Chemistry actor in GATE 10

D.E Kwon, **A.Pereda, G.R. Fois, H.N. Tran, G.Blain, S.Terfas, and L. Maigne**

PhD. student

daeun.kwon@clermont.in2p3.fr

LPCA, CNRS-UCA, France

The FLASHMOD collaboration
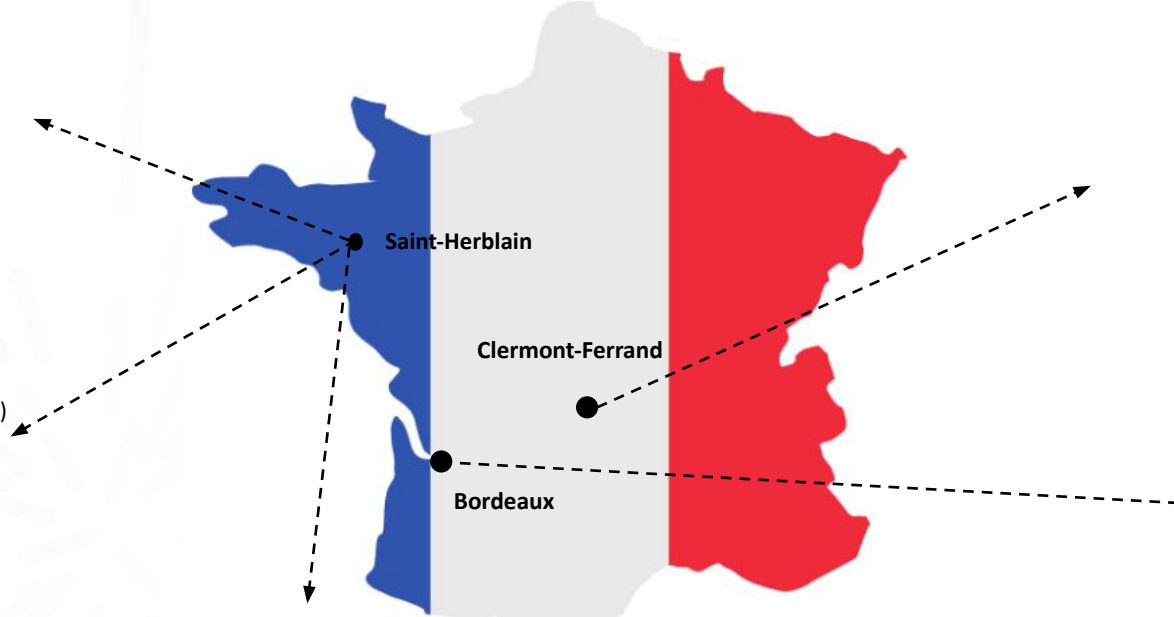
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Stéphane SUPIOT, MD, PhD (radiation therapy)
Gaelle Saade (radiobiology)
Mathieu Chocry, PhD, (radiobiology)

Saint-Herblain

Clermont-Ferrand

Bordeaux

LPC

Lydia MAIGNE, PhD (medical physics)
Giovanna FOIS, PhD (applied physics)
Daeun Kwon, (applied physics)

LP2i Bordeaux

Hoang Tran (G4-DNA)

Subatech

Guillaume BLAIN, PhD (radiochemistry)
Johan VANDENBORRE, PhD (radiochemistry)
Emeline Craff, PhD (radiochemistry)
Noël SERVAGENT, PhD (robotics)
Vincent METIVIER, PhD (nuclear physics)
Vincent Fiegel, PhD (radiochemistry)
Manon Evin (medical physics)
Sarra Terfas (radiochemistry)

