Chemistry examples

geant4-dna.org

Chem3 example

Presenter: Serena Fattori
INFN - LNS, Catania, Italy
serena.fattori@lns.infn.it

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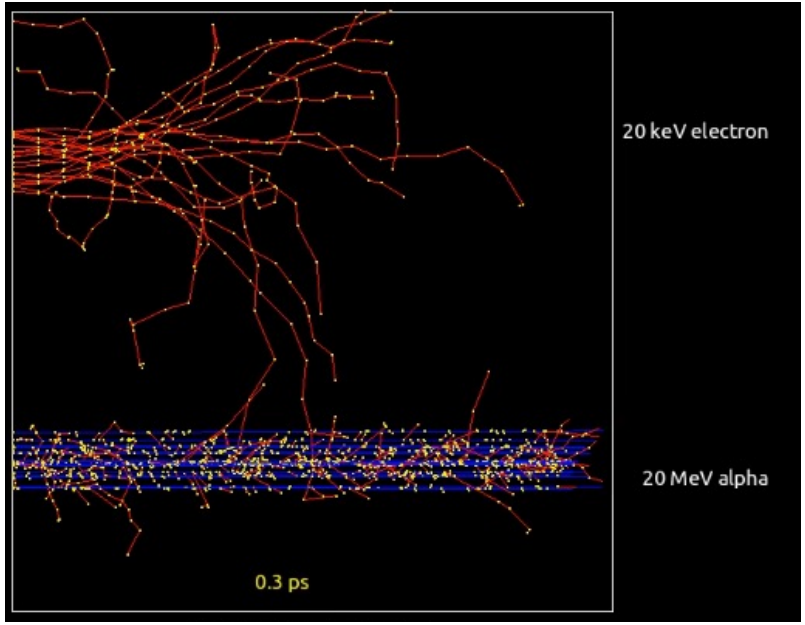
Processes in the Physical Stage

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

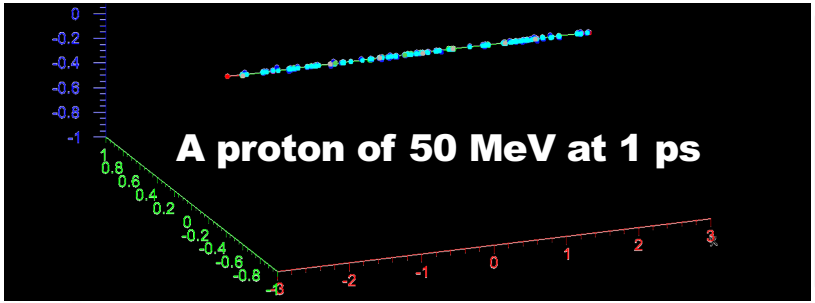
→ Water Dissociation

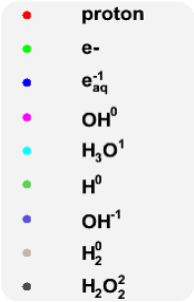
Chemical Species: DIFFUSION

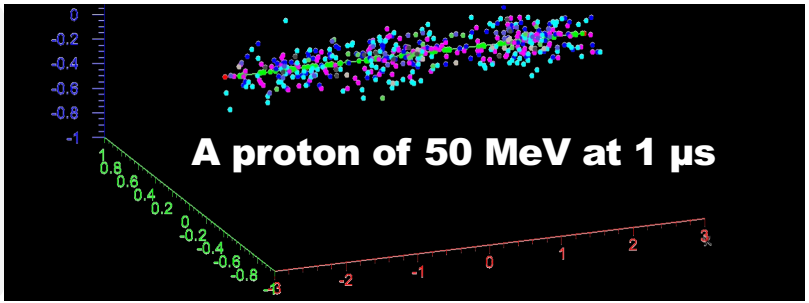
Species	Diffusion coefficient D (10^{-9} m^2 s^{-1})
H_3O^+	9.0
H•	7.0
OH^-	5.0
e^-_{aq}	4.9
H_2	5.0
•OH	2.8
H_2O_2	1.4

REACTIONS

Reactants	Products	Rate [1e-3 * m3 / (mole * s)]
$e^-_{aq} + e^-_{aq} + 2H2O$	$H_2 + 2OH^-$	0.5e10
e^-_{aq} + •OH	OH^-	2.95e10
e^-_{aq} + H• + H_2O	$H_2 + OH^-$	2.65e10
$e^-_{aq} + H_3O^+$	H• + H_2O	2.11e10
$e^-_{aq} + H_2O_2$	OH^- + •OH	1.41e10
•OH + •OH	H_2O_2	0.44e10
*OH + •H	H_2O	1.44e10
*H + •H	H_2	1.20e10
$H_3O^+ + OH^-$	2H2O	1.43e11







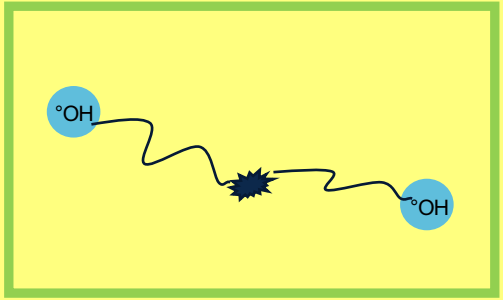
Chemistry Models

- 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.



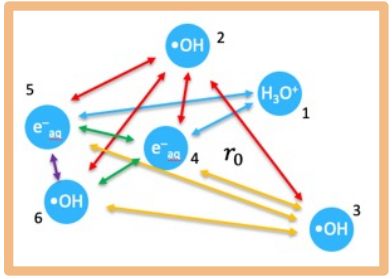
Karamitros, M. et al. (**2014**) Diffusion-controlled reactions modeling in Geant4-DNA. Journal of Computational Physics, 274, 841-882. https://doi.org/10.1016/j.jcp.2014.06.011

- 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.



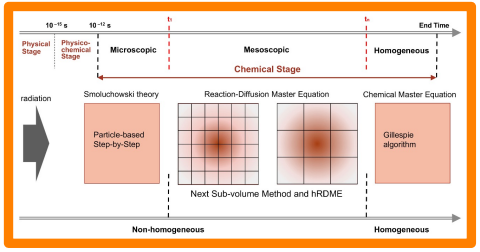
Karamitros, M. et al. (**2020**) Implementing the Independent Reaction Time method in Geant4 for radiation chemistry simulations. https://doi.org/10.48550/arXiv.2006.14225

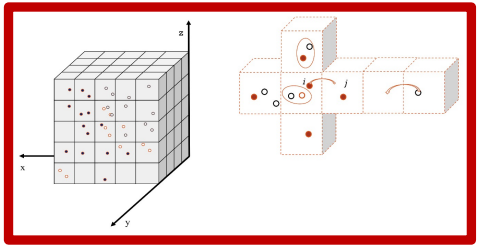
Ramos-Méndez, J. et al. (**2020**) Independent reaction times method in Geant4-DNA: Implementation and performance. https://doi.org/10.1002/mp.14490

- 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.

