Chemistry examples

geant4-dna.org

Chem6 example

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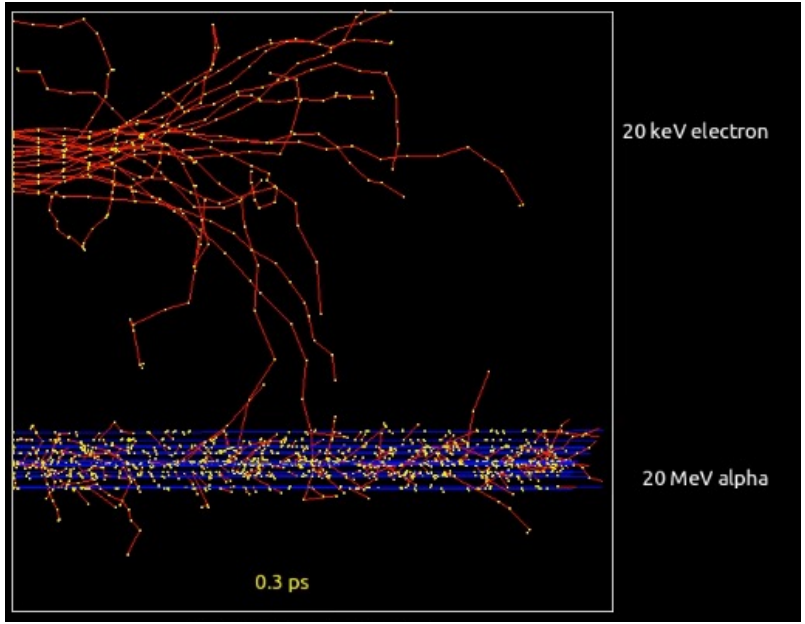
Pre-Chemistry Processes

Geant4-DNA simulation



			Branching ratio (%)		
Ionization	H_2O^+	$H_3O^+ + {}^{\bullet}OH$	100	100	Ionization
Excitation	A^1B_1	$H^{\bullet} + {}^{\bullet}OH$	65	65	A1B1_DissociationDecay
		$H_2O + \Delta E$	35	35	No displacement
	B^1A_1	$H_3O^+ + {}^{\bullet}OH + e_{aq}^-$	50	55	Auto-Ionization
		$H^{\bullet} + {}^{\bullet}OH$	25.35	-	A1B1_DissociationDecay
		$H_2 + 2{}^{\bullet}OH$	3.25	15	B1A1_DissociationDecay
		$2H^{\bullet} + O(^3P)^*$	3.9	-	B1A1_DissociationDecay2
		$H_2O + \Delta E$	17.5	30	No displacement
	Rydberg A+B, C+D, Diffuse bands	$H_3O^+ + {}^{\bullet}OH + e_{aq}^-$	50	50	Auto-Ionization
		$H_2O + \Delta E$	50	50	No displacement
Electron capture	DEA	$OH^- + {}^{\bullet}OH + H_2$	100	100	Dissociative attachment
	Recombinat -ion	$H^{\bullet} + {}^{\bullet}OH$	35.75	55	A1B1_DissociationDecay
		$H_2 + 2{}^{\bullet}OH$	13.65	15	B1A1_DissociationDecay
		$2H^{\bullet} + O(^3P)$	15.6	-	B1A1_DissociationDecay2
		$H_2O + \Delta E$	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} m^2 s^{-1})
H_3O^+	9.0
H•	7.0
OH^-	5.0
e^-_{aq}	4.9
H_2	5.0
•OH	2.8
H_2O_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

*H + *H -> H2
e_aq + H* + H2O -> H2 + OH-
H + O(3p) -> OH
H + O- -> OH-
OH + O(3p) -> HO2
HO2 + O(3p) -> O2
O(3p) + O(3p) -> O2

Type II: 31 reactions

*OH + *H -> H2O
H + H2O2 -> OH
H + OH- -> eaq-
H + O2 -> HO2
H + HO2 -> H2O2
H + O2- -> HO2-
*OH + *OH -> H2O2
OH + H2O2 -> HO2
OH + H2 -> H
e_aq + *OH -> OH-
OH + OH- -> O-
OH + HO2 -> O2
OH + O2- -> O2 + OH-
OH + HO2- -> HO2 + OH-
OH + O- -> HO2-
OH + O3- -> O2- + HO2
e_aq + H2O2 -> OH- + *OH
H2O2 + OH- -> HO2-
H2O2 + O(3p) -> HO2 + OH
H2O2 + O- -> HO2 + OH-
H2 + O(3p) -> H + OH
H2 + O- -> H + OH-
eaq- + O2 -> O2-
eaq + HO2 -> HO2-
OH- + HO2 -> O2-
OH- + O(3p) -> HO2-
O2 + O(3p) -> O3
O2 + O- -> O3-
HO2 + HO2 -> H2O2 + O2
HO2 + O2- -> HO2- + O2
HO2- + O(3p) -> O2- + OH

Type III: 3 reactions

e_aq + e_aq + 2H2O -> H2 + 2OH-
H3O+ + OH- -> 2H2O
H3O+ + O3- -> OH + O2

Type IV: 11 reactions

e_aq + H3O+ -> H* + H2O
e_aq + O2- -> H2O2 + OH- + OH-
e_aq + HO2- -> O- + OH-
e_aq + O- -> OH- + OH-
H3O+ + O2- -> HO2
H3O+ + HO2- -> H2O2
H3O+ + HO2- -> H2O2
O2- + O- -> O2 + OH- + OH-
HO2- + O- -> O2- + OH-
O- + O- -> H2O2 + OH- + OH-
O- + O3- -> O2- + O2-

Type VI: 20 reactions

O3- -> O- + O2
HO2 + H2O -> H3O+ + O2-
H + H2O -> eaq- + H3O+
eaq- + H2O -> H + OH-
O2- + H2O -> HO2 + OH-
HO2- + H2O -> H2O2 + OH-
O(3p) + H2O -> OH + OH
O- + H2O -> OH + OH-
eaq- + H3O+(B) -> H + H2O
O2- + H3O+(B) -> HO2 + H2O
OH- + H3O+(B) -> 2H2O
H3O+ + OH-(B) -> 2H2O
HO2- + H3O+(B) -> H2O2 + H2O
O- + H3O+(B) -> OH + H2O
O3- + H3O+(B) -> OH + O2 + H2O
H + OH-(B) -> H2O + eaq-
OH + OH-(B) -> O- + H2O
H2O2 + OH-(B) -> HO2- + H2O
HO2 + OH-(B) -> O2- + H2O
O(3p) + OH-(B) -> HO2-