Arronax Nantes

Charbel KOUMEIR, PhD (nuclear physics)
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Ferid HADDAD, PhD (nuclear physics)
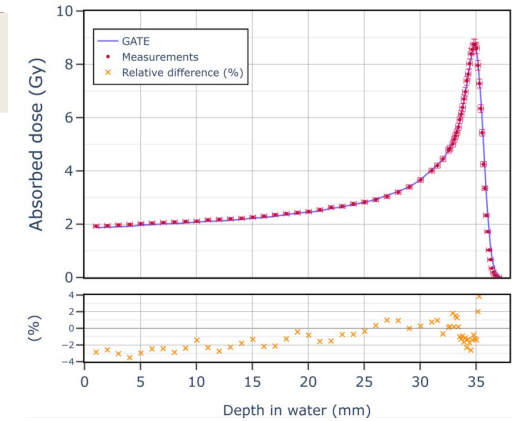Quentin Mouchard, PhD (nuclear physics)
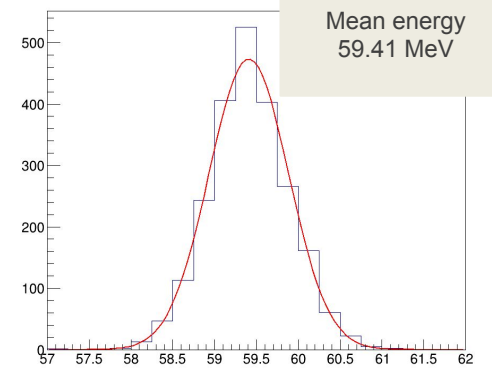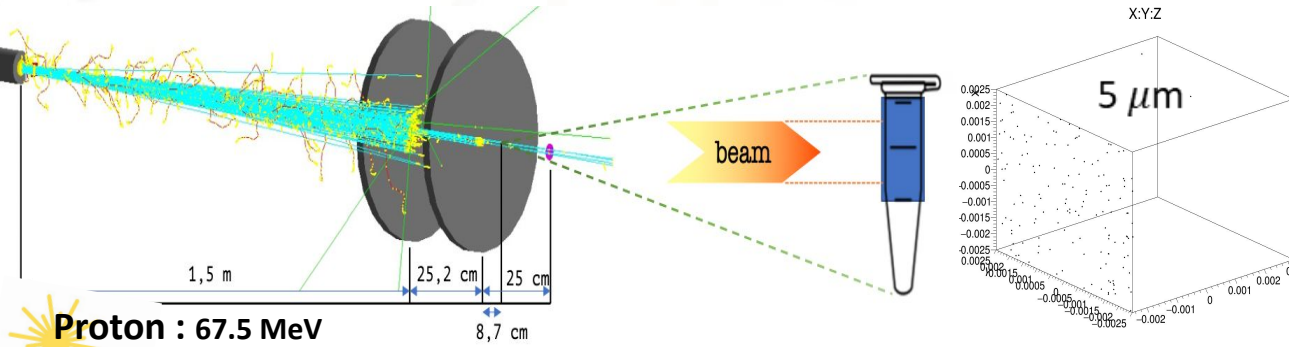

- ❑ IBA Cyclone® 70

- ❑ Protons, deuterons and helium ion particles

  - ❑ 30-70 MeV Protons
    (range in water 8 – 38mm)

  - ❑ 68 MeV Helium ions
    (range in water 3mm)

- ❑ Dose rates : 0.2 Gy/s to 60 kGy/s

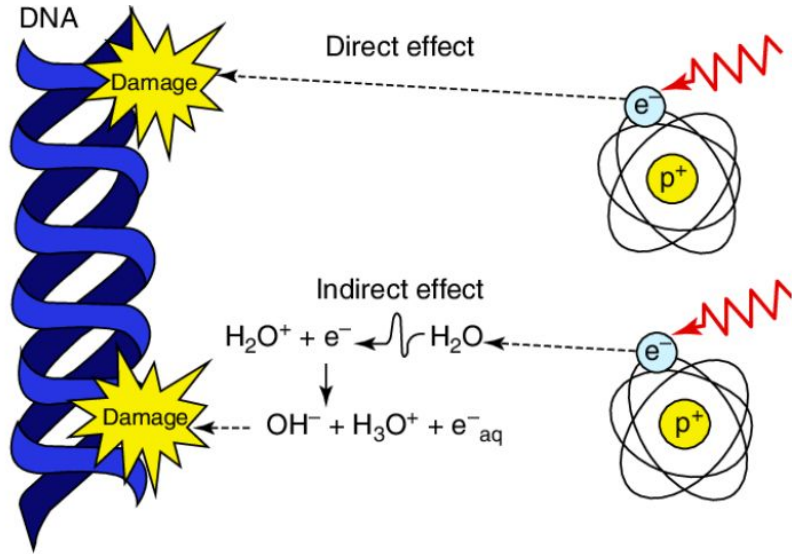# ARRONAX Alpha and proton beamlines using GATE 10

