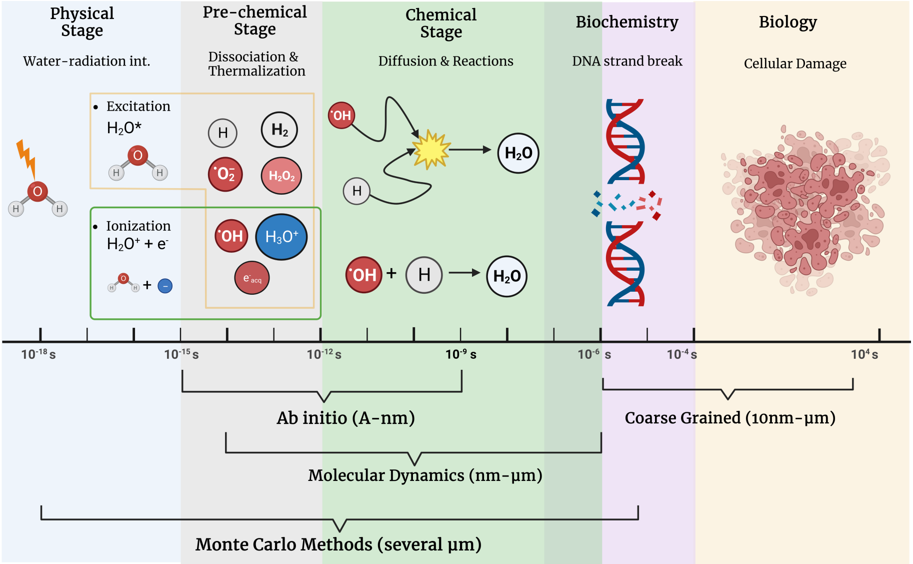
Multitrack extension tests

Lorenzo Castelli

University of Pisa

29 March 2023

Overview



Physical Stage
Water-radiation int.
Pre-chemical Stage
Dissociation & Thermalization
Chemical Stage
Diffusion & Reactions
Biochemistry
DNA strand break
Biology
Cellular Damage
Excitation
H_2O^*
Ionization
$H_2O^+ + e^-$
H
H_2
$^{\bullet}O_2^-$
H_2O_2
$^{\bullet}OH$
H_3O^+
e^-_{acq}
H_2O
$^{\bullet}OH$ + H → H_2O
10^{-18} s
10^{-15} s
10^{-12} s
10^{-9} s
10^{-6} s
10^{-4} s
10^{4} s
Ab initio (A-nm)
Coarse Grained (10nm-μm)
Molecular Dynamics (nm-μm)
Monte Carlo Methods (several μm)

MC Track Structure

Monte Carlo Methods

MC methods are particularly suitable for the study of radiation interactions with a target material since their stochastic nature

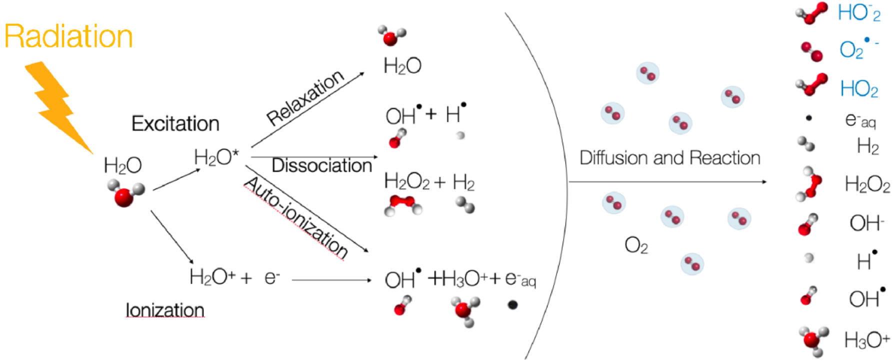
Two main approaches have been adopted by these simulation tools, the macroscopic or condensed history transport method and the event-by-event track structure approach

$\Downarrow$

- **Macroscopic:** computationally fast and perfectly reliable for high energy and large scales
- **Track Structure:** computationally expensive and thus inefficient to simulate the whole ion trajectory.

TRAX water radiolysis

Physical	Pre-chemical	Chemical
(~fs)	(fs-ps)	(ps-μs)
$\Downarrow$	$\Downarrow$	$\Downarrow$



Daria Boscolo: *Nanoscale insights on hypoxia radiosensitization with ion beams*

Physics

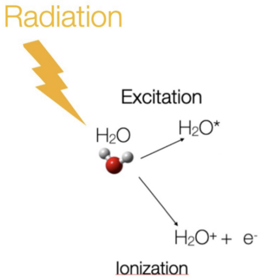
INPUT

Cross sections for shell-specific ionization (5) and excitation (8)

↓

The tracks of incident proj. are followed **event by event** until reaching a cutoff

↓



Physical stage

OUTPUT

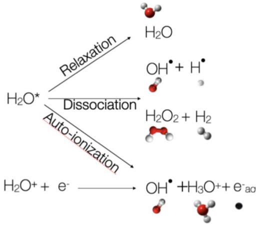
Spatial distribution of all the shell-specific ionization and excitation events and of all the sub-excitation electrons

Pre-chemical (fs - ps)

INPUT

Distribution of H_2O^+, H_2O^* and e^-_{aq} and their kinetic energy.

