Istituto Nazionale di Fisica Nucleare

GEANT4-DNA
A SIMULATION TOOLKIT

UHDR example: overview, updates & perspectives

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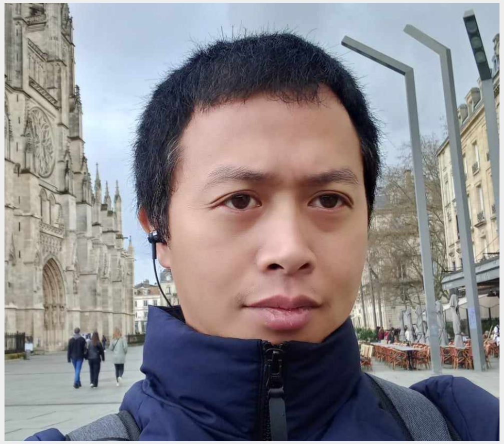
on behalf of Geant4-DNA collaboration

Geant4-DNA Extended example: UHDR

- The UHDR example and the Mesoscopic approach
- The new IRT-sync
- The pH validation
- More improvments later on



UHDR: General Overview

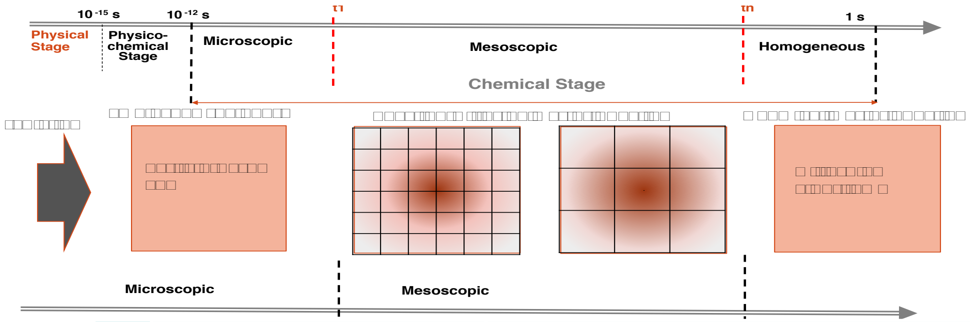
- Use new « mesoscopic » approach
- Simulation from heterogeneous to homogeneous states until about 15 minutes
- pH-dependence of hydroperoxyl radical / superoxide anion radical ($HO_2^{\bullet}$/ $O_2^{\bullet -}$) kinetics in water
- Dissolved Oxygen in Water
- Acid-base reactions associated with pKa at 25 °C.
- Implemented periodic boundary condition « PBC » for physical stage

AECL-11073, COG-94-167

Rate Constants and G-Values for the Simulation of the Radiolysis of Light Water over the Range 0-300°C

Constantes de vitesse et rendements g pour la simulation de la radiolyse de l'eau ordinaire entre les températures 0 et 300°C

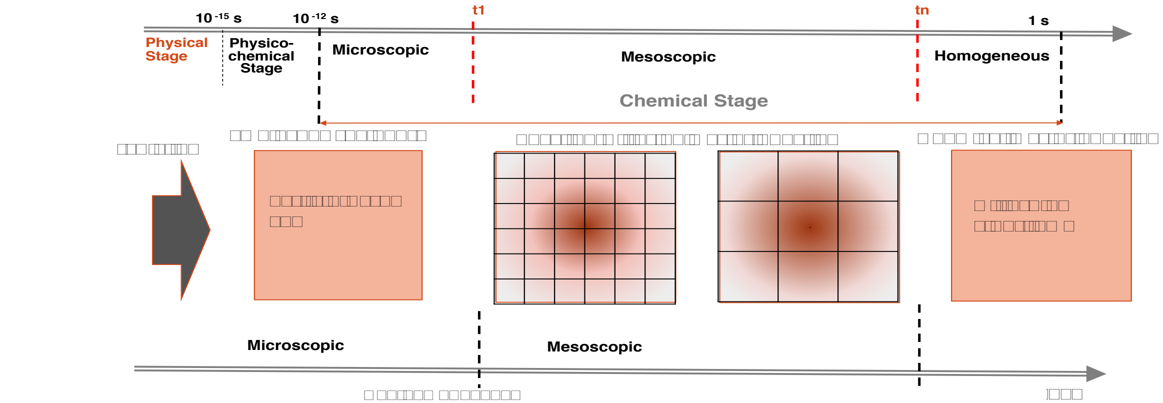
A.J. Elliot

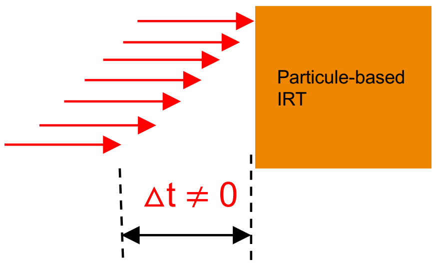


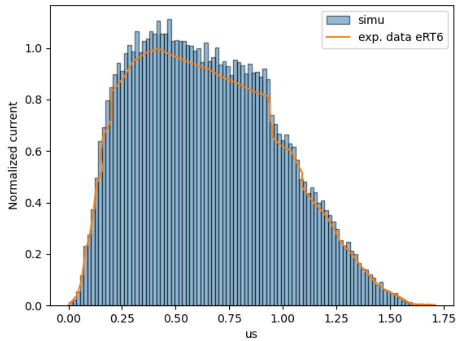
Tran et al., Int. J. Mol. Sci. (2021) 22