Chem3 example

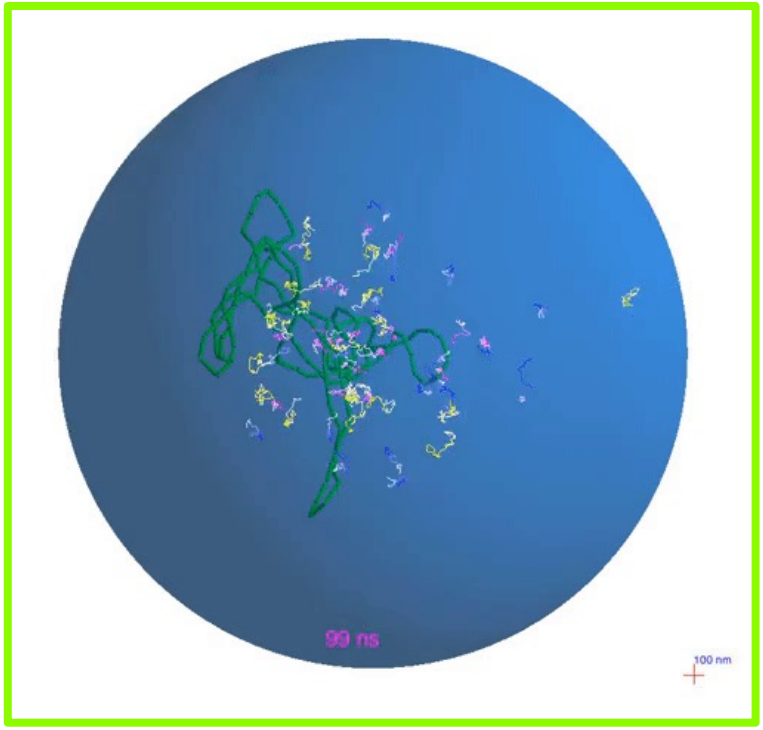
AUTHOR: Mathieu Karamitros

MAINTEINER: Hoang N. Tran

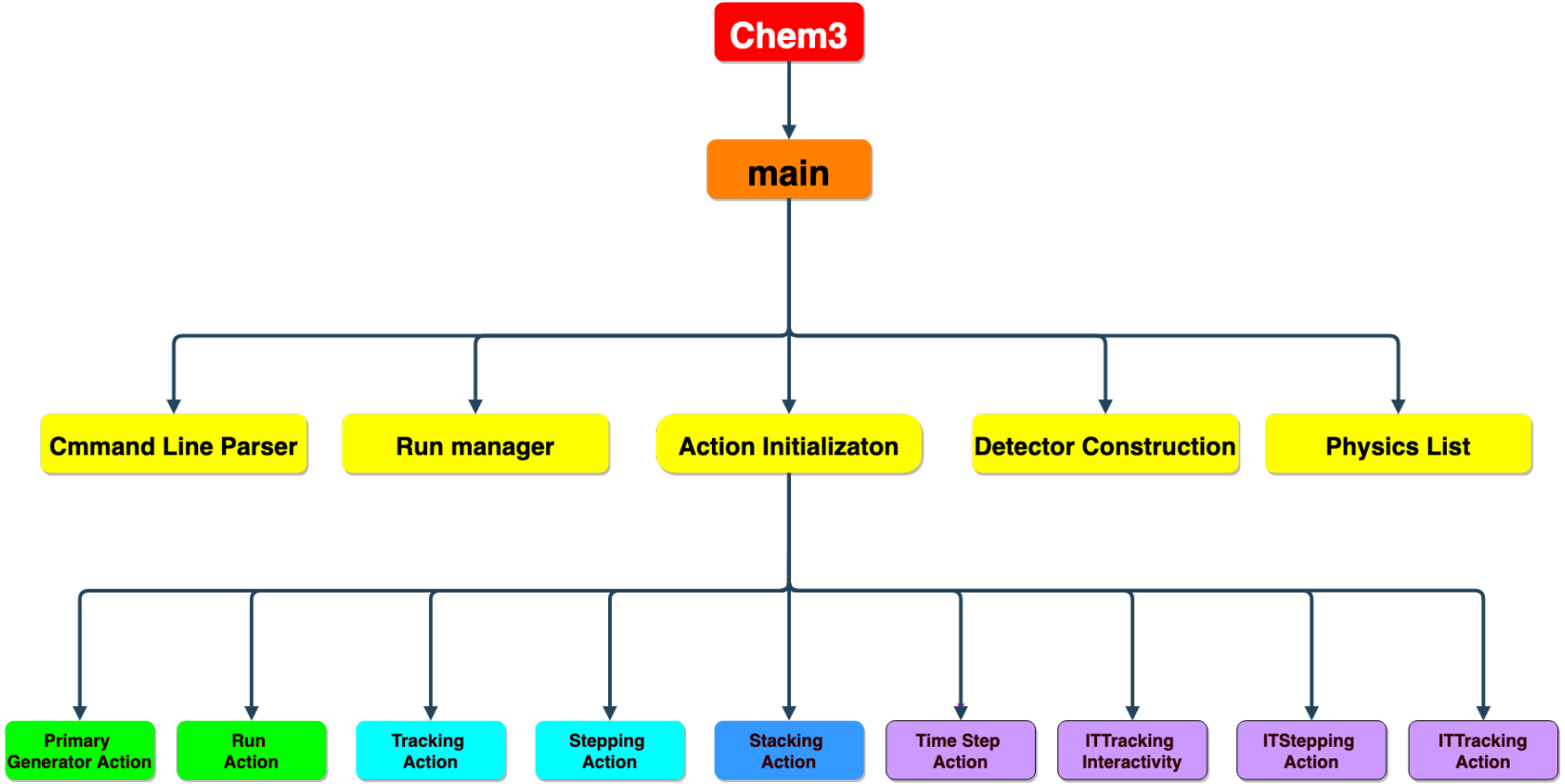
Chem3 Example

Illustrates how to implement user actions in the chemistry module using the step-by-step model.

Users can also visualize the trajectories of the chemical species in time and space using the graphical user interface.



Chem3 Application Code Structure



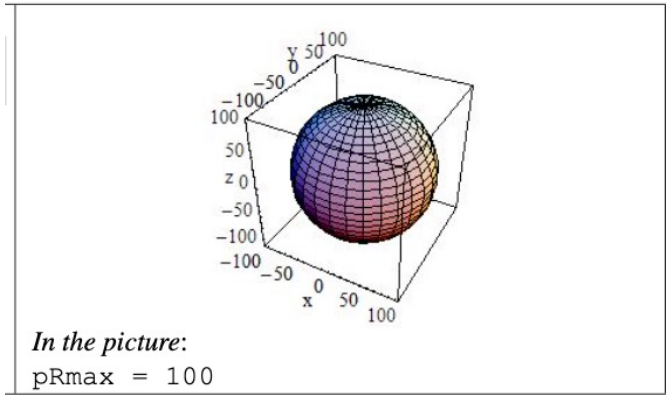
Chem3 Application Code Structure

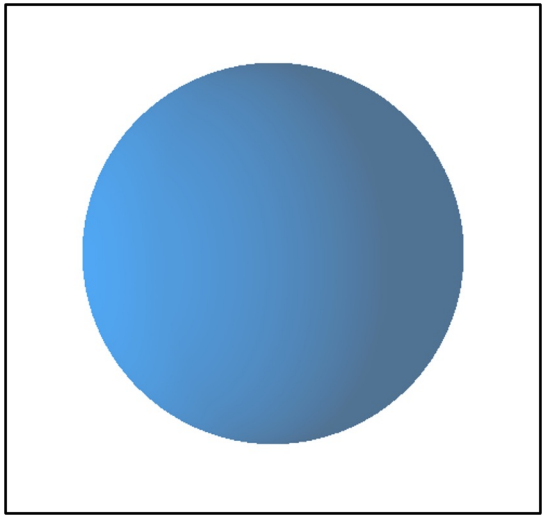
chem3.cc	Main file ⇒ creation **of RunManager, DetectorConstruction, PhysicsList, PrimaryGeneratorAction, ActionInitialization**
→ **RunManager**	Management of all the calls to Geant4 kernel and the threads in MT mode
→ **DetectorConstruction**	Definition of the geometry: World as **semi-transparent sphere**
→ **PhysicsList**	Choice of the physics & chemistry lists Default Physics ➔ **G4EmDNAPhysics** Default Chemistry ➔ **G4EmDNAChemistry** Chemistry Model ➔ **SBS**
→ **ActionInitialization**	**Build()** ⇒ creation of **PrimaryGeneratorAction** & optional user action classes: **RunAction**, **TrackingAction**, **SteppingAction**, **StackingAction**, **TimeStepAction**, **ITTrackingInteractivity**, **ITTrackingAction**, **ITSteppingAction**
→ **PrimaryGeneratorAction**	Choice of the primary particle. Default: **30 MeV Proton**

Chem3 Application Code Structure

→ **RunAction**	To retrieve information in the Beginning and in the End of Run. → In the EndOfRun gives in output the Seed used.
→ **TrackingAction**	To retrieve information of the Track. At the end of the Primary Track it gives in output the final kinetic energy of the primary.
→ **SteppingAction**	To retrieve information from a given "step".
→ **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...).
→ **ITTrackingInteractivity**	Mandatory to visualize chemical tracks and use stepping/tracking actions.
→ **ITTrackingAction**	To retrieve information from a given track. Similar to TrackingAction but for chemistry.
→ **ITSteppingAction**	To retrieve information from a given track. Similar to SteppingAction but for chemistry.

Geometry Definition





- The World Volume is a G4ORB

- Two parameters define the geometry :
  - the material of the Sphere → for Geant4-DNA it has to be water.
  - the radius of the Sphere: double worldRadius = 0.3*micrometer;

Physics / Chemistry List

Physics Models Included:

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

Chemistry Models Included:

- G4EmDNAChemistry ← default
- G4EmDNAChemistry_option1

N.B.

If the CommandLineParser has the flag "chemOFF" the chemistry is switched off.

