

Chemistry examples



geant4-dna.org

Chem6 example

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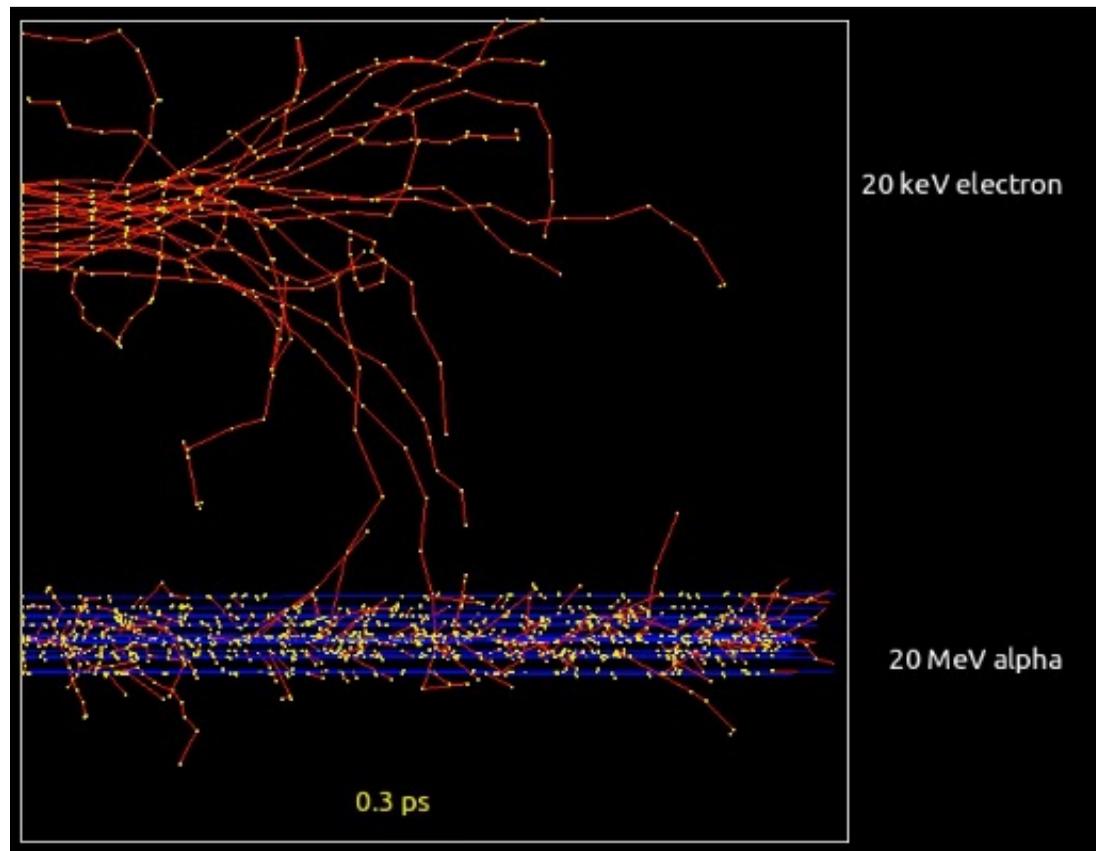
tran@lp2ib.in2p3.fr

Geant4-DNA tutorial, Bangkok, Thailand,
March 18-20, 2026.

Geant4 version 11.4
Released in December 2025

Pre-Chemistry Processes

Geant4-DNA simulation



		Branching ratio (%)			
Ionization	H ₂ O ⁺	H ₃ O ⁺ + ·OH	100	100	Ionization
Excitation	A ¹ B ₁	H [·] + ·OH	65	65	A1B1_DissociationDecay
		H ₂ O + ΔE	35	35	No displacement
	B ¹ A ₁	H ₃ O ⁺ + ·OH + e _{aq} ⁻	50	55	Auto-Ionization
		H [·] + ·OH	25.35	-	A1B1_DissociationDecay
		H ₂ + 2·OH	3.25	15	B1A1_DissociationDecay
		2H [·] + O(³ P)*	3.9	-	B1A1_DissociationDecay2
		H ₂ O + ΔE	17.5	30	No displacement
	Rydberg A+B, C+D, Diffuse bands	H ₃ O ⁺ + ·OH + e _{aq} ⁻	50	50	Auto-Ionization
		H ₂ O + ΔE	50	50	No displacement
	Electron capture	DEA	OH [·] + ·OH + H ₂	100	100
Recombinat -ion		H [·] + ·OH	35.75	55	A1B1_DissociationDecay
		H ₂ + 2·OH	13.65	15	B1A1_DissociationDecay
		2H [·] + O(³ P)	15.6	-	B1A1_DissociationDecay2
		H ₂ O + ΔE	35	30	No displacement

W.-G. Shin, et al., Phys. Med. (2021)

Processes in the Chemical Stage

Water Molecules:

- Electron Hole Recombination
- Water Dissociation

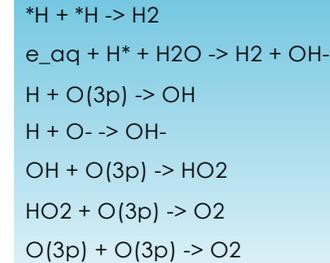
Chemical Species DIFFUSION

Species	Diffusion coefficient D ($10^{-9} \text{ m}^2 \text{ s}^{-1}$)
H ₃ O ⁺	9.0
H•	7.0
OH ⁻	5.0
e ⁻ _{aq}	4.9
H ₂	5.0
•OH	2.8
H ₂ O ₂	1.4

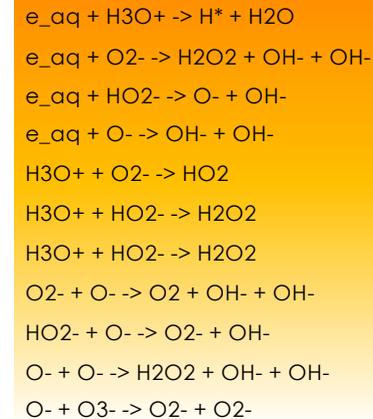
Chemical Species: **72 CHEMICAL REACTIONS !!**

Type	Description
I	Totally diffusion-controlled reactions: their reaction rates are completely governed by diffusion
II	Partially diffusion-controlled reactions: their reaction rates are governed by diffusion but also by the reaction rates of reactive loss
III	Totally diffusion-controlled reactions but the reactants are both ions so electrical interactions must be considered
IV	Partially diffusion-controlled reactions but the reactants are both ions so electrical interactions must be considered
V	Totally diffusion-controlled reactions in which the molecular spin is taken into account
VI	Non-diffusion controlled reactions: - first order reactions: decay of species - pseudo-first order reactions: those where one of the reactant has a considerably higher concentration than the other and it is considered to be a "background molecule"

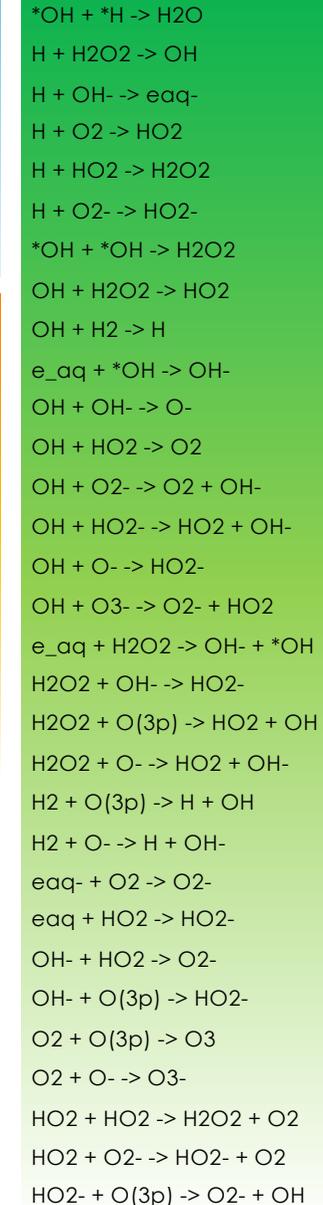
Type I: 7 reactions



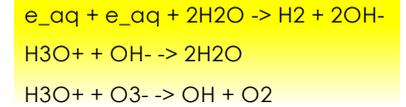
Type IV: 11 reactions



Type II: 31 reactions



Type III: 3 reactions



Type VI: 20 reactions



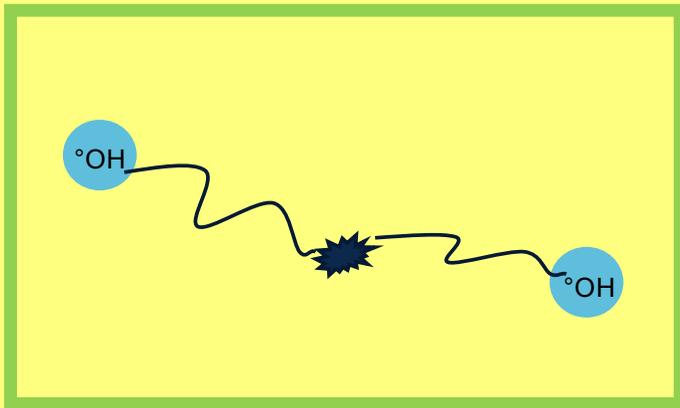
Chemistry Models

SBS model

At each step (bigger than a Minimum Time Step) the separation distance "d" of all pairs of reactants is checked.

Two species react with each other when d is below a given threshold "R", called reaction radius.

The Brownian bridge technique compensate for possible missed reactions.



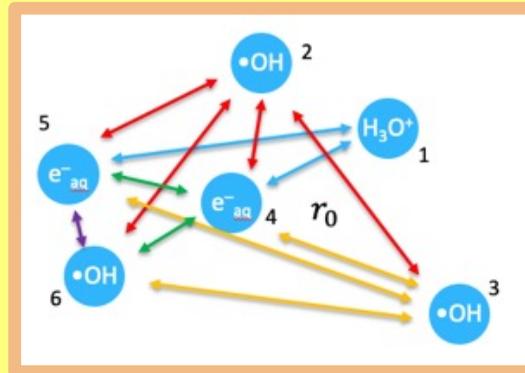
Karamitros, M. et al. (2014) Diffusion-controlled reactions modeling in Geant4-DNA. Journal of Computational Physics, 274, 841-882. <https://doi.org/10.1016/j.jcp.2014.06.011>

IRT model

An event table is constructed with the initial chemical species positions and reaction times (calculated with probability functions) for each reactant pair of interest.

Table's entries are sorted in ascending reaction time order and then processed.

Reaction product positions are randomly sampled within a sphere centred at the reaction site.



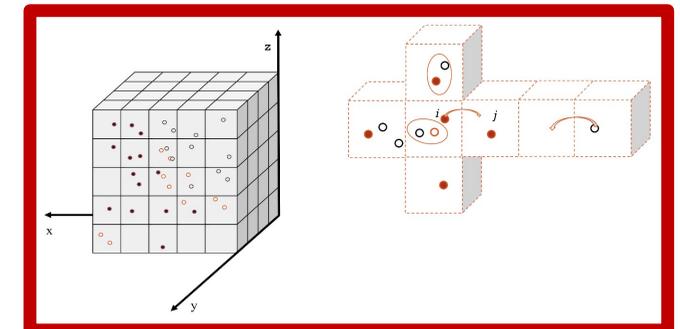
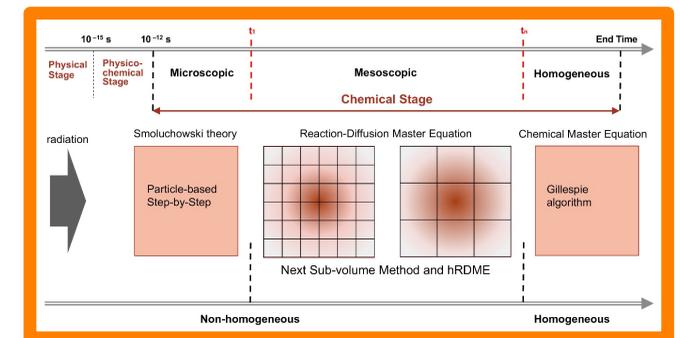
Karamitros, M. et al. (2020) Implementing the Independent Reaction Time method in Geant4 for radiation chemistry simulations. <https://doi.org/10.48550/arXiv.2006.14225>

Ramos-Méndez, J. et al. (2020) Independent reaction times method in Geant4-DNA: Implementation and performance. <https://doi.org/10.1002/mp.14490>

SBS-RDME model

Combination of:

- SBS model
- Compartment-based model using RDME (Reaction-Diffusion Master Equation)



Tran, H. N. et al. (2021) Geant4-DNA Modeling of Water Radiolysis beyond the Microsecond: An On-Lattice Stochastic Approach. International Journal of Molecular Sciences, 22(11), 6023. <https://doi.org/10.3390/ijms22116023>

The Chemistry Examples

example/extended/medical/dna

- The « chem1 » example illustrates how to activate the simulation of water radiolysis (step-by-step method).
- The « chem2 » example illustrates how to set minimum time step limits on water radiolysis (step-by-step method).
- The « chem3 » example illustrates how to implement user actions in the chemistry module (step-by-step method).
- The « chem4 » example illustrates how to compute radiochemical yields ("G") versus time, including a dedicated ROOT graphical interface (step-by-step method).
- The « chem5 » example illustrates how to compute radiochemical yields ("G") versus time, using alternative physics and chemistry lists (step-by-step method).
- The « chem6 » example illustrates how to compute radiochemical yields ("G") versus time and LET using IRT method.
- The « scavenger » example illustrates how to simulate scavenging using an easy-to-use interface and the IRT method.
- The « UHDR » extended/medical/dna example illustrates how to activate the chemistry mesoscopic model in combination with the step-by-step model, and allows to simulate chemical reactions beyond 1 us post-irradiation.