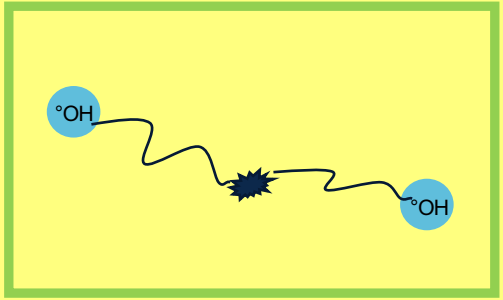
Chemistry Models

- 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.



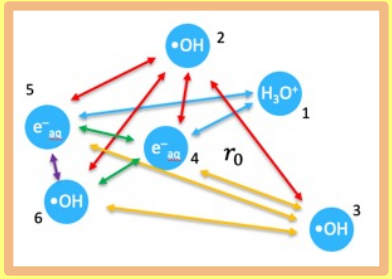
Karamitros, M. et al. (**2014**) Diffusion-controlled reactions modeling in Geant4-DNA. Journal of Computational Physics, 274, 841-882. https://doi.org/10.1016/j.jcp.2014.06.011

- 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.



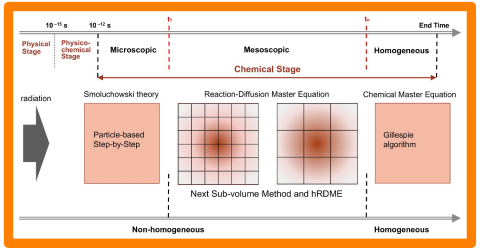
Karamitros, M. et al. (**2020**) Implementing the Independent Reaction Time method in Geant4 for radiation chemistry simulations. https://doi.org/10.48550/arXiv.2006.14225

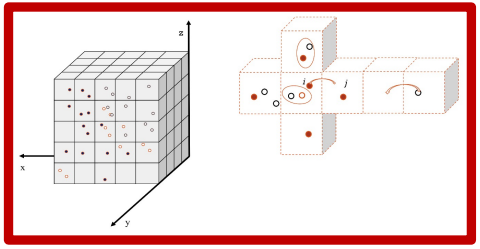
Ramos-Méndez, J. et al. (**2020**) Independent reaction times method in Geant4-DNA: Implementation and performance. https://doi.org/10.1002/mp.14490

- 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
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Chem6 Example

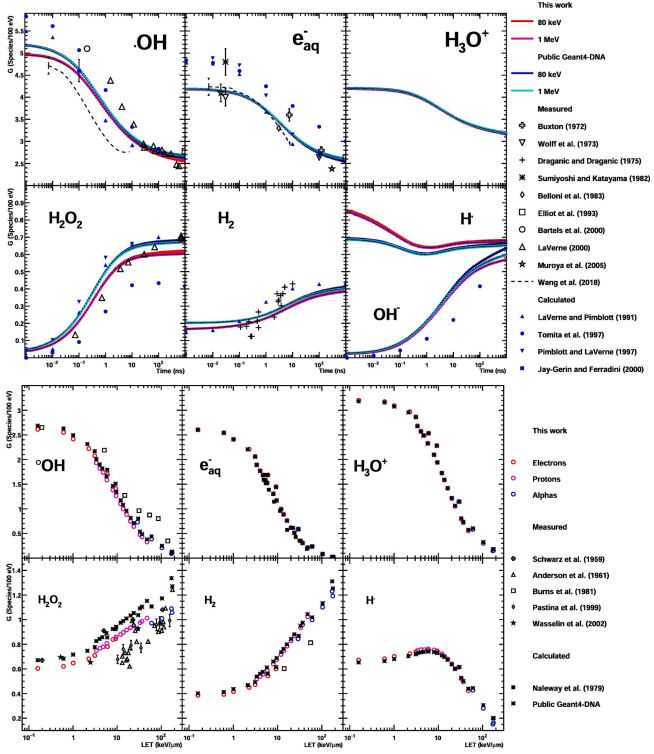
Based on chem4 and chem5 provides scoring of the radiochemical yield G:

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

as a function of time and LET.