Primary Generator

- The primary kinematic consists of a single particle starting at the center of the sphere.

default: 30 MeV Proton

- 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 1 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 chem3 example in "*my-simulations*"
- Create a build folder for chem3, i.e. "*chem3-build*"
- Enter inside "*chem3-build*" and execute the cmake command:
  cmake path-of-geant4-install path of chem3
- Source the geant4.sh:
  cd *path-of-geant4-install/bin*
  source geant4.sh
  cd –
- Compile the example:
  make –jn *(with n = number of cores available in your machine)*
- In the terminal window, inside your chem3-build folder:
  ./chem3 -gui tcsh or *./chem3 -gui qt*
- In the gui window:
  /control/execute beam.in

beam.in Macro Commands

```
#/tracking/verbose 1
/gun/position 0 0 0 micrometer
/gun/direction 0 0 1
/gun/particle e-
/gun/energy 1 keV
#
#============================================
# NB: comment lines when the flag chemOFF is used
#/scheduler/verbose 2
#/scheduler/whyDoYouStop
#============================================
#
/run/beamOn 1
```

=> Print information

=> Define the source

=> Print additinal chemistry information

=> Define the number of primary events

Output

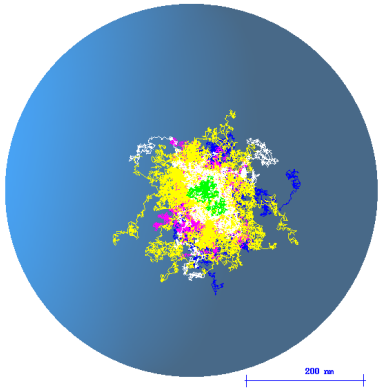
Defined reaction table

```
Physics stage ends
Number of chemical species involved in reactions = 6
Reaction                                        Reaction Rate [dm3/(mol*s)]   Interaction Range for chosen reaction model [nm]
-------------------------------------------------------------------------------------------------------------------------------
H3O^1 + e_aq^-1 -> H^0                          2.11e+10                      0.200589
-------------------------------------------------------------------------------------------------------------------------------
H3O^1 + OH^-1 -> No product                     1.43e+11                      1.34973
-------------------------------------------------------------------------------------------------------------------------------
OH^0 + e_aq^-1 -> OH^-1                         2.95e+10                      0.506256
-------------------------------------------------------------------------------------------------------------------------------
OH^0 + OH^0 -> H2O2^0                           4.4e+09                       0.207651
-------------------------------------------------------------------------------------------------------------------------------
OH^0 + H^0 -> No product                        1.44e+10                      0.194167
-------------------------------------------------------------------------------------------------------------------------------
e_aq^-1 + e_aq^-1 -> OH^-1 + OH^-1 + H_2^0      5e+09                         0.134838
-------------------------------------------------------------------------------------------------------------------------------
e_aq^-1 + H^0 -> OH^-1 + H_2^0                  2.65e+10                      0.294265
-------------------------------------------------------------------------------------------------------------------------------
e_aq^-1 + H2O2^0 -> OH^-1 + OH^0                1.41e+10                      0.295745
-------------------------------------------------------------------------------------------------------------------------------
H^0 + H^0 -> H_2^0                              1.2e+10                       0.226528
-------------------------------------------------------------------------------------------------------------------------------
DNAMolecularStepByStepModel will be used
```

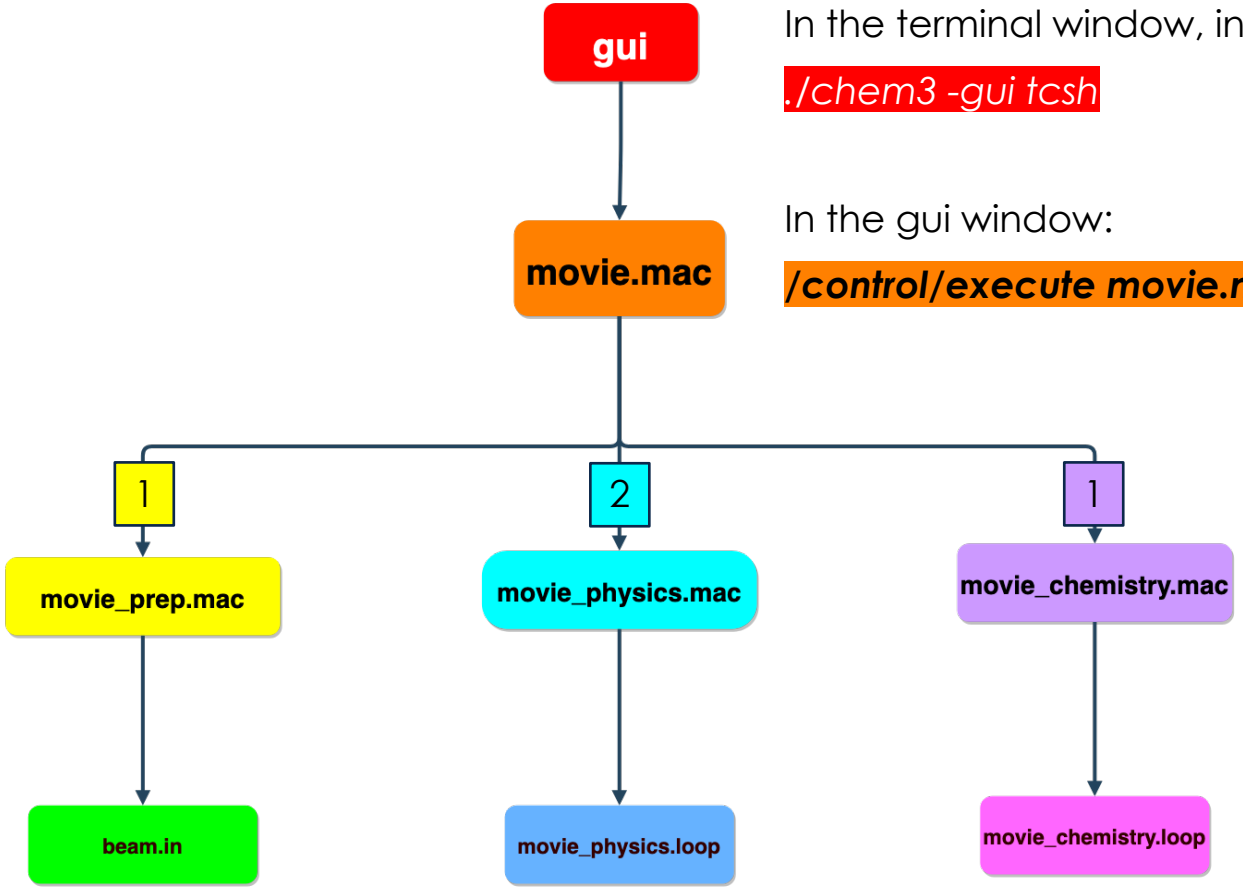
Chemical reactions

```
Physics stage ends
*** G4Scheduler starts processing
At time :        1 ps  Reaction : OH^-1 (-112) + H3O^1 (-166) -> No product
At time :    24.53 ps  Reaction : OH^0 (-145) + OH^0 (-173) -> H2O2^0 (-220)
At time :   37.218 ps  Reaction : OH^0 (-157) + e_aq^-1 (-72) -> OH^-1 (-221)
At time :   58.705 ps  Reaction : H^0 (-211) + H^0 (-215) -> H_2^0 (-222)
At time :   84.673 ps  Reaction : OH^0 (-167) + OH^0 (-175) -> H2O2^0 (-223)
At time :   86.673 ps  Reaction : OH^0 (-153) + OH^0 (-127) -> H2O2^0 (-224)
At time :   90.673 ps  Reaction : OH^0 (-151) + H^0 (-217) -> No product
At time :   132.29 ps  Reaction : OH^0 (-143) + OH^0 (-183) -> H2O2^0 (-225)
At time :   171.29 ps  Reaction : H3O^1 (-148) + OH^-1 (-221) -> No product
At time :    401.3 ps  Reaction : OH^0 (-185) + OH^0 (-161) -> H2O2^0 (-226)
At time :   486.46 ps  Reaction : OH^0 (-155) + e_aq^-1 (-20) -> OH^-1 (-227)
At time :   489.46 ps  Reaction : H3O^1 (-184) + OH^-1 (-227) -> No product
At time :   549.27 ps  Reaction : OH^0 (-141) + e_aq^-1 (-94) -> OH^-1 (-228)
At time :   582.27 ps  Reaction : OH^0 (-205) + e_aq^-1 (-99) -> OH^-1 (-229)
At time :    637.1 ps  Reaction : OH^0 (-137) + OH^0 (-218) -> H2O2^0 (-230)
At time :   726.44 ps  Reaction : e_aq^-1 (-190) + OH^0 (-181) -> OH^-1 (-231)
At time :   774.65 ps  Reaction : OH^0 (-216) + OH^0 (-206) -> H2O2^0 (-232)
At time :  1.0033 ns  Reaction : H3O^1 (-130) + OH^-1 (-229) -> No product
At time :  1.4536 ns  Reaction : OH^0 (-197) + OH^0 (-209) -> H2O2^0 (-233)
At time :  2.0366 ns  Reaction : H3O^1 (-182) + e_aq^-1 (-44) -> H^0 (-234)
At time :   2.801 ns  Reaction : OH^0 (-179) + OH^0 (-121) -> H2O2^0 (-235)
At time :   3.004 ns  Reaction : H3O^1 (-198) + e_aq^-1 (-73) -> H^0 (-236)
At time :  3.4335 ns  Reaction : e_aq^-1 (-199) + OH^0 (-169) -> OH^-1 (-237)
At time :  3.5283 ns  Reaction : H3O^1 (-160) + OH^-1 (-237) -> No product
At time :  3.9539 ns  Reaction : H3O^1 (-186) + OH^-1 (-231) -> No product
At time :  4.2798 ns  Reaction : e_aq^-1 (-88) + H^0 (-203) -
> OH^-1 (-238) + H_2^0 (-239)
At time :  4.6319 ns  Reaction : OH^-1 (-228) + H3O^1 (-134) -> No product
At time :   4.776 ns  Reaction : H3O^1 (-146) + e_aq^-1 (-39) -> H^0 (-240)
At time :  5.1574 ns  Reaction : OH^0 (-147) + e_aq^-1 (-110) -> OH^-1 (-241)
At time :  6.4734 ns  Reaction : H3O^1 (-172) + e_aq^-1 (-51) -> H^0 (-242)
At time :  7.4096 ns  Reaction : e_aq^-1 (-108) + H^0 (-219) -
> OH^-1 (-243) + H_2^0 (-244)
At time :  8.1618 ns  Reaction : OH^0 (-113) + OH^0 (-115) -> H2O2^0 (-245)
At time :  11.903 ns  Reaction : H3O^1 (-174) + OH^-1 (-241) -> No product
At time :  13.103 ns  Reaction : e_aq^-1 (-24) + H2O2^0 (-233) -
> OH^-1 (-246) + OH^0 (-247)
At time :  16.403 ns  Reaction : e_aq^-1 (-22) + OH^0 (-165) -> OH^-1 (-248)
At time :  17.403 ns  Reaction : OH^0 (-133) + OH^0 (-214) -> H2O2^0 (-249)
At time :  21.626 ns  Reaction : e_aq^-1 (-87) + OH^0 (-125) -> OH^-1 (-250)
At time :  25.091 ns  Reaction : OH^0 (-187) + e_aq^-1 (-37) -> OH^-1 (-251)
At time :  25.291 ns  Reaction : H3O^1 (-132) + OH^-1 (-246) -> No product
At time :  33.488 ns  Reaction : H3O^1 (-195) + OH^-1 (-251) -> No product
At time :  33.588 ns  Reaction : H2O2^0 (-226) + e_aq^-1 (-50) -
> OH^-1 (-252) + OH^0 (-253)
At time :  43.671 ns  Reaction : H3O^1 (-142) + OH^-1 (-250) -> No product
At time :  56.551 ns  Reaction : e_aq^-1 (-85) + OH^0 (-208) -> OH^-1 (-254)
*** G4Scheduler ends at time : 100 ns
```

