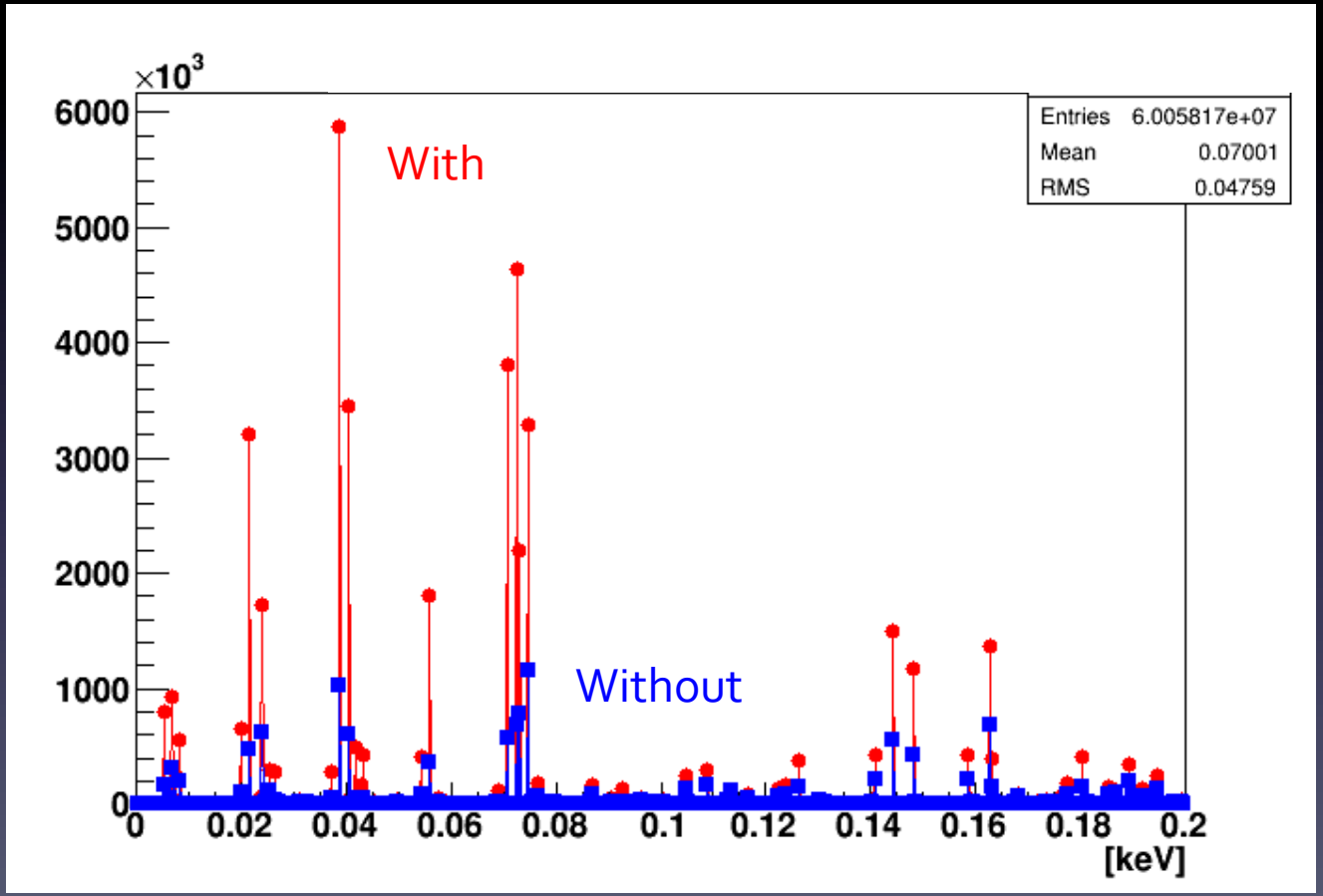




Ge 71 decay in Xe prop. counter
- Simulation smeared with Gaussian
- Measurements

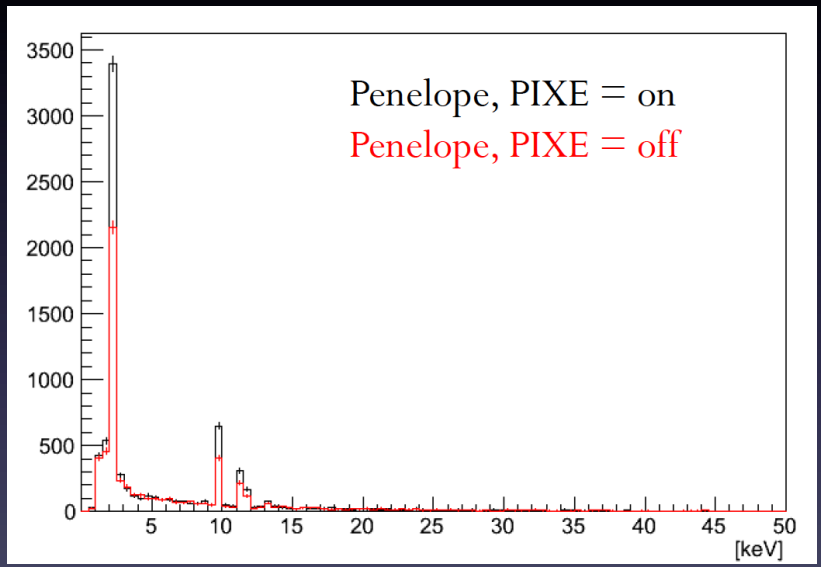
Atomic deexcitation: Auger cascade simulation

Example
- Release 10.2 BETA
- TestEm5
- pixe.mac
- 10^7 gammas
- 100 keV
- 50 um-thick Au target



Atomic Deexcitation: fixing of Penelope deexcitation

- Bugzilla #1761 by M. Maire
- The Penelope Ionisation model has a built-in management of the atomic de-excitation
- If the PIXE flag is TRUE, the Penelope model produces de-excitation cascade twice
  - Once via the internal mechanism and once via the PIXE universal interface
  - The net result is an over-production of x-rays
- Fix: the Penelope ionisation model will
  - use its own internal mechanism for atomic de-excitation when PIXE is FALSE
  - use the G4 EM unified atomic deexcitation interface when PIXE is TRUE



50 keV electrons in Au

4) ICRU'73 files for ions

- Updated ICRU'73 files for the computation of ions stopping powers
  - Reminder
    - Z>2
    - 25 atomic elements
    - 31 simple compounds (a few revised compounds by P. Sigmund)
  - This year, substituted 2016 files (new files for atomic elements and old files for compounds) by new PASS computations provided by A. Schinner in collaboration with P. Truscott (>=G4EMLOW6.44).
  - Located in $G4LEDATA/ion_stopping_data

5) Verification and validation: gamma models

- Verification of gamma attenuation coefficients in a variety of element and materials
  - 18 elements from Z=4 to 92
  - 3 compounds: water, PMMA, BGO (+other plastic phantoms)
- Performed by S. Guatelli, Wollongong U., as in IEEE TNS 52 (2005) 910 by Amako et al.
- Comparison with XCOM/NIST
- 5 EM Physics constructors

  opto, op3, opt4, Livermore, Penelope
- Attenuation coefficients to test
  - Total, Rayleigh, Compton, photoelec, conversion

Provided by Susanna Guatelli, Wollongong U.

Results: discussion

- In the last year, added:
  - New materials
  - Rayleigh scattering
  - Regression test
  - Standard_option0

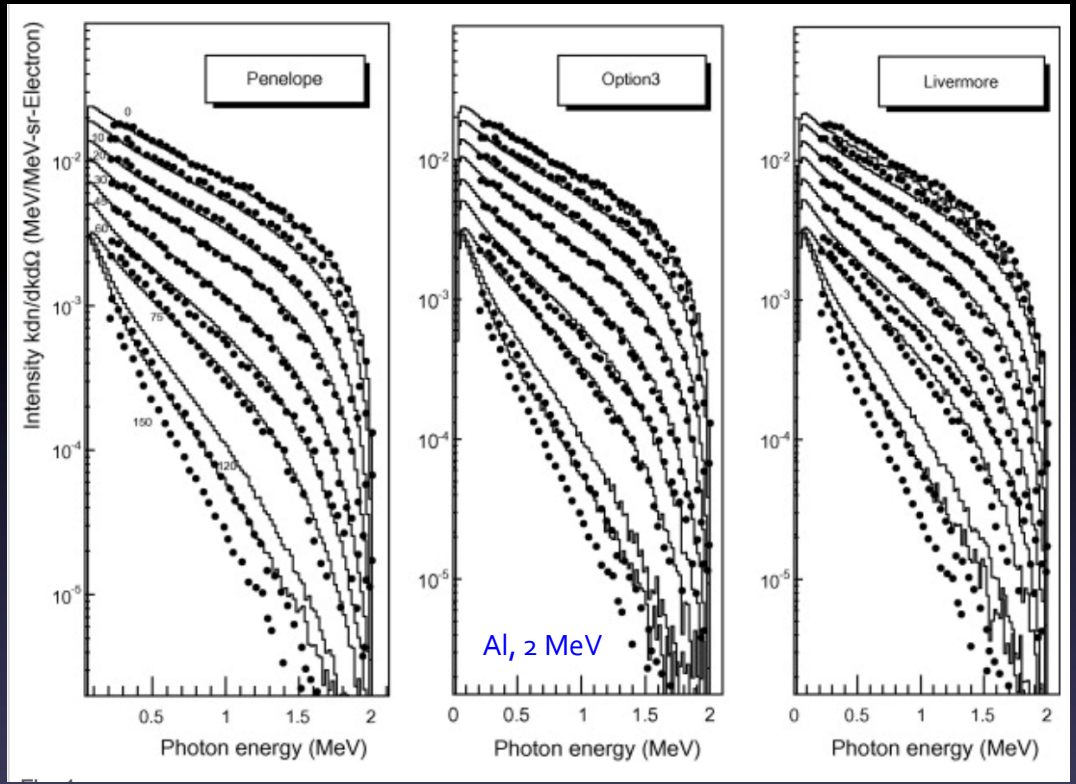
- Regression test: Geant4 10.1 agrees with Geant4 10.0 within statistical error bars.

- In general good agreement with NIST (within 5%, which is the NIST uncertainty).