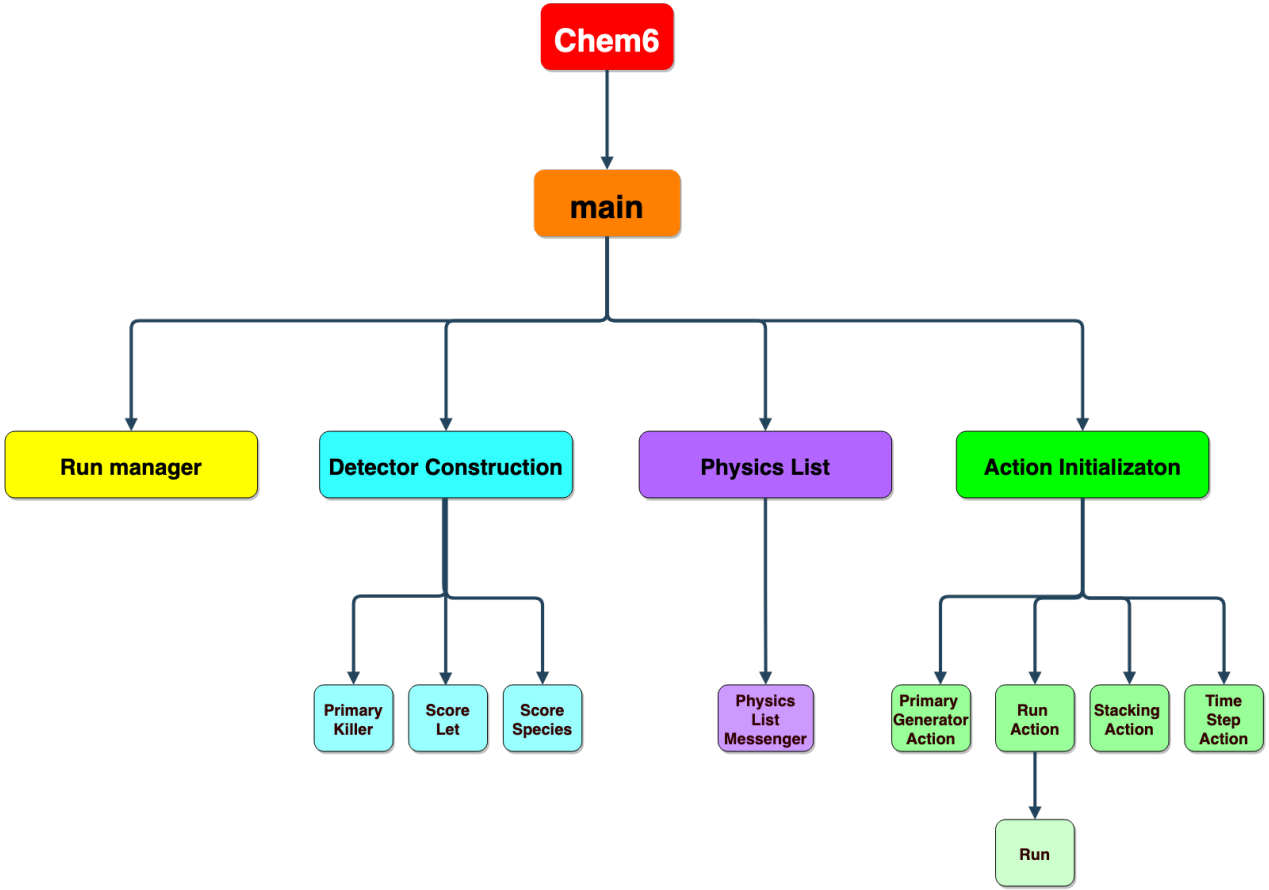
The example uses IRT by default.

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



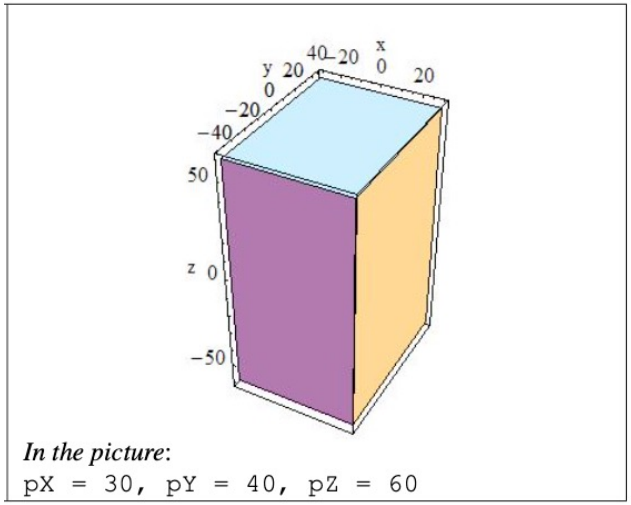
Chem6 Application Code Structure

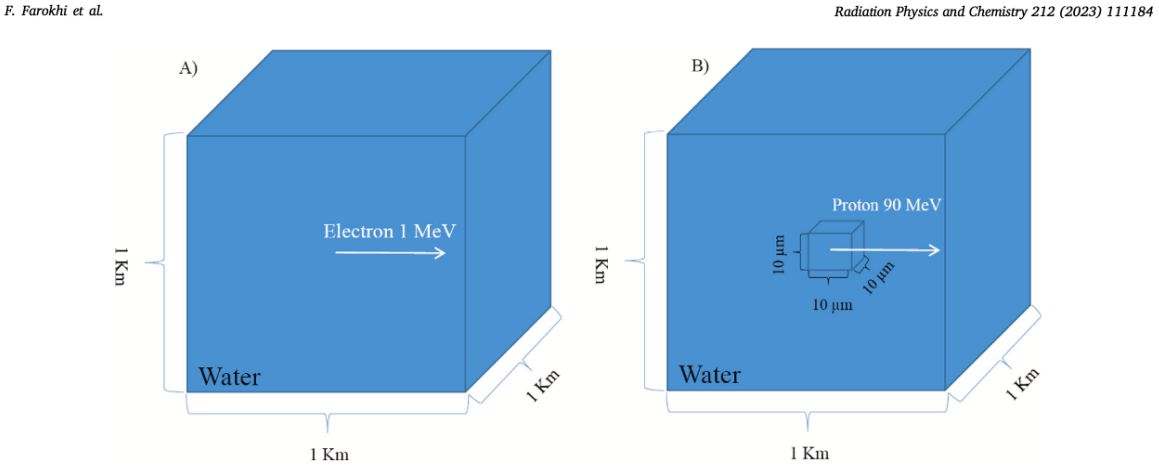
chem6.cc	Main file ⇒ creation **of RunManager, DetectorConstruction, PhysicsList, PrimaryGeneratorAction, ActionInitialization**
→RunManager	Management of all the calls to Geant4 kernel and the threads in MT mode
→DetectorConstruction	Definition of the geometry: World volume is a **water box** representing 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





- The World Volume is a G4Box
- Two parameters define the geometry :
  - the material of the Cube → G4Water
  - the half-lengths pX = pY = pZ = 500 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.

default: 100 keV Electron

- 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.

/gun/particle e-

/gun/energy 30 keV

/gun/position 0 0 0 micrometer

/gun/direction 0 0 1

- The chemistry module is triggered in the StackingAction class when all physical tracks have been processed.