- G4Physics initialization and the defined reaction table are printed.
- ITStepManager processes the chemical stage time step after time step.
- Chemical reactions are printed.
- In the GUI window a cumulative trajectory of the chemical species is drawn.



Movie Macros Scheme



In the terminal window, inside chem3-build folder:

./chem3 -gui tcsh

In the gui window:

/control/execute movie.mac

Time Evolution Visualization

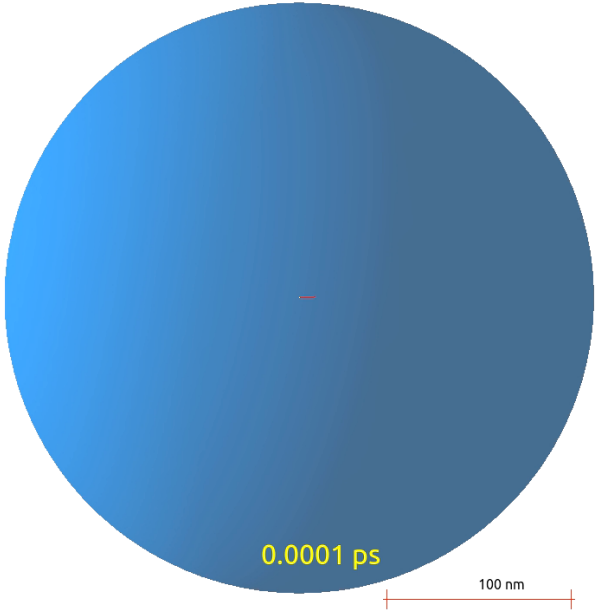
- User can start a visualization of the chemical track evolution in time and space using **/control/execute movie.mac**

- Note, that in default setup the simulation requires machine with 6 GB of RAM.

- To lower memory requirements, either:
  - decrease energy of the incident electron in **beam.in**

  or/and

  - shorten the simulation using **SetEndTime** setting in
    src/ActionInitialization.cc → default 100 ns
    and in
    movie_chemistry.mac



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

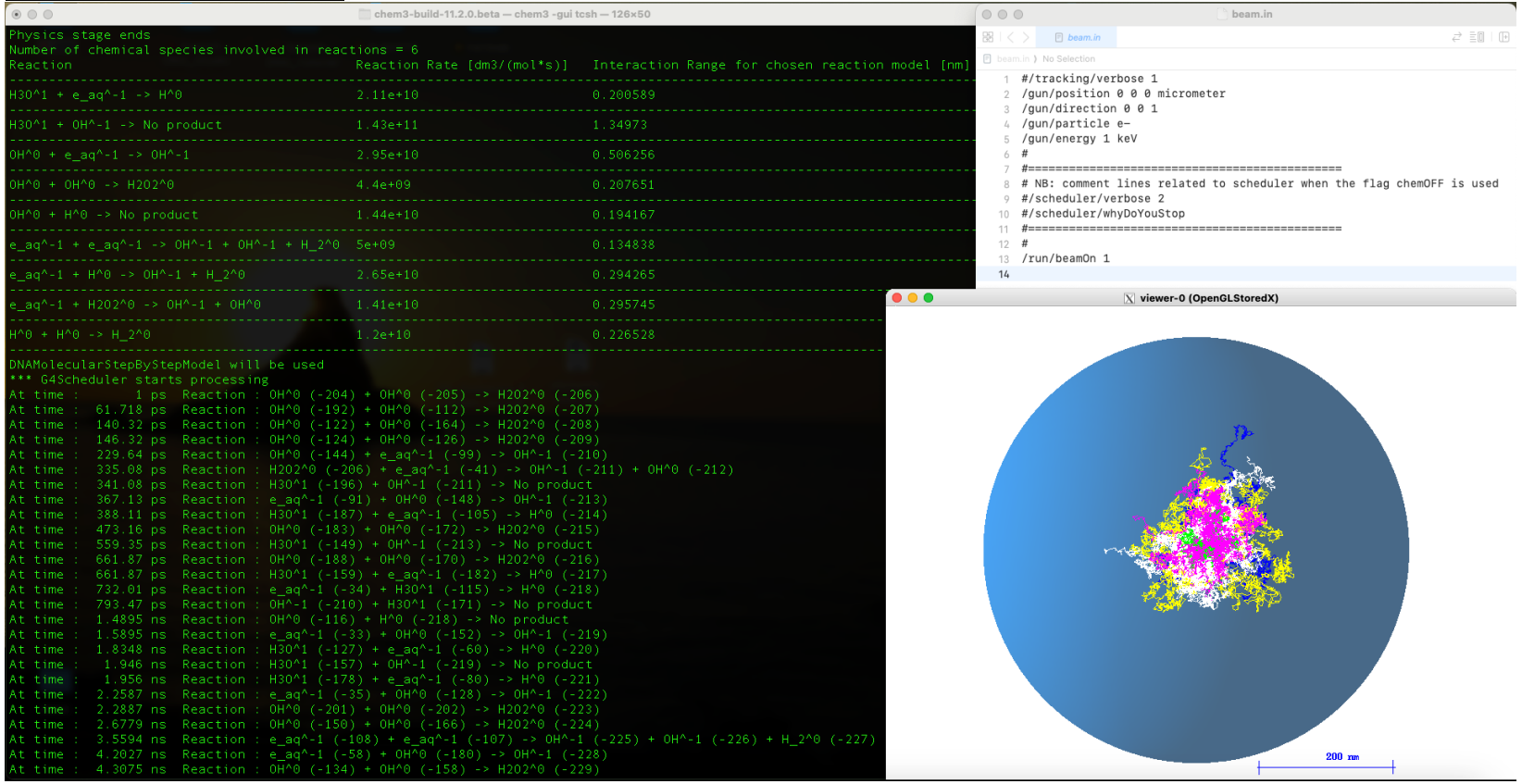
June 27th, 2023 : **Geant4 11.1.2** LP2i Virtual Machine has been released, see link.