- Penelope approach, Standard Option 0 and 3 Compton scattering report differences below ~20 keV, where this process is negligible

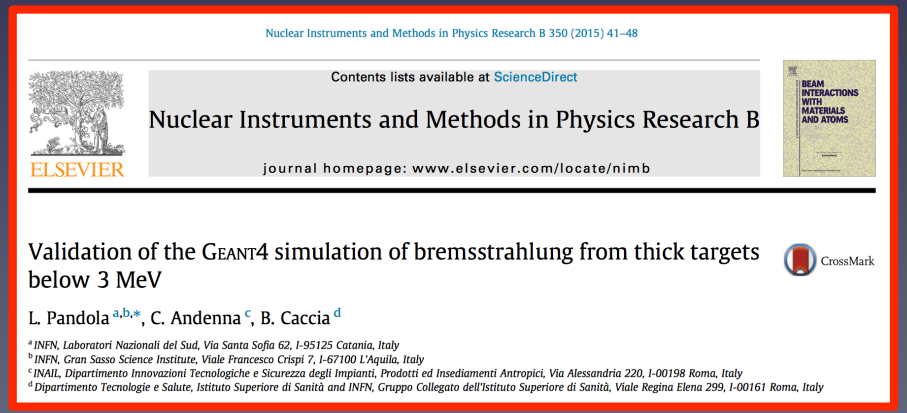
Verification and validation: bremsstrahlung

- Validation activity of Geant4 bremsstrahlung for thick targets, < 3 MeV, by L. Pandola et al.
- Too much energy/photon irradiated in the backward direction
- Good quantitative agreement for the forward direction



« The Penelope model shows the best agreement with measurements for incident electrons energies in the MeV range, but the choice is much less evident at lower energy (below 100 keV) ».

http://dx.doi.org/10.1016/j.nimb.2015.03.033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ELSEVIER

Validation of the GEANT4 simulation of bremsstrahlung from thick targets below 3 MeV

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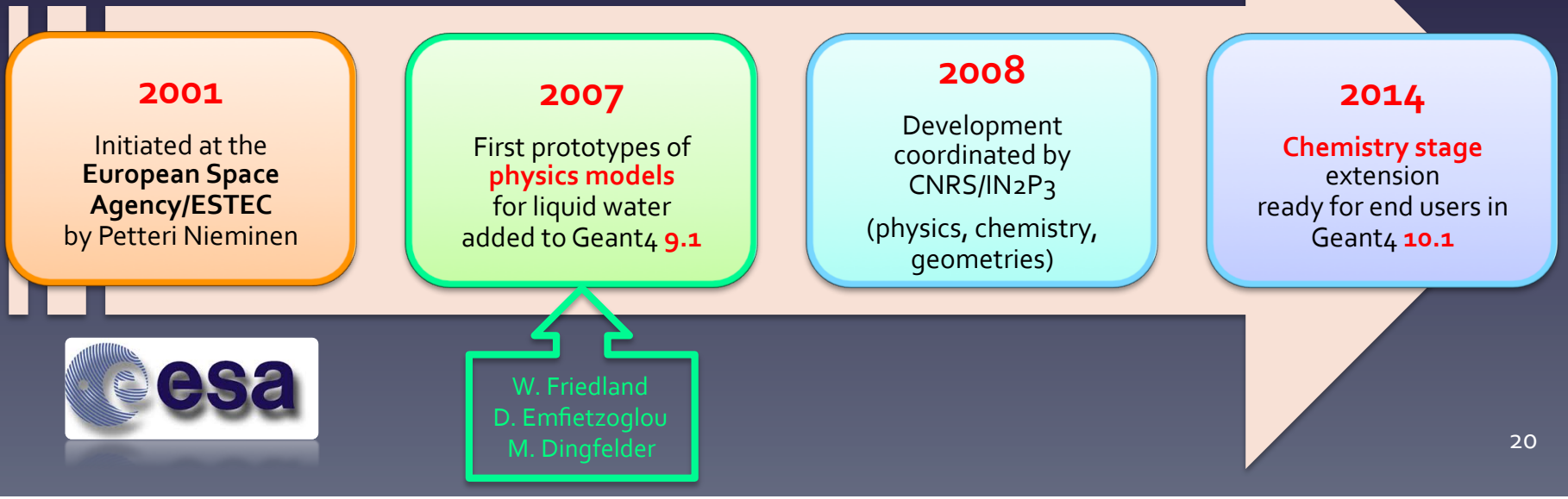
6) Status of Geant4-DNA

Main objective

Extend the general purpose Geant4 Monte Carlo toolkit for the simulation of interactions of radiation with biological systems at the cellular and DNA level in order to predict early DNA damage in the context of manned space exploration missions (« bottom-up » approach).

Designed to be developed and delivered in a FREE software spirit under Geant4 license, easy to upgrade and improve.



How can Geant4-DNA model early DNA damage ?

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

t=0 t=10^{-15}s t=10^{-6}s

10.2 BETA

Overview of physics models for liquid water

- **Electrons**
  - **Elastic scattering**
    - Screened Rutherford and Brenner-Zaider below 200 eV
    - Updated alternative version by Uehara from 10.2B
    - Partial wave framework model by C. Champion et al., 3 contributions to the interaction potential
  - **Ionisation**
    - 5 levels for H_2O
    - Dielectric formalism & FBA using H. Heller optical data up to 1 MeV, and low energy corrections, derived from the work of D. Emfietzoglou et al.
    - Improved alternative version by D. Emfietzoglou and I. Kyriakou from 10.2B
  - **Excitation (*)**
    - 5 levels for H_2O
    - Dielectric formalism & FBA using H. Heller optical data and semi-empirical low energy corrections, , derived from the work of D. Emfietzoglou et al.
    - Improved alternative version by D. Emfietzoglou and I. Kyriakou from 10.2B
  - **Vibrational excitation (*)**
    - M. Michaud *et al.* xs measurements in amorphous ice
    - Factor 2 to account for phase effect
  - **Dissociative attachment (*)**
    - C. Melton xs measurements
- **G4LowECapture process for capture**

See Med. Phys. 37 (2010) 4692-4708 (link)
Appl. Radiat. Isot. 69 (2011) 220-226 (link)
Med. Phys. 42 (2015) 3870 (link)

(*) 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 M. Dingfelder *et al.*
  - **Ionisation**
    - Rudd semi-empirical approach by M. Dingfelder *et al.* and Born and Bethe theories & dielectric formalism above 500 keV (relativistic + Fermi density)
  - **Charge change (*)**
    - Analytical parametrizations by M. 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 M. Dingfelder *et al.*
  - **Charge change (*)**
    - Semi-empirical models from M. 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)

Geant4-DNA Physics constructors

6 constructors are available (4 new as BETA)

Constructor name	Content
G4EmDNAPhysics	Default models
G4EmDNAPhysics_option1 (beta)	Same as G4EmDNAPhysics but uses New multiple scattering model G4LowEWentzelVIModel
G4EmDNAPhysics_option2	Same as G4EmDNAPhysics but faster (usage of CDCS for ionisation processes)
G4EmDNAPhysics_option3 (beta)	Same as G4EmDNAPhysics but includes nuclear scattering for protons and alphas
G4EmDNAPhysics_option4 (beta)	New electron ionisation and excitation models by Ioannina team
G4EmDNAPhysics_option5 (beta)	Same but usage of CDCS

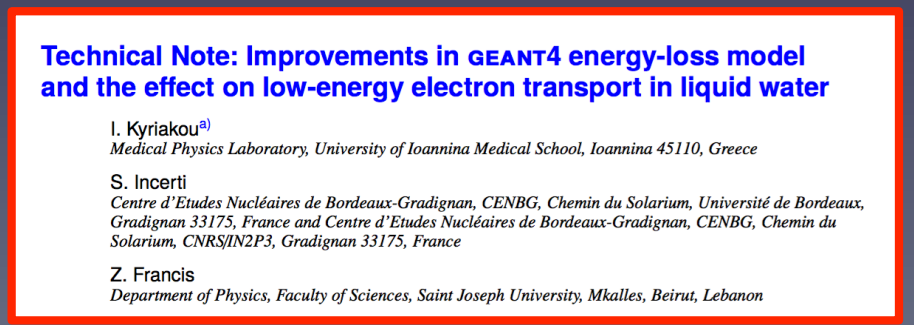
All are located in
$G4INSTALL/source/physics_lists/constructors/electromagnetic

New DRF models for electrons

- Some deficiencies in Geant4-DNA physics have been reported by collaboration members and users, for incident electrons
  - Too low electronic excitation cross section compared to experimental data or other MC codes (see for eg. Med. Phys. 37 (2010) 4692)
  - Too low average energy transferred per ion pair W (see for eg. Phys. Med. Biol 57 (2012) 3657)
  - Dose Point Kernels simulated with the current Screened Rutherford elastic model are not reliable (see for eg. Appl. Radiat. Isot. 83 (2014) 137)

- Thanks to I. Kyriakou et al. at Univ of Ioannina, Greece, these electron models have been improved
  - Inelastic models (based on the DRF theory by D. Emfietzoglou et al.)
    - inclusion of a truncation algorithm which accounts for broadened ionization thresholds; the truncated part is re-partitioned leading to higher excitation yield
    - Refinement of exchange and Coulomb corrections
  - Elastic: screening factor proposed by Uehara from vapor experimental data, instead of Grosswendt-Waibel

http://dx.doi.org/10.1118/1.4921613



Technical Note: Improvements in GEANT4 energy-loss model and the effect on low-energy electron transport in liquid water

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Z. Francis
Department of Physics, Faculty of Sciences, Saint Joseph University, Mkalles, Beirut, Lebanon