TimeStepAction

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

Methods

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

AddTimeStep(1 * picosecond, 0.1 * picosecond);	*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.*
AddTimeStep(10 * picosecond, 1 * picosecond);	*From 1 ps to 10 ps in simulation time, the minimal time step will be of 1 ps.*

TimeStepAction

In ActionInitilialisation: 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*"
- Create a build folder for chem6, i.e. "*chem6-build*"
- Source the geant4.sh:
  cd path-of-geant4-install/bin
  source geant4.sh
  cd –
- Enter inside "*chem6-build*" and execute the cmake command:
  cmake path-of-geant4-install path of chem6
- Compile the example:
  make –jn *(with n = number of cores available in your machine)*
- In the terminal window, inside your chem3-build folder:
  ./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),
# SBS ( is only for TDC, set 0 )
/chem6/TimeStepModel IRT
#/chem6/TimeStepModel IRT_syn
#/chem6/TimeStepModel SBS

/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- Solvatation 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 greated 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 greated 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 greated 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 greated 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 greated 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 greated 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 greated 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

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

Output

Defined Species Table

Molecular Config	Diffusion Coefficient (m2 / s)	Radius (nm)
H3O^1	9.46e-09	0.25
OH^0	2.2e-09	0.22
OH^-1	5.3e-09	0.33
e_aq^-1	4.9e-09	0.5
H^0	7e-09	0.19
H_2^0	4.8e-09	0.14
H2O2^0	2.3e-09	0.21
HO_2^0	2.3e-09	0.21
HO_2^-1	1.4e-09	0.25
O^0	2e-09	0.2
O^-1	2e-09	0.25
O_2^0	2.4e-09	0.17
O_2^-1	1.75e-09	0.22
O_3^0	2e-09	0.2
O_3^-1	2e-09	0.2

Defined Reactions Table

Number of chemical species involved in reactions = 6

Reaction	Reaction Rate [dm3/(mol*s)]
H3O^1 + OH^-1 -> No product	1.13e+11
H3O^1 + e_aq^-1 -> 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^-1 -> OH^-1	2.95e+10
e_aq^-1 + H^0 -> H_2^0 + OH^-1	2.5e+10
e_aq^-1 + e_aq^-1 -> H_2^0 + OH^-1 + OH^-1	6.36e+09
e_aq^-1 + H2O2^0 -> OH^-1 + OH^0	1.1e+10
H^0 + H^0 -> H_2^0	5.03e+09

Chemical reactions

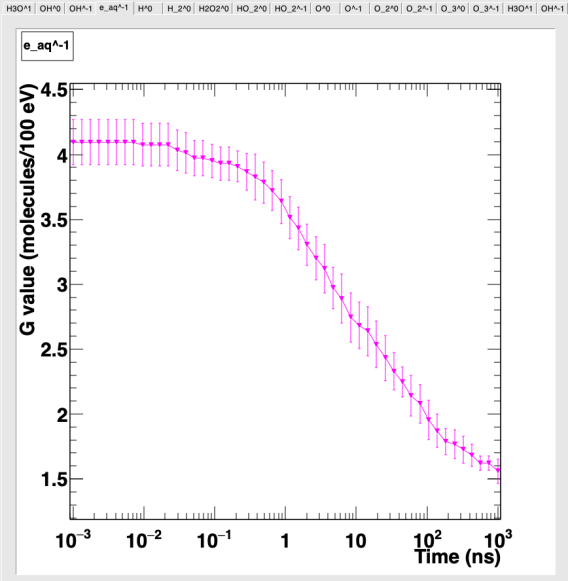
```
### Run 5 starts.
### Run 5 starts.
--> Event 0 starts.
*** G4Scheduler starts processing
At time :       1 ps  Reaction : OH^0 (-1341) + OH^0 (-1357) -> H2O2^0 (-1752)
At time :       1 ps  Reaction : e_aq^-1 (-865) + H3O^1 (-1514) -> H^0 (-1753)
At time :       1 ps  Reaction : OH^0 (-1554) + e_aq^-1 (-1556) -> OH^-1 (-1754)
At time :       1 ps  Reaction : OH^0 (-1656) + OH^0 (-1655) -> H2O2^0 (-1755)
At time :       1 ps  Reaction : OH^0 (-1698) + OH^0 (-1699) -> H2O2^0 (-1756)
At time :       1 ps  Reaction : OH^0 (-1682) + OH^0 (-1683) -> H2O2^0 (-1757)
At time :       1 ps  Reaction : OH^0 (-1610) + OH^0 (-1748) -> H2O2^0 (-1758)
At time :       1 ps  Reaction : OH^0 (-1730) + OH^0 (-1365) -> H2O2^0 (-1759)
At time :       1 ps  Reaction : e_aq^-1 (-137) + OH^0 (-917) -> OH^-1 (-1760)
At time :       1 ps  Reaction : H3O^1 (-916) + OH^-1 (-1760) -> No product
At time :       1 ps  Reaction : OH^0 (-1003) + OH^0 (-939) -> H2O2^0 (-1761)
At time :       1 ps  Reaction : OH^0 (-1009) + OH^0 (-1193) -> H2O2^0 (-1762)
At time :       1 ps  Reaction : H3O^1 (-1168) + OH^-1 (-874) -> No product
At time :   1.836 ps  Reaction : OH^0 (-1746) + OH^0 (-1747) -> H2O2^0 (-1763)
At time :  7.5883 ps  Reaction : OH^0 (-1325) + OH^0 (-1363) -> H2O2^0 (-1764)
At time :  10.258 ps  Reaction : e_aq^-1 (-445) + OH^0 (-1551) -> OH^-1 (-1765)
At time :  10.258 ps  Reaction : OH^-1 (-1765) + H3O^1 (-1552) -> No product
At time :  12.579 ps  Reaction : e_aq^-1 (-673) + OH^0 (-1213) -> OH^-1 (-1766)
At time :  12.579 ps  Reaction : H3O^1 (-1212) + OH^-1 (-1766) -> No product
At time :  13.175 ps  Reaction : H^0 (-1724) + OH^0 (-1373) -> No product
At time :  14.941 ps  Reaction : H^0 (-1608) + OH^0 (-1540) -> No product
At time :  19.462 ps  Reaction : OH^0 (-1249) + OH^0 (-1261) -> H2O2^0 (-1767)
At time :   20.08 ps  Reaction : OH^0 (-953) + OH^0 (-1375) -> H2O2^0 (-1768)
At time :  23.916 ps  Reaction : H3O^1 (-1522) + e_aq^-1 (-1523) -> H^0 (-1769)
At time :  24.295 ps  Reaction : OH^-1 (-871) + H3O^1 (-938) -> No product
At time :  24.573 ps  Reaction : OH^0 (-1253) + OH^0 (-1617) -> H2O2^0 (-1770)
At time :  30.568 ps  Reaction : OH^0 (-1263) + H^0 (-1618) -> No product
At time :  38.075 ps  Reaction : H^0 (-1572) + OH^0 (-1573) -> No product
At time :  43.326 ps  Reaction : OH^0 (-875) + OH^0 (-1169) -> H2O2^0 (-1771)
At time :  43.821 ps  Reaction : OH^0 (-1709) + e_aq^-1 (-291) -> OH^-1 (-1772)
At time :  43.821 ps  Reaction : OH^-1 (-1772) + H3O^1 (-1354) -> No product
At time :   43.99 ps  Reaction : H^0 (-1749) + OH^0 (-1607) -> No product
At time :  46.655 ps  Reaction : H3O^1 (-960) + e_aq^-1 (-168) -> H^0 (-1773)
At time :  47.871 ps  Reaction : H^0 (-1727) + H^0 (-1728) -> H_2^0 (-1774)
At time :  49.601 ps  Reaction : e_aq^-1 (-364) + OH^0 (-1323) -> OH^-1 (-1775)
At time :  49.601 ps  Reaction : OH^-1 (-1775) + H3O^1 (-1322) -> No product
At time :  50.198 ps  Reaction : H^0 (-1580) + OH^0 (-1670) -> No product
At time :  54.217 ps  Reaction : OH^0 (-1702) + e_aq^-1 (-401) -> OH^-1 (-1776)
At time :  56.466 ps  Reaction : OH^-1 (-868) + H3O^1 (-902) -> No product
At time :  57.404 ps  Reaction : OH^0 (-1241) + OH^0 (-1245) -> H2O2^0 (-1777)
At time :   70.1 ps  Reaction : OH^0 (-1581) + H^0 (-1582) -> No product
At time :  76.874 ps  Reaction : OH^0 (-1161) + OH^0 (-1167) -> H2O2^0 (-1778)
At time :  81.262 ps  Reaction : OH^-1 (-892) + H3O^1 (-1736) -> No product
At time :  85.681 ps  Reaction : OH^0 (-1659) + OH^0 (-1179) -> H2O2^0 (-1779)
At time :  96.932 ps  Reaction : OH^0 (-1648) + H^0 (-1649) -> No product
At time :  107.06 ps  Reaction : OH^0 (-1527) + e_aq^-1 (-1529) -> OH^-1 (-1780)
```