Exercises

- **Exercise 1**: Run as it is the beam.in macro
- **Exercise 2**: Change the type of particle and re-run the beam.in
- **Exercise 3**: Change the particle energy and re-run beam.in
- **Exercise 4**: Change the dimension of the sphere and re-run the beam.in
- **Exercise 5**: Run as it is the movie.mac macro
- **Exercise 6**: Change the type of particle and re-run the movie.mac
- **Exercise 7**: Change the particle energy and re-run movie.mac
- **Exercise 8**: Change the dimension of the sphere and re-run the movie.mac
- **Exercise 9**: Change the "endTime" of the chemistry movie (suggestion: via macro)
- **Exercise 10**: Change the EndTime of the chemistry execution (suggestion: in the proper class…)

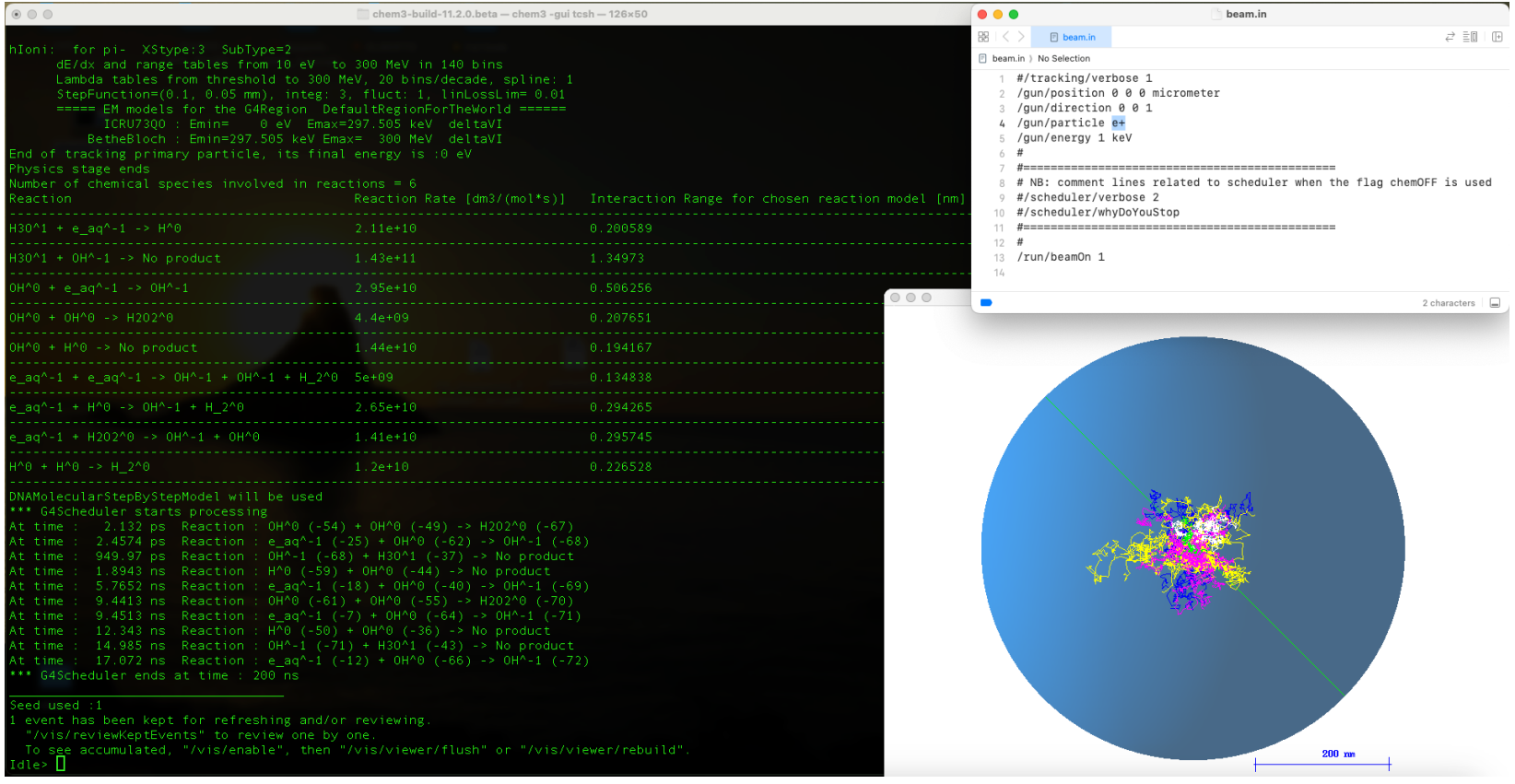
Exercise 1: Run as it is the beam.in macro

```
./chem3 -gui tcsh
```



Exercise 2: Change the type of particle and re-run the beam.in

```
./chem3 -gui tcsh
```



Exercise 3: Change the particle energy and re-run beam.in

```
./chem3 -gui tcsh
```

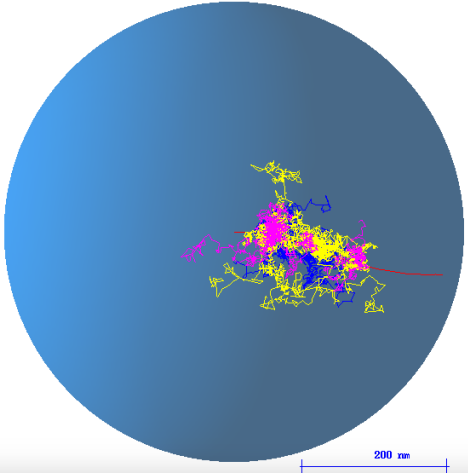
chem3-build-11.2.0.beta — chem3 -gui tcsh — 126×50

```
        BetheBloch : Emin=297.505 keV Emax=  300 MeV  deltaVI

msc:  for pi-  SubType= 10
      ===== EM models for the G4Region  DefaultRegionForTheWorld ======
        WentzelVIUni : Emin=    0 eV  Emax=  300 MeV
          StepLim=Minimal Rfact=0.2 Gfact=2.5 Sfact=0.6 DispFlag:0 Skin=3 Llim=1 mm

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
End of tracking primary particle, its final energy is :9.79727 keV
Physics stage ends
Number of chemical species involved in reactions = 6
Reaction                                    Reaction Rate [dm3/(mol*s)]   Interaction Range for chosen reaction model [nm]
-------------------------------------------------------------------------------------------------------------------------
H3O^1 + e_aq^-1 -> H^0                      2.11e+10                      0.200589
-------------------------------------------------------------------------------------------------------------------------
H3O^1 + OH^-1 -> No product                 1.43e+11                      1.34973
-------------------------------------------------------------------------------------------------------------------------
OH^0 + e_aq^-1 -> OH^-1                     2.95e+10                      0.506256
-------------------------------------------------------------------------------------------------------------------------
OH^0 + OH^0 -> H2O2^0                       4.4e+09                       0.207651
-------------------------------------------------------------------------------------------------------------------------
OH^0 + H^0 -> No product                    1.44e+10                      0.194167
-------------------------------------------------------------------------------------------------------------------------
e_aq^-1 + e_aq^-1 -> OH^-1 + OH^-1 + H_2^0  5e+09                         0.134838
-------------------------------------------------------------------------------------------------------------------------
e_aq^-1 + H^0 -> OH^-1 + H_2^0              2.65e+10                      0.294265
-------------------------------------------------------------------------------------------------------------------------
e_aq^-1 + H2O2^0 -> OH^-1 + OH^0            1.41e+10                      0.295745
-------------------------------------------------------------------------------------------------------------------------
H^0 + H^0 -> H_2^0                          1.2e+10                       0.226528
-------------------------------------------------------------------------------------------------------------------------
DNAMolecularStepByStepModel will be used
*** G4Scheduler starts processing
At time :  228.93 ps  Reaction : OH^0 (-35) + H^0 (-45) -> No product
At time :  1.6143 ns  Reaction : OH^0 (-46) + H^0 (-47) -> No product
At time :  6.9922 ns  Reaction : e_aq^-1 (-10) + OH^0 (-39) -> OH^-1 (-48)
At time :  14.667 ns  Reaction : e_aq^-1 (-23) + OH^0 (-43) -> OH^-1 (-49)
*** G4Scheduler ends at time : 200 ns
_____________________________
Seed used :1
1 event has been kept for refreshing and/or reviewing.
  "/vis/reviewKeptEvents" to review one by one.
  To see accumulated, "/vis/enable", then "/vis/viewer/flush" or "/vis/viewer/rebuild".
Idle> 
```

beam.in

```
1  #/tracking/verbose 1
2  /gun/position 0 0 0 micrometer
3  /gun/direction 0 0 1
4  /gun/particle e-
5  /gun/energy 10 keV
6  #
7  #============================================
8  # NB: comment lines related to scheduler when the flag chemOFF is used
9  #/scheduler/verbose 2
10 #/scheduler/whyDoYouStop
11 #============================================
12 #
13 /run/beamOn 1
14
```

viewer-0 (OpenGLStoredX)