Illustration of new DRF models

Contributions of ionisation & excitation

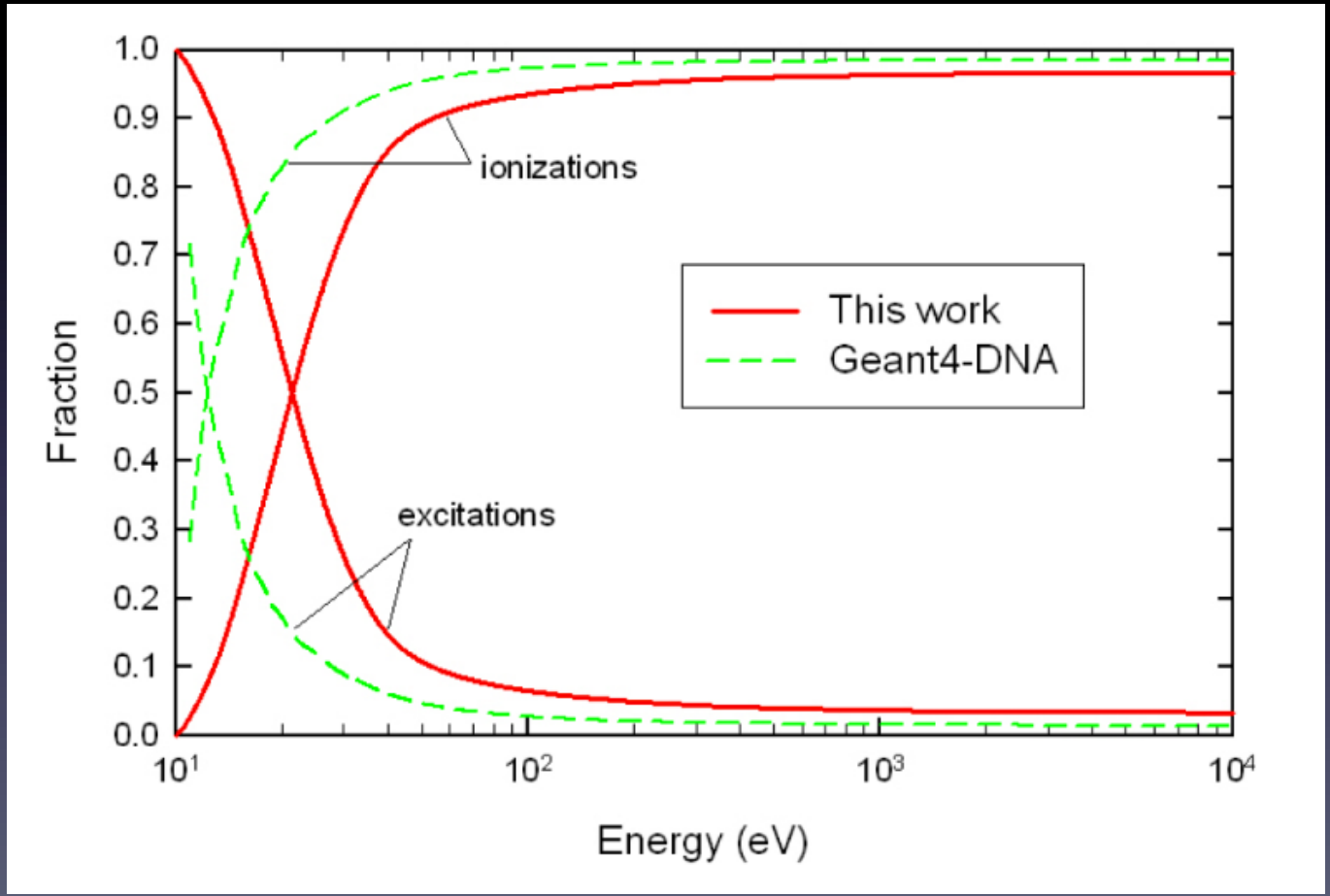


Illustration of new DRF models

DPK

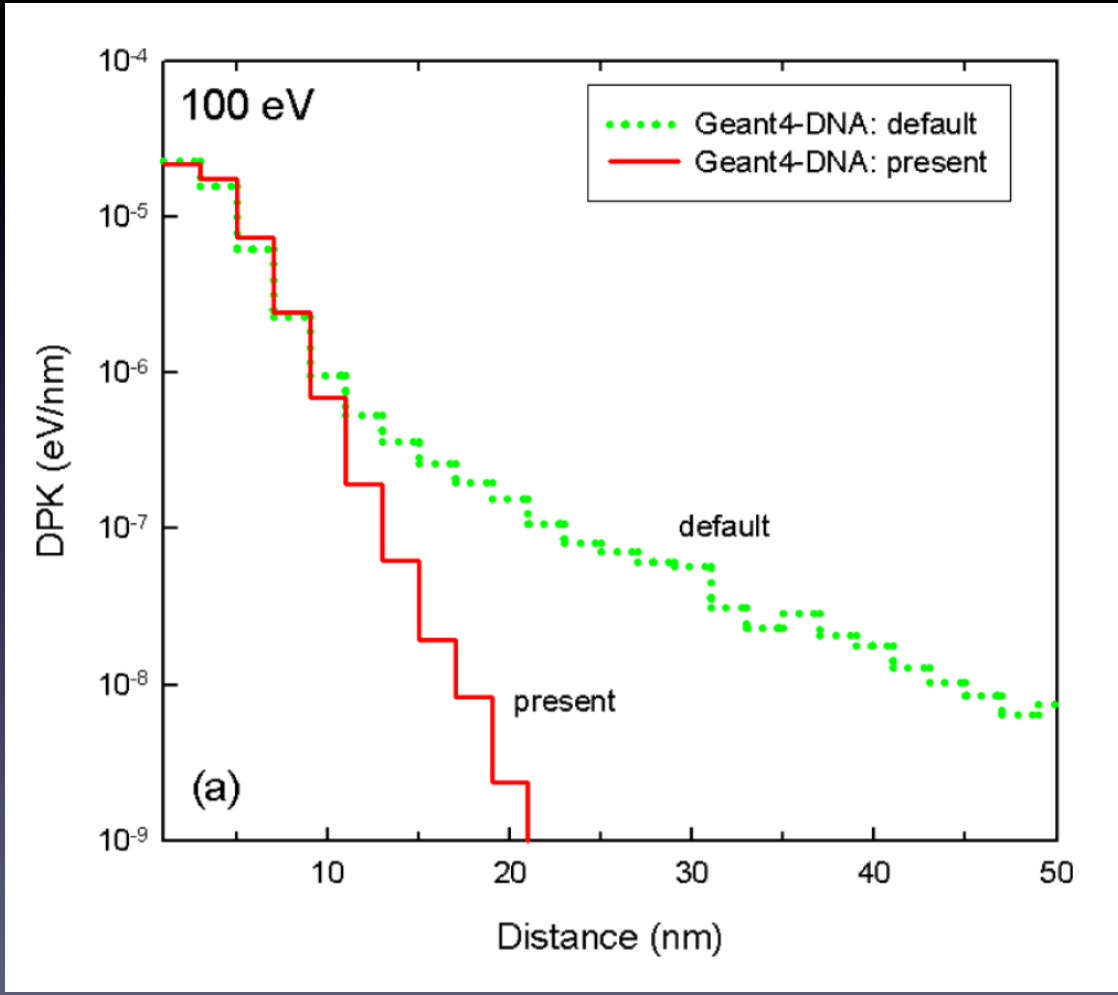
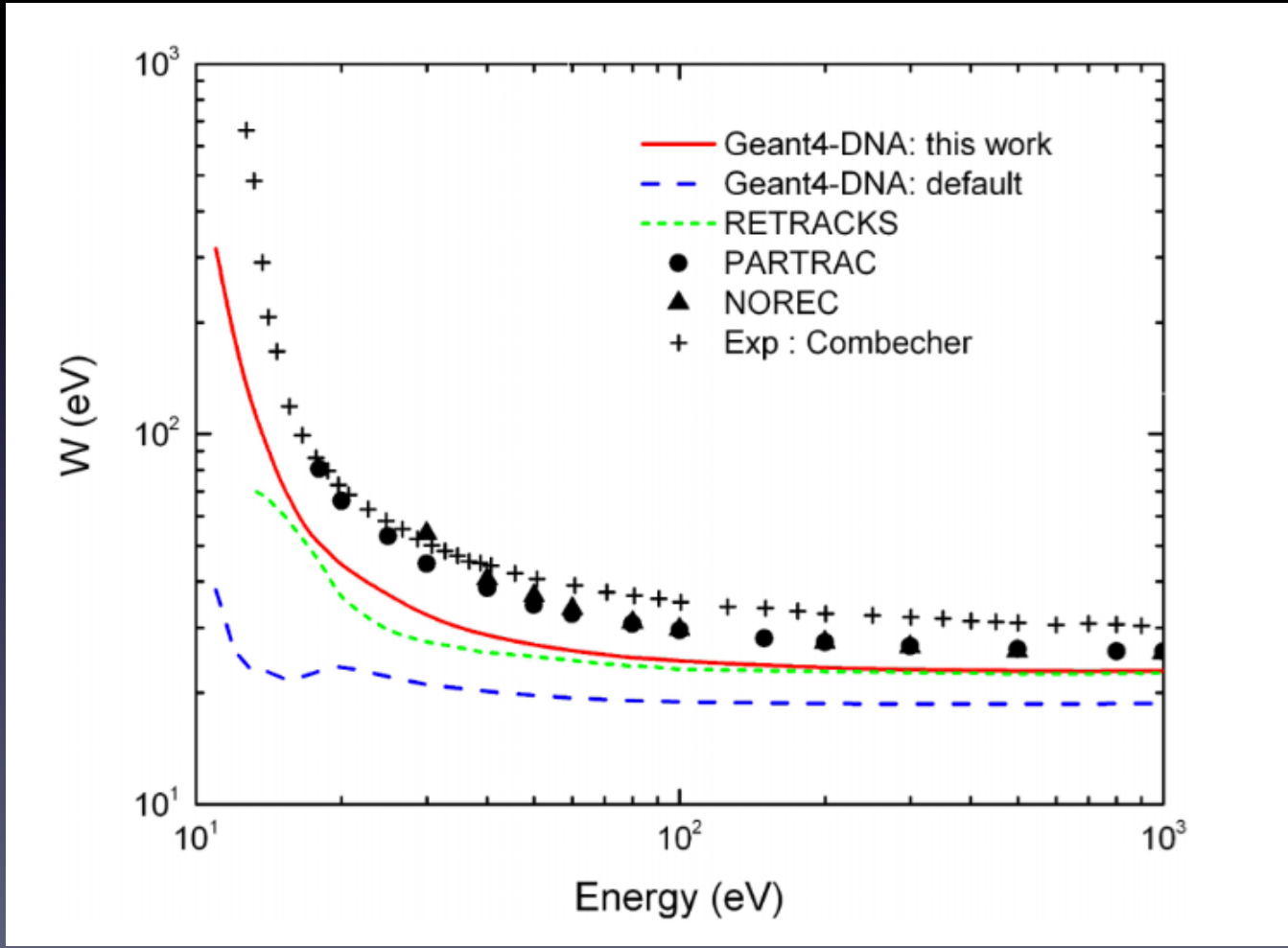


Illustration of new DRF models

W-value



Elastic scattering for protons and alphas

Classical mechanics approach: scattering angle may be numerically calculated and expressed in the CM frame (Everhart *et al.*, 1955)

$$\theta = \pi - 2(p / r_s)\int_0^{z_0} \frac{1}{\sqrt{1 - \frac{p^2}{r_s^2} z^2 - \frac{b}{r_s} z F_s(1/z)}}\, dz$$

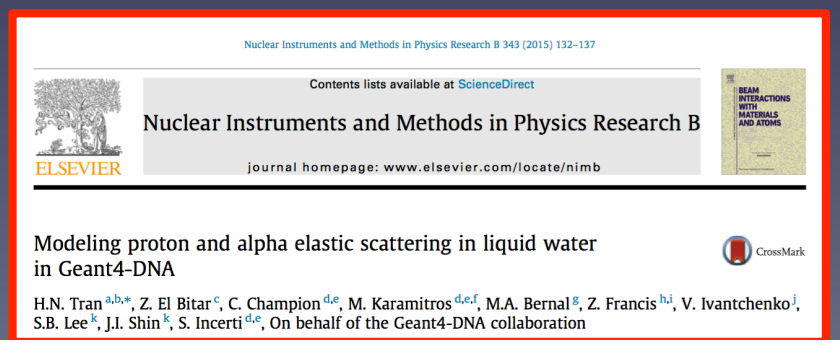
The screening function used for proton projectiles is that reported from ICRU49