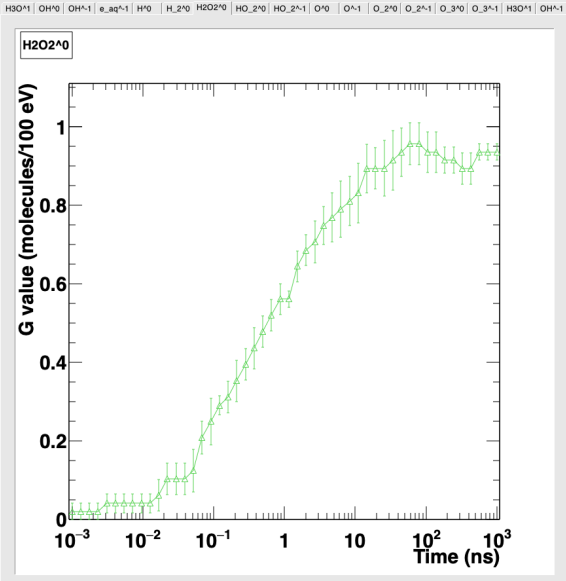
- Defined Species table is printed: /chem/PrintSpeciesTable
- Defined reaction table is printed: /chem/reaction/print
- G4Scheduler processes the chemical stage time step after time step.
- Molecular chemical reactions as a function of the elapsed time are printed: /scheduler/verbose 1