#	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 $M^{-1}s^{-1}$

UHDR: new developments (IRT-RDME)







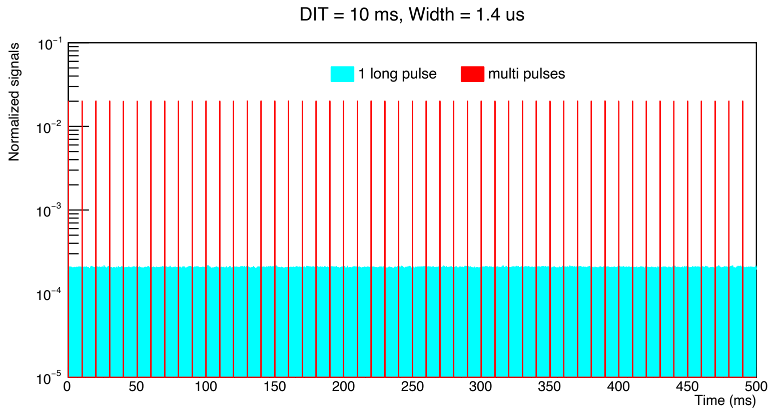
Jorge et al., Med Phys. 2022;49

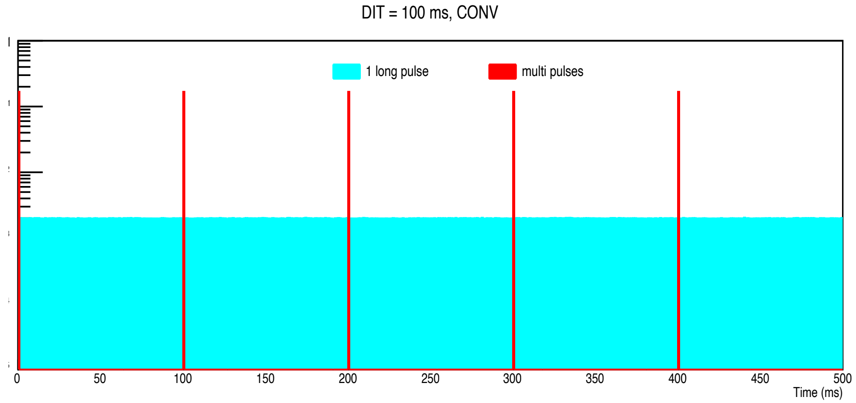
« Time structure » pulse

- Electron irradiated until the total energy deposition reaches 0.1-5 Gy
- Pulse duration (duration of the train) alterable until 1 second (t1)
- « Time structure » pulse have been sampled from a real raw signal

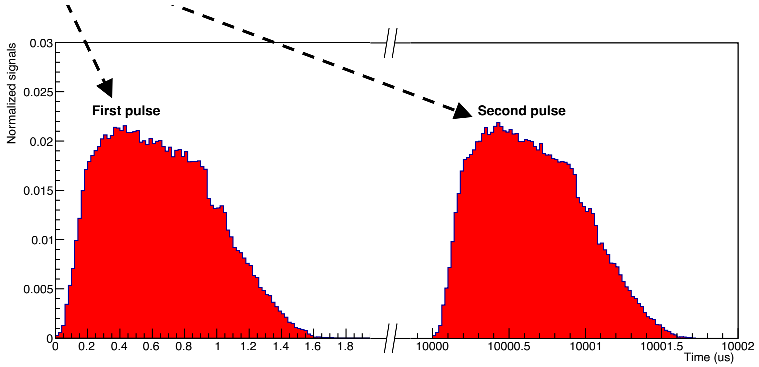
UHDR: new developments (IRT-RDME)