$$F_s(r / r_s) = 0.10e^{-6r/r_s} + 0.55e^{-1.2r/r_s} + 0.35e^{-0.3r/r_s}$$

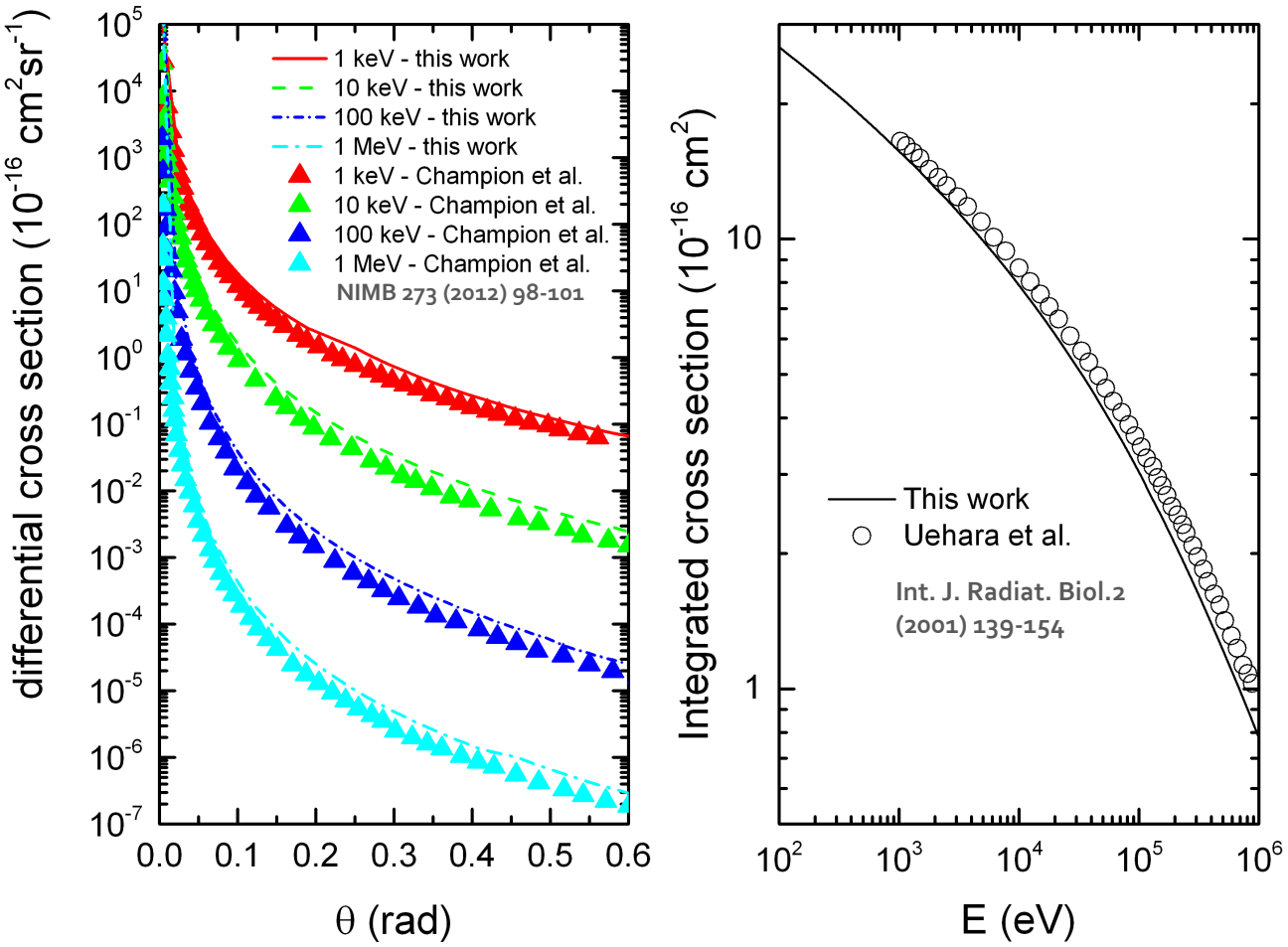
The integral elastic scattering cross section is obtained from

$$\frac{d\sigma_{el}}{d\Omega} = -\frac{p}{\sin\theta}\frac{dp}{d\theta} \qquad \sigma_{el}(T) = 2\pi\int_{\theta_{cut}}^{\pi} \frac{d\sigma_{el}}{d\Omega}\sin\theta d\theta$$

http://dx.doi.org/10.1016/j.nimb.2014.10.016

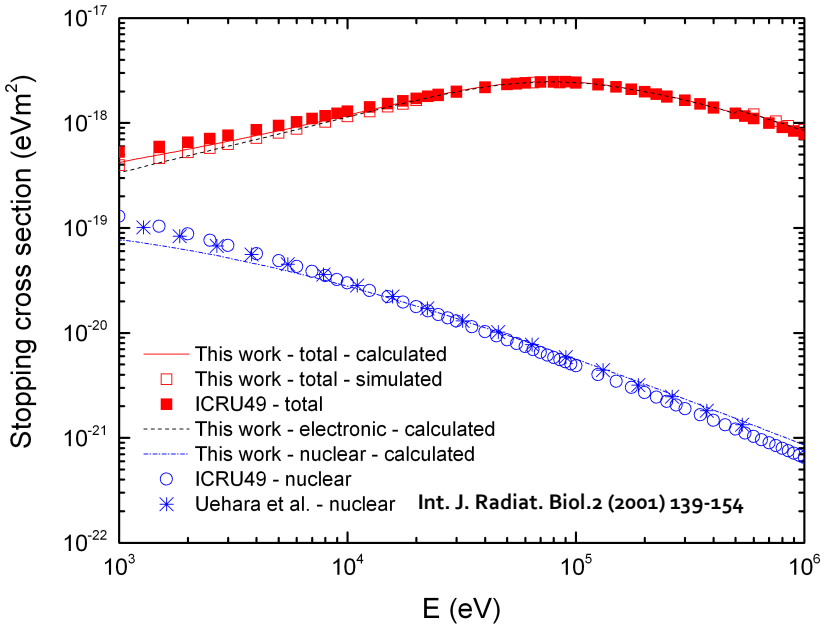


Differential cross section and Integral cross section for protons

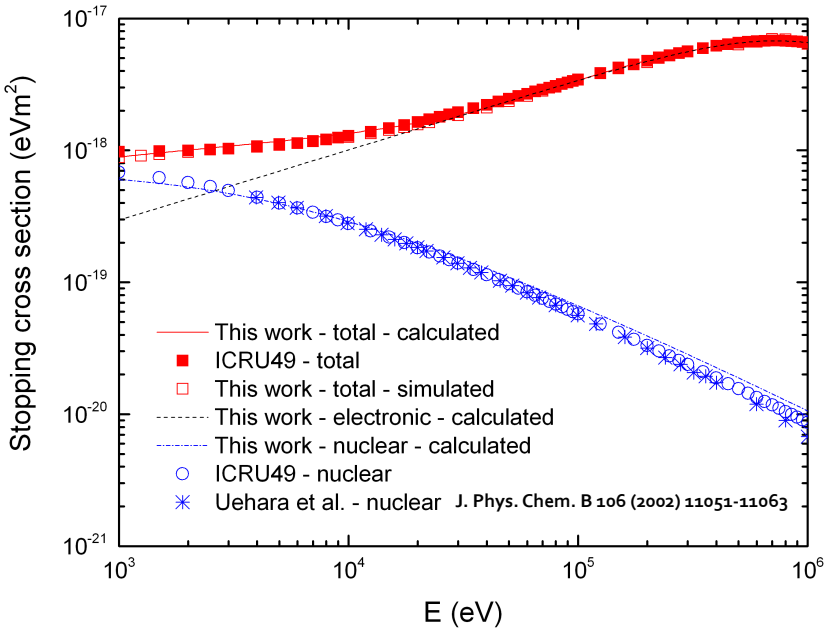


Stopping cross section

Protons



Alphas



Total, electronic and nuclear stopping cross sections

- calculated from Geant4-DNA cross sections
- simulated with Geant4-DNA

compared to ICRU49 and Uehara et al. Monte Carlo simulations

Other changes in models

- Handling of G4IonTable
  - Li, Be, B, C, N, O, Si, Fe
- Possibility to switch to a stationary regime in all energy loss models directly from PhysicsList
- While loops performance has been verified
  - For Geant4-DNA physics
  - For Penelope physics
  - Dedicated Twiki page

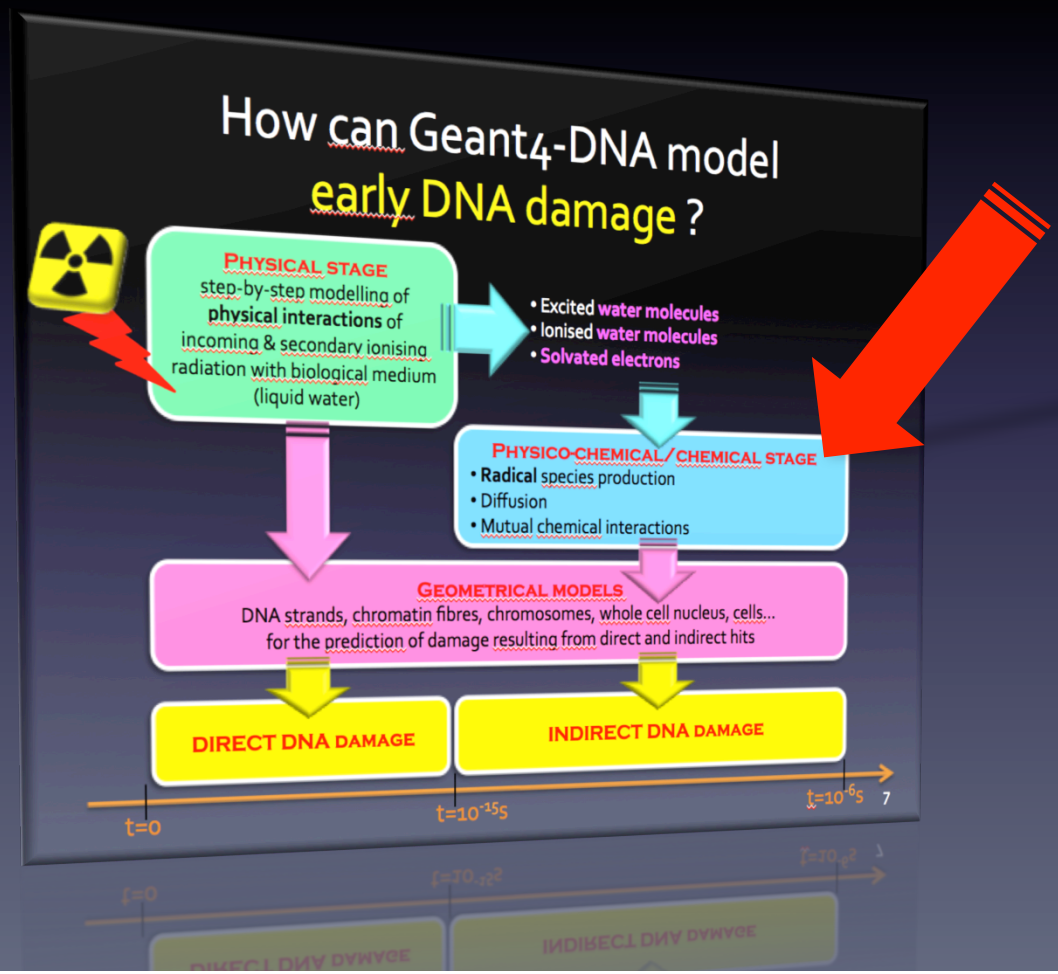
https://twiki.cern.ch/twiki/bin/view/Geant4/LoweSystemTesting