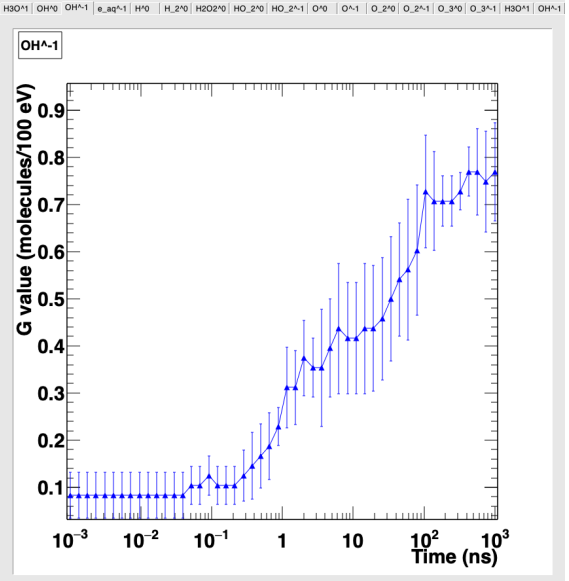
Root Analysis: G values vs. time

- 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



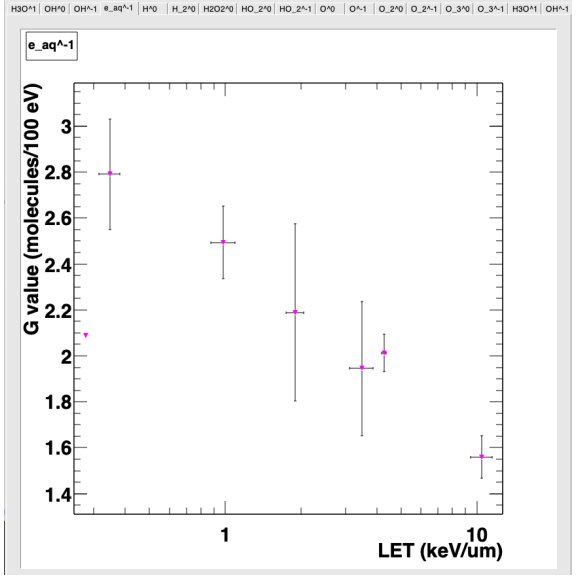


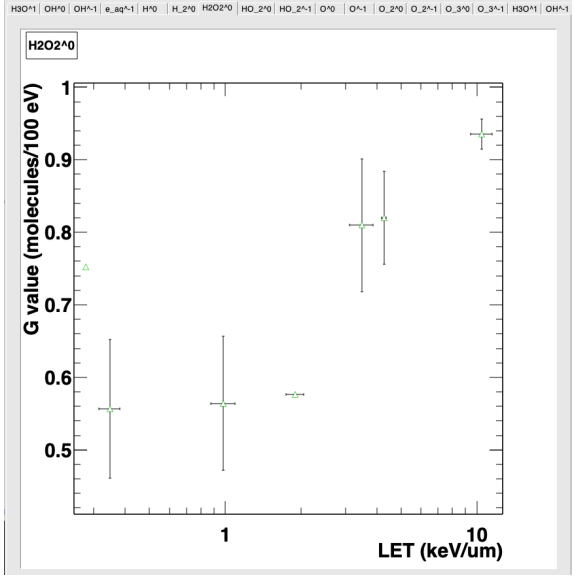


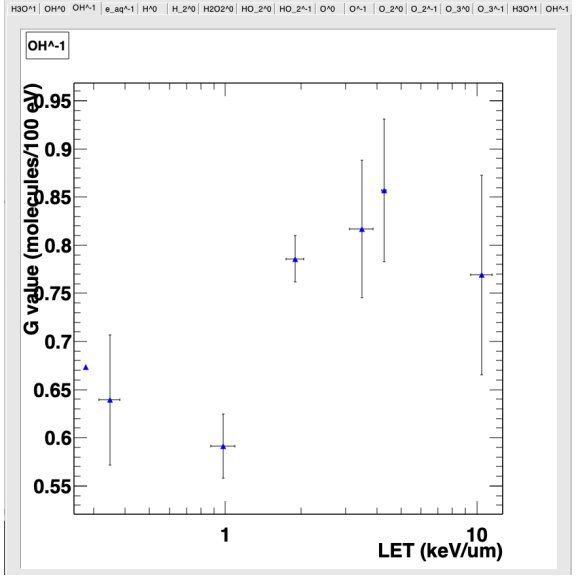
Root Analysis: G values vs. LET

- 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

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.

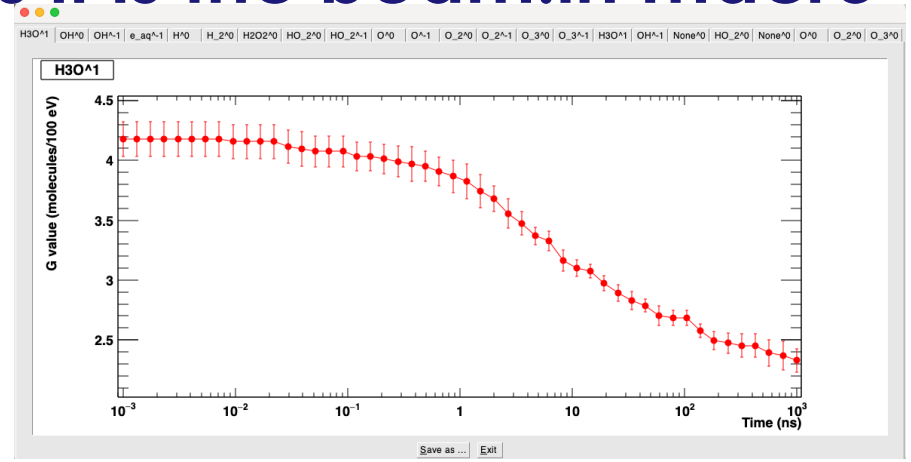
Exercises

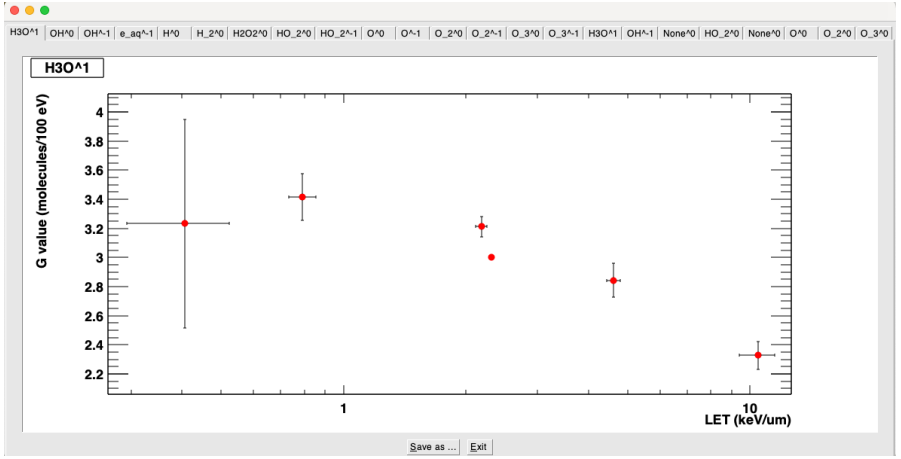
- **Exercise 1**: Run as it is the beam.in macro
- **Exercise 2**: Change the e- Solvatation Sub Type Process and re-run the beam.in macro
- **Exercise 3**: Change the chemical model and re-run the beam.in macro
- **Exercise 4**: Change the reaction rate of a chemical reaction and re-run beam.in macro
- **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
```

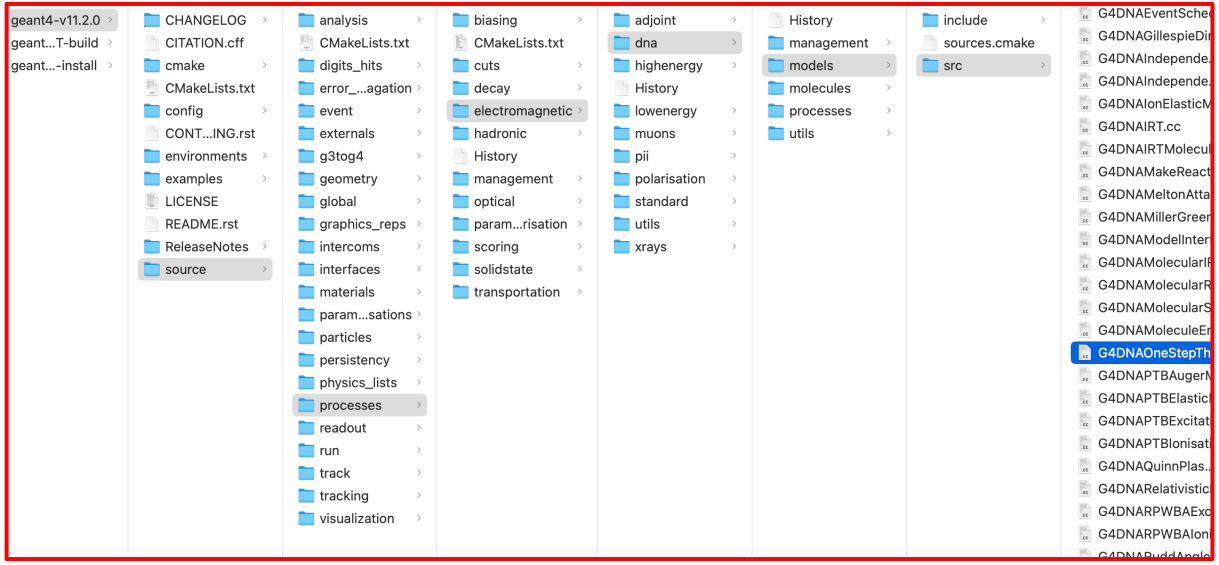




Exercise 2: Change the e- Solvatation Sub Type Process and re-run the beam.in macro

beam.in 〉 No Selection