Chem6 example

CORRESPONDING AUTHORS

W. G. Shin, S. Incerti

Chem6 Example

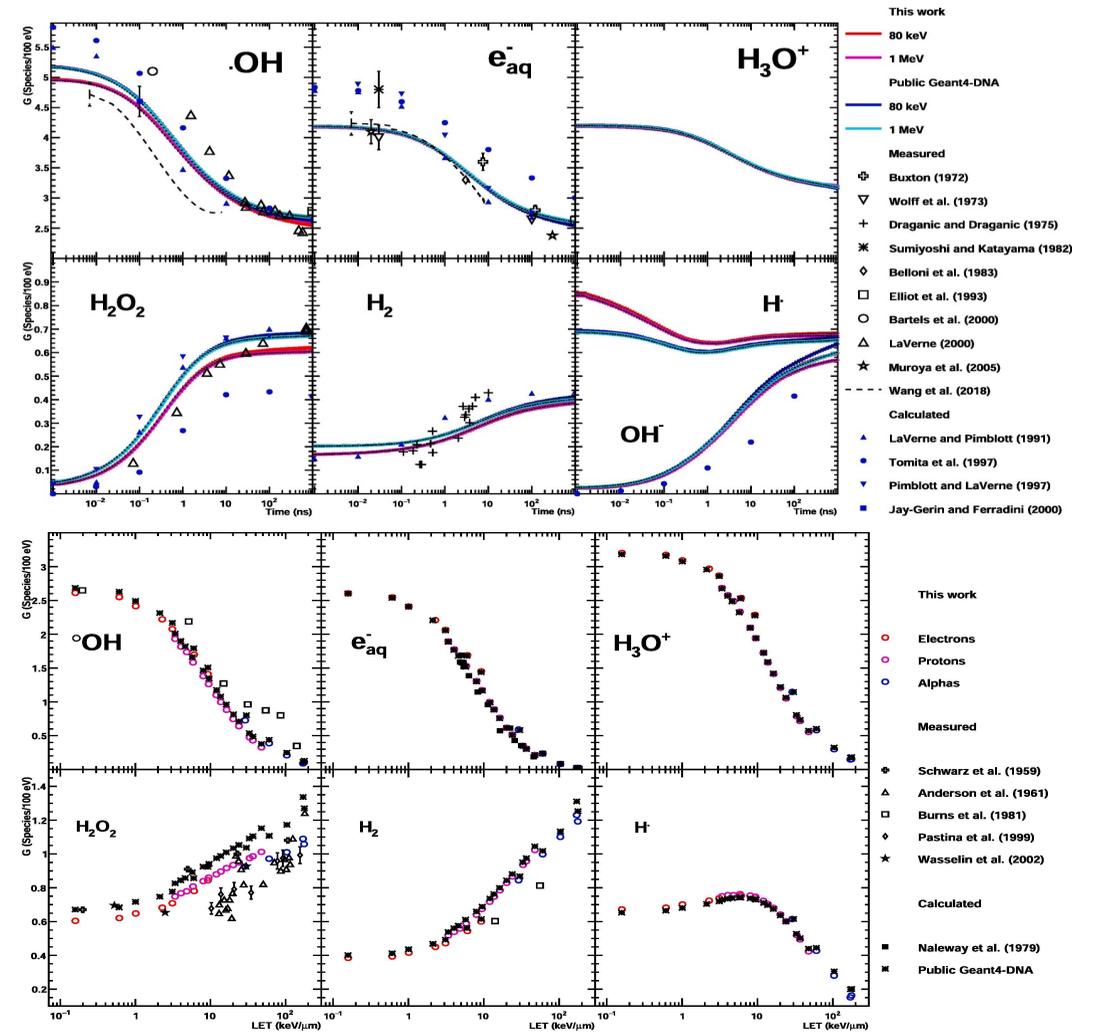
Based on **chem4** and **chem5** provides scoring of the radiochemical yield G :

$$G = \frac{\text{Number of species } X}{100 \text{ eV of deposited energy}}$$

as a function of **time** and **LET**.

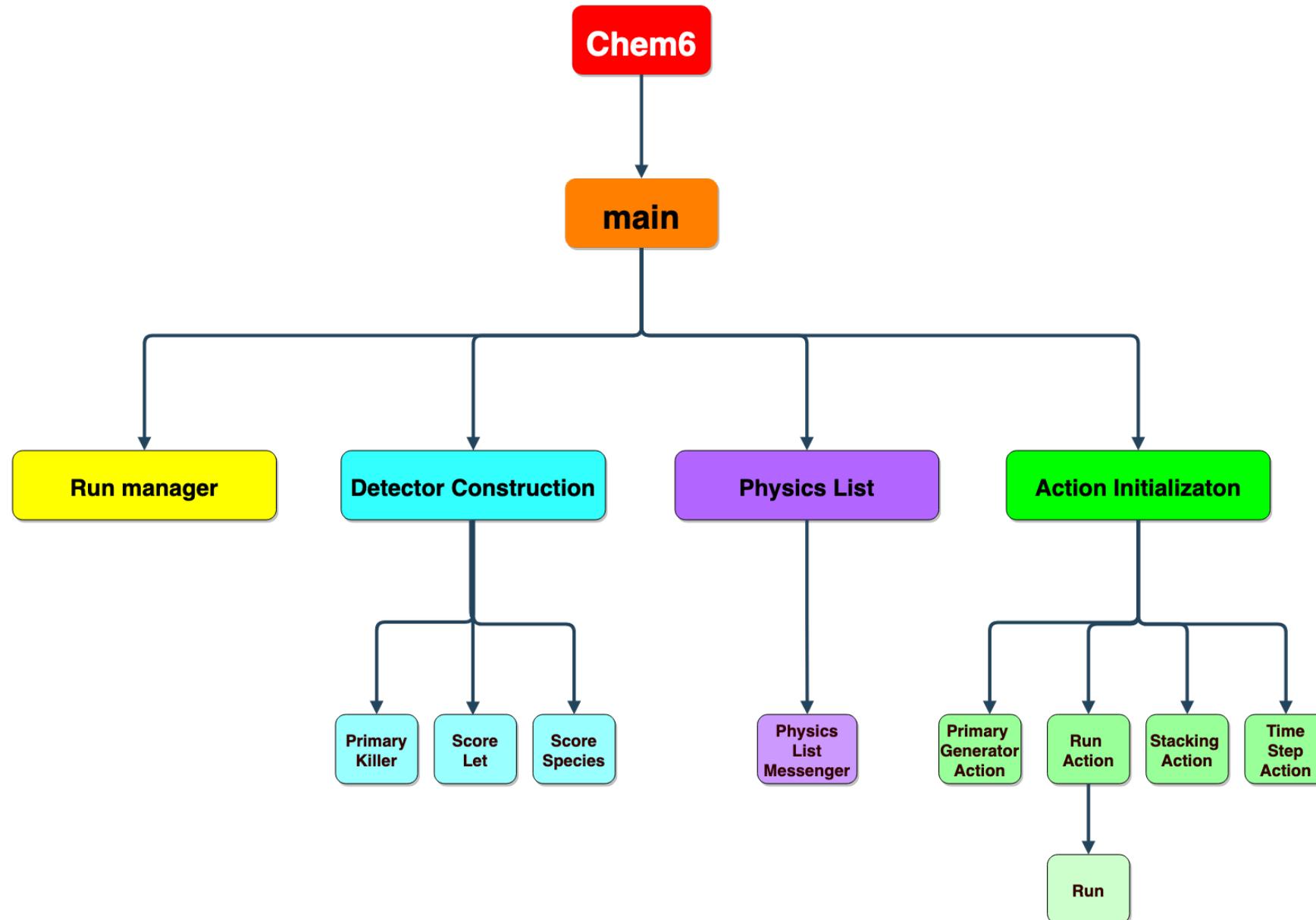
The example uses **IRT** by default.

UI for **species** and **reactions** manual definition



Shin W. G. et al. "Geant4-DNA simulation of the pre-chemical stage of water radiolysis and its impact on initial radiochemical yields" *Physica Medica*, Volume 88, (2021), Pages 86-90
<https://doi.org/10.1016/j.ejmp.2021.05.029>

Chem6 Application Code Structure



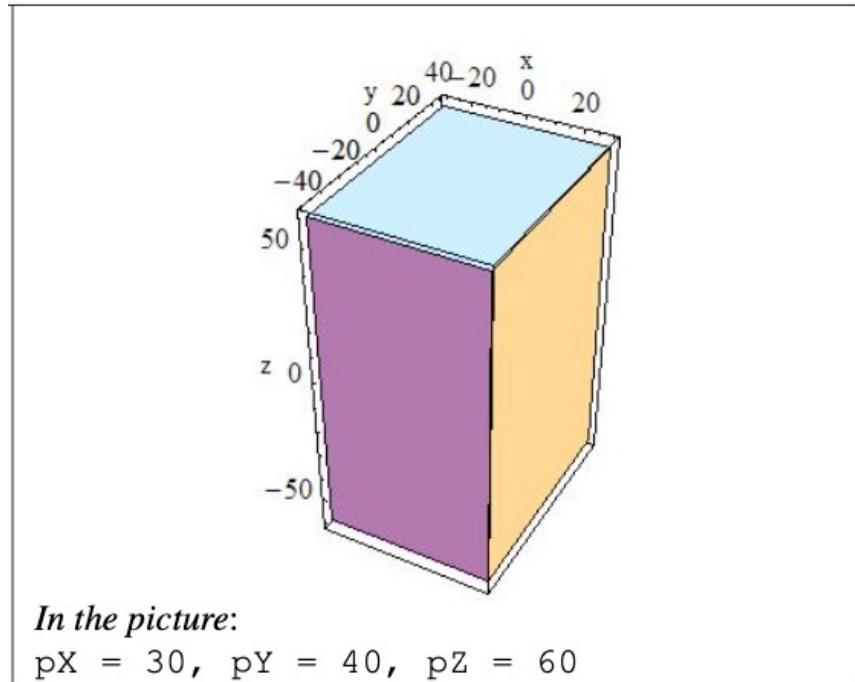
Chem6 Application Code Structure

chem6.cc	Main file ⇒ creation of RunManager, DetectorConstruction, PhysicsList, PrimaryGeneratorAction, ActionInitialization
→RunManager	Management of all the calls to Geant4 kernel and the threads in MT mode
→DetectorConstruction	Definition of the geometry: World volume is a water box representing a 'pseudo infinite' homogeneous medium. SD volume is controlled through the PrimaryKiller
→→PrimaryKiller	G-values are computed for a range of deposited energy. Primary is killed once it has deposited more energy than a minimum value . Event is aborted once the primary has deposited more energy than a maximum value . The SD can be controlled also setting the boundaries: killing outside primary and secondaries
→→ScoreLet	To obtain G versus LET results, LET values are simultaneously calculated during the run.
→→ScoreSpecies	Computes the energy deposition and the number of species along time to extract the radiochemical yields as in chem4 example.
→PhysicsList	Choice of the physics & chemistry lists Default Physics List → G4EmDNAPhysics_option2 Default Chemistry List → G4EmDNAChemistry_option3 Default Chemistry Model → IRT

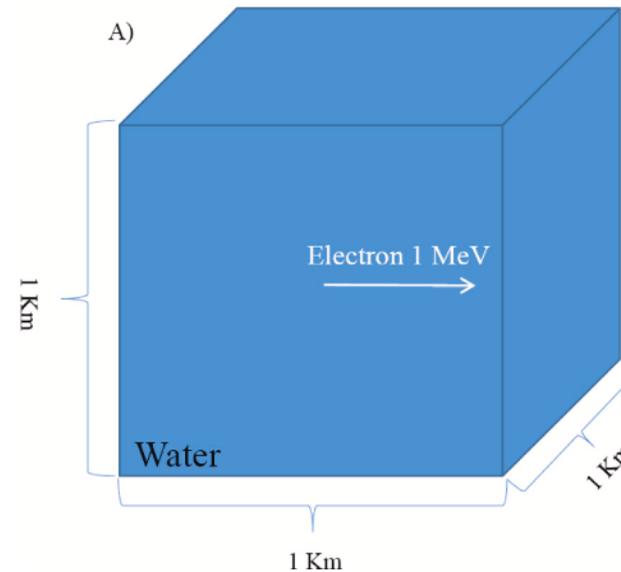
Chem6 Application Code Structure

→→PhysicsList Messenger	Defines commands to switch by macro the chemistry model between: SBS, IRT, IRT_syn
→ActionInitialization	Build() ⇒ creation of PrimaryGeneratorAction & optional user action classes: RunAction, StackingAction, TimeStepAction
→→PrimaryGeneratorAction	Choice of the primary particle. Default: 100 keV Electron
→→RunAction	To retrieve information in the Beginning and in the End of Run. → In the EndOfRun gives in output the number of events, the LET_mean, the LET_square, the total energy deposited in the world volume.
→→→ Run	Records event values and merges them between all the threads (energy deposited, LET)
→→StackingAction	When no more “physical tracks” remain, the method StackingAction::NewStage is called → The Chemistry Stage starts.
→→TimeStepAction	Allows the user to set minimal time step values and to retrieve information from a given time step (molecule names, reaction products, etc...).

