GEANT4-DNA
A SIMULATION TOOLKIT

# UHDR example

geant4-dna.org

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

Hoang TRAN
LP2i/In2p3/CNRS, Bordeaux, France
tran@lp2ib.in2p3.fr

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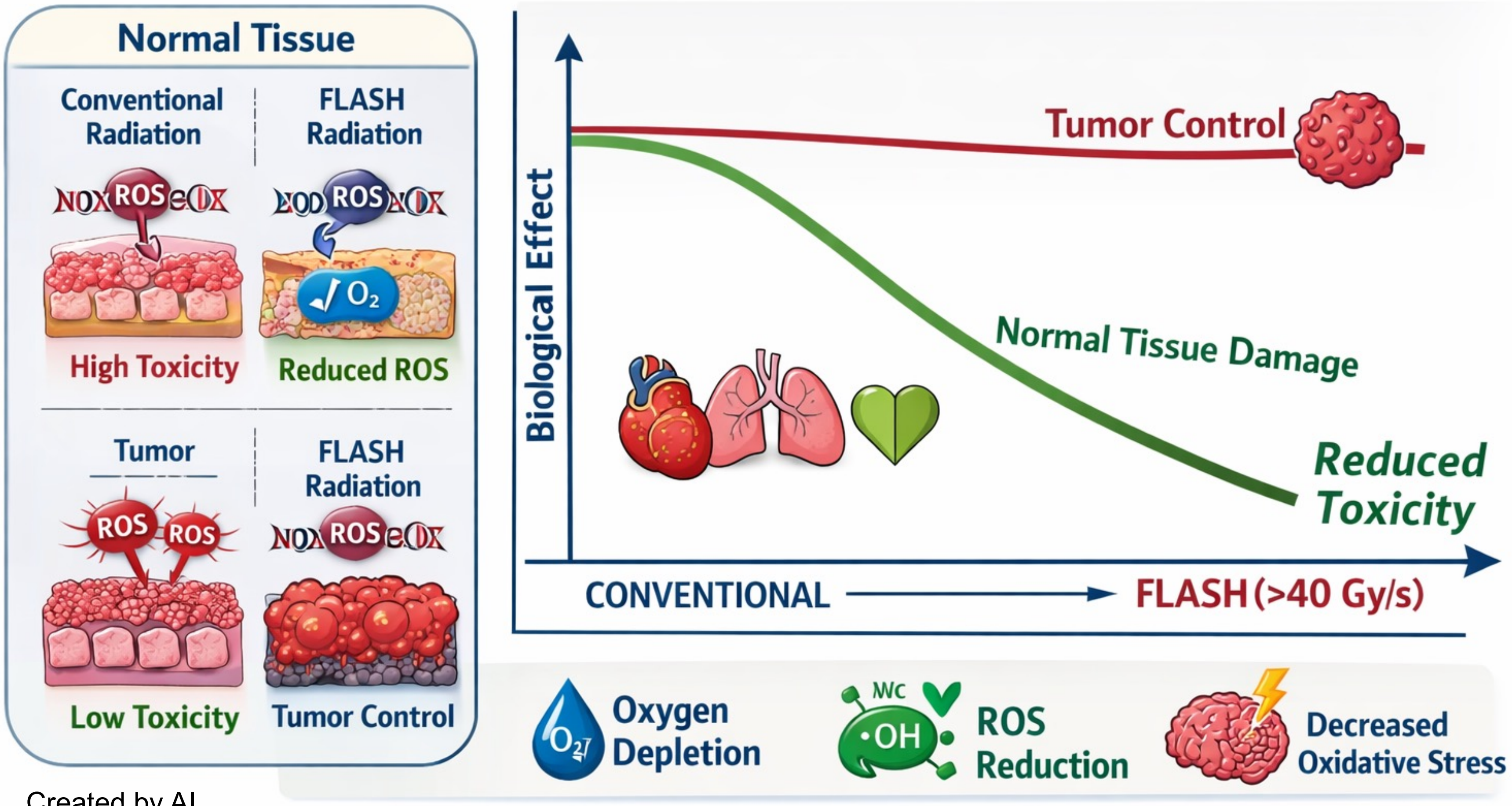
# The *FLASH Effect* in Radiobiology




Created by AI

# UHDR Example

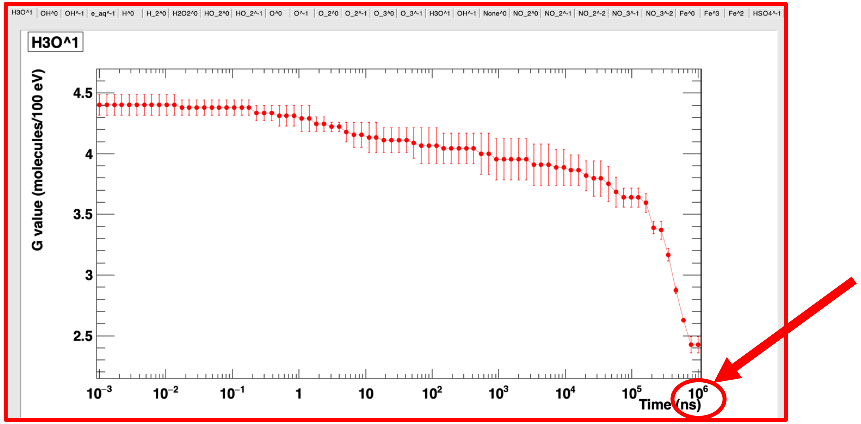
**Tran, H. N.** et al. (**2021**) Geant4-DNA Modeling of Water Radiolysis beyond the Microsecond: An On-Lattice Stochastic Approach. International Journal of Molecular Sciences, 22(11), 6023. https://doi.org/10.3390/ijms22116023

- ✅ The world is a water box with two possible optimized dimensions
- ✅ The example implements the mesoscopic approach (SBS-RDME)
- ✅ Chemical reactions implemented by builders for specific applications)
- ✅ Scavenger molecules
- ✅ Chemical evolution vs. ph
- ✅ Each event consists of multiple incident particles