- **Dissociation:** Depends on ionization type and excitation state
- **Thermalization:** fragments release the kinetic energy (cannot interact until thermalized).



Pre-chemical stage

$\downarrow$

OUTPUT

The initial position of all the chemical species generated by water radiolysis

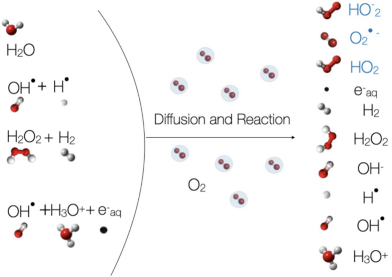
Chemical (ps - μs)

INPUT

Dissociation products distribution

↓

All radiolytic products diffuse and interact with each other with a **step by step approach** (Δt changes during evolution)



Chemical stage

↓

OUTPUT

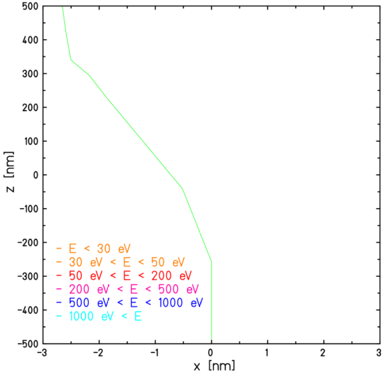
It is possible to determine the position of each chemical species at every step of the simulation.

Radiation type

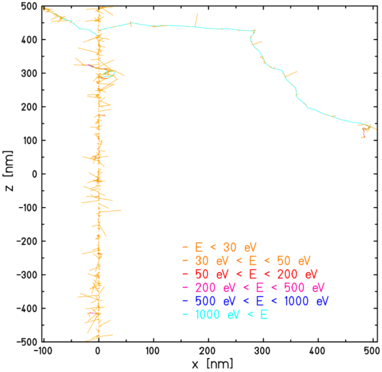
Different radiation qualities, i.e. radiation type and energy, vary in their **energy deposition patterns** $\hookrightarrow$ **Different ionization density**

$$\Downarrow$$

Electron 500**keV**



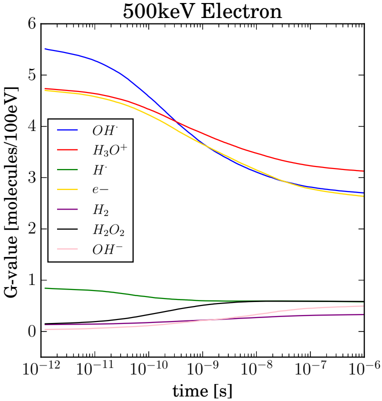
Carbon ion 40**MeV/u**

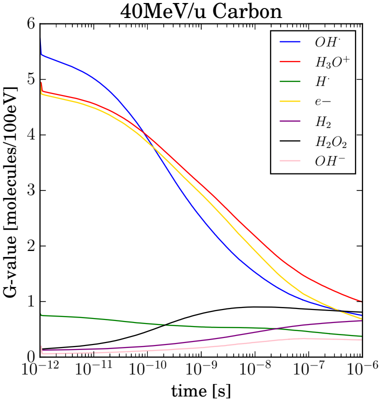


TRAX-CHEM simulation

G-value:*the number of molecules produced per* $100eV$ *of energy deposited.*

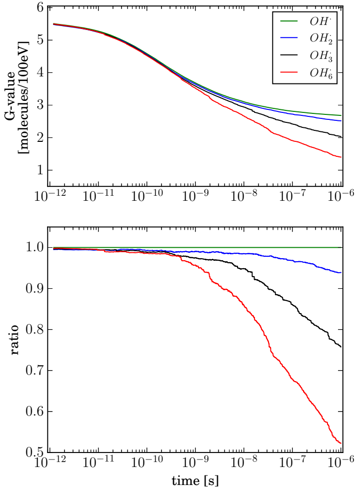
- **Point-like Source :** monoenergetic 500keV electrons and 40MeV/u carbon ions.
- **Target geo:** Cylinder with 5μm radius and 1μm depth