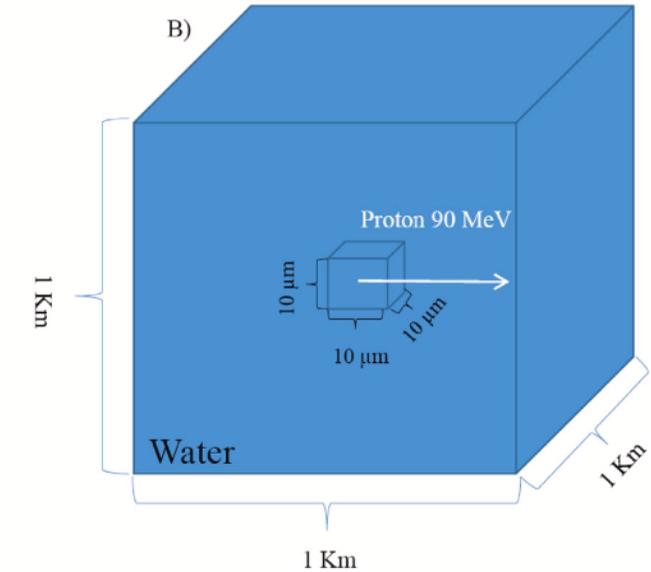
Geometry Definition



F. Farokhi et al.



Radiation Physics and Chemistry 212 (2023) 111184



- The World Volume is a **G4Box**
- Two parameters define the geometry :
 - the material of the Cube → **G4Water**
 - the half-lengths $pX = pY = pZ = 500 \text{ m}$;

The SD is controlled in two ways in the PrimaryKiller:

- With the **low** and **high Edep thresholds**;
- With the **geometrical boundaries**.

Physics / Chemistry List

Physics Models Included:

- G4EmDNAPhysics
- G4EmDNAPhysics_option1
- G4EmDNAPhysics_option2 ← default
- G4EmDNAPhysics_option3
- G4EmDNAPhysics_option4
- G4EmDNAPhysics_option5
- G4EmDNAPhysics_option6
- G4EmDNAPhysics_option7
- G4EmDNAPhysics_option8

Chemistry Models Included:

- G4EmDNAChemistry
- G4EmDNAChemistry_option1
- G4EmDNAChemistry_option2
- G4EmDNAChemistry_option3 ← default

This chemistry constructor is based on the pre-chemical stage of PARTRAC and chemical parameters of RITRACKS. It uses independent reaction time method as a default

Primary Generator

- The primary kinematic consists of a single particle starting at the center of the cube.
- Particle type
Particle energy
Particle initial position
Particle initial direction
are set in the PrimaryGeneratorAction class, and can be changed via the G4 build-in commands of G4ParticleGun class.
- The chemistry module is triggered in the StackingAction class when all physical tracks have been processed.

default: 100 keV Electron

/gun/particle e-

/gun/energy 30 keV

/gun/position 0 0 0 micrometer

/gun/direction 0 0 1

TimeStepAction

In ActionInitialisation: `G4Scheduler::Instance()->SetUserAction(new TimeStepAction());`

Methods

- **TimeStepAction():** Constructor of the TimeStepAction class. Inside it you can set the minimal time steps of your simulation.

<code>AddTimeStep(1 * picosecond, 0.1 * picosecond);</code>	<i>During the first simulated picosecond the minimal time step will be of 0.1 picosecond. If molecules are too close and can react before that time limit: Brownian bridge.</i>
<code>AddTimeStep(10 * picosecond, 1 * picosecond);</code>	<i>From 1 ps to 10 ps in simulation time, the minimal time step will be of 1 ps.</i>

TimeStepAction

In ActionInitialisation: `G4Scheduler::Instance()->SetUserAction(new TimeStepAction());`

Methods

- **StartProcessing()**: Beginning of the chemistry simulation.
- **EndProcessing()**: End of the chemistry simulation.
- **UserPreTimeStepAction()**: If the user wants to do something before the start of the current time step.
- **UserPostTimeStepAction()**: If the user wants to do something after the end of the current time step. Called once after stepping all the tracks.
- **UserReactionAction(Reactif1, Reactif2, Products)**: will be called just after a reaction happened.

How to start?

- Create your own simulation folder, i.e. "*my-simulations*"
- Copy the chem6 example in "*my-simulations*"

```
cd my-simulations
```

```
cp -R $G4EXAMPLES/extended/medical/dna/chem6/ .
```

```
mkdir chem6-build //Create a build folder for chem6
```

```
cd chem6-build // go to the build folder
```

```
cmake ../chem6 // config the example
```

```
make // compile the example
```

```
./chem6 beam.in
```

- *./chem6 beam.in*
electrons from the center of the
water phantom

or

```
./chem6 beam_HCP.in  
protons and alphas from the edge  
of a 5x5x5 um3 water phantom
```

beam.in Macro Commands/1

```
/run/numberOfThreads 2  
/process/dna/e-SolvationSubType Meesungnoen2002  
#/process/dna/e-SolvationSubType Ritchie1994  
#/process/dna/e-SolvationSubType Terrisol1990
```

```
# use Step-by-Step (SBS), independent reaction time (IRT)  
# or synchronized IRT (IRT_syn),  
/process/chem/TimeStepModel IRT  
#/process/chem/TimeStepModel SBS  
#/process/chem/TimeStepModel IRT_syn
```

```
/run/initialize
```

```
# species definition  
# username [ molecule | charge | D(m2/s) | Radius(nm) ]  
#/chem/species O2 [ O2 | 0 | 2.4e-9 | 0.17 ]
```

```
/chem/PrintSpeciesTable
```

```
# reset reaction table  
/chem/reaction/UI
```

=> Choice of e- Solvation Sub Type Process

=> Choice of chemical model

UI species are definition, where:
username is decided by users, *molecule* is used by Geant4,
D is diffusion constant,
Radius is reaction radius.
Spaces between characters are needed.

beam.in Macro Commands/2

```
# totally diffusion-controlled (TDC) | Fix | reactionRate[dm3/(mol*s)] | TDC (0)
/chem/reaction/add H + H -> H2 | Fix | 0.503e10 | 0
/chem/reaction/add e_aq + H -> H2 + OHm | Fix | 2.50e10 | 0
/chem/reaction/add e_aq + e_aq -> H2 + OHm + OHm | Fix | 0.636e10 | 0
/chem/reaction/add H3Op + OHm -> H2O | Fix | 1.13e11 | 0

# partially diffusion-controlled (PDC) | Fix | reactionRate[dm3/(mol*s)] | PDC (1)
/chem/reaction/add OH + H -> H2O | Fix | 1.55e10 | 1
/chem/reaction/add OH + OH -> H2O2 | Fix | 0.55e10 | 1
/chem/reaction/add e_aq + OH -> OHm | Fix | 2.95e10 | 1
/chem/reaction/add e_aq + H2O2 -> OHm + OH | Fix | 1.10e10 | 1
/chem/reaction/add e_aq + H3Op -> H + H2O | Fix | 2.11e10 | 1
```

```
/chem/reaction/print
```

```
/gun/position 0 0 0
/gun/direction 0 0 1
/gun/particle e-
```

```
# in order to reproduce LET values of NIST data
# please see the spower example using stationary mode
```

```
# select cutoff energy for restricted LET
#/scorer/LET/cutoff 100 eV
```

```
#/scorer/species/addTimeToRecord 1 ps
#/scorer/species/addTimeToRecord 10 ps
#/scorer/species/addTimeToRecord 100 ps
#/scorer/species/addTimeToRecord 1 ns
#/scorer/species/addTimeToRecord 10 ns
#/scorer/species/addTimeToRecord 100 ns
#/scorer/species/addTimeToRecord 1 us
```

```
/scorer/species/nOfTimeBins 50
```

```
/tracking/verbose 0
/scheduler/verbose 0
/scheduler/endTime 1 microsecond
```

```
/run/printProgress 100
```

UI reactions definition, where:

H is species username;

0.503e10 is reaction rate;

0 is reaction type.

Spaces between characters are needed.

=> Definition the source:

an e- from the water phantom center, shot straight forward

=> cutoff for restricted LET

=> set times to record the chemical species yields

=> Set the end Time of the chemistry stage

beam.in Macro Commands/3

```
/primaryKiller/eLossMin 1.2 keV # primary is killed if deposited E is greater than this value
/primaryKiller/eLossMax 1.212 keV # event is aborted if deposited E is greater than this value
/gun/energy 2 keV
/run/beamOn 15

/primaryKiller/eLossMin 1.6 keV # primary is killed if deposited E is greater than this value
/primaryKiller/eLossMax 1.616 keV # event is aborted if deposited E is greater than this value
/gun/energy 3.5 keV
/run/beamOn 15

/primaryKiller/eLossMin 2.3 keV # primary is killed if deposited E is greater than this value
/primaryKiller/eLossMax 2.323 keV # event is aborted if deposited E is greater than this value
/gun/energy 7.5 keV
/run/beamOn 15

/primaryKiller/eLossMin 3.8 keV # primary is killed if deposited E is greater than this value
/primaryKiller/eLossMax 3.838 keV # event is aborted if deposited E is greater than this value
/gun/energy 12.5 keV
/run/beamOn 5

/primaryKiller/eLossMin 6.0 keV # primary is killed if deposited E is greater than this value
/primaryKiller/eLossMax 6.06 keV # event is aborted if deposited E is greater than this value
/gun/energy 30 keV
/run/beamOn 5

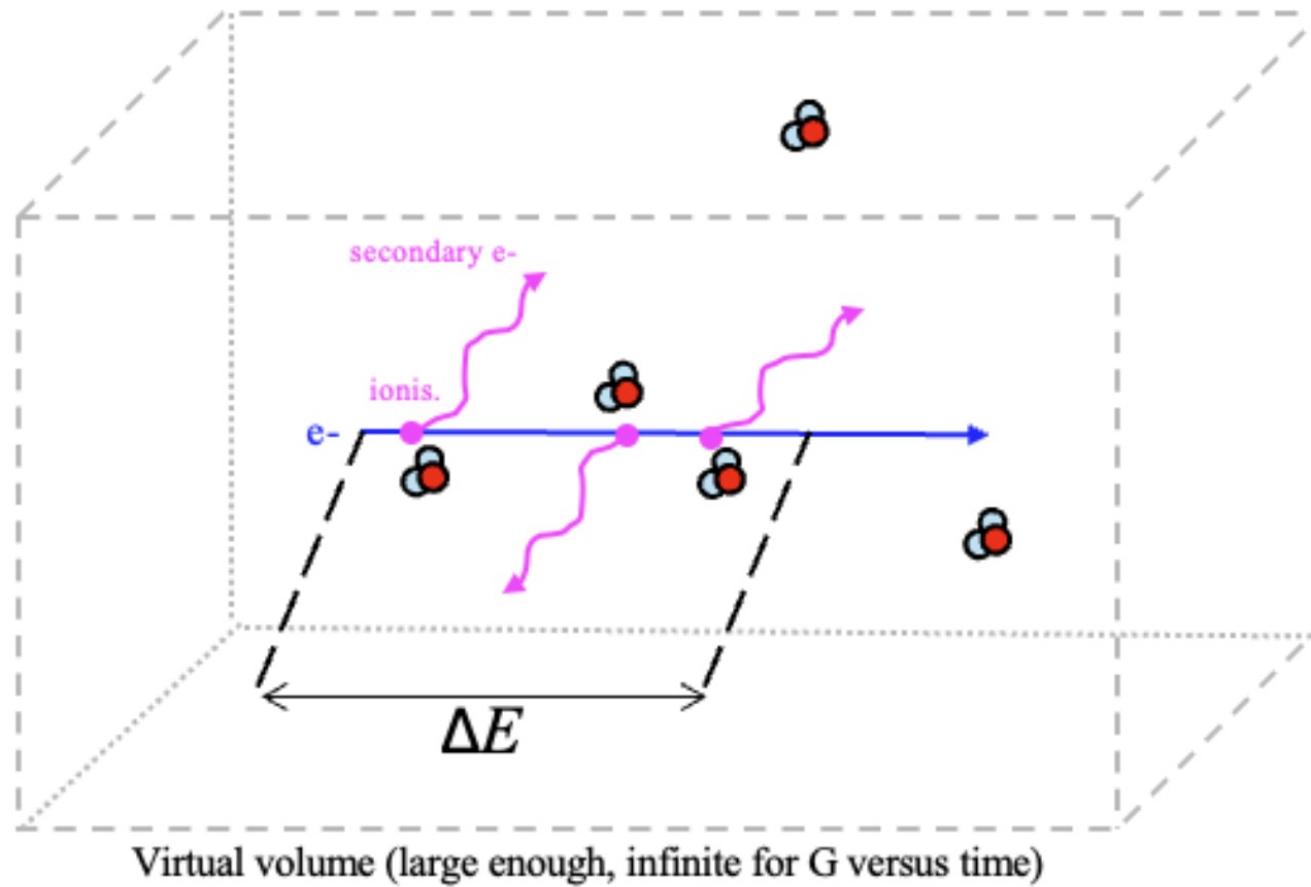
/primaryKiller/eLossMin 8.0 keV # primary is killed if deposited E is greater than this value
/primaryKiller/eLossMax 8.08 keV # event is aborted if deposited E is greater than this value
/gun/energy 80 keV
/run/beamOn 5

/primaryKiller/eLossMin 10 keV # primary is killed if deposited E is greater than this value
/primaryKiller/eLossMax 10.1 keV # event is aborted if deposited E is greater than this value
/gun/energy 999.999 keV
/run/beamOn 2
```