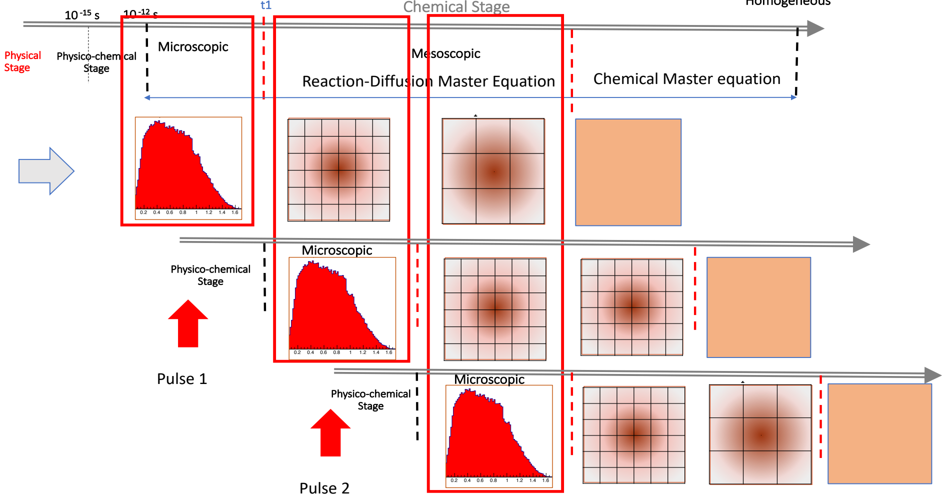
As chem6 provides scoring of the radiochemical yield G:

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

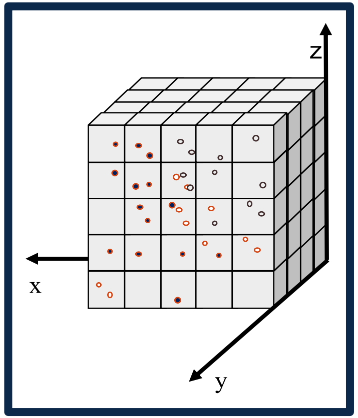
as a function of time.



# New « UHDR » example

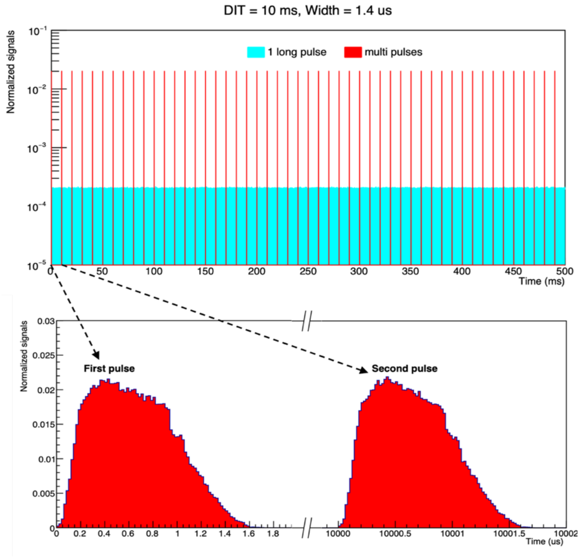



- Use a new « mesoscopic » approach to study the production and evolution of reactive oxygen species generated under irradiation with different dose rate conditions, such as in FLASH RT
- Coarse-grained model: "compartment-based"
- Simulation from heterogeneous (microsecond) to homogeneous states (beyond)
- Multiple pulses simulation




1. *Well mixed species in voxels*
2. *Species can react with each other in the voxels*
3. *Diffusion is modelled by jumps between adjacent voxels*

Voxelization of the simulation volume into smaller sub-volumes. Species are represented by different types of circles

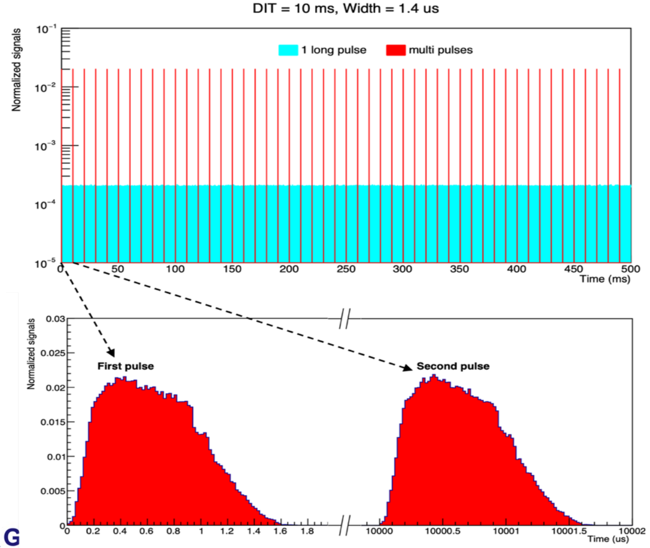



GEANT4-DNA

# User interface

UHDR example provides a user interface to control the simulation :

- Irradiated geometries
- pH control
- Oxygen concentration
- cut-off dose




UHDR.in

```
/run/numberOfThreads 10

# initialize geo and phys
/control/execute initialize.in

# time structure
/UHDR/pulse/pulseOn true
# push structure file
/UHDR/pulse/pulseFile 1.4us

# pulse structure
/UHDR/pulse/multiPulse true
/UHDR/pulse/pulsePeriod 10 ms
/UHDR/pulse/numberOfPulse 2
#/UHDR/pulse/pulseInHisto pulseHisto.txt

/run/initialize

#/run/verbose 1
/tracking/verbose 0
/scheduler/verbose 0
/scheduler/endTime 1000 s

# medium is configured in this file (scavengers.in)
/control/execute scavengers.in

/scorer/Dose/cutoff 1 Gy
/UHDR/source/particle e-
/UHDR/source/energy 0.999 MeV
/run/beamOn 10
```