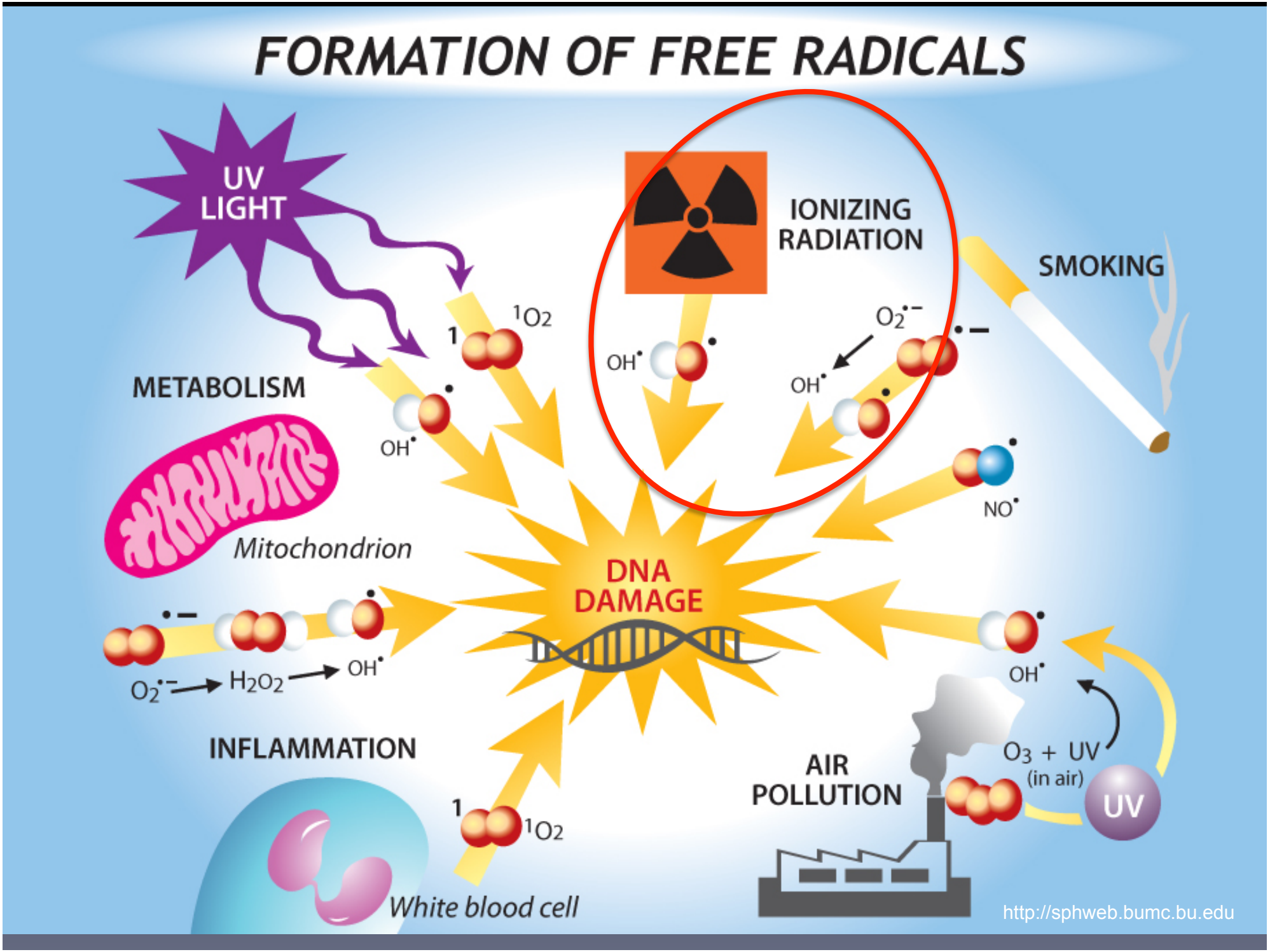
While loops

Verification of the performance of "while loops" is on-going. The following classes have been checked:

Directory	Class name	G4 version	line numbers of loop	Fix by tag ?	Verifier name
dna/models/src	G4DNABornExcitationModel1.cc	Geant4 10.2Beta	238, 248	no	SI
dna/models/src	G4DNABornExcitationModel2.cc	Geant4 10.2Beta	303	not used	SI
dna/models/src	G4DNAEmfietzoglouExcitationModel.cc	Geant4 10.2Beta	284, 295	no	SI
dna/models/src	G4DNABornIonisationModel1.cc	Geant4 10.2Beta	180, 244, 448, 590, 608 (longest for e- when fasterCode is false), 638, 937, 948	no	SI
dna/models/src	G4DNABornIonisationModel2.cc	Geant4 10.2Beta	194, 331, 473, 491 (longest for e- when fasterCode is false), 521, 765, 776	no	SI
dna/models/src	G4DNAEmfietzoglouIonisationModel.cc	Geant4 10.2Beta	175, 481, 494, 731, 742	no	SI
dna/models/src	G4DNAChampionElasticModel.cc	Geant4 10.2Beta	168	no	SI

Geant4-DNA: PHYSICO-CHEMICAL & CHEMICAL STAGE

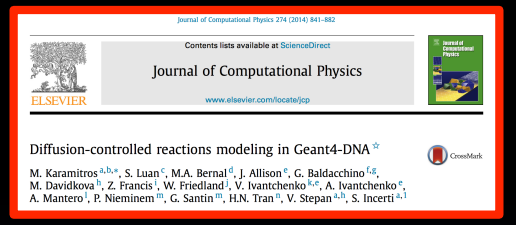



FORMATION OF FREE RADICALS
UV LIGHT
IONIZING RADIATION
SMOKING
METABOLISM
Mitochondrion
DNA DAMAGE
NO•
INFLAMMATION
White blood cell
AIR POLLUTION
O3 + UV (in air)
UV
http://sphweb.bumc.bu.edu

$t=10^{-15}s$ $t=10^{-12}s$

Physico-chemical stage

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


Journal of Computational Physics 274 (2014) 841–882

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Diffusion-controlled reactions modeling in Geant4-DNA ☆

M. Karamitros [a,b,*], S. Luan [c], M.A. Bernal [d], J. Allison [e], G. Baldacchino [f,g], M. Davidkova [h], Z. Francis [i], W. Friedland [j], V. Ivantchenko [k,e], A. Ivantchenko [e], A. Mantero [l], P. Nieminem [m], G. Santin [m], H.N. Tran [n], V. Stepan [a,h], S. Incerti [a,1]

http://dx.doi.org/10.1016/j.jcp.2014.06.011

Electronic state	Dissociation channels	Fraction (%)
All single ionization states	$H_3O^+ + \bullet OH$	100
Excitation state A1B1: (1b1) → (4a1/3s)	$\bullet OH + H\bullet$ $H_2O + DE$	65 35
Excitation state B1A1: (3a1) → (4a1/3s)	$H_3O^+ + \bullet OH + e^-_{aq}$ (AI) $\bullet OH + \bullet OH + H_2$ $H_2O + DE$	55 15 30
Excitation state: Rydberg, diffusion bands	$H_3O^+ + \bullet OH + e^-_{aq}$ (AI) $H_2O + DE$	50 50
Dissociative attachment	$^\bullet OH + OH^- + H_2$	100

- Products thermalize down to their energy of diffusion at equilibrium

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

Chemical stage

Species	Diffusion coefficient D (10^{-9} m^2 s^{-1})
H_3O^+	9.0
$H^\bullet$	7.0
OH^-	5.0
e^-_{aq}	4.9
H_2	4.8
$^\bullet OH$	2.8
H_2O_2	2.3

InConstructMolecules()

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

Reaction	Reaction rate (10^{10} M^{-1} s^{-1})
$H_3O^+ + OH^- \rightarrow 2\,H_2O$	14.3
$^\bullet OH + e^-_{aq} \rightarrow OH^-$	2.95
$H^\bullet + e^-_{aq} + H_2O \rightarrow OH^- + H_2$	2.65
$H_3O^+ + e^-_{aq} \rightarrow H^\bullet + H_2O$	2.11
$H^\bullet + {}^\bullet OH \rightarrow H_2O$	1.44
$H_2O_2 + e^-_{aq} \rightarrow OH^- + {}^\bullet OH$	1.41
$H^\bullet + H^\bullet \rightarrow H_2$	1.20
$e^-_{aq} + e^-_{aq} + 2\,H_2O \rightarrow 2\,OH^- + H_2$	0.50
$^\bullet OH + {}^\bullet OH \rightarrow H_2O_2$	0.44

InConstructReactionTable()

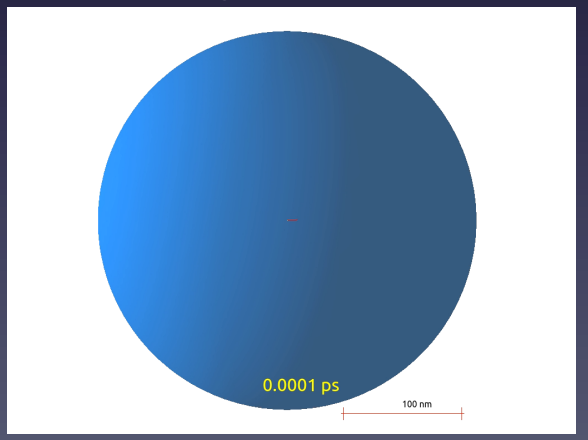
Kreipl *et al*, 2009

How to use Geant4-DNA for radiation chemistry ?

- Three examples have been released publicly in Geant4 10.1 in the « extended examples/medical/dna » category of Geant4 examples
  - CHEM1: activating chemistry
    - Display of chemical reactions at initialization
    - Illustration of usage of radiolysis macro commands « /scheduler/… »:
      - Verbosity
      - Stop of simulation after a certain time duration
      - Or after a maximum number of steps in time
  - CHEM2: altering chemistry run
    - How to access information at the time step level
    - How to set user minimum time step limits using a G4UserTimeStepAction user action class (TimeStepAction)
    - How to retrieve information from a given time step
      - Molecule names, reaction products…
  - CHEM3: user interactivity and visualization
    - How to handle user interactivity
      - SteppingAction, TrackingAction, visualization
    - Enables drawing of cumulative trajectory of species

Work in MT + G4_WATER

Chem3 for 1 keV e-



http://dx.doi.org/10.6084/m9.figshare.978887

10.2 BETA

Chemistry is activated using 3 instructions only…

PhysicsList

- Register the G4EmDNAChemistry « physics-chemistry list »

```
RegisterConstructor( "G4EmDNAChemistry" );
```