Different runs are started sequentially, changing:

- the low energy threshold to kill the primary
- the high energy threshold to abort the event
- the primary particle initial energy
- the number of events of the run

Energy thresholds



- track segment G-value

$$G(x) = \frac{n(x)}{\bar{\epsilon}}$$

beam_HCP.in Macro Commands

```
/run/numberOfThreads 2
/process/dna/e-SolvationSubType Meesungnoen2002
#/process/dna/e-SolvationSubType Ritchie1994
#/process/dna/e-SolvationSubType Terrisol1990

/run/initialize

/chem/reaction/print

/primaryKiller/setSize 5 5 5 um
/gun/position 0 0 -2.5 um
/gun/direction 0 0 1
/gun/particle proton

# in order to reproduce LET values of NIST data
# please see the spower example using stationary mode

# select cutoff energy for restricted LET
#/scorer/LET/cutoff 100 eV

#/scorer/species/addTimeToRecord 1 ps
#/scorer/species/addTimeToRecord 10 ps
#/scorer/species/addTimeToRecord 100 ps
#/scorer/species/addTimeToRecord 1 ns
#/scorer/species/addTimeToRecord 10 ns
#/scorer/species/addTimeToRecord 100 ns
#/scorer/species/addTimeToRecord 1 us

/scorer/species/nOfTimeBins 50

/tracking/verbose 0
/scheduler/verbose 0
/scheduler/endTime 1 microsecond

/run/printProgress 10

/gun/energy 500 keV
/run/beamOn 10
```

=> Kills primary and secondary particles outside of the virtual volume

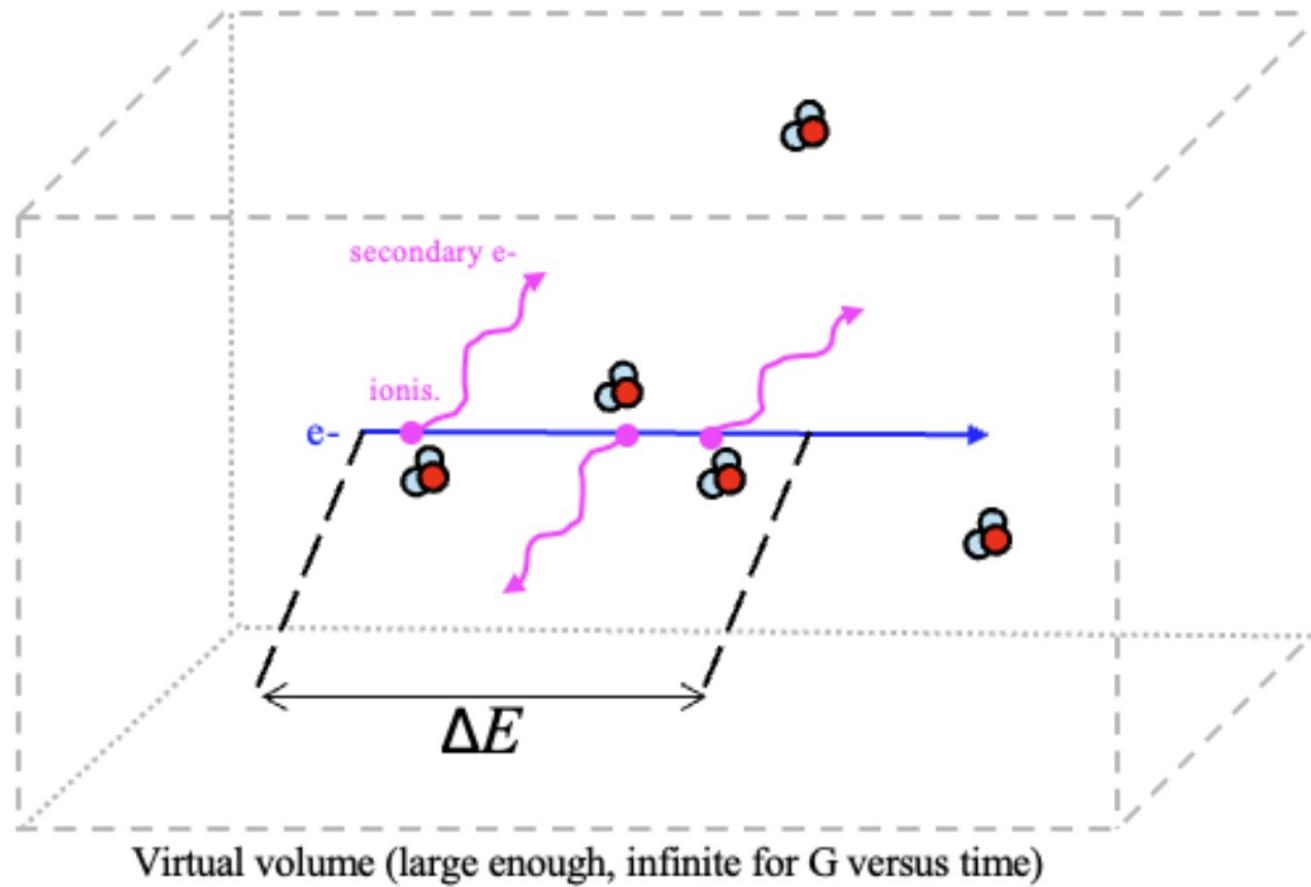
=> Source:

a proton from the edge of a 5x5x5 um³ water phantom, shoot forward

..... After different runs of protons (changing energy and # of events),

the macro continues with a set of runs of alphas:
same geometry, changing energy and # of events

Energy thresholds



- track segment G-value

$$G(x) = \frac{n(x)}{\bar{\epsilon}}$$

Output

Defined Species Table

Molecular Config	Diffusion Coefficient (m ² / s)	Radius (nm)
H3O ⁺	9.46e-09	0.25
OH ⁺	2.2e-09	0.22
OH ⁻	5.3e-09	0.33
e _{aq} ⁻	4.9e-09	0.5
H ⁺	7e-09	0.19
H ₂ ⁺	4.8e-09	0.14
H2O ⁺	2.3e-09	0.21
HO ₂ ⁺	2.3e-09	0.21
HO ₂ ⁻	1.4e-09	0.25
O ⁺	2e-09	0.2
O ⁻	2e-09	0.25
O ₂ ⁺	2.4e-09	0.17
O ₂ ⁻	1.75e-09	0.22
O ₃ ⁺	2e-09	0.2
O ₃ ⁻	2e-09	0.2

Defined Reactions Table

Number of chemical species involved in reactions = 6	
Reaction	Reaction Rate [dm ³ /(mol*s)]
H3O ⁺ + OH ⁻ -> No product	1.13e+11
H3O ⁺ + e _{aq} ⁻ -> H ⁺	2.11e+10
OH ⁺ + H ⁺ -> No product	1.55e+10
OH ⁺ + OH ⁺ -> H2O ⁺	5.5e+09
OH ⁺ + e _{aq} ⁻ -> OH ⁻	2.95e+10
e _{aq} ⁻ + H ⁺ -> H ₂ ⁺ + OH ⁻	2.5e+10
e _{aq} ⁻ + e _{aq} ⁻ -> H ₂ ⁺ + OH ⁻ + OH ⁻	6.36e+09
e _{aq} ⁻ + H2O ⁺ -> OH ⁻ + OH ⁺	1.1e+10
H ⁺ + H ⁺ -> H ₂ ⁺	5.03e+09

Chemical reactions

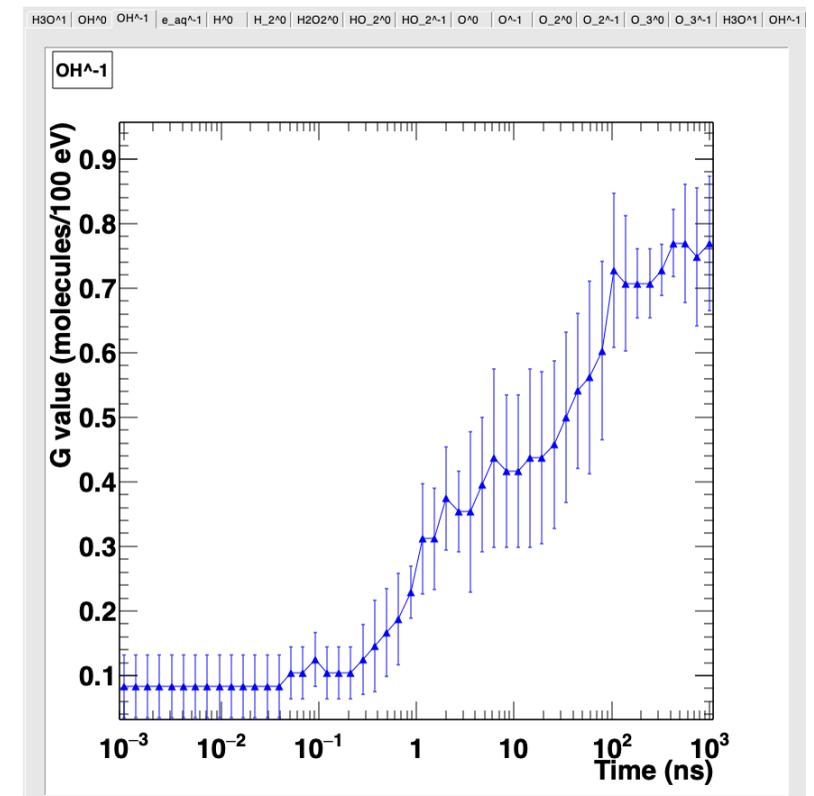
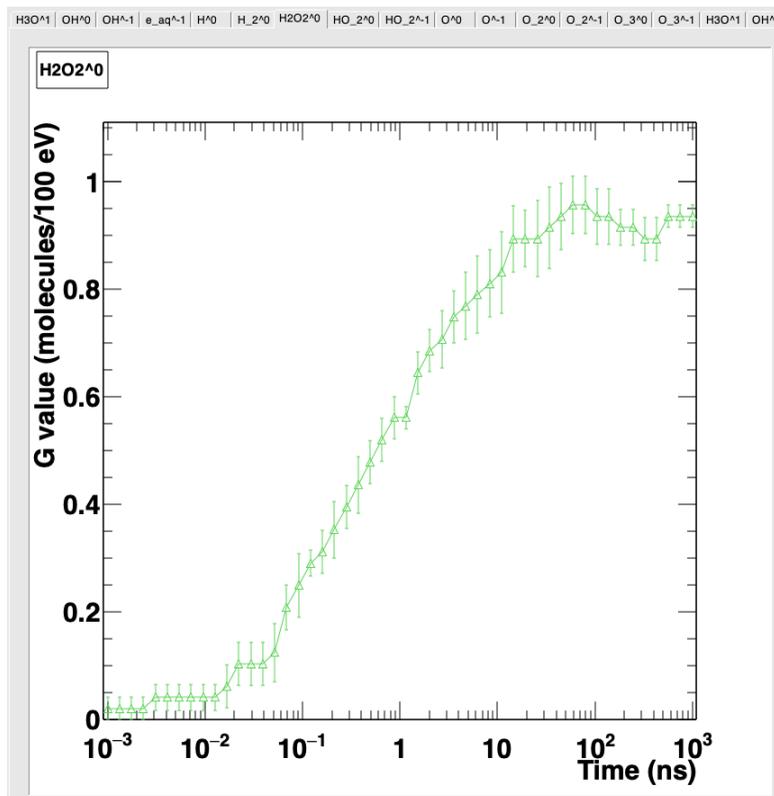
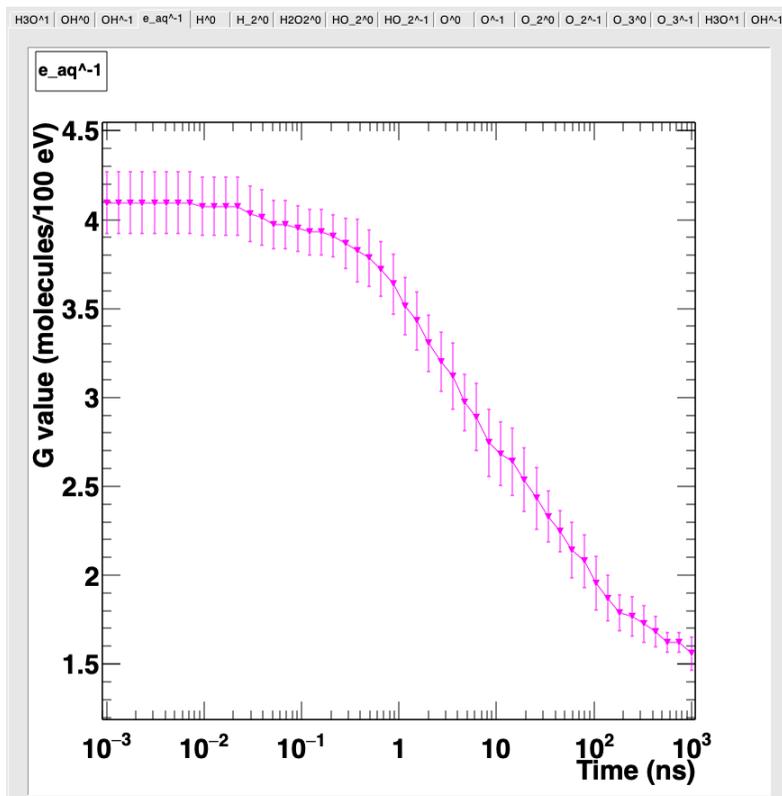
```
### Run 5 starts.
### Run 5 starts.
--> Event 0 starts.
*** G4Scheduler starts processing
At time : 1 ps Reaction : OH+ (-1341) + OH+ (-1357) -> H2O+ (-1752)
At time : 1 ps Reaction : eaq- (-865) + H3O+ (-1514) -> H+ (-1753)
At time : 1 ps Reaction : OH+ (-1554) + eaq- (-1556) -> OH- (-1754)
At time : 1 ps Reaction : OH+ (-1656) + OH+ (-1655) -> H2O+ (-1755)
At time : 1 ps Reaction : OH+ (-1698) + OH+ (-1699) -> H2O+ (-1756)
At time : 1 ps Reaction : OH+ (-1682) + OH+ (-1683) -> H2O+ (-1757)
At time : 1 ps Reaction : OH+ (-1610) + OH+ (-1748) -> H2O+ (-1758)
At time : 1 ps Reaction : OH+ (-1730) + OH+ (-1365) -> H2O+ (-1759)
At time : 1 ps Reaction : eaq- (-137) + OH+ (-917) -> OH- (-1760)
At time : 1 ps Reaction : H3O+ (-916) + OH- (-1760) -> No product
At time : 1 ps Reaction : OH+ (-1003) + OH+ (-939) -> H2O+ (-1761)
At time : 1 ps Reaction : OH+ (-1009) + OH+ (-1193) -> H2O+ (-1762)
At time : 1 ps Reaction : H3O+ (-1168) + OH- (-874) -> No product
At time : 1.836 ps Reaction : OH+ (-1746) + OH+ (-1747) -> H2O+ (-1763)
At time : 7.5883 ps Reaction : OH+ (-1325) + OH+ (-1363) -> H2O+ (-1764)
At time : 10.258 ps Reaction : eaq- (-445) + OH+ (-1551) -> OH- (-1765)
At time : 10.258 ps Reaction : OH- (-1765) + H3O+ (-1552) -> No product
At time : 12.579 ps Reaction : eaq- (-673) + OH+ (-1213) -> OH- (-1766)
At time : 12.579 ps Reaction : H3O+ (-1212) + OH- (-1766) -> No product
At time : 13.175 ps Reaction : H+ (-1724) + OH+ (-1373) -> No product
At time : 14.941 ps Reaction : H+ (-1608) + OH+ (-1540) -> No product
At time : 19.462 ps Reaction : OH+ (-1249) + OH+ (-1261) -> H2O+ (-1767)
At time : 20.08 ps Reaction : OH+ (-953) + OH+ (-1375) -> H2O+ (-1768)
At time : 23.916 ps Reaction : H3O+ (-1522) + eaq- (-1523) -> H+ (-1769)
At time : 24.295 ps Reaction : OH- (-871) + H3O+ (-938) -> No product
At time : 24.573 ps Reaction : OH+ (-1253) + OH+ (-1617) -> H2O+ (-1770)
At time : 30.568 ps Reaction : OH+ (-1263) + H+ (-1618) -> No product
At time : 38.075 ps Reaction : H+ (-1572) + OH+ (-1573) -> No product
At time : 43.326 ps Reaction : OH+ (-875) + OH+ (-1169) -> H2O+ (-1771)
At time : 43.821 ps Reaction : OH+ (-1709) + eaq- (-291) -> OH- (-1772)
At time : 43.821 ps Reaction : OH- (-1772) + H3O+ (-1354) -> No product
At time : 43.99 ps Reaction : H+ (-1749) + OH+ (-1607) -> No product
At time : 46.655 ps Reaction : H3O+ (-960) + eaq- (-168) -> H+ (-1773)
At time : 47.871 ps Reaction : H+ (-1727) + H+ (-1728) -> H2+ (-1774)
At time : 49.601 ps Reaction : eaq- (-364) + OH+ (-1323) -> OH- (-1775)
At time : 49.601 ps Reaction : OH- (-1775) + H3O+ (-1322) -> No product
At time : 50.198 ps Reaction : H+ (-1580) + OH+ (-1670) -> No product
At time : 54.217 ps Reaction : OH+ (-1702) + eaq- (-401) -> OH- (-1776)
At time : 56.466 ps Reaction : OH- (-868) + H3O+ (-902) -> No product
At time : 57.404 ps Reaction : OH+ (-1241) + OH+ (-1245) -> H2O+ (-1777)
At time : 70.1 ps Reaction : OH+ (-1581) + H+ (-1582) -> No product
At time : 76.874 ps Reaction : OH+ (-1161) + OH+ (-1167) -> H2O+ (-1778)
At time : 81.262 ps Reaction : OH- (-892) + H3O+ (-1736) -> No product
At time : 85.681 ps Reaction : OH+ (-1659) + OH+ (-1179) -> H2O+ (-1779)
At time : 96.932 ps Reaction : OH+ (-1648) + H+ (-1649) -> No product
At time : 107.06 ps Reaction : OH+ (-1527) + eaq- (-1529) -> OH- (-1780)
```