Irradiated geometries

media

pH control

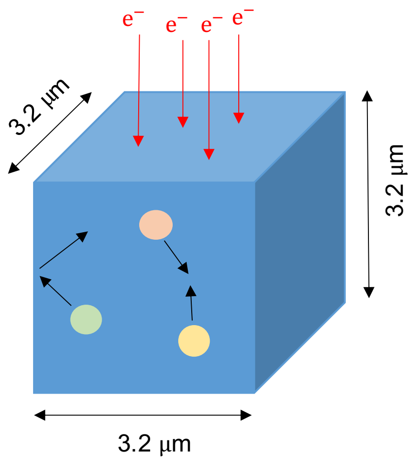
oxygen control

Chemistry simulation controls

Cut-off Dose

# Geometry

- Two cubic water volumes of 3.2 x 3.2 x 3.2 µm3 and 1.6 x 1.6 x 1.6 µm3 are used for UHDR and CONV simulations
- Chemical molecules diffuse and react in a bound volume that is, the diffusion is limited by geometrical boundaries.
- The bouncing of chemical molecules on the volume border is applied for both microscopic and mesoscopic sub-stages, depicting a closed system of test cells for in vitro measurements




initialize.in

```
# Set the simulation volume (half Side Length)
#/UHDR/env/volume 0.8 um # for UHDR
/UHDR/env/volume 1.6 um # for CONV
```

# pH and Scavenger

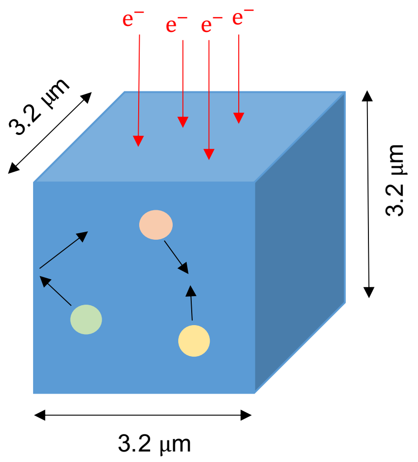
- Define the pH
- The scavengers : O2, CO2, $NO_3^+$, …

scavenger.in

```
# pH and Scavenger
/UHDR/env/pH 5.5

# air concentration
/UHDR/env/scavenger O2 21 %
/UHDR/env/scavenger CO2 0.041 %
/UHDR/env/scavenger HCO3m 2.4 uM
# NO3-/NO2- concentration
#/UHDR/env/scavenger NO3m 1 mM
#/UHDR/env/scavenger NO2m 10 uM
#/UHDR/env/scavenger N2O 0.1 mM
#/UHDR/env/scavenger CH3OH 10 mM


/chem/reaction/print

# set false if many beamOn in medium
/scheduler/ResetScavengerForEachBeamOn true

/scorer/Gvalues/nOfTimeBins 80

/run/printProgress 10
```

# Particle source

## Modelling of ultra-high dose rate (UHDR) electron beams



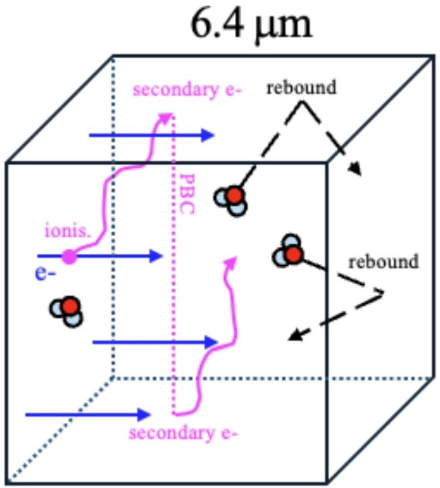

- Source: 1 MeV electron beam
- Primary electrons are shot at the same time until the sum of all energy deposits in the volume reaches a given absorbed dose ("instantaneous pulse").
- By cumulating the dose until 0.01 Gy (cut-off dose), we define a conventional irradiation (or CONV) and from 1-10 Gy, we define a higher dose rate (or UHDR).
- Electron irradiation until the total energy deposition reaches 1-10 Gy (UHDR) or ~ 0.01 Gy (conventional)
- Instantaneous pulse (all species are produced simultaneously). Pulse duration is not considered. All species are produced simultaneously at 1 ps.

| Modalities | Volume ($\mu m^3$) | Dose rates (Gy/pulse) | Incident electrons (tracks) | deposit energy (keV) |
|---|---|---|---|---|
| CONV | 3.2 x 3.2 x 3.2 | 0.0109812 | 6 | 2.246 |
| UHDR | 1.6 x 1.6 x 1.6 | 1.00273 | 110 | 25.637 |
| | | 5.01636 | 562 | 128.254 |
| | | 10.0076 | 1063 | 255.866 |

*Table 1. An example of simulation setup at different irradiations where the deposit energy and incident electrons are recorded until the dose per pulse corresponding with the irradiated volumes.*

# « mesoscopic » approach

$t_1$



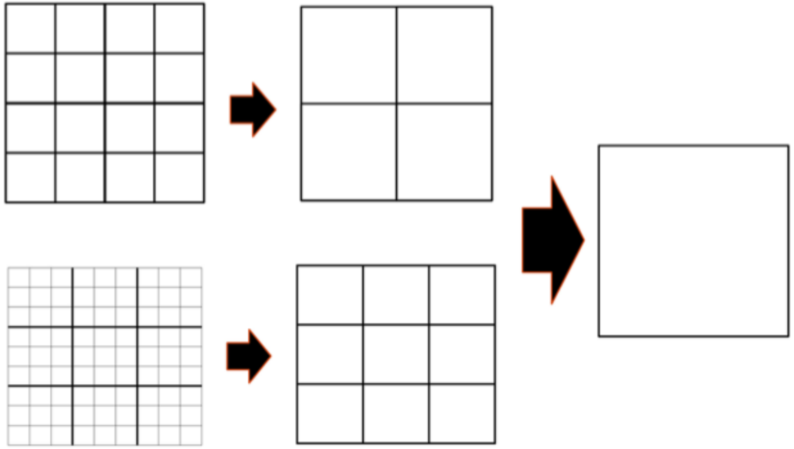



**Figure 4.** The hRDME approach, here represented in 2D. The mesh of $4^3$ voxels (**top**) is moved to $2^3$, and then to one voxel. The mesh of $9^3$ voxels (**bottom**) is moved to $3^3$ and then to one voxel.