❖ **Alpha**
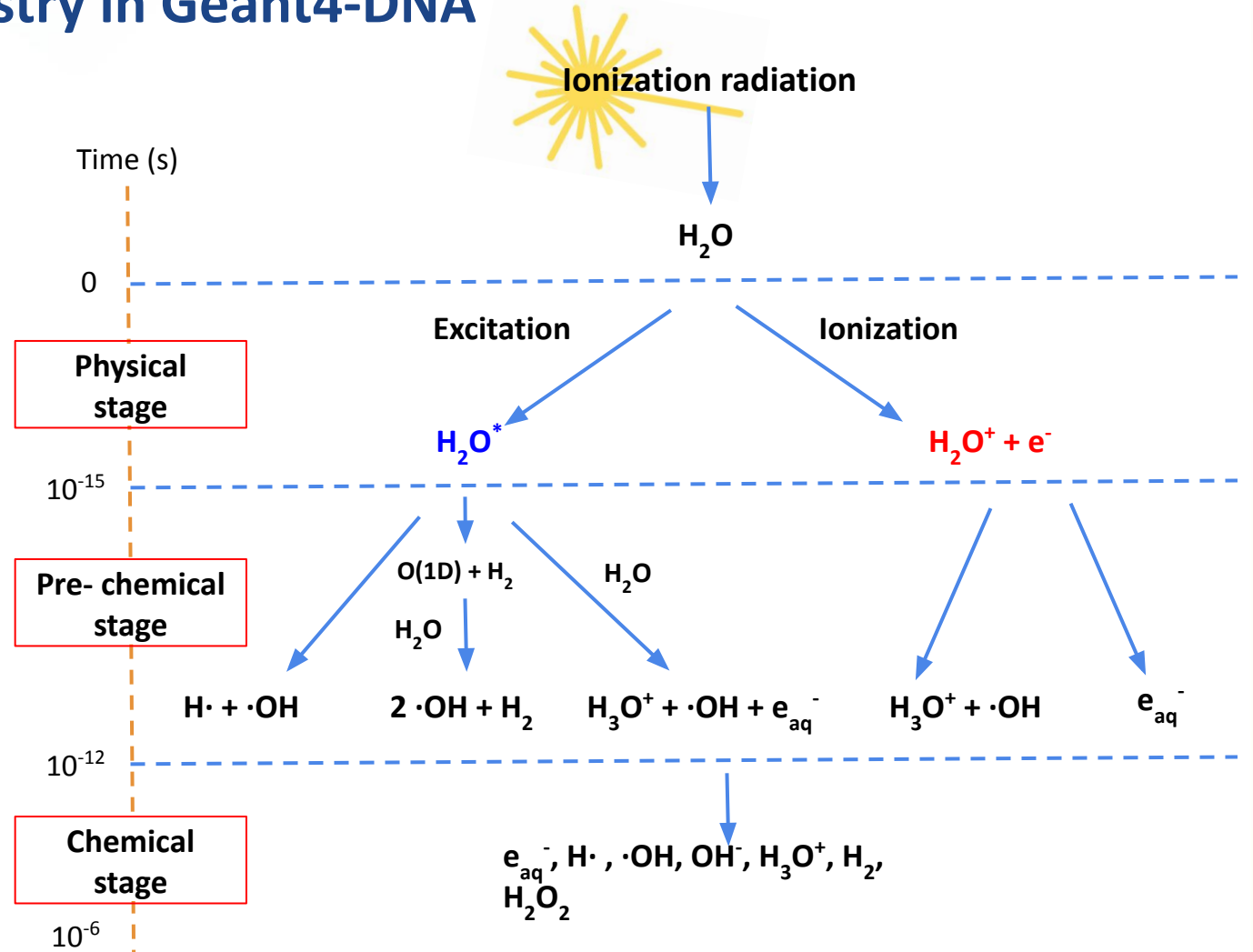

❖ **Proton**

Proton : 67.5 MeV

Mean energy
59.41 MeV
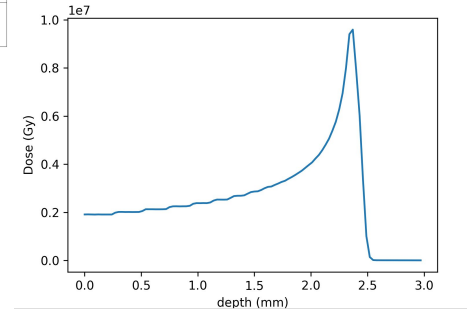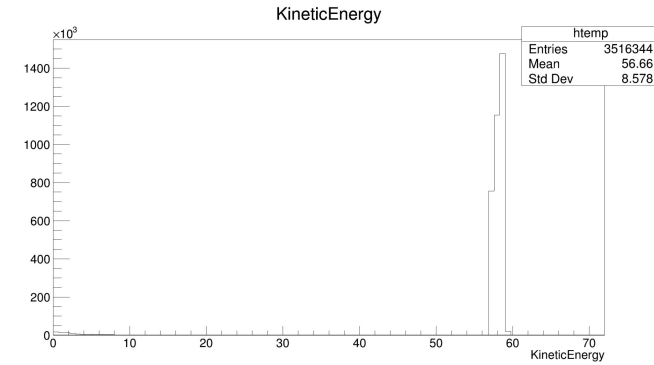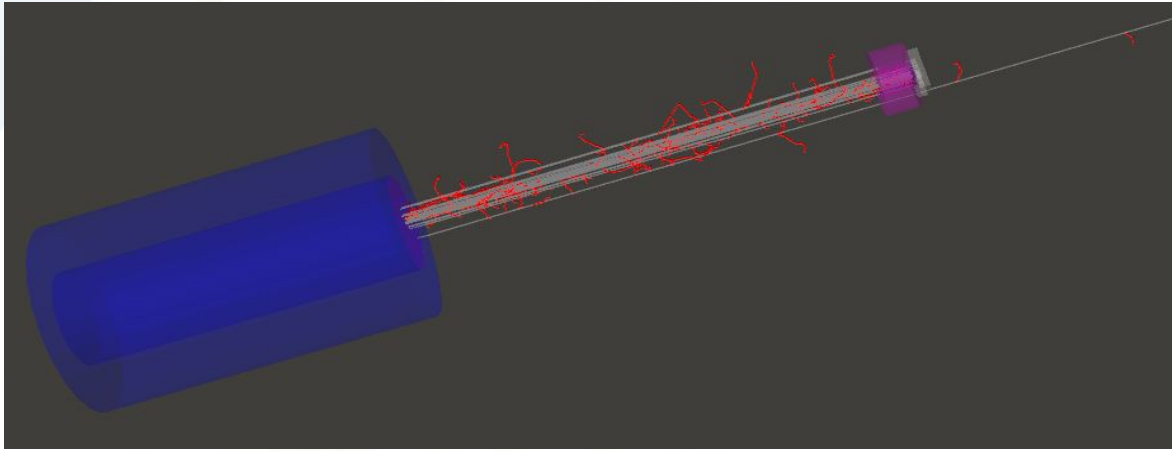
Water radiolysis chemistry in Geant4-DNA

■ Indirect Damage: DNA damage type cause by reactive species such as OH radical which created from *radiolysis of water molecule*

Ionization radiation

H_2O

Time (s)

0

| Physical stage |

Excitation   Ionization

H_2O^* $H_2O^+ + e^-$

10^{-15}

| Pre- chemical stage |

$O(1D) + H_2$ H_2O

H_2O

$H\cdot + \cdot OH$ $2\ \cdot OH + H_2$ $H_3O^+ + \cdot OH + e_{aq}^-$ $H_3O^+ + \cdot OH$ e_{aq}^-

10^{-12}

| Chemical stage |

e_{aq}^-, $H\cdot$, $\cdot OH$, OH^-, H_3O^+, H_2, H_2O_2

10^{-6}

Step by Step (SBS) or Independence Reaction Time (IRT)

SBS (step by step) model

Debye-Smoluchowski Brownian diffusion model from which encounters between reactants are dynamically sampled.