Action Initialization

- In Build() method, creation of a StackingAction

The chemistry module is triggered when all physical tracks have been processed

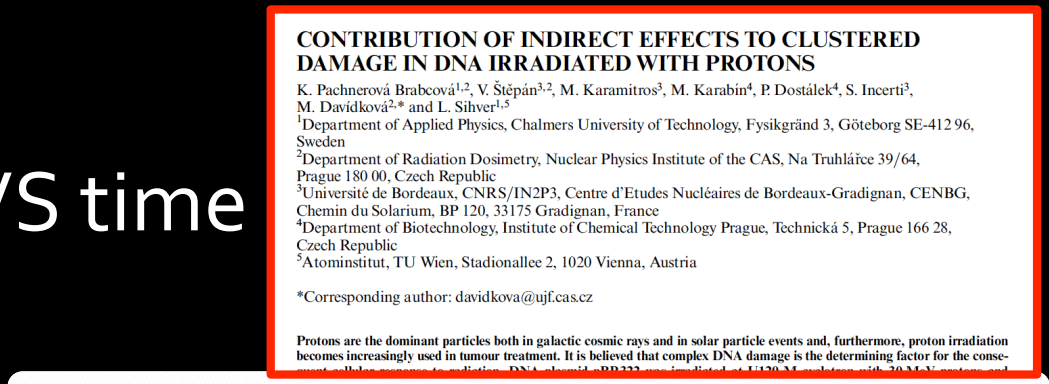
StackingAction

- Start handling of chemistry tracks at new stage

```
G4DNAChemistryManager::Instance()->Run();
```

Validation: radiochemical yields VS time

- We compared measured G values of OH radicals in liquid water to Monte Carlo simulations
- Experiment
  - 30 MeV proton beam at NPI in Prague
  - Target is coumarin-3-carboxylic acid scavenger (C3CA), 3 concentrations (2, 20, 200 mM). C3CA forms fluorescent product with OH, 7-hydroxycoumarin-3-carboxylic acid (7-OH-C3CA) The inverse of the reaction rate k [C3CA] corresponds to the time scale of the reaction.
- Simulations
  - Geant4-DNA physics + RADAMOL for radiolysis (15 & 30 MeV) developed at NPI (M. Davidkova et al.)
  - Geant4-DNA physics + radiolysis (20 MeV)
  - Same geometry as in previous setup : we selected three energies in order to to cover the energy decrease of protons in the sample

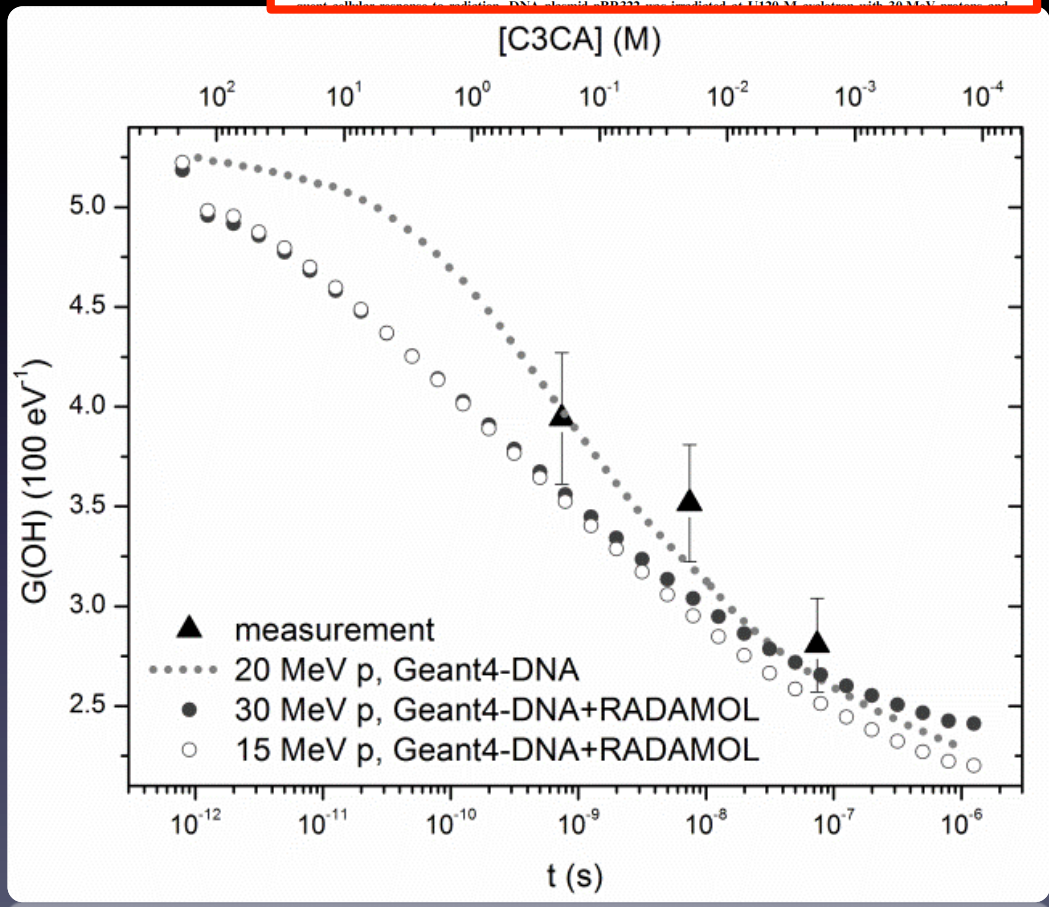


CONTRIBUTION OF INDIRECT EFFECTS TO CLUSTERED DAMAGE IN DNA IRRADIATED WITH PROTONS

K. Pachnerová Brabcová[1,2], V. Štěpán[3,2], M. Karamitros[3], M. Karabín[4], P. Dostálek[4], S. Incerti[3], M. Davídková[2,*] and L. Sihver[1,5]
[1]Department of Applied Physics, Chalmers University of Technology, Fysikgränd 3, Göteborg SE-412 96, Sweden
[2]Department of Radiation Dosimetry, Nuclear Physics Institute of the CAS, Na Truhlářce 39/64, Prague 180 00, Czech Republic
[3]Université de Bordeaux, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux-Gradignan, CENBG, Chemin du Solarium, BP 120, 33175 Gradignan, France
[4]Department of Biotechnology, Institute of Chemical Technology Prague, Technická 5, Prague 166 28, Czech Republic
[5]Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria

*Corresponding author: davidkova@ujf.cas.cz

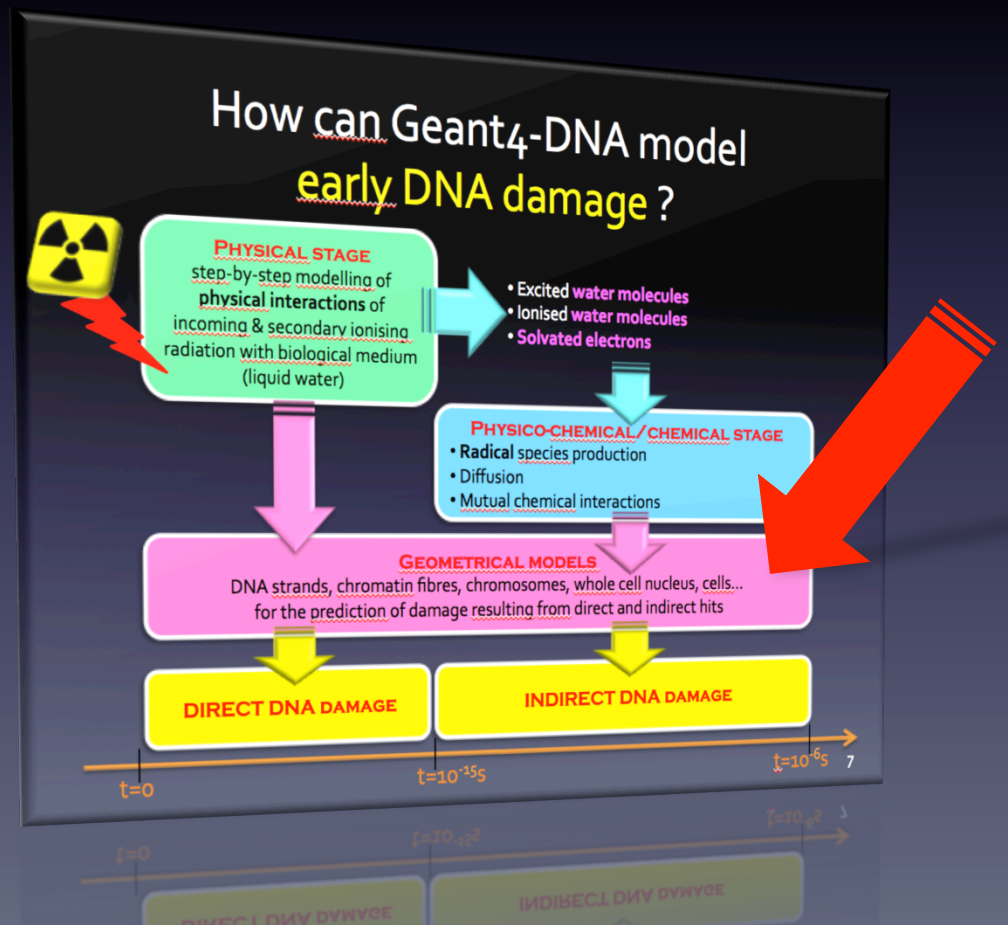
Protons are the dominant particles both in galactic cosmic rays and in solar particle events and, furthermore, proton irradiation becomes increasingly used in tumour treatment. It is believed that complex DNA damage is the determining factor for the conse-



Calculated OH radical yields in time are in acceptable agreement with the experimental data, notably when utilising Geant4-DNA chemistry simulation capabilities

Radiat. Prot. Dosim. 166 (2015) 44-48

Geant4-DNA: GEOMETRICAL MODELS



RCSB PDB PROTEIN DATA BANK

http://pdb4dna.in2p3.fr
http://geant4-dna.org

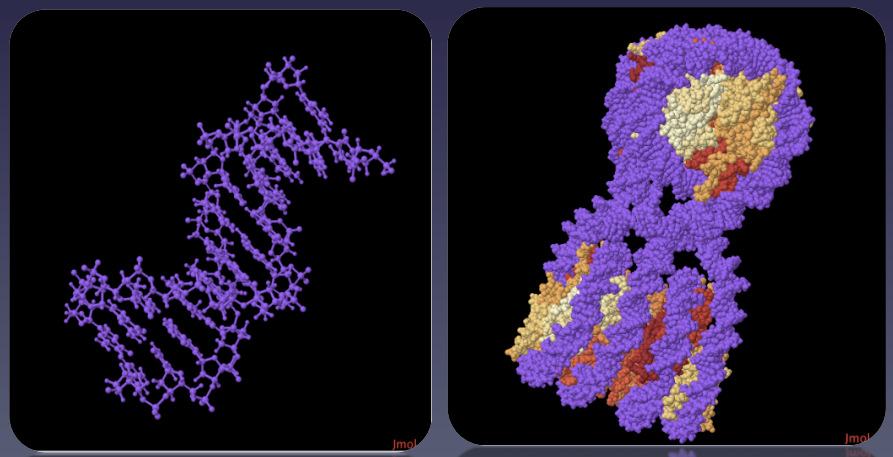
A new interface to describe geometries in Geant4-DNA