Int. J. Mol. Sci. 2021, 22, 6023

# Dissolved Oxygen in Water

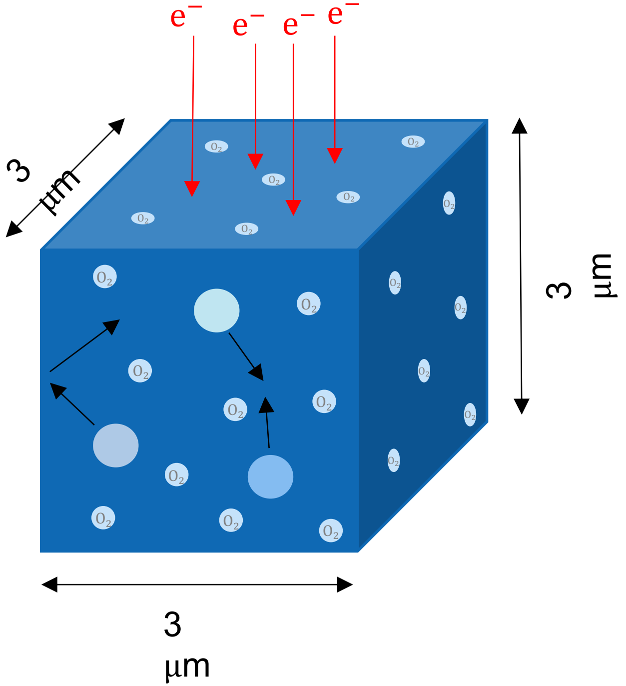
**Modelling oxygen as a continuum**

$$\frac{dX}{dt} = -k\,[O_2]\,X$$

$X$ = concentration of species $X$ $[M]$

$k$ = reaction rate $[M^{-1}s^{-1}]$

$[O_2]$ = concentration of oxygen $[M]$




- Homogeneous distribution of oxygen
- Variation of $[O_2]$ over time
- partially oxygenated water is converted to concentration

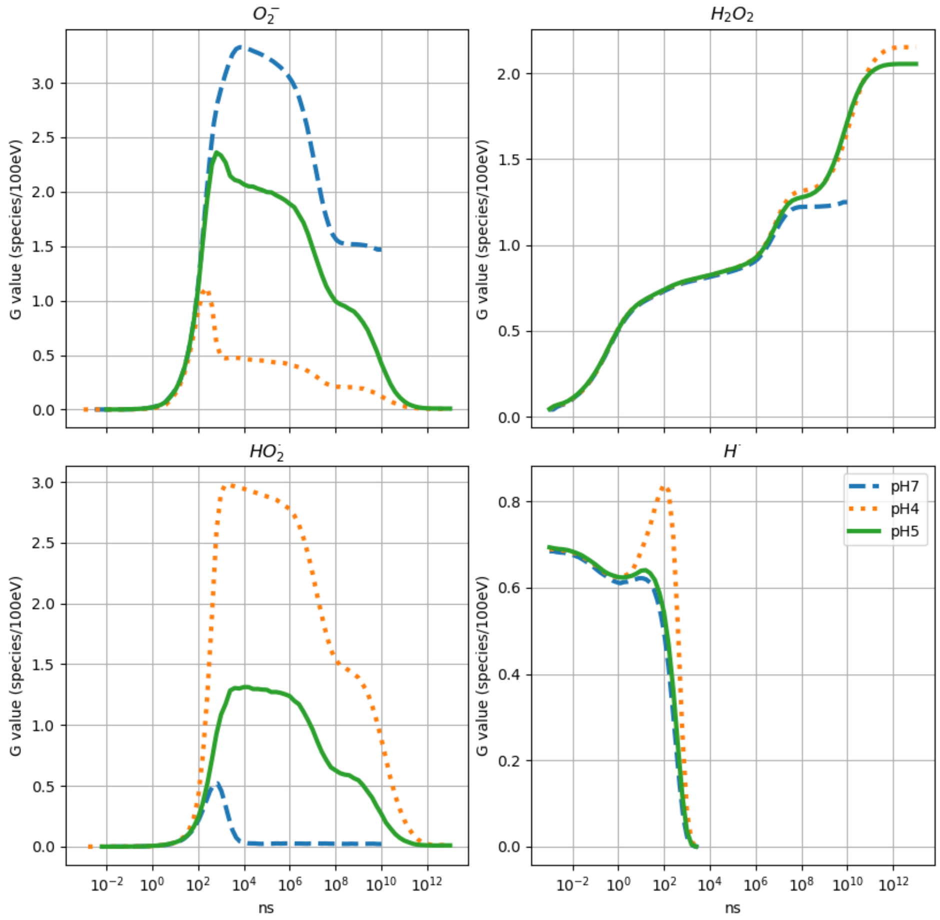
```
# Oxygen concentration
/UHDR/env/scavenger O2 19 %
```

# pH simulation

| # | Equilibrium | pKa |
|---|---|---|
| 1 | $2H_2O \leftrightarrow OH^- + H_3O^+$ | 13.999 |
| 2 | $H_2O_2 + H_2O \leftrightarrow HO_2^- + H_3O^+$ | 11.65 |
| 3 | $^{\bullet}OH + H_2O \leftrightarrow O^- + H_3O^+$ | 11.9 |
| 4 | $HO_2 + H_2O \leftrightarrow O_2^- + H_3O^+$ | 4.57 |
| 5 | $H + H_2O \leftrightarrow e^-_{aq} + H_3O^+$ | 9.77 |