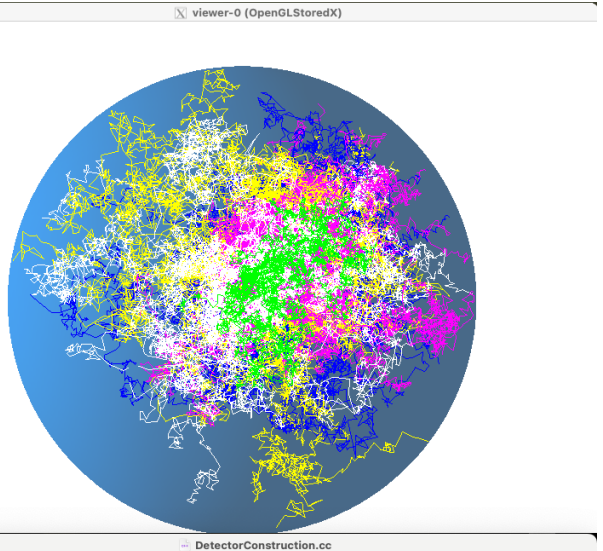


Exercise 4: Change the dimension of the sphere and re-run the beam.in

```
make
./chem3 -gui tcsh
```

chem3-build-11.2.0.beta — chem3 -gui tcsh — 126×50

```
*** G4Scheduler starts processing
At time :        1 ps  Reaction : OH^0 (-204) + OH^0 (-205) -> H2O2^0 (-206)
At time :   61.718 ps  Reaction : OH^0 (-192) + OH^0 (-112) -> H2O2^0 (-207)
At time :   140.32 ps  Reaction : OH^0 (-122) + OH^0 (-164) -> H2O2^0 (-208)
At time :   146.32 ps  Reaction : OH^0 (-124) + OH^0 (-126) -> H2O2^0 (-209)
At time :   229.64 ps  Reaction : e_aq^-1 (-99) + OH^0 (-144) -> OH^-1 (-210)
At time :   335.08 ps  Reaction : H2O2^0 (-206) + e_aq^-1 (-41) -> OH^-1 (-211) + OH^0 (-212)
At time :   341.08 ps  Reaction : H3O^1 (-196) + OH^-1 (-211) -> No product
At time :   367.13 ps  Reaction : e_aq^-1 (-91) + OH^0 (-148) -> OH^-1 (-213)
At time :   388.11 ps  Reaction : e_aq^-1 (-105) + H3O^1 (-187) -> H^0 (-214)
At time :   473.16 ps  Reaction : OH^0 (-183) + OH^0 (-172) -> H2O2^0 (-215)
At time :   559.35 ps  Reaction : OH^-1 (-213) + H3O^1 (-149) -> No product
At time :   661.87 ps  Reaction : OH^0 (-188) + OH^0 (-170) -> H2O2^0 (-216)
At time :   661.87 ps  Reaction : H3O^1 (-159) + e_aq^-1 (-182) -> H^0 (-217)
At time :   732.01 ps  Reaction : e_aq^-1 (-34) + H3O^1 (-115) -> H^0 (-218)
At time :   793.47 ps  Reaction : OH^-1 (-210) + H3O^1 (-171) -> No product
At time :  1.4895 ns  Reaction : OH^0 (-116) + H^0 (-218) -> No product
At time :  1.5895 ns  Reaction : e_aq^-1 (-33) + OH^0 (-152) -> OH^-1 (-219)
At time :  1.8348 ns  Reaction : e_aq^-1 (-60) + H3O^1 (-127) -> H^0 (-220)
At time :   1.946 ns  Reaction : H3O^1 (-157) + OH^-1 (-219) -> No product
At time :   1.956 ns  Reaction : e_aq^-1 (-80) + H3O^1 (-178) -> H^0 (-221)
At time :  2.2587 ns  Reaction : e_aq^-1 (-35) + OH^0 (-128) -> OH^-1 (-222)
At time :  2.2887 ns  Reaction : OH^0 (-201) + OH^0 (-202) -> H2O2^0 (-223)
At time :  2.6779 ns  Reaction : OH^0 (-150) + OH^0 (-166) -> H2O2^0 (-224)
At time :  3.5594 ns  Reaction : e_aq^-1 (-107) + e_aq^-1 (-108) -> OH^-1 (-225) + OH^-1 (-226) + H_2^0 (-227)
At time :  4.2027 ns  Reaction : e_aq^-1 (-58) + OH^0 (-180) -> OH^-1 (-228)
At time :  4.3075 ns  Reaction : OH^0 (-134) + OH^0 (-158) -> H2O2^0 (-229)
At time :  4.3881 ns  Reaction : OH^-1 (-228) + H3O^1 (-121) -> No product
At time :  4.7245 ns  Reaction : e_aq^-1 (-37) + e_aq^-1 (-64) -> OH^-1 (-230) + OH^-1 (-231) + H_2^0 (-232)
At time :  4.9113 ns  Reaction : OH^-1 (-231) + H3O^1 (-133) -> No product
At time :  7.2387 ns  Reaction : H3O^1 (-139) + e_aq^-1 (-179) -> H^0 (-233)
At time :  8.3472 ns  Reaction : OH^0 (-191) + OH^0 (-142) -> H2O2^0 (-234)
At time :  9.5549 ns  Reaction : OH^0 (-132) + OH^0 (-136) -> H2O2^0 (-235)
At time :  11.324 ns  Reaction : e_aq^-1 (-65) + e_aq^-1 (-73) -> OH^-1 (-236) + OH^-1 (-237) + H_2^0 (-238)
At time :  12.724 ns  Reaction : H2O2^0 (-215) + e_aq^-1 (-82) -> OH^-1 (-239) + OH^0 (-240)
At time :  19.528 ns  Reaction : OH^0 (-212) + e_aq^-1 (-54) -> OH^-1 (-241)
At time :  25.605 ns  Reaction : OH^0 (-240) + e_aq^-1 (-84) -> OH^-1 (-242)
At time :  26.805 ns  Reaction : OH^-1 (-236) + H3O^1 (-147) -> No product
At time :  29.187 ns  Reaction : OH^0 (-114) + OH^0 (-118) -> H2O2^0 (-243)
At time :  30.287 ns  Reaction : e_aq^-1 (-43) + e_aq^-1 (-63) -> OH^-1 (-244) + OH^-1 (-245) + H_2^0 (-246)
At time :  30.487 ns  Reaction : OH^0 (-197) + OH^0 (-194) -> H2O2^0 (-247)
At time :   31.69 ns  Reaction : e_aq^-1 (-77) + H2O2^0 (-209) -> OH^-1 (-248) + OH^0 (-249)
At time :   31.89 ns  Reaction : OH^-1 (-239) + H3O^1 (-117) -> No product
At time :  34.908 ns  Reaction : H3O^1 (-198) + OH^-1 (-237) -> No product
At time :  55.073 ns  Reaction : e_aq^-1 (-45) + H2O2^0 (-247) -> OH^-1 (-250) + OH^0 (-251)
At time :  75.197 ns  Reaction : OH^-1 (-245) + H3O^1 (-161) -> No product
At time :  91.857 ns  Reaction : H3O^1 (-111) + OH^-1 (-242) -> No product
At time :  169.23 ns  Reaction : OH^0 (-185) + OH^0 (-140) -> H2O2^0 (-252)
*** G4Scheduler ends at time : 200 ns
```

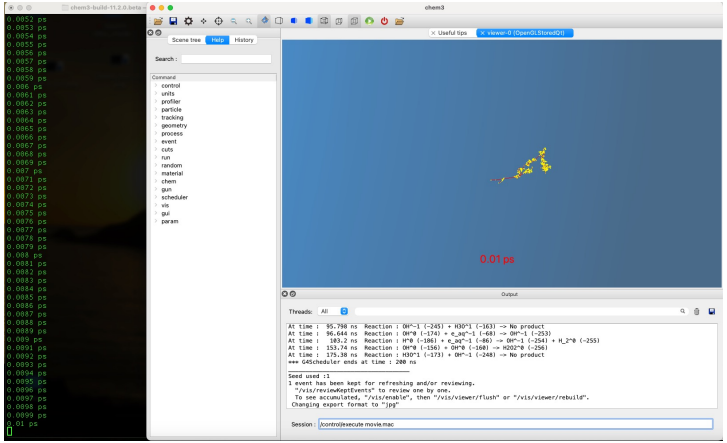


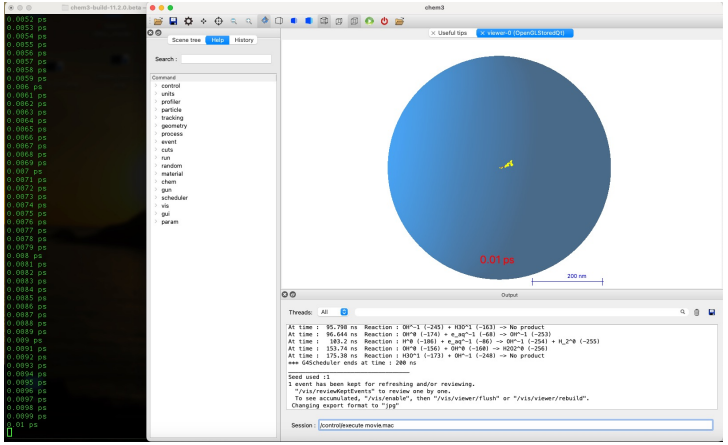
DetectorConstruction.cc

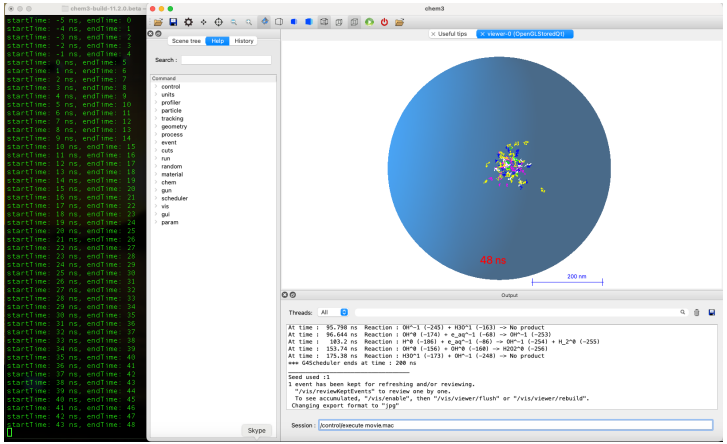
```
97  G4VPhysicalVolume* DetectorConstruction::ConstructDetector()
98  {
99    G4Material *water = OtherMaterial("G4_WATER");
100
101   // WORLD VOLUME = an G4ORB FULL OF LIQUID WATER
102
103   double worldRadius = 0.1*micrometer;
104
105   G4Orb* solidWorld = new G4Orb("World", worldRadius);
106
107   G4LogicalVolume* logicWorld =
108       new G4LogicalVolume(solidWorld,  //its solid
109           water,  //its material
```