- Defined Species table is printed: /chem/PrintSpeciesTable
- Defined reaction table is printed: /chem/reaction/print
- G4Scheduler processes the chemical stage time step after time step.
- Molecular chemical reactions as a function of the elapsed time are printed: /scheduler/verbose 1

Root Analysis: G values vs. time

- The information about all the molecular species is scored in a ROOT ntuple file Species(runID).root e.g.: **Species0.root** Species1.root ...
- A root macro is provided for the analysis: **plotG_time.C**
→ Plots G values vs. time according to the molecular species by importing **Species0.root**.

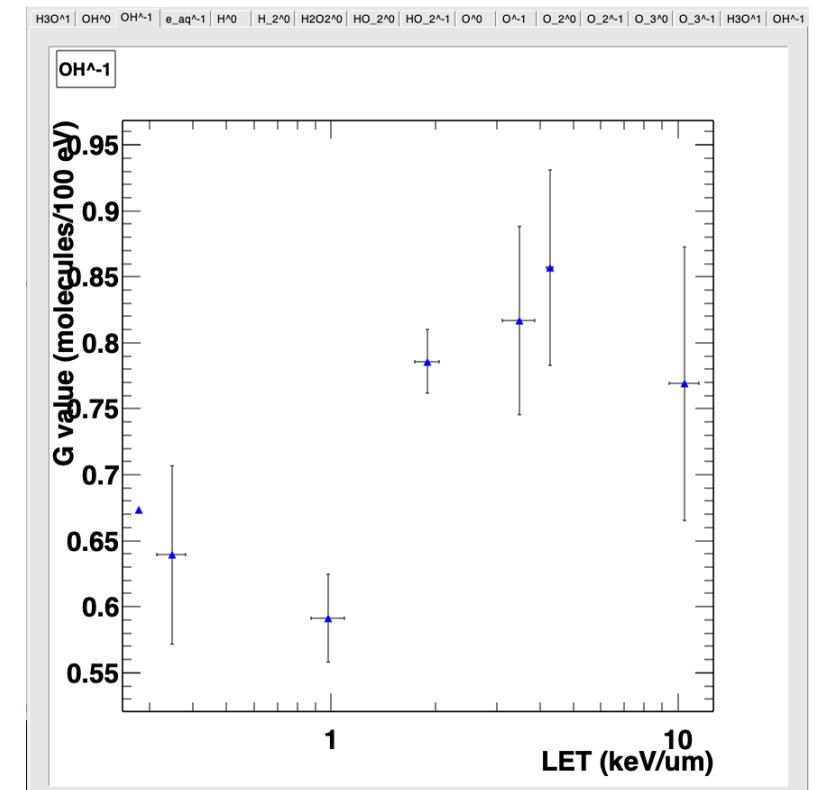
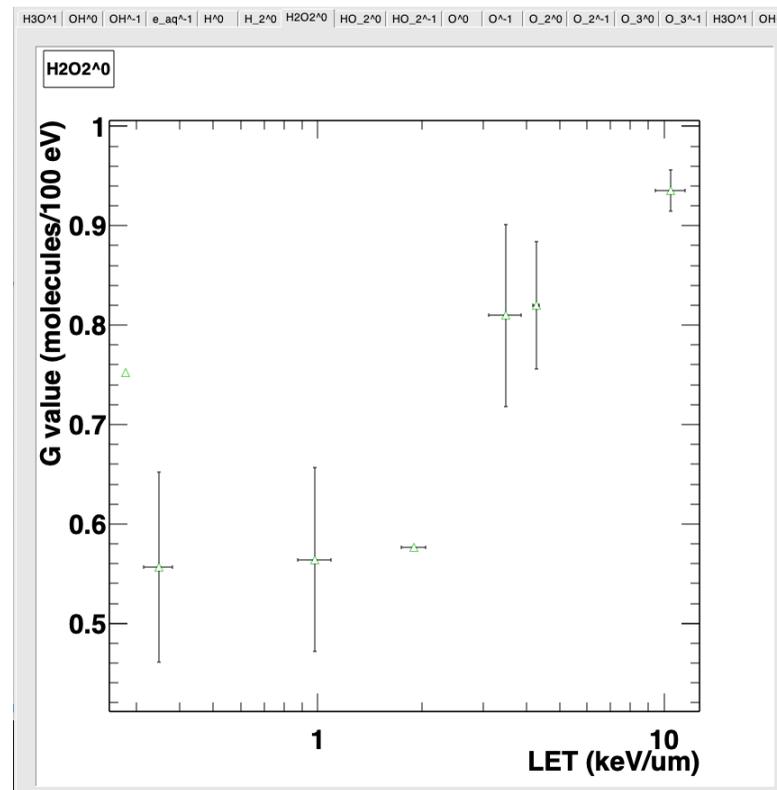
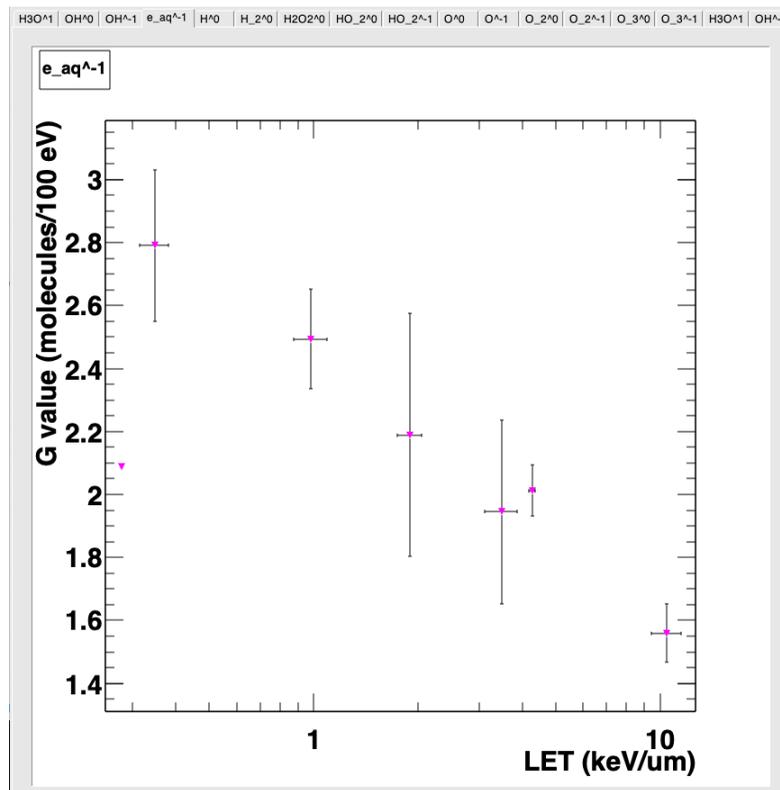
N.B.: To analyse all the run outputs, user should change manually the runID # into the root macro



Root Analysis: G values vs. LET

- G values at the last time bin are scored in a text file `Species.txt` in order to obtain G vs. LET results.
- A root macro is provided for the analysis: `plotG_LET.C`
 - Plot G values as a function of LET according to the molecular species by importing `Species.txt`

N.B. The G versus LET results are accumulated all along, thus, user should remove manually the `Species.txt` file in order to initialize the results.



More Information



GEANT4-DNA : EXTENDING THE GEANT4 MONTE CARLO SIMULATION TOOLKIT FOR RADIOBIOLOGY

Welcome to the web page of the Geant4-DNA project !

The [Geant4](#) general purpose particle-matter Monte Carlo simulation toolkit is being extended with processes for the **modeling of biological damage induced by ionising radiation at the DNA scale**. Such developments are on-going in the framework of the Geant4-DNA project. This project was originally initiated by the [European Space Agency \(ESA\)](#). Developments are undertaken by an [international collaboration](#), coordinated since 2008 by the [National Institute of Nuclear and Particle Physics \(IN2P3\)](#) of the [National Centre for Scientific Research \(CNRS\)](#) in France, in collaboration with the [Geant4@IN2P3](#) activities.

Once published, all developments are freely accessible in **full open access** through the [Geant4 toolkit](#) or through our freely accessible [Geant4 Virtual Machine](#).