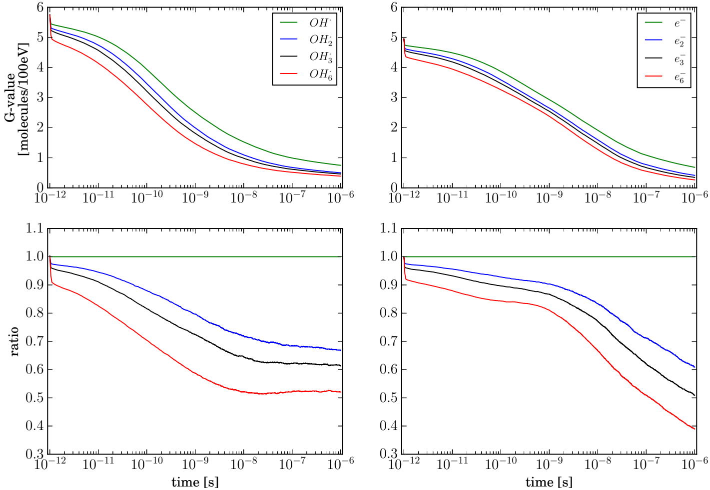
Intertrack simulation e⁻

- **Point-like Source :** monoenergetic 500keV electrons (2-3-6)
- **Target geo:** Cylinder with 5μm radius and 1μm depth



Intertrack simulation Carbon ion

- **Point-like Source :** monoenergetic 40MeV/u carbon ions (2-3-6)
- **Target geo:** Cylinder with 5μm radius and 1μm depth



Δx ; Δt

New Features

Recently, the option of examining the system while controlling the temporal and spatial separation of incident particles has been added.

$\hookrightarrow$ Combination of different Δx and Δt for 2 particles

·Proton 20MeV · Helium 5MeV/u

Δx [nm] \ Δt [ps]	0	1	10	10^2	10^3	10^4	10^5
0	✓	✓	✓	✓	✓	✓	✓
1	✓	✓	✓	✓	✓	✓	✓
10	✓	✓	✓	✓	✓	✓	✓
100	✓	✓	✓	✓	✓	✓	✓
1000	✓	✓	✓	✓	✓	✓	✓

Δx ; Δt

New Features

Recently, the option of examining the system while controlling the temporal and spatial separation of incident particles has been added.

$\hookrightarrow$ Combination of different Δx and Δt for 2 particles

- **Proton** 20**MeV** LET= 3keV/μm

Δt [ps] / Δx [nm]	0	1	10	10^2	10^3	10^4	10^5
0	✓	✓	✓	✓	✓	✓	✓
1	✓	✓	✓	✓	✓	✓	✓
10	✓	✓	✓	✓	✓	✓	✓
100	✓	✓	✓	✓	✓	✓	✓
1000	✓	✓	✓	✓	✓	✓	✓

Δx ; Δt

New Features

Recently, the option of examining the system while controlling the temporal and spatial separation of incident particles has been added.

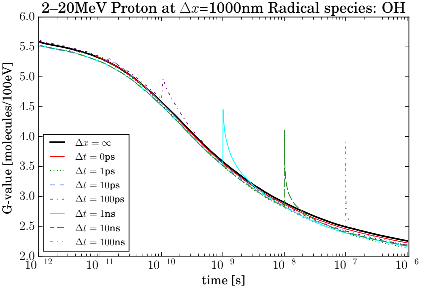
$\hookrightarrow$ Combination of different Δx and Δt for 2 particles

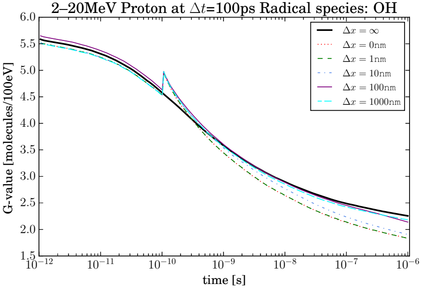
- **Proton 20MeV** LET= 3keV/μm

Δx [nm] \ Δt [ps]	0	1	10	10^2	10^3	10^4	10^5
0	✓	✓	✓	✓	✓	✓	✓
1	✓	✓	✓	✓	✓	✓	✓
10	✓	✓	✓	✓	✓	✓	✓
100	✓	✓	✓	✓	✓	✓	✓
1000	✓	✓	✓	✓	✓	✓	✓

20MeV Proton

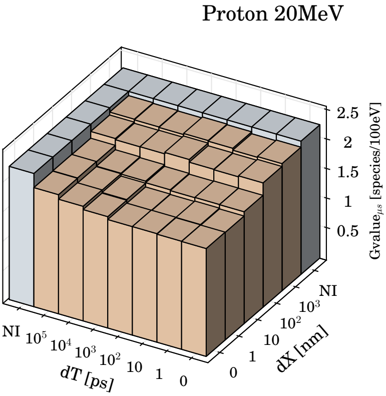
- **Point-like Source :** monoenergetic 20MeV Protons
- **Target geo:** box with 2.5μm depth and 5μm lenght