```
#
/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),
# SBS ( is only for TDC, set 0 )
/chem6/TimeStepModel IRT
#/chem6/TimeStepModel IRT_syn
#/chem6/TimeStepModel SBS

```



C* G4DNAOneStepThermalizationModel

C* G4DNAOneStepThermalizationModel 〉 No Selection

```
//---------------------------------------------------------------

namespace DNA {
namespace Penetration {

const double
Meesungnoen2002::gCoeff[13] =
{ -4.06217193e-08,  3.06848412e-06,  -9.93217814e-05,
  1.80172797e-03,  -2.01135480e-02,   1.42939448e-01,
  -6.48348714e-01,  1.85227848e+00,  -3.36450378e+00,
  4.37785068e+00,  -4.20557339e+00,   3.81679083e+00,
  -2.34869784e-01 };
// fit from Meesungnoen, 2002

const double
Meesungnoen2002_amorphous::gCoeff[7] =
{ 7.3144e-05,   -2.2474e-03,    3.4555e-02,
  -4.3574e-01,  2.8954e+00, -1.0381e+00,
  1.4300e+00 };
// fit from Meesungnoen, 2002

const double
Terrisol1990::gEnergies_T1990[11] =
{ 0.2, 0.5, 1, 2, 3, 4, 5, 6, 7,
  // The two last are not in the dataset
  8, 9}; // eV

const double
Terrisol1990::gStdDev_T1990[11] =
{ 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: Terrissol 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

```
#
/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),
# SBS ( is only for TDC, set 0 )
#/chem6/TimeStepModel IRT
/chem6/TimeStepModel IRT_syn
#/chem6/TimeStepModel SBS

/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

# 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
```

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

Annotate the time for the run in each case!!

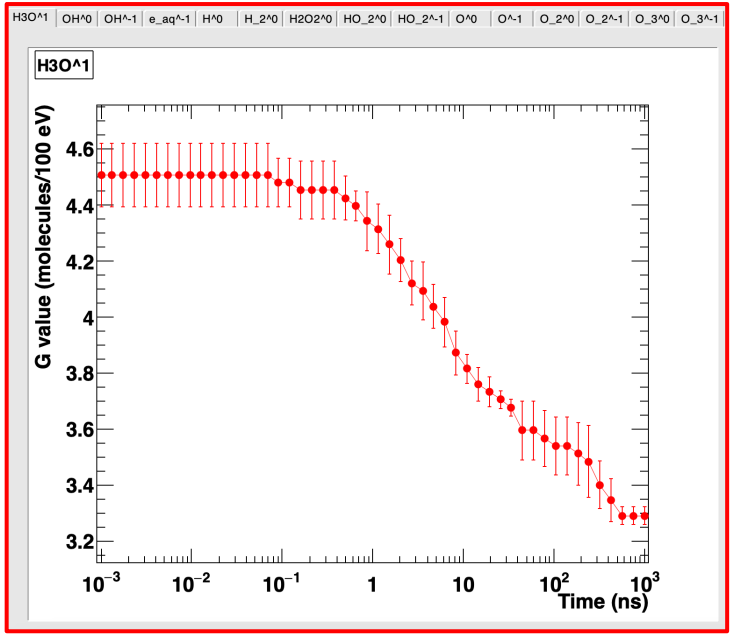
Exercise 4: Change the reaction rate of a chemical reaction and re-run the beam.in macro

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^1 + OH^-1 -> No product                       1.13e+10
-------------------------------------------------------------------------------
H3O^1 + e_aq^-1 -> 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^-1 -> OH^-1                           2.95e+10
-------------------------------------------------------------------------------
e_aq^-1 + H^0 -> H_2^0 + OH^-1                    2.5e+10
-------------------------------------------------------------------------------
e_aq^-1 + e_aq^-1 -> H_2^0 + OH^-1 + OH^-1        6.36e+09
-------------------------------------------------------------------------------
e_aq^-1 + H2O2^0 -> OH^-1 + 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

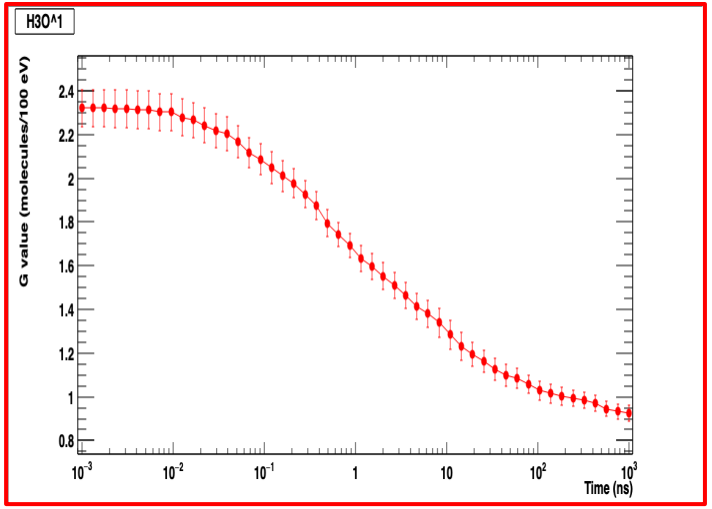
beam.in

beam.in ⟩ 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
```

```
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;
}
```

```
fpLETDir = new G4UIdirectory("/scorer/LET/");
fpLETDir->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.