- The products of primary and secondary reactions can participate in equilibrium reactions which are associated with pKa (see the table)
- Based on the H3O+ and OH- ion concentrations determined by the pH, acid-base reactions associated with these pKa are simulated

```
# pH and Scavenger
/UHDR/env/pH 5.5
```



# Acid-base reactions

Acid-base reactions associated with pKa at 25 °C. $[H_2O]$ = 55.3 M. $k_{-1}$ and $k_1$ represent opposite directions in the first equilibrium process.

| # | Acid-Base reactions | Rate coefficients and corresponding references | |
|---|---|---|---|
| 1 | $HO_2 \rightarrow H_3O^+ + O_2^-$ | $k_{-1} * K_4$ | 7.58e5 $s^{-1}$ |
| −1 | $H_3O^+ + O_2^- \rightarrow HO_2$ | [Elliot, 1994] | 4.78e10 $M^{-1}s^{-1}$ |
| 2 | $H \rightarrow e^-_{aq} + H_3O^+$ | $k_{-2} * K_5$ | 6.32 $s^{-1}$ |
| −2 | $e^-_{aq} + H_3O^+ \rightarrow H^\bullet$ | [Elliot, 1994] | 2.25e10 $M^{-1}s^{-1}$ |
| 3 | $e^-_{aq} + H_2O \rightarrow H^\bullet + OH^-$ | $k_{-3} * K_1 / (K_5 * [H_2O)])$ | 1.57e1 $M^{-1}s^{-1}$ |
| −3 | $H^\bullet + OH^- \rightarrow H_2O + e^-_{aq}$ | [Elliot, 1994] | 2.49e7 $M^{-1}s^{-1}$ |
| 4 | $O_2^- + H_2O \rightarrow HO_2 + OH^-$ | $k_{-4} * K_1 / (K_4 * [H_2O)])$ | 0.15 $M^{-1}s^{-1}$ |
| −4 | $HO_2 + OH^- \rightarrow O_2^- + H_2O$ | [Elliot, 1994] | 1.27e10 $M^{-1}s^{-1}$ |
| 5 | $HO_2^- + H_2O \rightarrow H_2O_2 + OH^-$ | $k_{-5} * K_1 / (K_2 * [H_2O)])$ | 1.36e6 $M^{-1}s^{-1}$ |
| −5 | $H_2O_2 + OH^- \rightarrow HO_2^- + H_2O$ | [Elliot, 1994] | 1.27e10 $M^{-1}s^{-1}$ |
| 6 | $O^- + H_2O \rightarrow OH + OH^-$ | $k_{-6} * K_1 / (K_3 * [H_2O)])$ | 1.8e6 $M^{-1}s^{-1}$ |
| −6 | $OH + OH^- \rightarrow O^- + H_2O$ | [Elliot, 1994] | 1.27e10 $M^{-1}s^{-1}$ |
| 7 | $H_2O_2 \rightarrow H_3O^+ + HO_2^-$ | $k_{-7} * K_2$ | 7.86e-2 $s^{-1}$ |
| −7 | $HO_2^- + H_3O^+ \rightarrow$ H2O2 | [Elliot, 1994] | 4.78e10 $M^{-1}s^{-1}$ |
| 8 | $^\bullet OH \rightarrow O^- + H_3O^+$ | $k_{-8} * K_3$ | 0.0602 $s^{-1}$ |
| −8 | $O^- + H_3O^+ \rightarrow OH$ | [Elliot, 1994] | 9.56e10 $M^{-1}s^{-1}$ |

# Chemistry Builders

Chemical reactions can be grouped by different chemistry builders. Depend on user application, these builder can be used. UHDR provides 5 default builders.

- ChemPureWaterBuilder::WaterScavengerReaction to simulate acid-base reactions associated with pH
- ChemOxygenWaterBuilder::OxygenScavengerReaction to simulate the reactions with oxygen.
- ChemOxygenWaterBuilder:: SecondOrderReactionExtended to simulate secondary reaction
- ChemNO2_NO3ScavengerBuilder::NO2_NO3ScavengerReaction to simulate NO2+/NO3+
- ChemFrickeReactionBuilder::FrickeDosimeterReaction to simulate Fricke dosimeter

# Exercises

- **Exercise 1**: Visualize the geometry
- **Exercise 2:** Print the reaction
- **Exercise 3**: Change pulse duration

- **Exercise 4**: Change the pulse distance

- **Exercise 5**: Change the oxygen concentration

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

# Exercise 1: Visualize the geometry

```
>cd
>cp $G4EXAMPLES/extended/medical/dna/UHDR/ .
>mkdir UHDR-build
>cd UHDR-build
>cmake ../UHDR
>make
```

# Exercise 1: Visualize the geometry

```
UHDR-build < 72 >gedit vis.mac
```

```
/chem/activate false

/scorer/Dose/abortedDose 100 Gy
/scorer/Dose/cutoff 10 Gy
/UHDR/source/particle proton
/UHDR/source/energy 100 MeV
```

```
/chem/activate false

/scorer/Dose/abortedDose 100 Gy
/scorer/Dose/cutoff 1 Gy
/UHDR/source/particle proton
/UHDR/source/energy 100 MeV
```