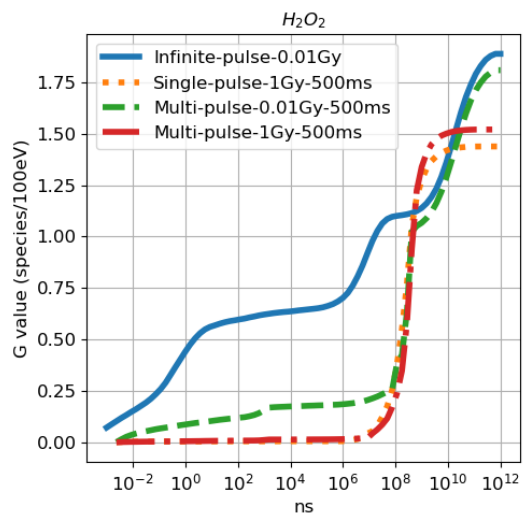
UHDR and CONV irradiations

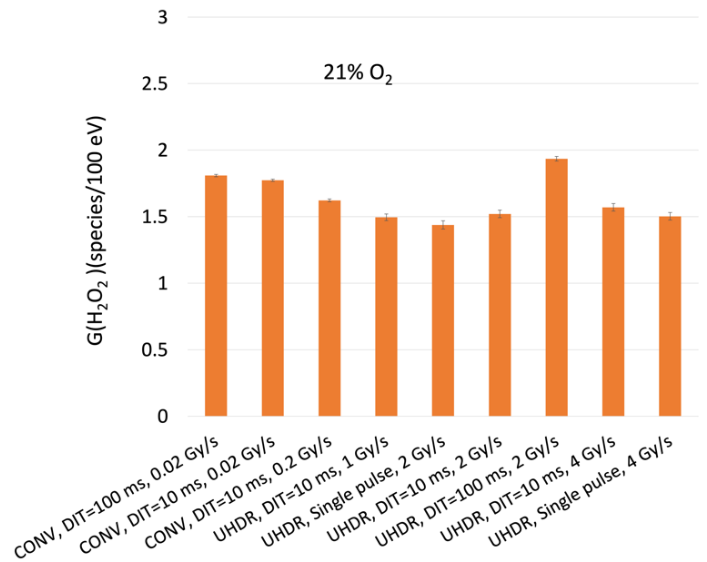




time structure
/UHDR/pulse/pulseOn true
/UHDR/pulse/multiPulse true
/UHDR/pulse/pulsePeriod 250 ms
/UHDR/pulse/numberOfPulse 2
/UHDR/pulse/pulseFile 1.4us