Exercise 5: Run as it is the movie.mac macro

```
./chem3 -gui qt

Idle>/control/execute movie.mac
```







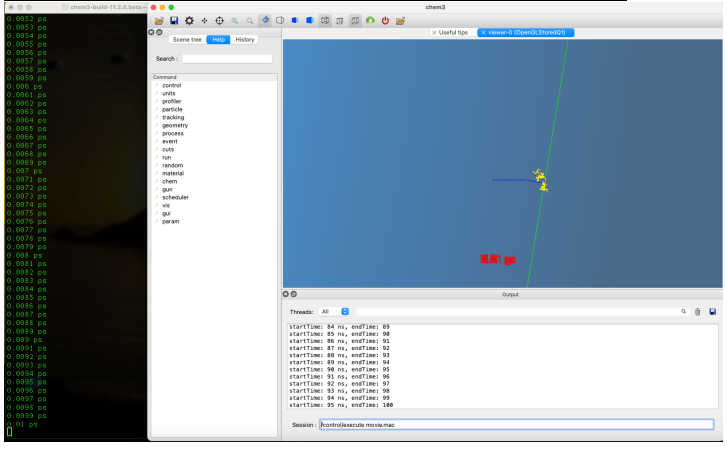
Exercise 6: Change the type of particle and re-run the movie.mac

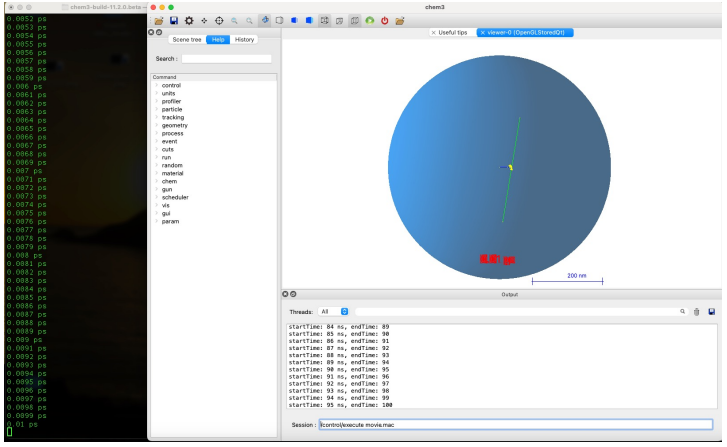
beam.in

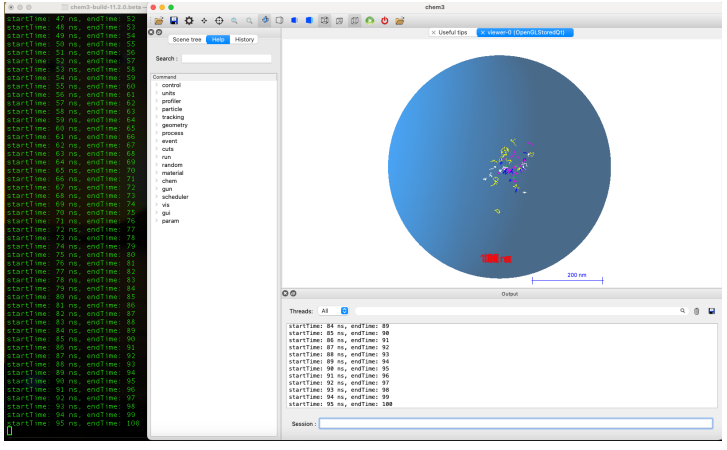
beam.in ⟩ No Selection

```
1  #/tracking/verbose 1
2  /gun/position 0 0 0 micrometer
3  /gun/direction 0 0 1
4  /gun/particle e+
5  /gun/energy 1 keV
6  #
7  #============================================
8  # NB: comment lines related to scheduler when the flag chemOFF is used
9  #/scheduler/verbose 2
10 #/scheduler/whyDoYouStop
11 #============================================
12 #
13 /run/beamOn 1
14
```

```
Idle>/control/execute movie.mac
```







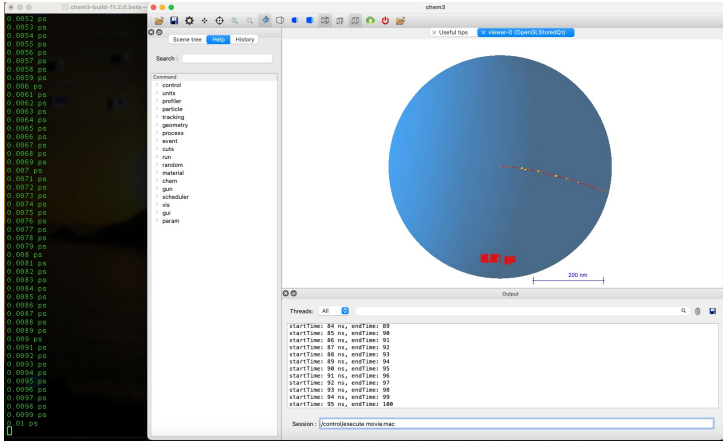
Exercise 7: Change the particle energy and re-run movie.mac

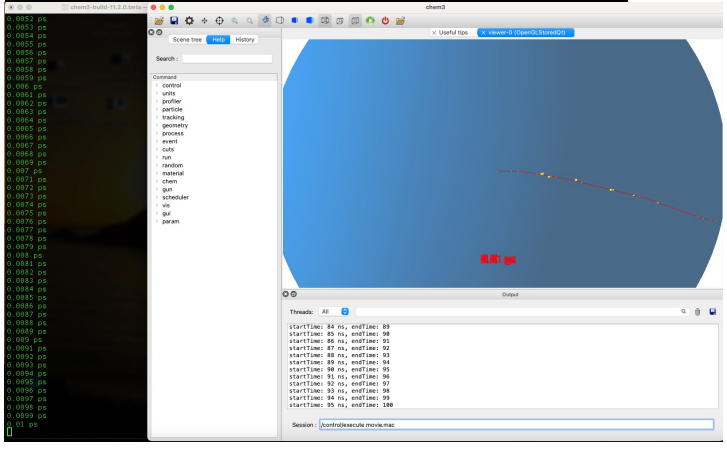
beam.in

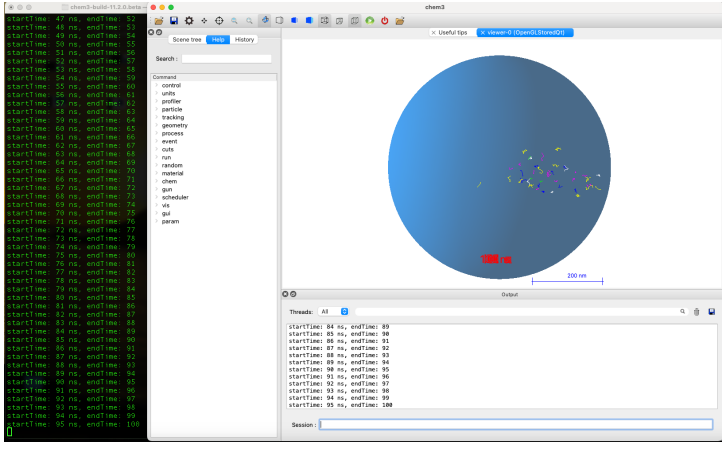
beam.in ⟩ No Selection

```
1  #/tracking/verbose 1
2  /gun/position 0 0 0 micrometer
3  /gun/direction 0 0 1
4  /gun/particle e-
5  /gun/energy 10 keV
6  #
7  #============================================
8  # NB: comment lines related to scheduler when the flag chemOFF is used
9  #/scheduler/verbose 2
10 #/scheduler/whyDoYouStop
11 #============================================
12 #
13 /run/beamOn 1
14
```

```
Idle>/control/execute movie.mac
```