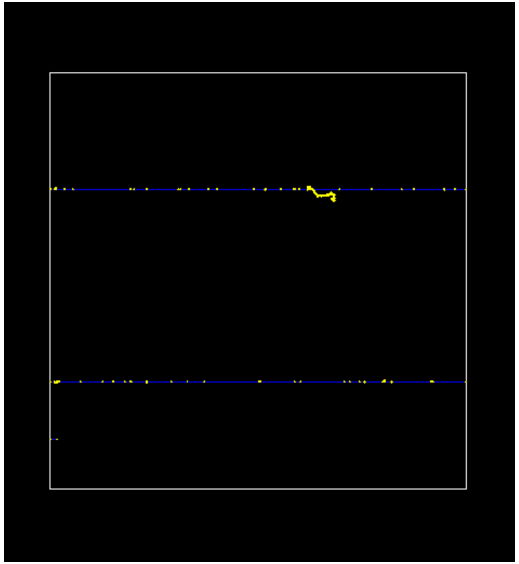
```
UHDR-build < 72 >./UHDR
```

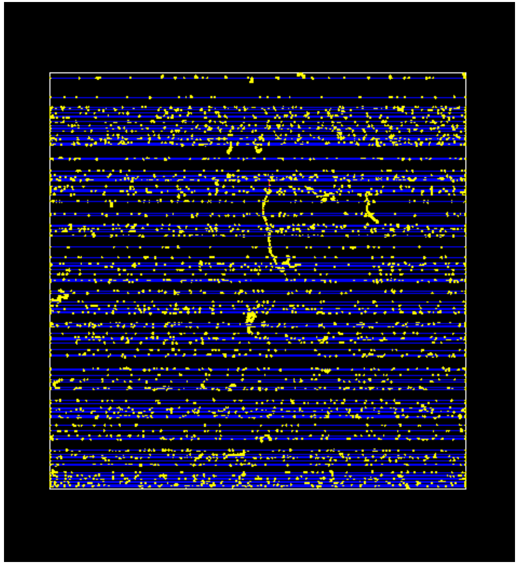
Proton,100 MeV: 0.01 Gy, 1 Gy, 10 Gy

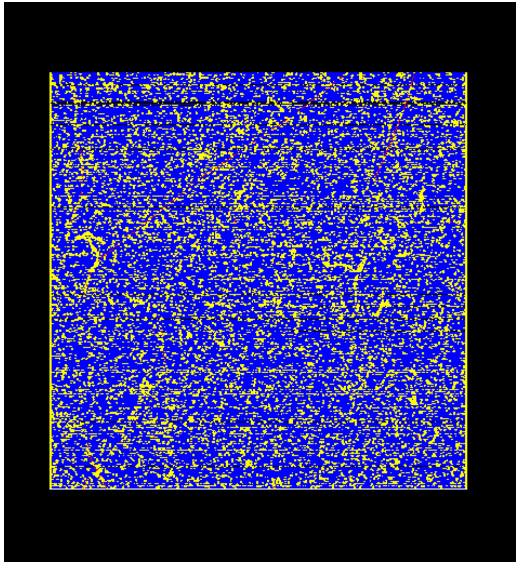
# Visualisation

- Proton,100 MeV: 0.01 Gy, 1 Gy, 10 Gy

```
/scorer/Dose/abortedDose 0.05 Gy

/scorer/Dose/cutoff 0.01 Gy
/UHDR/source/particle proton
/UHDR/source/energy 100 MeV
```







# Exercise 2: Print the reaction

```
# pH and Scavenger
/UHDR/env/pH 5.5
# air concentration
/UHDR/env/scavenger O2 21 %
/UHDR/env/scavenger CO2 0.041 %
/UHDR/env/scavenger HCO3m 2.4 uM
# NO3-/NO2- concentration
#/UHDR/env/scavenger NO3m 1 mM
#/UHDR/env/scavenger NO2m 10 uM
#/UHDR/env/scavenger N2O 0.1 mM
#/UHDR/env/scavenger CH3OH 10 mM
/chem/reaction/print
#/run/verbose 1
/tracking/verbose 0
/scheduler/verbose 0
/scheduler/endTime 1000 s
# set false if many beamOn in medium
/scheduler/ResetScavengerForEachBeamOn true
/scorer/Gvalues/nOfTimeBins 80
/run/printProgress 10
```

>gedit scavenger.in

/scheduler/verbose 1

/UHDR-build ./UHDR UHDR.in

# $T_1$ = 5 ns

```
G4WT0 > At time :  4.1792 ns  Reaction : °OH^0 (-1964) + °OH^0 (-1804) -> H2O2^0 (-2672)
G4WT0 > At time :  4.2158 ns  Reaction : H3O^1 (-1429) + HO_2^-1 (-2578) -> H2O2^0 (-2673)
G4WT0 > At time :  4.2261 ns  Reaction : °OH^0 (-1922) + °OH^0 (-1896) -> H2O2^0 (-2674)
G4WT0 > At time :  4.2605 ns  Reaction : °OH^0 (-1874) + °OH^0 (-1328) -> H2O2^0 (-2675)
G4WT0 > At time :  4.2978 ns  Reaction : °OH^0 (-1356) + °OH^0 (-1268) -> H2O2^0 (-2678)
G4WT0 > At time :  4.3392 ns  Reaction : H2O2^0 (-2538) + OH^-1 (-2478) -> HO_2^-1 (-2679)
G4WT0 > At time :  4.6044 ns  Reaction : H3O^1 (-1673) + O^-1 (-2588) -> °OH^0 (-2680)
G4WT0 > At time :  4.7143 ns  Reaction : °OH^0 (-2034) + e_aq^-1 (-1213) -> OH^-1 (-2681)
G4WT0 > At time :  4.7683 ns  Reaction : °OH^0 (-1860) + e_aq^-1 (-426) -> OH^-1 (-2682)
G4WT0 > At time :  4.9583 ns  Reaction : H^0 (-2294) + e_aq^-1 (-1096) -> OH^-1 (-2684) + H_2^0 (-2685)
G4WT0 > At time :  4.9863 ns  Reaction : H3O^1 (-1505) + OH^-1 (-2599) -> No product
G4WT0 > At Time :  5.0025 ns  the Mesh has 512 x 512 x 512 voxels with Resolution 6.25 nm  during next 93.006 ns
G4WT0 > At time :  5.0641 ns  Reaction : e_aq^-1 + °OH^0 -> OH^-1
G4WT0 > At time :  5.1518 ns  Reaction : e_aq^-1 + H3O^1 -> H^0
G4WT0 > At time :  5.1824 ns  Reaction : e_aq^-1 + °OH^0 -> OH^-1
G4WT0 > At time :  5.1916 ns  Reaction : e_aq^-1 + °OH^0 -> OH^-1
G4WT0 > At time :  5.2799 ns  Reaction : H3O^1 + OH^-1 -> No product
G4WT0 > At time :  5.3877 ns  Reaction : e_aq^-1 + °OH^0 -> OH^-1
G4WT0 > At time :  5.4311 ns  Reaction : e_aq^-1 + O_2^0 -> O_2^-1
G4WT0 > At time :   5.434 ns  Reaction : e_aq^-1 + °OH^0 -> OH^-1
G4WT0 > At time :  5.5869 ns  Reaction : e_aq^-1 + °OH^0 -> OH^-1
G4WT0 > At time :   5.632 ns  Reaction : e_aq^-1 + e_aq^-1 -> OH^-1 + OH^-1 + H_2^0
G4WT0 > At time :  5.7071 ns  Reaction : e_aq^-1 + °OH^0 -> OH^-1
G4WT0 > At time :  5.7311 ns  Reaction : H3O^1 + OH^-1 -> No product
G4WT0 > At time :  5.7387 ns  Reaction : e_aq^-1 + H3O^1 -> H^0
```