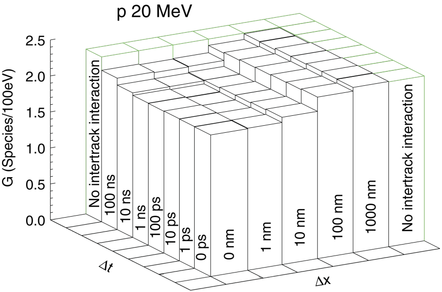




Comparison with Kreipl

G-value for $OH^{\bullet}$ at $1\mu s$ (left mine, right Kreipl)





Δx ; Δt

New Features

Recently, the option of examining the system while controlling the temporal and spatial separation of incident particles has been added.

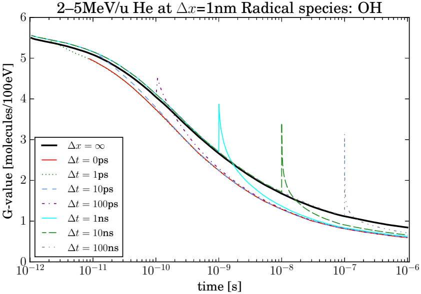
$\hookrightarrow$ Combination of different Δx and Δt for 2 particles

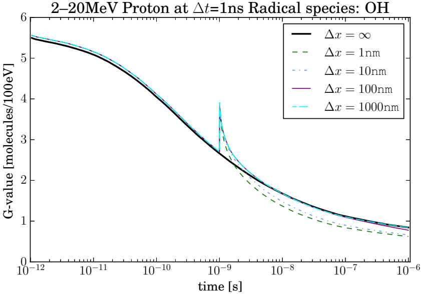
- **Helium 5MeV/u** LET= 38keV/μm

Δx [nm] \ Δt [ps]	0	1	10	10^2	10^3	10^4	10^5
0	✓	✓	✓	✓	✓	✓	✓
1	✓	✓	✓	✓	✓	✓	✓
10	✓	✓	✓	✓	✓	✓	✓
100	✓	✓	✓	✓	✓	✓	✓
1000	✓	✓	✓	✓	✓	✓	✓

5MeV/u Helium

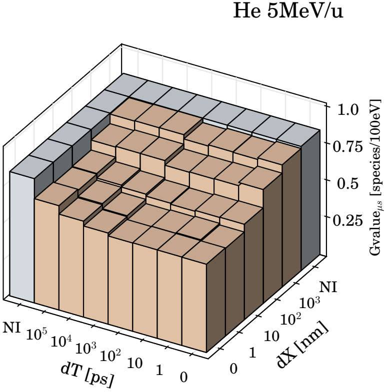
- **Point-like Source :** monoenergetic 5MeV/u Helium
- **Target geo:** box with 1.5μm depth and 5μm lenght

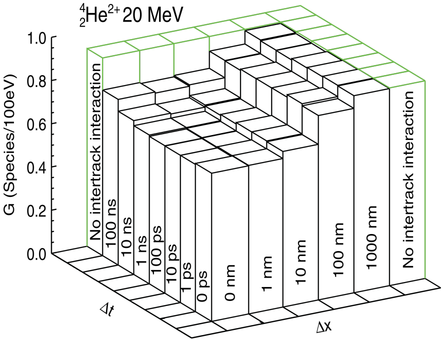




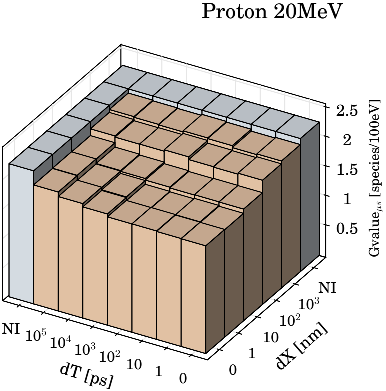
Comparison with Kreipl

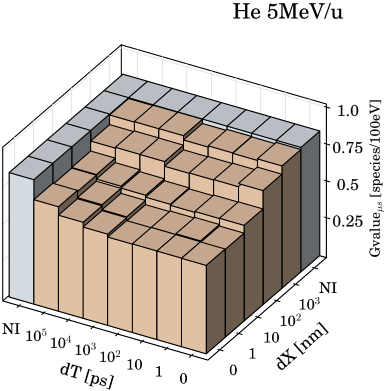
G-value for $OH^{\bullet}$ at $1\mu s$ (left mine, right Kreipl)





Conclusion





Carbon?