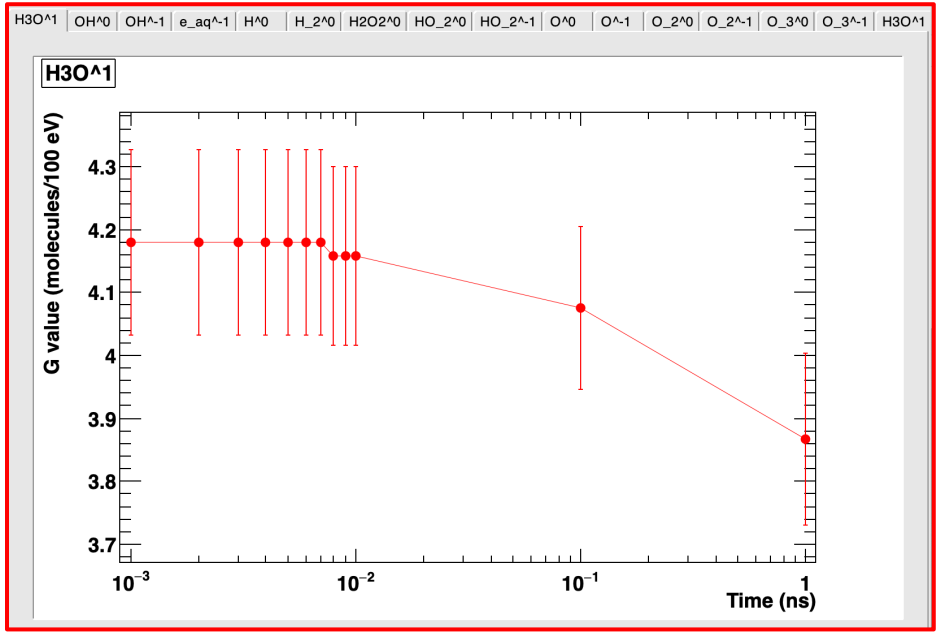
```
./chem6 beam.in
root plotG_time.C
root plotG_LET.C
```

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

beam.in 〉 No Selection

```
/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 2 ps
/scorer/species/addTimeToRecord 3 ps
/scorer/species/addTimeToRecord 4 ps
/scorer/species/addTimeToRecord 5 ps
/scorer/species/addTimeToRecord 6 ps
/scorer/species/addTimeToRecord 7 ps
/scorer/species/addTimeToRecord 8 ps
/scorer/species/addTimeToRecord 9 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
```

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



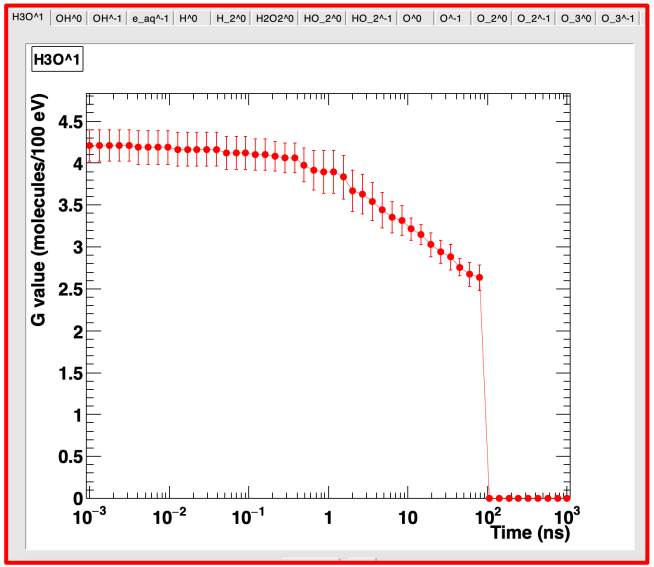
Exercise 8: Change the end of the chemical stage and re-run beam.in

beam.in

beam.in 〉 No Selection

```
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
```

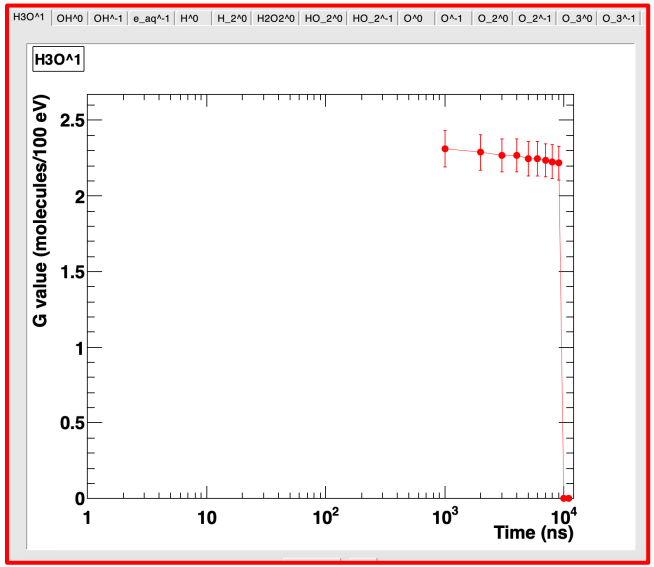


beam.in

beam.in 〉 No Selection

```
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
```



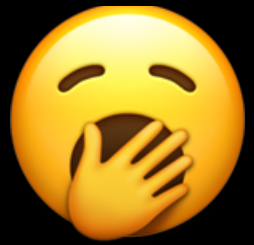
Be careful to use the proper Time to Score Species!!!

```
/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 ======
             ICRU73QO : 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

```
#

/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 1

/gun/energy 5000 keV
/run/beamOn 10
```

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

```
G4VisManager: Using G4TrajectoryDrawByCharge as fallback trajector
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 %
```