# Exercise 3: Change pulse duration

cd ../UHDR/include

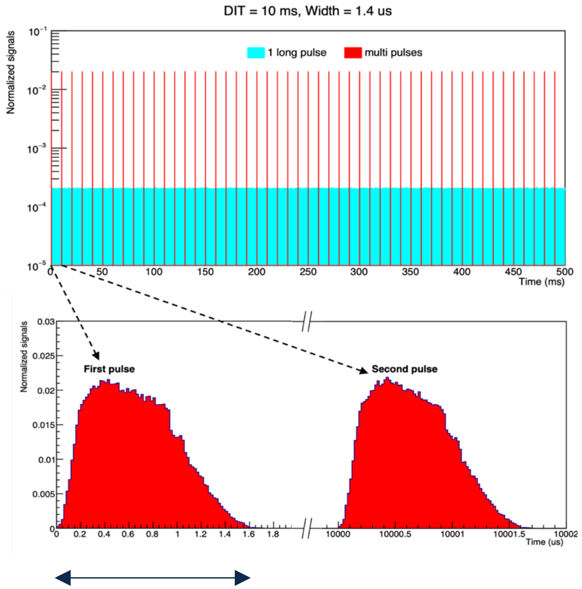
```
    inline void SetPulse(const G4bool& pulse) { fActivePulse = pulse; }

    inline G4bool IsActivedPulse() const { return fActivePulse; }
    // L.T. Anh added getter/setter for interpulse class:
    void SetLonggestDelayedTime(G4double lt) { fLonggestDelayedTime = lt; }
    const G4String GetPulseFileName() { return fFileName; }
    G4int GetVerbose() { return fVerbose; }
    G4double GetPulseLarger() const;

  protected:
    G4int fVerbose = 2;
    G4double fDelayedTime = 0;

private:
    void InitializeForHistoInput();
    std::unique_ptr<PulseInfo> fpPulseInfo;
```

Verbose number : 2

/UHDR-build make

/UHDR-build ./UHDR UHDR.in

# Exercise 3: Change pulse duration




```
/home/local1/Geant4/UHDR/PulseStructure
total 56
-rw-r--r-- 1 local1 local1  695 11 mars  15:28 100ms
-rw-r--r-- 1 local1 local1  560 11 mars  15:28 100us
-rw-r--r-- 1 local1 local1  608 11 mars  15:28 10ms
-rw-r--r-- 1 local1 local1  532 11 mars  15:28 10us
-rw-r--r-- 1 local1 local1  500 11 mars  15:28 1.4us
-rw-r--r-- 1 local1 local1  581 11 mars  15:28 1ms
-rw-r--r-- 1 local1 local1  695 11 mars  15:28 1s
-rw-r--r-- 1 local1 local1  418 11 mars  15:28 2.4us
-rw-r--r-- 1 local1 local1  695 11 mars  15:28 2s
-rw-r--r-- 1 local1 local1  462 11 mars  15:28 3.5us
-rw-r--r-- 1 local1 local1  695 11 mars  15:28 500ms
-rw-r--r-- 1 local1 local1  581 11 mars  15:28 5ms
-rw-r--r-- 1 local1 local1 1708 11 mars  15:28 80ns
-rw-r--r-- 1 local1 local1  557 11 mars  15:28 pulseHisto.txt
```

```
# time structure
/UHDR/pulse/pulseOn true
# push structure file
/UHDR/pulse/pulseFile 1.4us
```

# Exercise 3: Change pulse duration

UHDR.in

```
/run/numberOfThreads 10

# initialize geo and phys
/control/execute initialize.in

# time structure
/UHDR/pulse/pulseOn true
# push structure file
/UHDR/pulse/pulseFile 10ms

# pulse structure
/UHDR/pulse/multiPulse true
/UHDR/pulse/pulsePeriod 10 ms
/UHDR/pulse/numberOfPulse 1
#/UHDR/pulse/pulseInHisto pulseHisto.txt

/run/initialize

# medium is configured in this file (scavengers.in)
/control/execute scavengers.in

/scorer/Dose/cutoff 1 Gy
/UHDR/source/particle e-
/UHDR/source/energy 0.999 MeV
/run/beamOn 1
```

```
15:28 100ms
15:28 100us
15:28 10ms
15:28 10us
15:28 1.4us
15:28 1ms
15:28 1s
15:28 2.4us
15:28 2s
15:28 3.5us
15:28 500ms
15:28 5ms
15:28 80ns
15:28 pulseHisto.txt
```