- PDB : Protein Data Bank

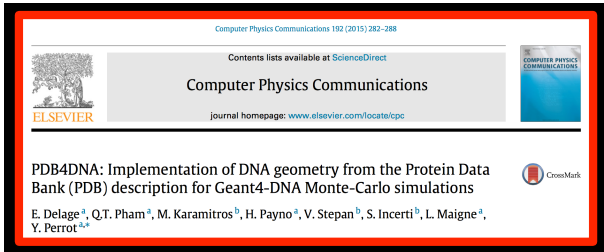
  http://www.rcsb.org/pdb/

  - 3D structure of molecules
  - Proteins
  - Nucleic acids
- Description of DNA molecules
  - 1FZX.pdb
    - Dodecamer
    - 12 DNA base pairs
    - (2,8 x 2,3 x 4,01 nm^3)
  - 1ZBB.pdb
    - Tetranucleosome
    - 2 nucloosomes : 347 pairs of bases
    - (9,5 x 15,0 x 25,1 nm^3)

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



1FZX.pdb 1ZBB.pdb


Computer Physics Communications 192 (2015) 282–288

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

PDB4DNA: Implementation of DNA geometry from the Protein Data Bank (PDB) description for Geant4-DNA Monte-Carlo simulations

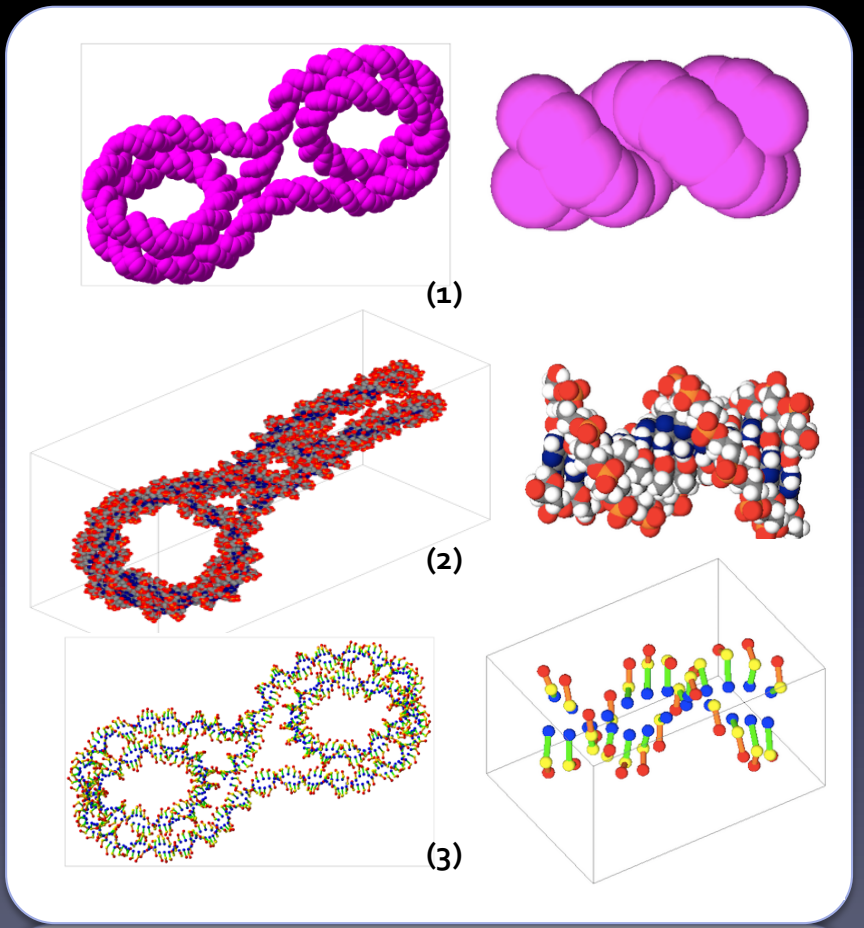
E. Delage [a], Q.T. Pham [a], M. Karamitros [b], H. Payno [a], V. Stepan [b], S. Incerti [b], L. Maigne [a], Y. Perrot [a,*]

http://dx.doi.org/10.1016/j.cpc.2015.02.026

http://pdb4dna.in2p3.fr
http://geant4-dna.org

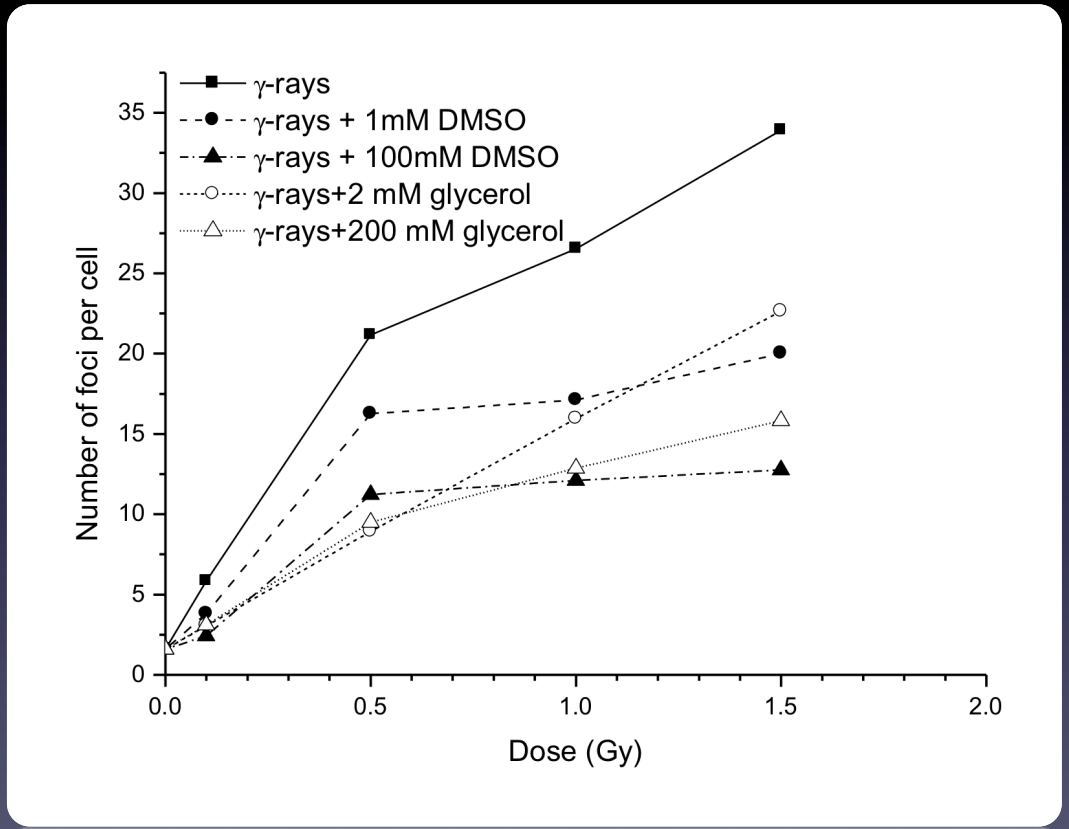
« PDB4DNA » suite

- 1) A C++ library
  - Reading of PDB files
  - Build bounding boxes from atom coordinates
  - Search for closest atom from a given point
  - Geometry and visualization : 3 granularities
    - (1) Barycenter of nucleotides
    - (2) Atomistic
    - (3) Barycenter of nucleotide components
- 2) A Geant4-DNA example
  - Water box surrounding the molecule
  - The output results consists in a ROOT file, containing for each event:
    - energy deposit in bounding boxes
    - number of single strand breaks (SSB)
    - number of double strand breaks (DSB)
- Available on-line under Geant4 license



Biological damage: validation on-going

- On-going validation activity for the prediction of direct damage under gamma and proton irradiation of biological cells
- Two °OH scavengers @ increasing concentration
  - DMSO
  - Glycerol
- Several cancer cell lines
  - Eg. MCF-7 (breast)
- University of Belgrade : A. Ristic-Fira and I. Petrovic



Geant4-DNA examples included in Geant4

Example code name	Purpose	Location
dnaphysics	• Usage of Geant4-DNA Physics processes • variable density	$G4INSTALL/examples/extended/medical/dna
microdosimetry	Combination of Standard EM or Low Energy EM processes with Geant4-DNA Physics processes	$G4INSTALL/examples/extended/medical/dna
range	Usage of Geant4-DNA Physics processes for range simulation	$G4INSTALL/examples/extended/medical/dna
svalue	Usage of Geant4-DNA Physics processes in spheres for S-value calculation	$G4INSTALL/examples/extended/medical/dna
wvalue	Usage of Geant4-DNA Physics processes for W-value caculation	$G4INSTALL/examples/extended/medical/dna
chem1, chem2, chem3	Usage of Geant4-DNA chemistry	$G4INSTALL/examples/extended/medical/dna
wholeNuclearDNA	Cell nucleus	$G4INSTALL/examples/extended/medical/dna
pdb4dna	Interface to PDB database	$G4INSTALL/examples/extended/medical/dna
(microbeam)	(3D cellular phantom)	($G4INSTALL/examples/advanced)

Summary

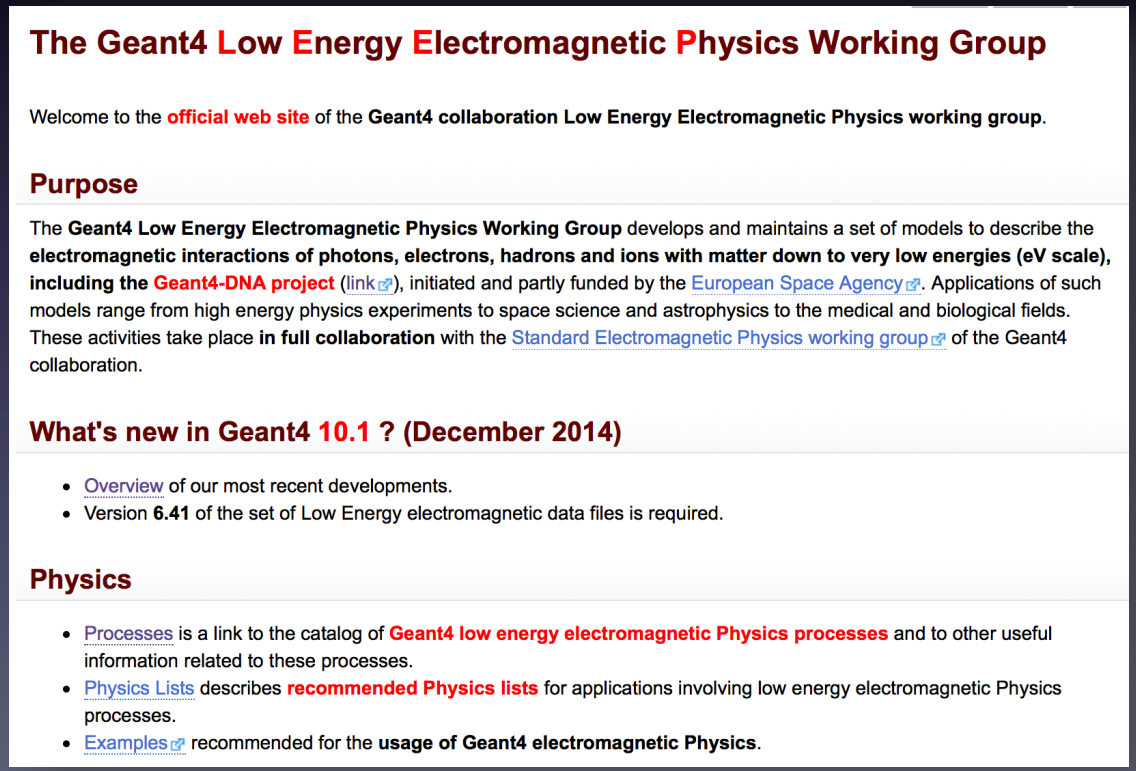
- Low energy EM Physics
  - Low energy limit treatment of gamma models
  - New Monash models
  - Update of atomic de-excitation
  - Update of ICRU73
  - Further verification & validation activities
- Geant4-DNA
  - New electron models
  - Chemistry prototype + 3 examples
  - Geometries : pdb4dna
  - New extended/medical/dna examples

Thanks for your attention

and specials thanks to

J.M.C. Brown, S. Guatelli, V. Ivantchenko, S. Paltani, L. Pandola, B. Suerfu, the Geant4-DNA Collaboration

P. Nieminen and G. Santin @ ESA



The Geant4 Low Energy Electromagnetic Physics Working Group

Welcome to the **official web site** of the **Geant4 collaboration Low Energy Electromagnetic Physics working group**.