Reactions happen when A diffuse close to B within a distance R_0 **(Diffusion-controlled reactions)**

Simulation time needed for calculating the distance between species at every time step is a _huge computational burden._
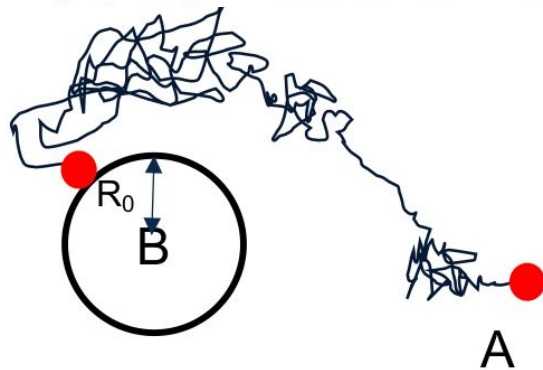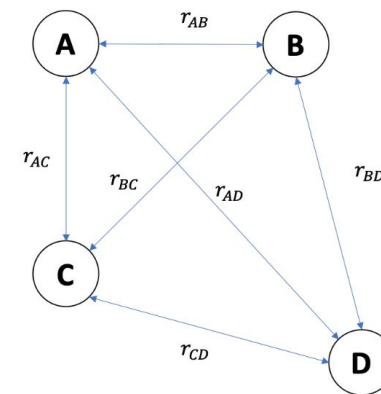

**IRT (Independent Reaction Times)
model**

An event table is constructed with the **initial chemical species positions and reaction times** for each reactant pair of interest

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

No spatial information

Reaction	Time (ps)	Order of reactions
A+B	63	X
A+C	3	1
A+D	111	X
B+C	192	X
B+D	15	2
C+D	90	X

Geant4-DNA Chemistry constructors

**The chemistry constructors in Geant4-DNA specify the dissociation scheme and chemical reactions in water radiolysis.**

❏ **G4EmDNAChemistry** : First constructor implemented with parameter values from Karamitros et al.

– from PARTRAC

❏ **G4EmDNAChemistry_option1** : Implements a revisited set of chemistry parameters from Shin et al.

– from TRACs + Burns et al. (1981) + Rowe et al. (1988)

❏ **G4EmDNAChemistry_option2** : Includes chemistry parameters for reactions with DNA components

– from Buxton et al. (1988)

❏ **G4EmDNAChemistry_option3** : Implements the **IRT approach** from Ramos-Mendez et al. (2020)

– from RITRACKS & Elliot et al. (1994)

List of Geant4-DNA chemistry examples

Several examples are provided in order to test water radiolysis in Geant4-DNA

Chemistry example	Purpose	Reference
chem1	Activation of chemical module	Karamitros et al (2011)
chem2	Selection of time steps	Karamitros et al (2011)
chem3	Visualization of chemical stage as a function of time	Karamitros et al (2011)
chem4	Calculation of G-value as a function of time	Karamitros et al (2011)
chem5	Calculation of G-value as a function of time specific constructors	Ramos-Mendez et al (2018)
chem6	IRT approach	Ramos-Mendez et al (2022)

SBS

IRT

SBS

GATE 10 (Chemistry module) vs Geant4-DNA (chem6 example)

❖ C ++ side StackingAction/NewStage to run chemistry

❖ Python interface to:

-> select timestep _model (IRT, SBS)

-> configure time_step (end_time , bins_count)

-> list chemical reaction to consider

$$H_3O^+ + OH^- -> 2H_2O$$
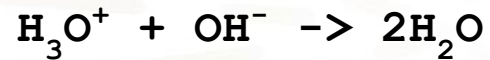
reactant	H_3O^+
reactant	OH^-
product	$2H_2O$
reaction rate	1.3e11
type of reaction	0

```python
# Geometry Definition
world = sim.world
world.size = [3.2 * um, 3.2 * um, 3.2 * um]
world.material = "G4_WATER"

# physics

sim.physics_manager.physics_list_name =  "G4EmDNAPhysics_option2"
sim.physics_manager.special_physics_constructors.G4EmDNAChemistry_option3 = True

# source
source = sim.add_source("GenericSource", "beam1d")
source.energy.mono = 59.4 * MeV
source.particle = "proton"

# chemistry actor
chem = sim.add_actor("ChemistryActor", "Chem")
chem.timestep_model = "IRT"  # or "SBS"
chem.end_time = 1 * us
chem.time_bins_count = 50
chem.reactions = [
    # totally diffusion-controlled (TDC)
    [["H", "H"], ["H2"], "Fix", 0.5e10, 0],
    [["e_aq", "H"], ["H2", "OHm"], "Fix", 2.5e10, 0],
    [["e_aq", "e_aq"], ["H2", "OHm", "OHm"], "Fix", 0.636e10, 0],
    [["H3Op", "OHm"], ["2H2O"], "Fix", 1.13e11, 0]
```