Recent posts

June 27th, 2023 : Geant4 11.1.2 LP2i Virtual Machine has been released, see [link](#).

Exercises

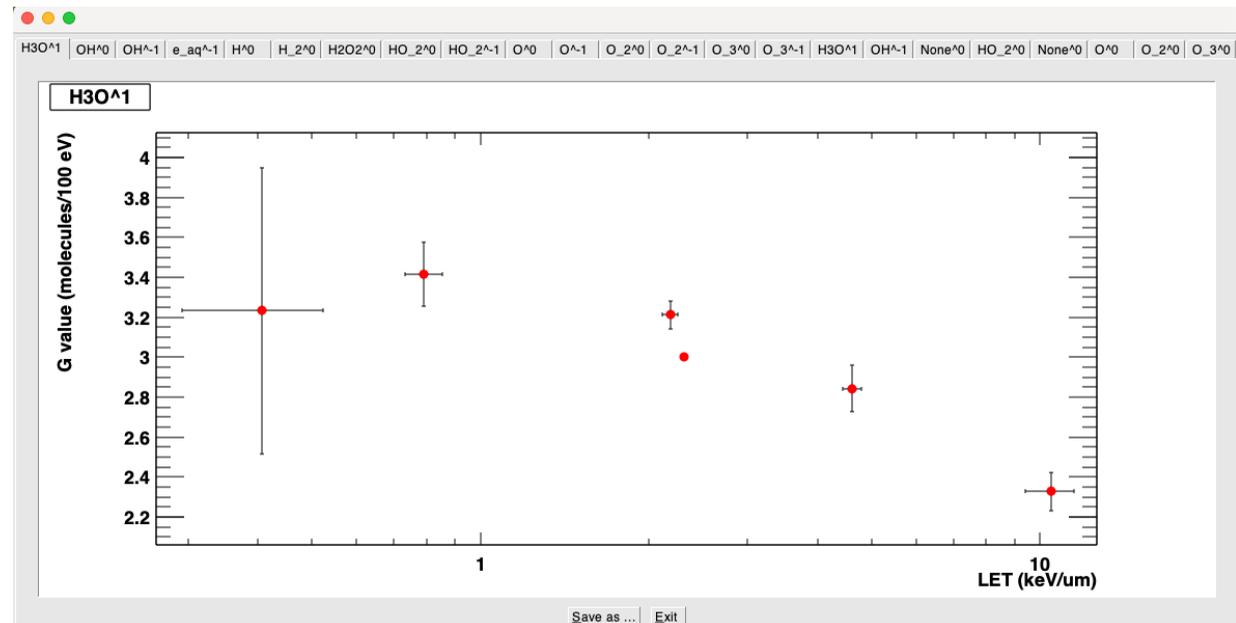
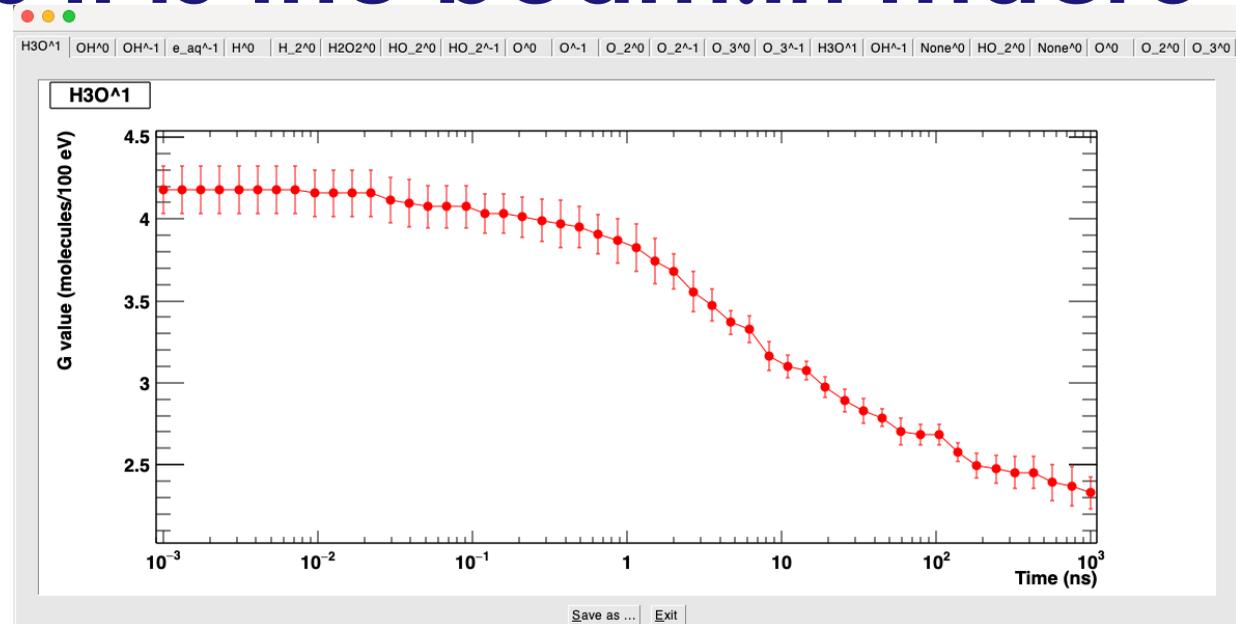
- **Exercise 1:** Run as it is the beam.in macro
- **Exercise 2:** Change the e- Solvation Sub Type Process and re-run the beam.in macro
- **Exercise 3:** Change the chemical model and re-run the beam.in macro
- **Exercise 4:** Change the reaction rate of a chemical reaction and re-run beam.in macro
- **Exercise 5:** Change position / direction / type of source and re-run beam.in macro
- **Exercise 6:** Set and change the cutoff for restricted LET and re-run beam.in macro
- **Exercise 7:** Set and change the times to record the chemical species yields and re-run beam.in macro
- **Exercise 8:** Change the end (not too much!) of the chemical stage and re-run beam.in macro
- **Exercise 9:** Run as it is the beam_HCP.in macro...when you get bored of waiting: go to Exercise 10
- **Exercise 10:** Try to change parameters in the HCP.in macro and re-run it

After each run, start root and analyse data with the root macros provided: **plotG_time.C** and **plotG_LET.C**

Exercise 1: Run as it is the beam.in macro

```
./chem6 beam.in  
root plotG_time.C  
root plotG_LET.C
```

- Species0.root
- Species1.root
- Species2.root
- Species3.root
- Species4.root
- Species5.root

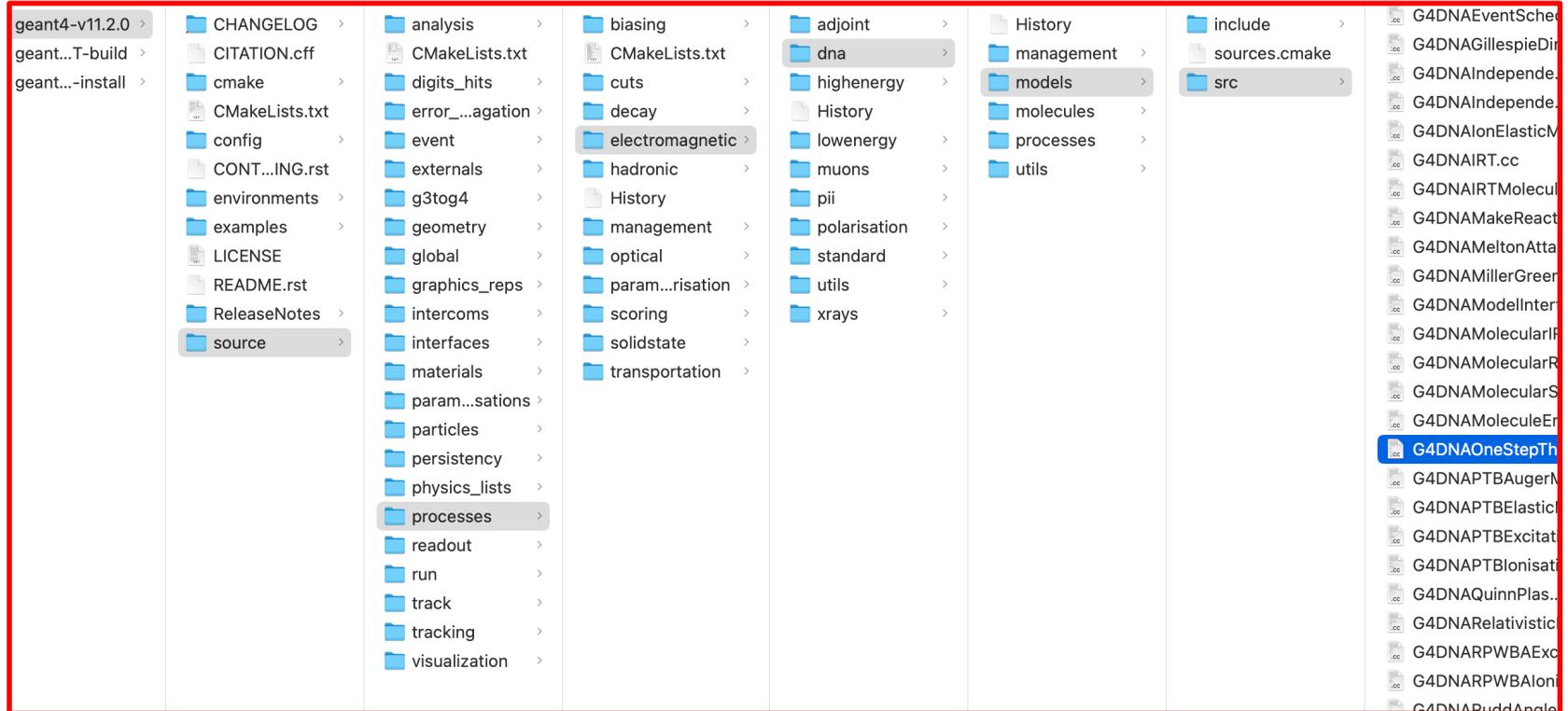


Exercise 2: Change the e- Solvation Sub Type Process and re-run the beam.in macro

```

1 #
2 /run/numberOfThreads 2
3 /process/dna/e-SolvationSubType Meesungnoen2002
4 #/process/dna/e-SolvationSubType Ritchie1994
5 #/process/dna/e-SolvationSubType Terrisol1990
6
7 # use Step-by-Step (SBS), independent reaction time (IRT)
8 # or synchronized IRT (IRT_syn),
9 # SBS ( is only for TDC, set 0 )
10 /chem6/TimeStepModel IRT
11 #/chem6/TimeStepModel IRT_syn
12 #/chem6/TimeStepModel SBS
13

```



```

45 //-----
46
47
48 namespace DNA {
49 namespace Penetration {
50
51 const double
52 Meesungnoen2002::gCoeff[13] =
53 { -4.06217193e-08, 3.06848412e-06, -9.93217814e-05,
54 1.80172797e-03, -2.01135480e-02, 1.42939448e-01,
55 -6.48348714e-01, 1.85227848e+00, -3.36450378e+00,
56 4.37785068e+00, -4.20557339e+00, 3.81679083e+00,
57 -2.34069784e-01 };
58 // fit from Meesungnoen, 2002
59
60 const double
61 Meesungnoen2002_amorphous::gCoeff[7] =
62 { 7.3144e-05, -2.2474e-03, 3.4555e-02,
63 -4.3574e-01, 2.8954e+00, -1.0381e+00,
64 1.4300e+00 };
65 // fit from Meesungnoen, 2002
66
67 const double
68 Terrisol1990::gEnergies_T1990[11] =
69 { 0.2, 0.5, 1, 2, 3, 4, 5, 6, 7,
70 // The two last are not in the dataset
71 8, 9 }; // eV
72
73 const double
74 Terrisol1990::gStdDev_T1990[11] =
75 { 17.68*CLHEP::angstrom,

```

Article: Jintana Meesungnoen, Jean-Paul Jay-Gerin, Abdelali Filali-Mouhim, and Samlee Mankhetkorn (2002) Low-Energy Electron Penetration Range in Liquid Water. Radiation Research: November 2002, Vol. 158, No. 5, pp.657-660

Article: Terrisol M, Beaudre A (1990) Simulation of space and time evolution of radiolytic species induced by electrons in water. Radiat Prot Dosimetry 31:171-175

Article: Ritchie RH, Hamm RN, Turner JE, Bolch WE (1994) Interaction of low-energy electrons with condensed matter: relevance for track structure. Computational approaches in molecular radiation biology, Plenum, New York, Vol. 63, pp. 155-166
Note: also used in Ballarini et al., 2000