Purpose

The **Geant4 Low Energy Electromagnetic Physics Working Group** develops and maintains a set of models to describe the **electromagnetic interactions of photons, electrons, hadrons and ions with matter down to very low energies (eV scale), including the Geant4-DNA project** (link), initiated and partly funded by the European Space Agency. Applications of such models range from high energy physics experiments to space science and astrophysics to the medical and biological fields. These activities take place **in full collaboration** with the Standard Electromagnetic Physics working group of the Geant4 collaboration.

What's new in Geant4 10.1 ? (December 2014)

- Overview of our most recent developments.
- Version **6.41** of the set of Low Energy electromagnetic data files is required.

Physics

- Processes is a link to the catalog of **Geant4 low energy electromagnetic Physics processes** and to other useful information related to these processes.
- Physics Lists describes **recommended Physics lists** for applications involving low energy electromagnetic Physics processes.
- Examples recommended for the **usage of Geant4 electromagnetic Physics**.

Backup

chem1

Initialization of chemistry: List of chemical reactions & reaction rates

Reaction	Reaction Rate [dm3/(mol*s)]
H3O^1 + e_aq^1 -> H^0	2.11e+10
H3O^1 + OH^-1 -> No product	1.43e+11
OH^0 + e_aq^1 -> OH^-1	2.95e+10
OH^0 + OH^0 -> H2O2^0	4.4e+09
OH^0 + H^0 -> No product	1.44e+10
e_aq^1 + e_aq^1 -> OH^-1 + OH^-1 + H_2^0	5e+09
e_aq^1 + H^0 -> OH^-1 + H_2^0	2.65e+10
e_aq^1 + H2O2^0 -> OH^-1 + OH^0	1.41e+10
H^0 + H^0 -> H_2^0	1.2e+10

Verbose(1) Occuring reactions

```
G4WT0 > Physics stage ends
G4WT0 > *** G4Scheduler starts processing
G4WT0 > At time :       1 ps  Reaction : OH^-1 (-69) + H3O^1 (-73) -> No product
G4WT0 > At time :       3 ps  Reaction : e_aq^1 (-64) + OH^0 (-72) -> OH^-1 (-142)
G4WT0 > At time :       3 ps  Reaction : H3O^1 (-71) + OH^-1 (-142) -> No product
G4WT0 > At time : 59.3971 ps  Reaction : OH^0 (-94) + H^0 (-141) -> No product
G4WT0 > At time :  103.14 ps  Reaction : e_aq^1 (-36) + OH^0 (-88) -> OH^-1 (-143)
G4WT0 > At time : 127.186 ps  Reaction : e_aq^1 (-65) + OH^0 (-78) -> OH^-1 (-144)
G4WT0 > At time : 169.258 ps  Reaction : H3O^1 (-85) + OH^-1 (-143) -> No product
G4WT0 > At time : 201.482 ps  Reaction : e_aq^1 (-49) + H3O^1 (-125) -> H^0 (-145)
G4WT0 > At time :  600.47 ps  Reaction : e_aq^1 (-46) + OH^0 (-104) -> OH^-1 (-146)
G4WT0 > At time : 4.96327 ns  Reaction : OH^0 (-82) + OH^0 (-106) -> H2O2^0 (-147)
G4WT0 > At time : 16.0101 ns  Reaction : e_aq^1 (-32) + H3O^1 (-129) -> H^0 (-148)
G4WT0 > At time : 96.4559 ns  Reaction : e_aq^1 (-22) + H3O^1 (-93) -> H^0 (-149)
G4WT0 > *** G4Scheduler ends at time : 1 mus
```

Verbose(2) Detail of time steps: reaction & duration

```
G4WT1 > Physics stage ends
G4WT1 > *** G4Scheduler starts processing
G4WT1 > *** End of step N°1      T_i= 1 ps       dt= 0 ps        T_f= 1 ps
At time :       1 ps  Reaction : OH^-1 (-69) + H3O^1 (-73) -> No product
G4WT1 > *** End of step N°2      T_i= 1 ps       dt= 0 ps        T_f= 1 ps
*** End of step N°3      T_i= 1 ps       dt= 1 ps        T_f= 2 ps       eCollisi
At time :       3 ps  Reaction : e_aq^1 (-64) + OH^0 (-72) -> OH^-1 (-142)
G4WT1 > *** End of step N°4      T_i= 2 ps       dt= 1 ps        T_f= 3 ps
At time :       3 ps  Reaction : H3O^1 (-71) + OH^-1 (-142) -> No product
G4WT1 > *** End of step N°5      T_i= 3 ps       dt= 0 ps        T_f= 3 ps
*** End of step N°6      T_i= 3 ps       dt= 3.19769 ps          T_f= 6.19769 ps
*** End of step N°7      T_i= 6.19769 ps         dt= 4.24303 ps          T_f= 10.
*** End of step N°8      T_i= 10.4407 ps         dt= 5.1737 ps   T_f= 15.6144 ps
```

Verbose(3) Detail of time step duration calculation

```
G4WT1 > Physics stage ends
G4WT1 > *** G4Scheduler starts processing
G4WT1 >
G4WT1 > ___________________________________________________________________
G4WT1 > *** Start Of Step N°1 ***
G4WT1 > Current Global time : 1 ps
G4WT1 > *** Time stepper returned : 1.54648 ps  ***
G4WT1 > *** The minimum time returned by the processes is : 0 ps  ***
G4WT1 > *** End of step N°1      T_i= 1 ps       dt= 0 ps        T_f= 1 ps
 has also reached the user time limit
___________________________________________________________________
 Start Of Step N°2 ***
G4WT1 > Current Global time : 1 ps
G4WT1 > *** Time stepper returned : 0 ps  ***
G4WT1 > *** The minimum time returned by the processes is : 4.32364 mus ***
G4WT1 > At time :       1 ps  Reaction : OH^-1 (-69) + H3O^1 (-73) -> No product
G4WT1 > *** End of step N°2      T_i= 1 ps       dt= 0 ps        T_f= 1 ps
It has also reached the user time limit
___________________________________________________________________
*** Start Of Step N°3 ***
G4WT1 > Current Global time : 1 ps
G4WT1 > *** Time stepper returned : 1 ps  ***
G4WT1 > *** The minimum time returned by the processes is : 4.32364 mus ***
G4WT1 > *** End of step N°3      T_i= 1 ps       dt= 1 ps        T_f= 2 ps
It has also reached the user time limit
```

(verbose level is selected using UI commands)

chem1

Verbose(4)

Maximum detail:

- trackID (<0)

- Pre & post-step positions

- Volumes

- Chemical processes

```
G4WT1 > Physics stage ends
G4WT1 > *** G4Scheduler starts processing
G4WT1 > ____________________________________________________________
G4WT1 > *** Start Of Step N°1 ***
G4WT1 > Current Global time : 1 ps
G4WT1 > *** Time stepper returned : 1.54648 ps  ***
G4WT1 > *** The minimum time returned by the processes is : 0 ps  ***
G4WT1 > *** G4Scheduler::DoIt ***
G4WT1 > #Name             trackID        Position                        Pre step volume         Post step volume        Process
G4WT1 > H2O^-1            -66            -0.0276062 -0.0635558 1.21083 um   World                   ---
G4WT1 > H2O^-1            -66            -0.0276062 -0.0635558 1.21083 um   ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -62            -0.0262441 -0.0657665 1.20832 um   World                   ---
G4WT1 > H2O^1             -62            -0.0262441 -0.0657665 1.20832 um   ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -61            -0.0266101 -0.0649094 1.21005 um   World                   ---
G4WT1 > H2O^1             -61            -0.0266101 -0.0649094 1.21005 um   ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -60            -0.0261657 -0.0652823 1.21039 um   World                   ---
G4WT1 > H2O^1             -60            -0.0261657 -0.0652823 1.21039 um   ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -59            -0.025907 -0.0673742 1.21049 um    World                   ---
G4WT1 > H2O^1             -59            -0.025907 -0.0673742 1.21049 um    ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -54            -0.0299001 -0.0945952 1.50938 um   World                   ---
G4WT1 > H2O^1             -54            -0.0299001 -0.0945952 1.50938 um   ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -51            -0.027727 -0.121723 1.93883 um     World                   ---
G4WT1 > H2O^1             -51            -0.027727 -0.121723 1.93883 um     ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -47            -0.0293585 -0.144776 2.24876 um    World                   ---
G4WT1 > H2O^1             -47            -0.0293585 -0.144776 2.24876 um    ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -34            -0.0322278 -0.233501 3.49242 um    World                   ---
G4WT1 > H2O^1             -34            -0.0322278 -0.233501 3.49242 um    ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -33            -0.030755 -0.233669 3.49276 um     World                   ---
G4WT1 > H2O^1             -33            -0.030755 -0.233669 3.49276 um     ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -25            -0.00715171 -0.317087 4.55492 um   World                   ---
G4WT1 > H2O^1             -25            -0.00715171 -0.317087 4.55492 um   ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -24            -0.00647864 -0.31762 4.55433 um    World                   ---
G4WT1 > H2O^1             -24            -0.00647864 -0.31762 4.55433 um    ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -20            0.0140478 -0.346855 4.89029 um     World                   ---
G4WT1 > H2O^1             -20            0.0140478 -0.346855 4.89029 um     ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -14            -0.0283664 -0.29422 4.15272 um     World                   ---
G4WT1 > H2O^1             -14            -0.0283664 -0.29422 4.15272 um     ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -12            -0.0294111 -0.228729 3.42316 um    World                   ---
G4WT1 > H2O^1             -12            -0.0294111 -0.228729 3.42316 um    ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -11            -0.0283104 -0.222311 3.33667 um    World                   ---
G4WT1 > H2O^1             -11            -0.0283104 -0.222311 3.33667 um    ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -9             -0.027194 -0.209459 3.1837 um      World                   ---
G4WT1 > H2O^1             -9             -0.027194 -0.209459 3.1837 um      ---                     World                   H2O_DNAMolecularDecay
G4WT1 > H2O^1             -7             -0.0277829 -0.147386 2.28426 um    World                   ---
```