Output (Chemistry module- GATE 10)

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

```python
def analysis(chem):
    times = chem.get_times()
    data = chem.get_data()

    for key in {'H2O2^0', 'e_aq^-1', 'OH^0', 'H3O^1', 'OH^-1', 'H^0',
'H_2^0', 'O^0'}:
        fig, ax = plt.subplots(figsize=(6.5, 5), dpi=300)
        ax.set_xlabel('time (ns)')
        ax.set_ylabel(r'G value (molecules / 100 eV)')
```
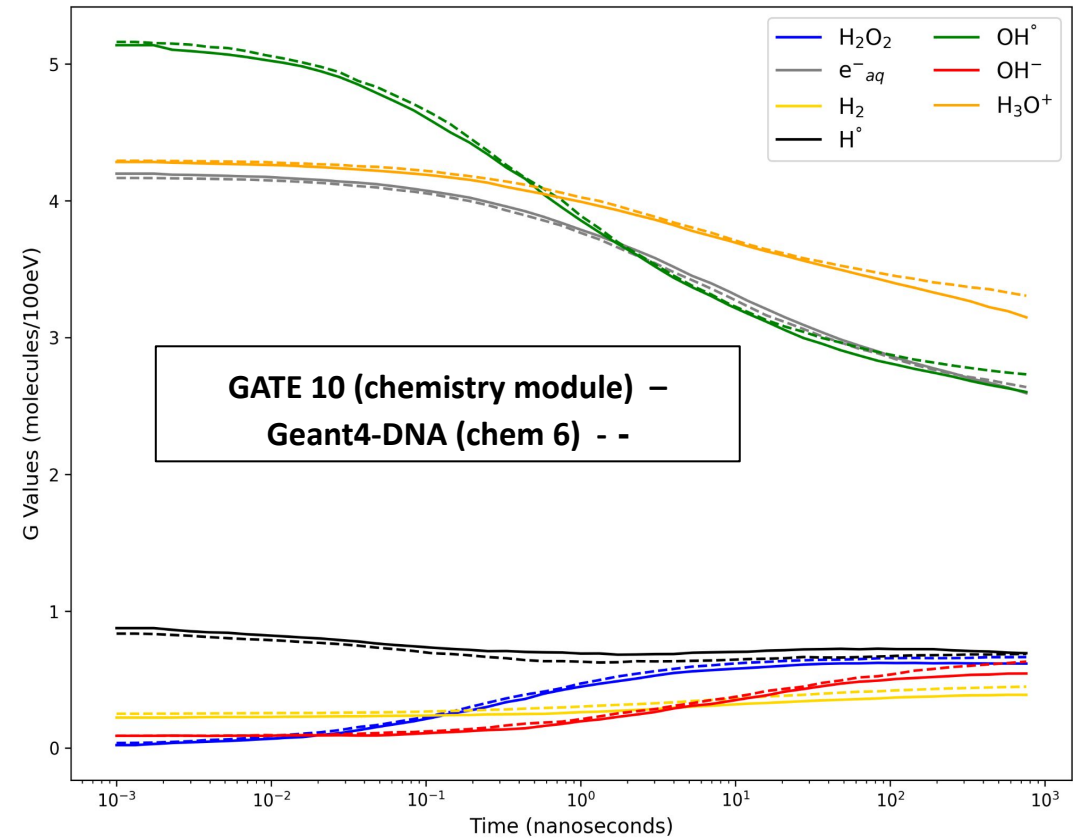
IRT