T.A. Le et al. - https://arxiv.org/abs/2409.11993

Ongoing: pH validation

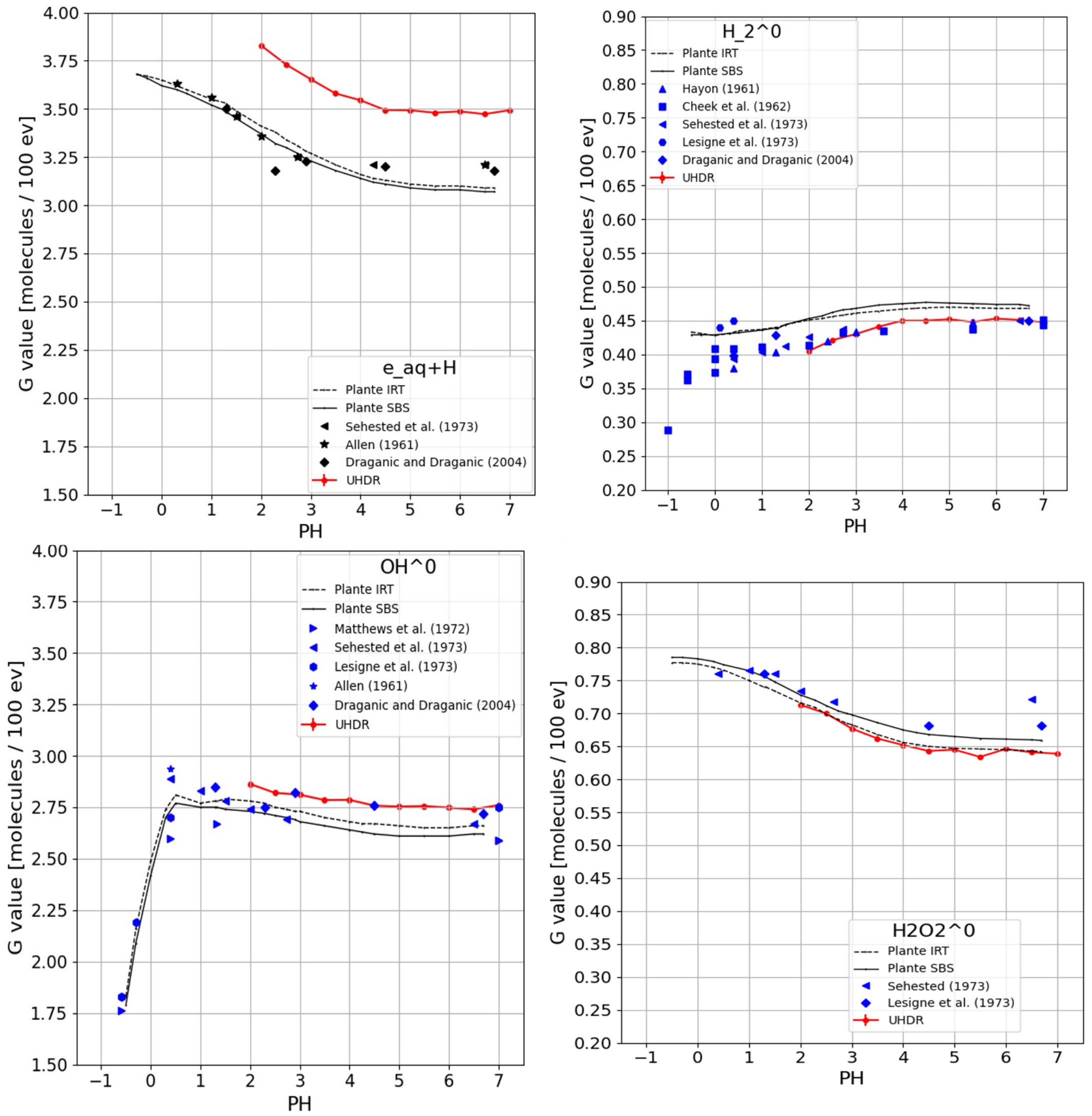
300 MeV proton

pH dependence during heterogeneous periode

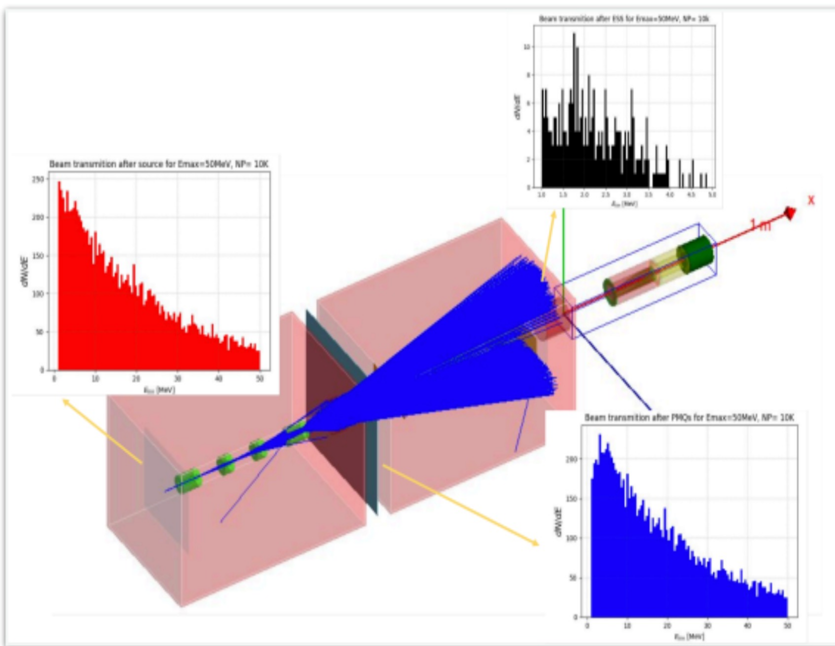
pH-dependence of $\mathbf{HO_2^{\bullet}/\ O_2^{\bullet-}}$ kinetics in water

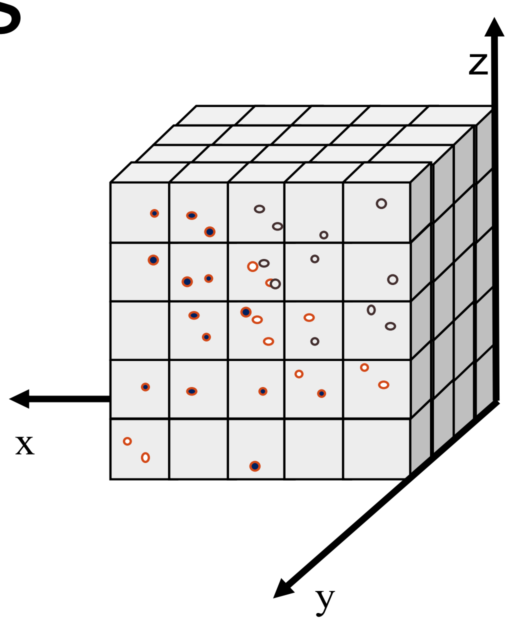
Currently:

- Very good agreement for most radiolitic species
- Divergency for e_aq and H
- Investigation are ongoing
- These species are very sensitive to the oxygen content



Future applications





- The **output** of the **Laser** driven appliaction (see “Hadrontherapy example:Current Status and Future Perspectives” G.Petringa)
- Will be the Phase Space in **Input** to the **UHDR** application

Thank you for your attention!