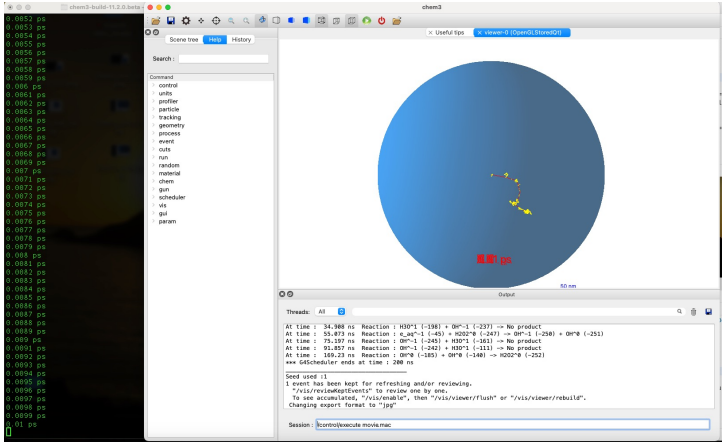


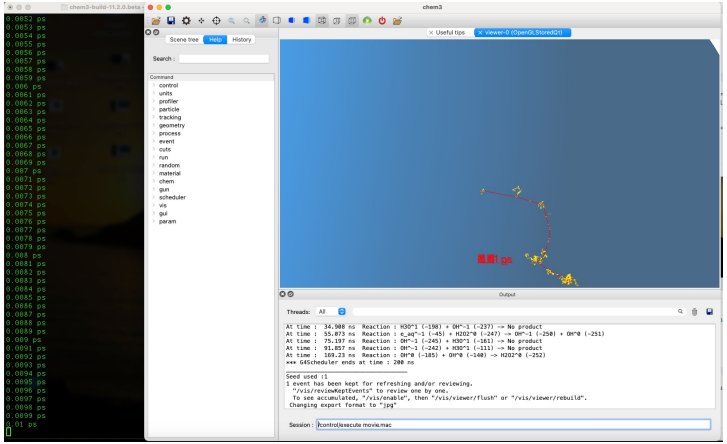
Exercise 8: Change the dimension of the sphere and re-run the movie.mac

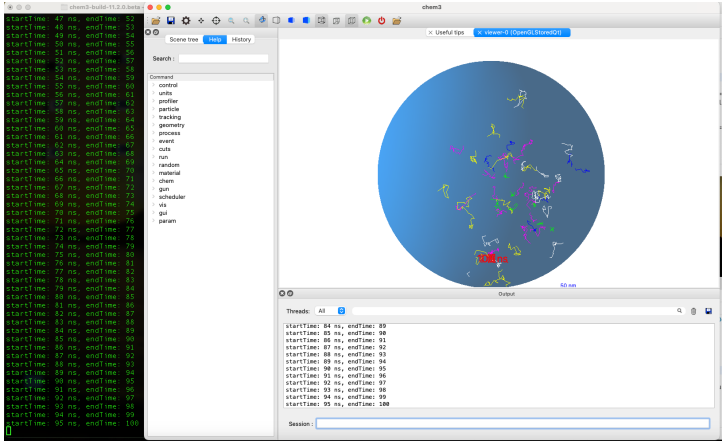
C* DetectorConstruction ⟩ M DetectorConstruction::ConstructDetector()

```
94
95  //....oooO0000ooo........oooO0000ooo........oooO0000ooo........oooO0000ooo......
96
97  G4VPhysicalVolume* DetectorConstruction::ConstructDetector()
98  {
99    G4Material *water = OtherMaterial("G4_WATER");
100
101   // WORLD VOLUME = an G4ORB FULL OF LIQUID WATER
102
103   double worldRadius = 0.1*micrometer;
104
105   G4Orb* solidWorld = new G4Orb("World", worldRadius);
```

```
make
./chem3 -gui tcsh
Idle>/control/execute movie.mac
```







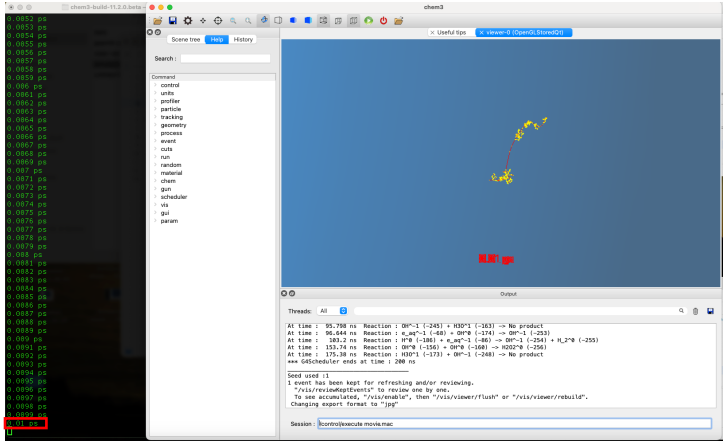
Exercise 9: Change the “endTime” of the chemistry movie

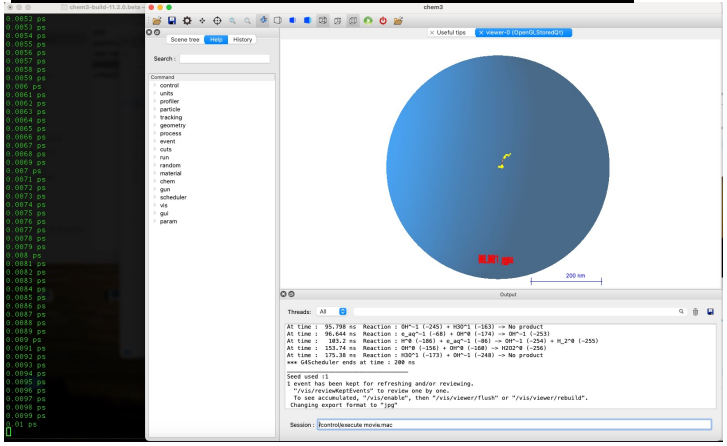
movie_chemistry.mac

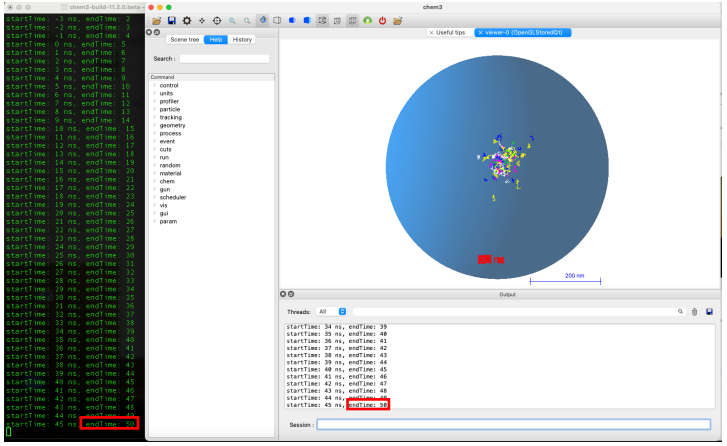
movie_chemistry.mac ⟩ No Selection

```
1  /vis/modeling/trajectories/drawByParticleID-0/default/setDrawStepPts false
2
3  # end time of chemistry in ns (change units in chemistry.loop
4  /control/alias endTime 45
5  /vis/viewer/set/timeWindow/startTime 0 ps
6  #/vis/viewer/set/timeWindow/endTime 1 ps
7
8  /vis/viewer/set/timeWindow/fadeFactor 0
9  /vis/viewer/set/timeWindow/displayHeadTime true -0.1 -0.8 24 1.0 0.0 0.0
10 /control/alias timeWindow 5
11 /control/loop movie_chemistry.loop startTime -{timeWindow} {endTime} 1
12
```

```
Idle>/control/execute movie.mac
```







Exercise 10: Change the EndTime of the chemistry execution

ActionInitialization.cc

```
72
73  //....oooO0000ooo........oooO0000ooo........oooO0000ooo........oooO0000ooo......
74
75  ActionInitialization::~ActionInitialization()
76  {}
77
78  //....oooO0000ooo........oooO0000ooo........oooO0000ooo........oooO0000ooo......
79
80  void ActionInitialization::BuildForMaster() const
81  {
82   // In MT mode, to be clearer, the RunAction class for the master thread might
83   // be different than the one used for the workers.
84   // This RunAction will be called before and after starting the
85   // workers.
86   // For more details, please refer to :
87   // https://twiki.cern.ch/twiki/bin/view/Geant4/Geant4MTForApplicationDevelopers
88   //
89   // RunAction* runAction= new RunAction();
90   // SetUserAction(runAction);
91  }
92
93  void ActionInitialization::Build() const
94  {
95    PrimaryGeneratorAction* primGenAction = new PrimaryGeneratorAction;
96    SetUserAction(primGenAction);
97
98    // Set optional user action classes
99    SetUserAction(new RunAction());
100   SetUserAction(new TrackingAction());
101   SetUserAction(new SteppingAction());
102   SetUserAction(new StackingAction());
103
104   // chemistry part
105   if(G4DNAChemistryManager::IsActivated()){
106     G4Scheduler::Instance()->SetUserAction(new TimeStepAction());
107
108     // Uncomment and set to stop chemistry stage after:
109     // ...given number of time steps
110     //G4Scheduler::Instance()->SetMaxNbSteps(1000);
111
112     // ...OR reaching this time
113     G4Scheduler::Instance()->SetEndTime(50*nanosecond);
114
```

```
make
./chem3 -gui tcsh
Idle>/control/execute movie.mac
```