SBS

GATE 10 (chemistry module) –
Geant4-DNA (chem 6) - -

Conclusion
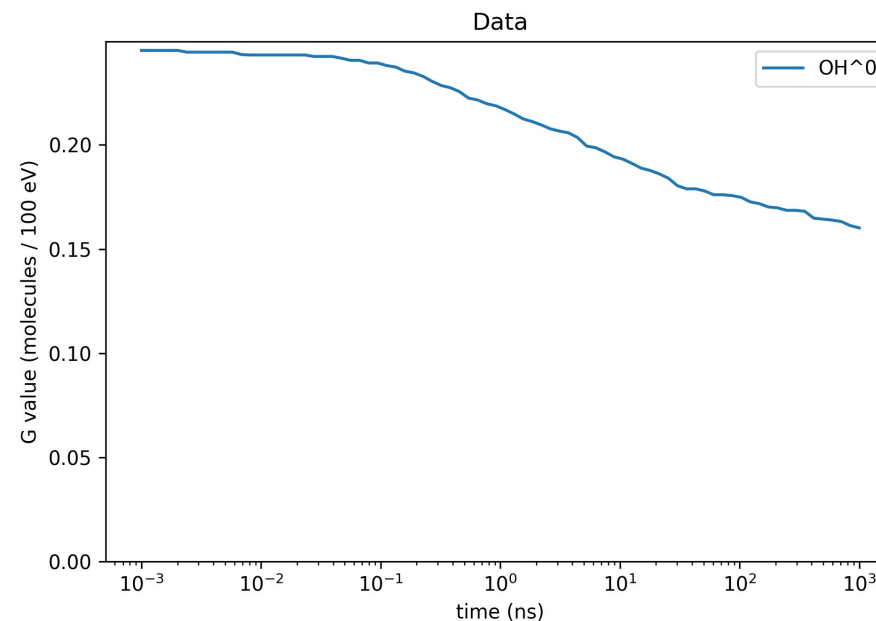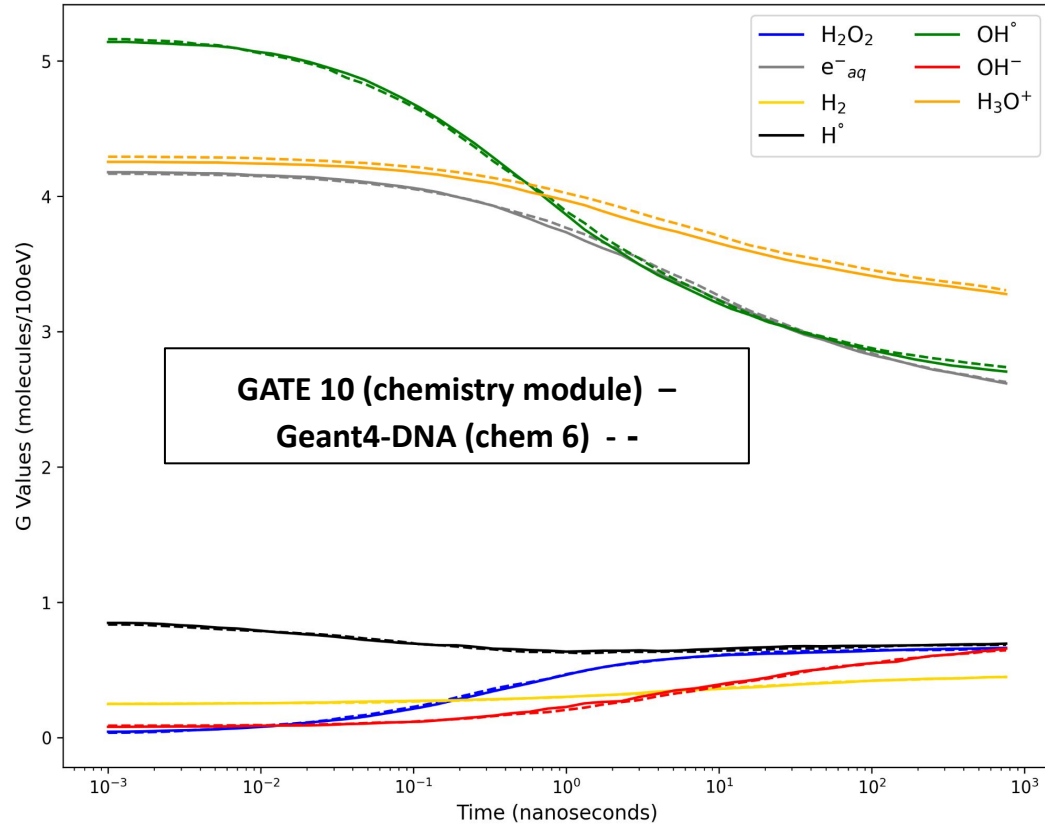
Chemistry actor

❖   Chemistry actor validated in GATE 10

❖   Chemistry model: SBS (Step by Step) and IRT (Independent reaction time)

Next

❖   UHDR example in GATE 10

   - ph level, Oxygen concentration, Scavenger, dose rate and so on…

❖   Chemistry model: SBS-RDME

Thank you