Exercise 3: Change the chemical model and re-run the beam.in macro

```
beam.in
beam.in > No Selection
1 #
2 /run/numberOfThreads 2
3 /process/dna/e-SolvationSubType Meesungnoen2002
4 #/process/dna/e-SolvationSubType Ritchie1994
5 #/process/dna/e-SolvationSubType Terrisol1990
6
7 # use Step-by-Step (SBS), independent reaction time (IRT)
8 # or synchronized IRT (IRT_syn),
9 # SBS ( is only for TDC, set 0 )
10 #/chem6/TimeStepModel IRT
11 /chem6/TimeStepModel IRT_syn
12 #/chem6/TimeStepModel SBS
13
14 /run/initialize
15
16 # species definition
17 # username [ molecule | charge | D(m2/s) | Radius(nm) ]
18 #/chem/species O2 [ O2 | 0 | 2.4e-9 | 0.17 ]
19
20 /chem/PrintSpeciesTable
21
22 # reset reaction table
23 /chem/reaction/UI
24
25 # totally diffusion-controlled (TDC) | Fix | reactionRate[dm3/(mol*s)] | TDC (0)
26 /chem/reaction/add H + H -> H2 | Fix | 0.503e10 | 0
27 /chem/reaction/add e_aq + H -> H2 + OHm | Fix | 2.50e10 | 0
28 /chem/reaction/add e_aq + e_aq -> H2 + OHm + OHm | Fix | 0.636e10 | 0
29 /chem/reaction/add H3Op + OHm -> H2O | Fix | 1.13e11 | 0
30
31 # partially diffusion-controlled (PDC) | Fix | reactionRate[dm3/(mol*s)] | PDC (1)
32 /chem/reaction/add OH + H -> H2O | Fix | 1.55e10 | 1
33 /chem/reaction/add OH + OH -> H2O2 | Fix | 0.55e10 | 1
34 /chem/reaction/add e_aq + OH -> OHm | Fix | 2.95e10 | 1
35 /chem/reaction/add e_aq + H2O2 -> OHm + OH | Fix | 1.10e10 | 1
36 /chem/reaction/add e_aq + H3Op -> H + H2O | Fix | 2.11e10 | 1
37
38 /chem/reaction/print
39
```

```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```

Annotate the time
for the run in
each case!!

Exercise 4: Change the reaction rate of a chemical reaction and re-run the beam.in macro

```

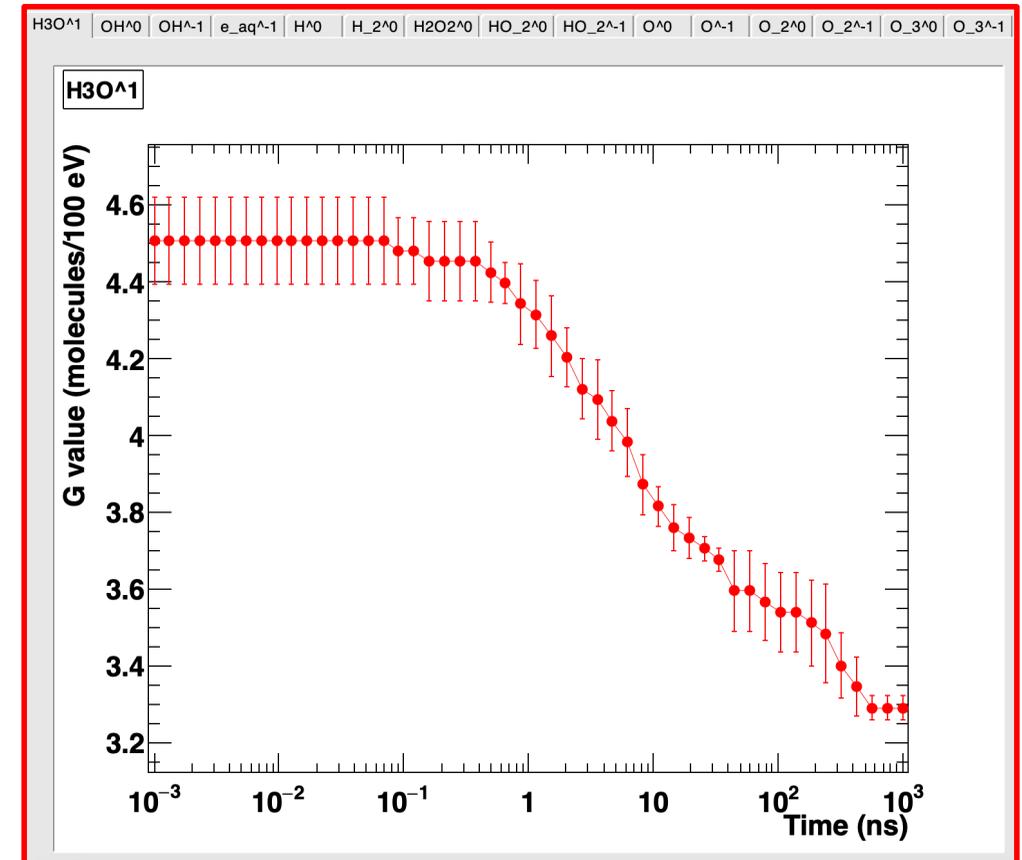
beam.in ) No Selection
24
25 # totally diffusion-controlled (TDC)          | Fix | reactionRate[dm3/(mol*s)] | TDC (0)
26 /chem/reaction/add H + H -> H2              | Fix | 0.503e10 | 0
27 /chem/reaction/add e_aq + H -> H2 + OHm     | Fix | 2.50e10  | 0
28 /chem/reaction/add e_aq + e_aq -> H2 + OHm + OHm | Fix | 0.636e10 | 0
29 /chem/reaction/add H3Op + OHm -> H2O       | Fix | 1.13e10  | 0
30
31 # partially diffusion-controlled (PDC)       | Fix | reactionRate[dm3/(mol*s)] | PDC (1)
32 /chem/reaction/add OH + H -> H2O           | Fix | 1.55e10  | 1
33 /chem/reaction/add OH + OH -> H2O2        | Fix | 0.55e10  | 1
34 /chem/reaction/add e_aq + OH -> OHm       | Fix | 2.95e10  | 1
35 /chem/reaction/add e_aq + H2O2 -> OHm + OH | Fix | 1.10e10  | 1
36 /chem/reaction/add e_aq + H3Op -> H + H2O  | Fix | 2.11e10  | 1
  
```

```

./chem6 beam.in
root plotG_time.C
root plotG_LET.C
  
```

Number of chemical species involved in reactions = 6

Reaction	Reaction Rate [dm3/(mol*s)]
H3O ⁺ + OH ⁻ -> No product	1.13e+10
H3O ⁺ + e _{aq} ⁻ -> H ⁰	2.11e+10
OH ⁰ + H ⁰ -> No product	1.55e+10
OH ⁰ + OH ⁰ -> H2O2 ⁰	5.5e+09
OH ⁰ + e _{aq} ⁻ -> OH ⁻	2.95e+10
e _{aq} ⁻ + H ⁰ -> H ₂ ⁰ + OH ⁻	2.5e+10
e _{aq} ⁻ + e _{aq} ⁻ -> H ₂ ⁰ + OH ⁻ + OH ⁻	6.36e+09
e _{aq} ⁻ + H2O2 ⁰ -> OH ⁻ + OH ⁰	1.1e+10
H ⁰ + H ⁰ -> H ₂ ⁰	5.03e+09

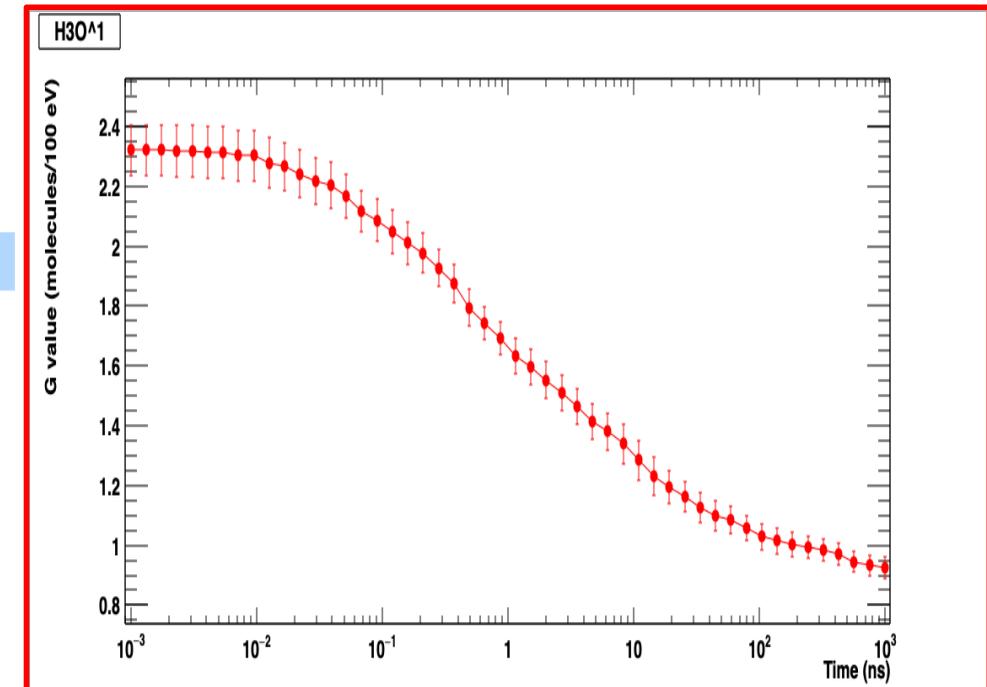


Exercise 5: Change position / direction / type of source and re-run the beam.in macro

```
beam.in |< > | beam.in | ↷ | ☰ | ☰ | ☰ |
beam.in > No Selection
18 #/chem/species O2 [ O2 | 0 | 2.4e-9 | 0.17 ]
19
20 /chem/PrintSpeciesTable
21
22 # reset reaction table
23 /chem/reaction/UI
24
25 # totally diffusion-controlled (TDC) | Fix | reactionRate[dm3/(mol*s)] | TDC (0)
26 /chem/reaction/add H + H -> H2 | Fix | 0.503e10 | 0
27 /chem/reaction/add e_aq + H -> H2 + OHm | Fix | 2.50e10 | 0
28 /chem/reaction/add e_aq + e_aq -> H2 + OHm + OHm | Fix | 0.636e10 | 0
29 /chem/reaction/add H3Op + OHm -> H2O | Fix | 1.13e11 | 0
30
31 # partially diffusion-controlled (PDC) | Fix | reactionRate[dm3/(mol*s)] | PDC (1)
32 /chem/reaction/add OH + H -> H2O | Fix | 1.55e10 | 1
33 /chem/reaction/add OH + OH -> H2O2 | Fix | 0.55e10 | 1
34 /chem/reaction/add e_aq + OH -> OHm | Fix | 2.95e10 | 1
35 /chem/reaction/add e_aq + H2O2 -> OHm + OH | Fix | 1.10e10 | 1
36 /chem/reaction/add e_aq + H3Op -> H + H2O | Fix | 2.11e10 | 1
37
38 /chem/reaction/print
39
40 /gun/position 0 0 0
41 /gun/direction 0 0 1
42 /gun/particle e-
43
44 # in order to reproduce LET values of NIST data
45 # please see the spower example using stationary mode
46
47 # select cutoff energy for restricted LET
48 #/scorer/LET/cutoff 100 eV
49
50
```

```
39
40 /gun/position 0 0 0
41 /gun/direction 0 0 1
42 /gun/particle proton
43
```

```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```



Exercise 6: Set and change the cutoff for restricted LET and re-run the beam.in macro

```
G4bool ScoreLET::ProcessHits(G4Step* aStep,G4TouchableHistory* /*TH*/)
{
  // In order to follow the primary track
  // regardless charge increasing or decreasing
  if(aStep->GetTrack()->GetTrackID() != 1 &&
     aStep->GetTrack()->GetParticleDefinition()->GetPDGEncoding() != 11){
    G4int subType = aStep->GetTrack()->GetCreatorProcess()
      ->GetProcessSubType();
    if(subType == 56 || subType == 57){
      fTrackID = aStep->GetTrack()->GetTrackID();
    }
  }

  // Ignore the step if it is not primary.
  if(aStep->GetTrack()->GetTrackID() != fTrackID) return false;
  else{
    fStepL += aStep->GetStepLength()/um;
    fEdep += aStep->GetTotalEnergyDeposit()/keV;

    G4int subType = aStep->GetPostStepPoint()->
      GetProcessDefinedStep()->GetProcessSubType();

    // Don't add the kinetic energy of primary particle
    if(subType == 56 || subType == 57) return false;

    const std::vector<const G4Track*> secondary =
      aStep->GetSecondaryInCurrentStep();

    size_t nbtrk = (*secondary).size();

    if(nbtrk){
      for(size_t lp=0;lp<nbtrk;lp++){
        // Store the kinetic energy of secondaries
        // which less than cutoff energy.
        if((*secondary)[lp]->GetKineticEnergy()/eV<fCutoff){
          fEdep += (*secondary)[lp]->GetKineticEnergy()/keV;
        }
      }
    }
  }
  return true;
}
```

```
fpLETDDir = new G4UIdirectory("/scorer/LET/");
fpLETDDir->SetGuidance("LET scorer commands");

fpCutoff = new G4UicmdWithADoubleAndUnit("/scorer/LET/cutoff", this);
fCutoff = DBL_MAX;
```

```
void ScoreLET::SetNewValue(G4Uicommand* command, G4String newValue){
  if(command == fpCutoff) fCutoff = atof(newValue);
}
```

$$L_{\Delta} = \left(\frac{dE}{dl} \right)_{\Delta}$$

```
beam.in
beam.in > No Selection
46
47 # select cutoff energy for restricted LET
48 /scorer/LET/cutoff 100 eV
49
```

The following is the most recent definition given by ICRU (1968):