/UHDR-build ./UHDR UHDR.in

# Exercise 3: Change pulse duration

```
G4WT2 > -----------------------------------------------------
G4WT2 > Beam line               : (e-, 0.999 MeV)
G4WT2 > Cut-off dose            : 1 Gy
G4WT2 > Stop at actual dose     : 1.01866 Gy
G4WT2 > DIT                     : 10 ms
G4WT2 > Pulse number            : 1
G4WT2 > Beam duration           : 0.00989477 s
G4WT2 > Actual dose rate        : 102.949 Gy/s
G4WT2 > Track number            : 57 tracks
G4WT2 > Irradiated volume       : 4.096 um3 (1.6 x 1.6 x 1.6)
G4WT2 > O_2^0                   : 0.000273 M
G4WT2 > pH                      : 5.5
G4WT2 > CO_2^0                   : 1.394e-05 M
G4WT2 > HCO_3^-1                  : 2.4e-06 M
G4WT2 > Total deposit energy : 26044.2 eV
G4WT2 > Dose to abort           : 1.5 Gy
G4WT2 > -----------------------------------------------------
```

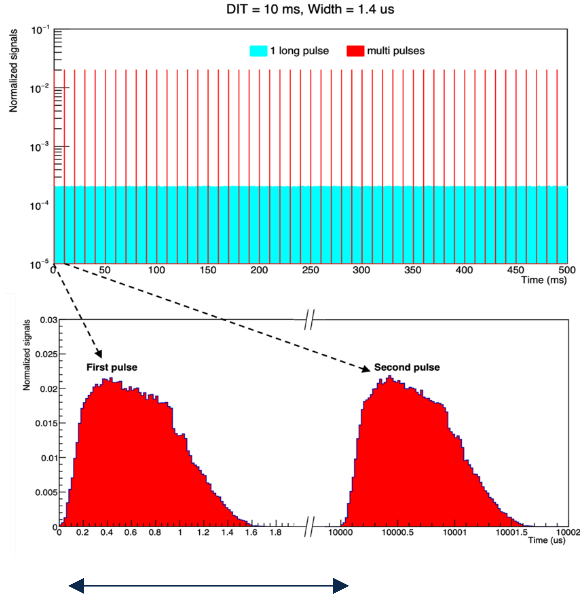
# Exercise 4: Change the pulse distance

UHDR.in

```
/run/numberOfThreads 10

# initialize geo and phys
/control/execute initialize.in

# time structure
/UHDR/pulse/pulseOn true
# push structure file
/UHDR/pulse/pulseFile 1.4us

# pulse structure
/UHDR/pulse/multiPulse true
/UHDR/pulse/pulsePeriod 100 ms
/UHDR/pulse/numberOfPulse 2
#/UHDR/pulse/pulseInHisto pulseHisto.txt

/run/initialize

# medium is configured in this file (scavengers.in)
/control/execute scavengers.in

/scorer/Dose/cutoff 1 Gy
/UHDR/source/particle e-
/UHDR/source/energy 0.999 MeV
/run/beamOn 1
```

```
>/UHDR-build ./UHDR UHDR.in
```

- pulsePeriod is the distance bewteen 2 pulses




pulsePeriod

# Exercise 5: Change the oxygen concentration

UHDR.in

```

# initialize geo and phys
/control/execute initialize.in

# time structure
/UHDR/pulse/pulseOn true
# push structure file
/UHDR/pulse/pulseFile 10ms

# pulse structure
/UHDR/pulse/multiPulse true
/UHDR/pulse/pulsePeriod 10 ms
/UHDR/pulse/numberOfPulse 1
#/UHDR/pulse/pulseInHisto pulseHisto.txt

/run/initialize

# medium is configured in this file (scavengers.in)
/control/execute scavengers.in

/scorer/Dose/cutoff 1 Gy
/UHDR/source/particle e-
/UHDR/source/energy 0.999 MeV
/run/beamOn 1
```

```

# pH and Scavenger
/UHDR/env/pH 5.5

# air concentration
/UHDR/env/scavenger O2 21 %
/UHDR/env/scavenger CO2 0.041 %
/UHDR/env/scavenger HCO3m 2.4 uM
# NO3-/NO2- concentration
#/UHDR/env/scavenger NO3m 1 mM
#/UHDR/env/scavenger NO2m 10 uM
#/UHDR/env/scavenger N2O 0.1 mM
#/UHDR/env/scavenger CH3OH 10 mM


/chem/reaction/print

#/run/verbose 1
/tracking/verbose 0
/scheduler/verbose 0
/scheduler/endTime 1000 s

# set false if many beamOn in medium
/scheduler/ResetScavengerForEachBeamOn true

/scorer/Gvalues/nOfTimeBins 80

/run/printProgress 10

```

/UHDR-build ./UHDR UHDR.in

# Exercise 5: Change the oxygen concentration

UHDR.in

```

# initialize geo and phys
/control/execute initialize.in

# time structure
/UHDR/pulse/pulseOn true
# push structure file
/UHDR/pulse/pulseFile 10ms

# pulse structure
/UHDR/pulse/multiPulse true
/UHDR/pulse/pulsePeriod 10 ms
/UHDR/pulse/numberOfPulse 1
#/UHDR/pulse/pulseInHisto pulseHisto.txt

/run/initialize

# medium is configured in this file (scavengers.in)
/control/execute scavengers.in

/scorer/Dose/cutoff 1 Gy
/UHDR/source/particle e-
/UHDR/source/energy 0.999 MeV
/run/beamOn 1
```

0.1 Gy

10

```

# pH and Scavenger
/UHDR/env/pH 5.5

# air concentration
/UHDR/env/scavenger O2 21 %
/UHDR/env/scavenger CO2 0.041 %
/UHDR/env/scavenger HCO3m 2.4 uM
# NO3-/NO2- concentration
#/UHDR/env/scavenger NO3m 1 mM
#/UHDR/env/scavenger NO2m 10 uM
#/UHDR/env/scavenger N2O 0.1 mM
#/UHDR/env/scavenger CH3OH 10 mM


/chem/reaction/print

#/run/verbose 1
/tracking/verbose 0
/scheduler/verbose 0
/scheduler/endTime 1000 s

# set false if many beamOn in medium
/scheduler/ResetScavengerForEachBeamOn true

/scorer/Gvalues/nOfTimeBins 80

/run/printProgress 10
```

4%