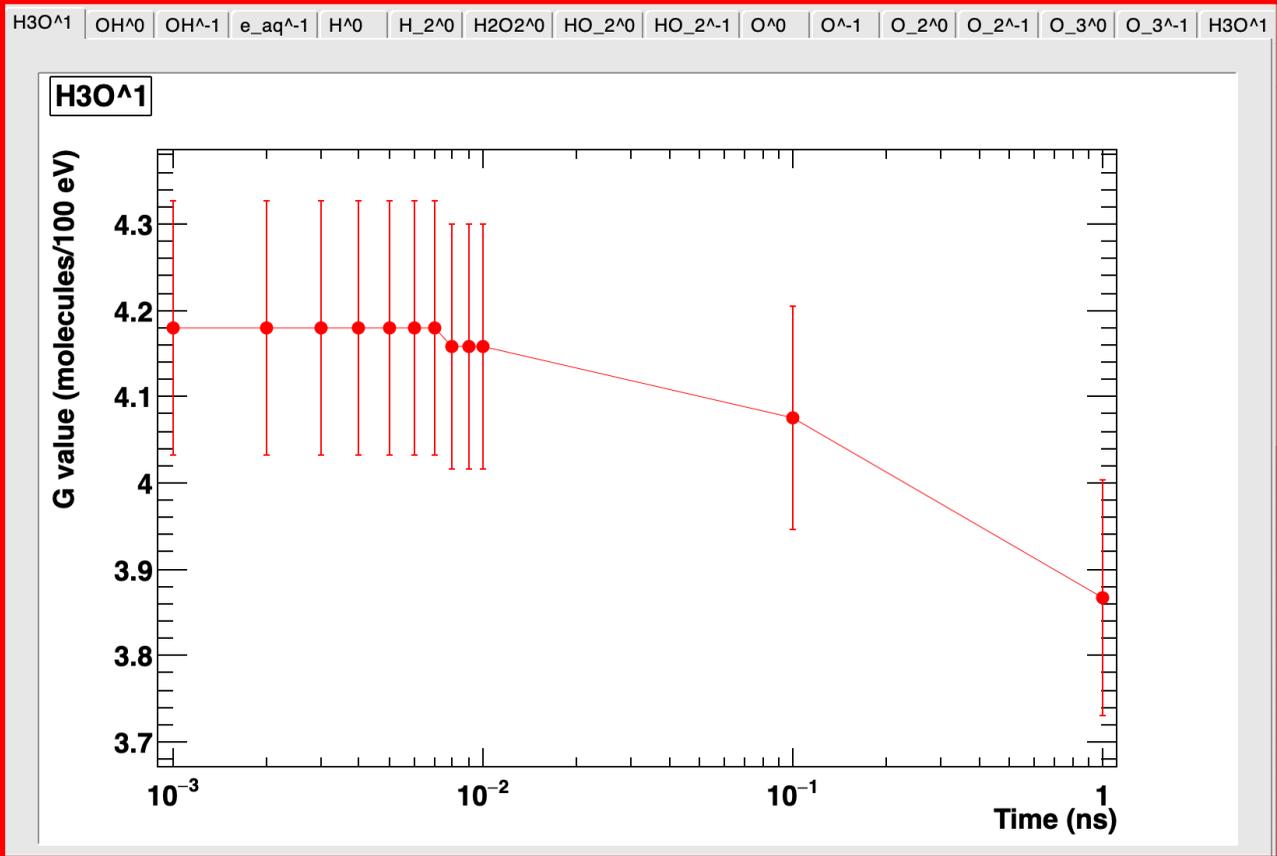
The *linear energy transfer* or *restricted linear collision stopping power* (L_{Δ}) of charged particles in a medium is the quotient of dE by dl , where dl is the distance traversed by the particle and dE is the mean energy-loss due to collisions with energy transfers less than some specified value Δ .

```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```

Exercise 7: Set and change the times to record the chemical species yields and re-run the beam.in macro

```
beam.in > No Selection
38 /chem/reaction/print
39
40 /gun/position 0 0 0
41 /gun/direction 0 0 1
42 /gun/particle e-
43
44 # in order to reproduce LET values of NIST data
45 # please see the spower example using stationary mode
46
47 # select cutoff energy for restricted LET
48 /scorer/LET/cutoff 100 eV
49
50 /scorer/species/addTimeToRecord 1 ps
51 /scorer/species/addTimeToRecord 2 ps
52 /scorer/species/addTimeToRecord 3 ps
53 /scorer/species/addTimeToRecord 4 ps
54 /scorer/species/addTimeToRecord 5 ps
55 /scorer/species/addTimeToRecord 6 ps
56 /scorer/species/addTimeToRecord 7 ps
57 /scorer/species/addTimeToRecord 8 ps
58 /scorer/species/addTimeToRecord 9 ps
59 /scorer/species/addTimeToRecord 10 ps
60 /scorer/species/addTimeToRecord 100 ps
61 /scorer/species/addTimeToRecord 1 ns
62 #/scorer/species/addTimeToRecord 10 ns
63 #/scorer/species/addTimeToRecord 100 ns
64 #/scorer/species/addTimeToRecord 1 us
65
66 #/scorer/species/nOfTimeBins 50
```

```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```



Exercise 8: Change the endTime of the chemical stage and re-run beam.in

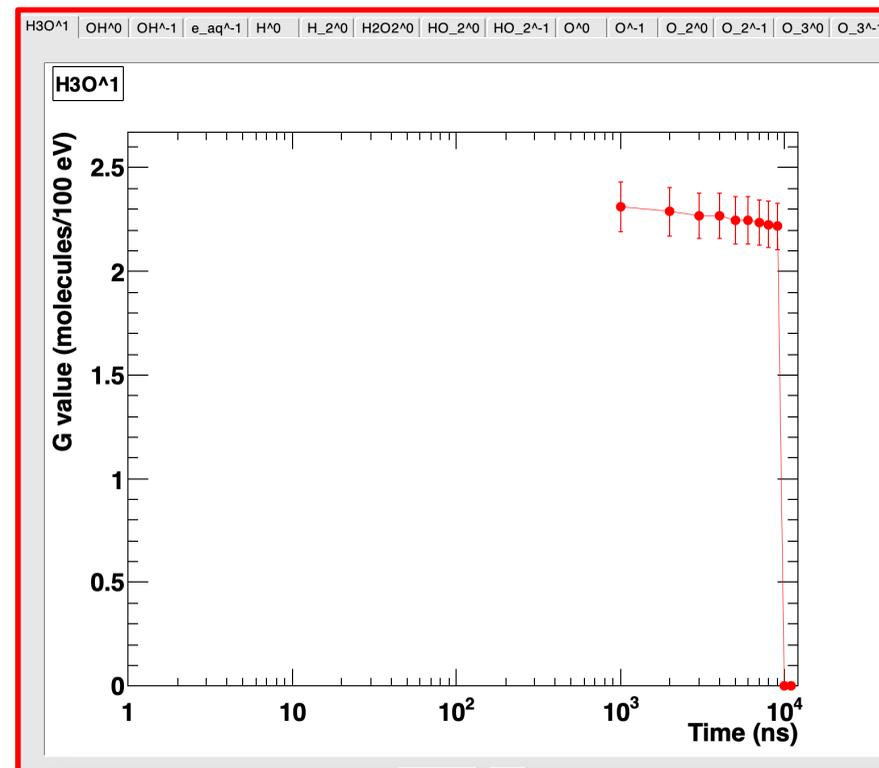
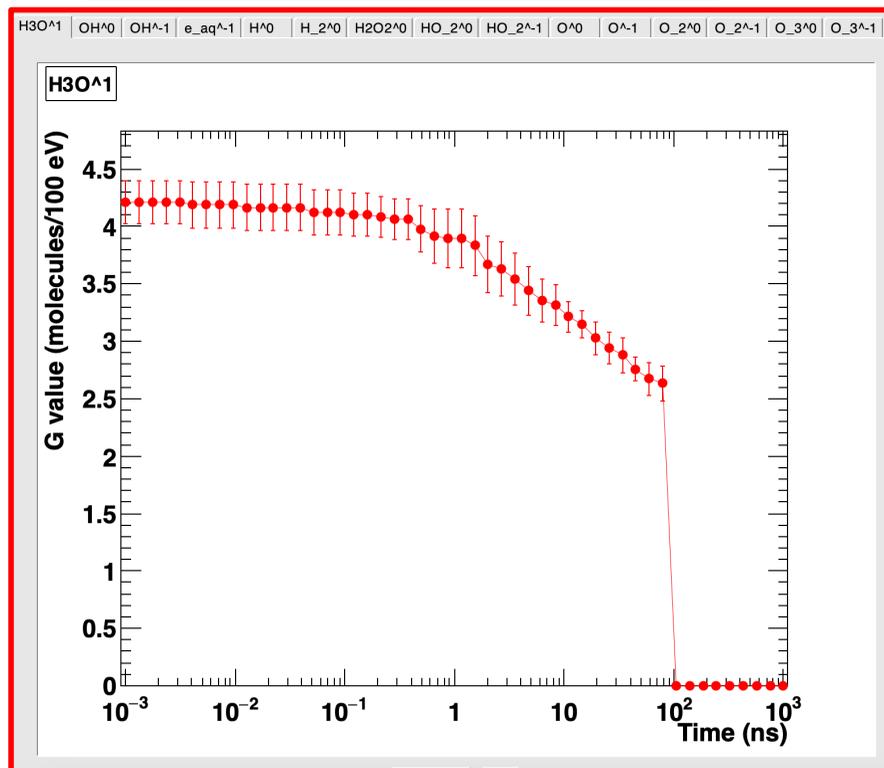
```
beam.in
59
60 /tracking/verbose 0
61 /scheduler/verbose 0
62 /scheduler/endTime 0.1 microsecond
63
```

```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```

```
beam.in
70 /tracking/verbose 0
71 /scheduler/verbose 0
72 /scheduler/endTime 10 microsecond
73
```

```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```

Be careful to use the proper Time to Score Species!!!



```
/scorer/species/addTimeToRecord 1 us
/scorer/species/addTimeToRecord 2 us
/scorer/species/addTimeToRecord 3 us
/scorer/species/addTimeToRecord 4 us
/scorer/species/addTimeToRecord 5 us
/scorer/species/addTimeToRecord 6 us
/scorer/species/addTimeToRecord 7 us
/scorer/species/addTimeToRecord 8 us
/scorer/species/addTimeToRecord 9 us
/scorer/species/addTimeToRecord 10 us
```

Exercise 9: Run as it is the beam_HCP.in macro

...when you get bored of waiting: go to Exercise 10

```
./chem6 beam.in
...
hIoni: for pi- XStype:3 SubType=2
      dE/dx and range tables from 10 eV to 300 MeV in 140 bins
      Lambda tables from threshold to 300 MeV, 20 bins/decade, spline: 1
      StepFunction=(0.1, 0.05 mm), integ: 3, fluct: 1, linLossLim= 0.01
      ===== EM models for the G4Region DefaultRegionForTheWorld =====
              ICRU73Q0 : Emin= 0 eV Emax=297.505 keV deltaVI
              BetheBloch : Emin=297.505 keV Emax= 300 MeV deltaVI
G4VisManager: Using G4TrajectoryDrawByCharge as fallback trajectory model.
See commands in /vis/modeling/trajectories/ for other options.
### Run 0 starts.
### Run 0 starts.
--> Event 0 starts.
DNAMolecularIRTModel will be used
█
```



Exercise 10: Try to change parameters in the HCP.in macro and re-run it

```
beam_HCP.in > No Selection
1 #
2
3 /run/numberOfThreads 2
4 /process/dna/e-SolvationSubType Meesungnoen2002
5 #/process/dna/e-SolvationSubType Ritchie1994
6 #/process/dna/e-SolvationSubType Terrisol1990
7
8 /run/initialize
9
10 /chem/reaction/print
11
12 /primaryKiller/setSize 5 5 5 um
13 /gun/position 0 0 -2.5 um
14 /gun/direction 0 0 1
15 /gun/particle proton
16
17 # in order to reproduce LET values of NIST data
18 # please see the spower example using stationary mode
19
20 # select cutoff energy for restricted LET
21 #/scorer/LET/cutoff 100 eV
22
23 #/scorer/species/addTimeToRecord 1 ps
24 #/scorer/species/addTimeToRecord 10 ps
25 #/scorer/species/addTimeToRecord 100 ps
26 #/scorer/species/addTimeToRecord 1 ns
27 #/scorer/species/addTimeToRecord 10 ns
28 #/scorer/species/addTimeToRecord 100 ns
29 #/scorer/species/addTimeToRecord 1 us
30
31 /scorer/species/nOfTimeBins 50
32
33 /tracking/verbose 0
34 /scheduler/verbose 0
35 /scheduler/endTime 1 microsecond
36
37 /run/printProgress 1
38
39 /gun/energy 5000 keV
40 /run/beamOn 10
41
42
```

```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```

```
G4VisManager: Using G4TrajectoryDrawByCharge as fallback trajectory
See commands in /vis/modeling/trajectories/ for other options.
### Run 0 starts.
### Run 0 starts.
--> Event 0 starts.
DNAMolecularIRTModel will be used
--> Event 1 starts.
--> Event 2 starts.
--> Event 3 starts.
--> Event 4 starts.
--> Event 5 starts.
--> Event 6 starts.
--> Event 7 starts.
--> Event 8 starts.
--> Event 9 starts.

-----End of Global Run-----
The run has 10 events
Number of events recorded by the species scorer = 10
Total energy deposited in the world volume : 4.3138e+05 eV
-----

serenafattori@MacBook-Air-di-Serena chem6-build-11.2.0.beta %
```

