

Overview of the Geant4-DNA Project



geant4-dna.org

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Geant4-DNA tutorial
INFN-LNS, Catania, Italy
9-10/10/2025

Geant4 version 11.3
Released in December 2024

Contents of this talk

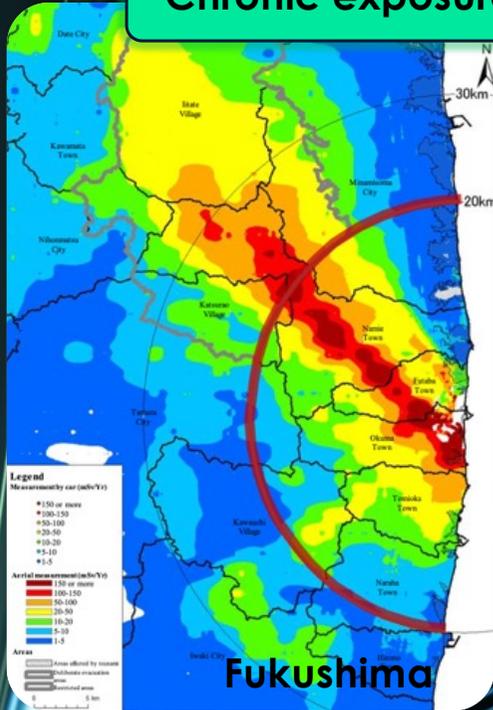
- Context of the Geant4-DNA project
- Physical stage
- Physico-chemical & chemical stage
- Geometrical models
- DNA damage and biological models
- More...

Contents of this talk

- Context of the Geant4-DNA project
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Modeling biological effects of ionising radiation remains a major scientific challenge

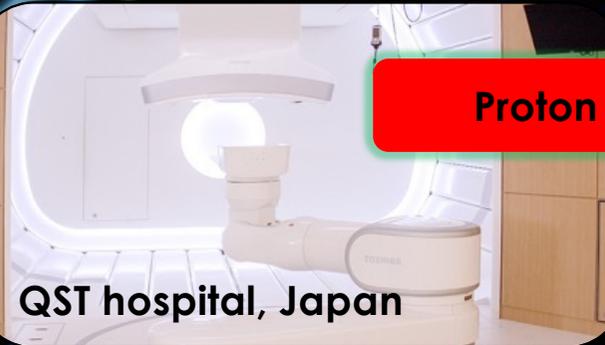
Chronic exposure



Diagnosis



Proton & ion-therapy



Moon



Space missions



Space exploration

ESA & NASA



Radiation effects scales



Human body: ~ 1cm - 100 cm

Radiation sickness (organ-level effects)

Tissue: ~ 1 mm - 10 mm

Radiation injury

Cell: ~ 1 μm - 10 μm

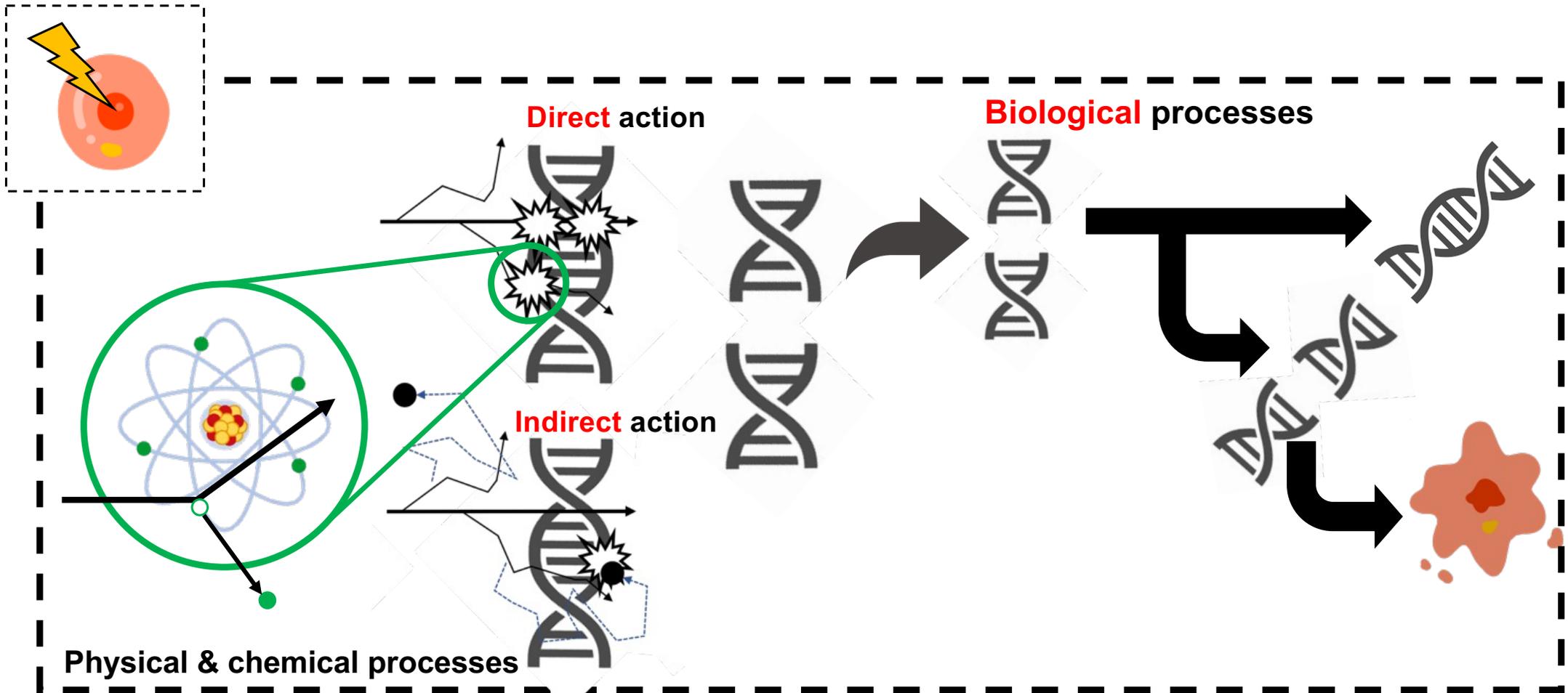
Cell death

DNA: ~ 1 nm - 10 nm

DNA damage, mutation, ...

Geant4-DNA main target

Radiobiological processes after irradiation

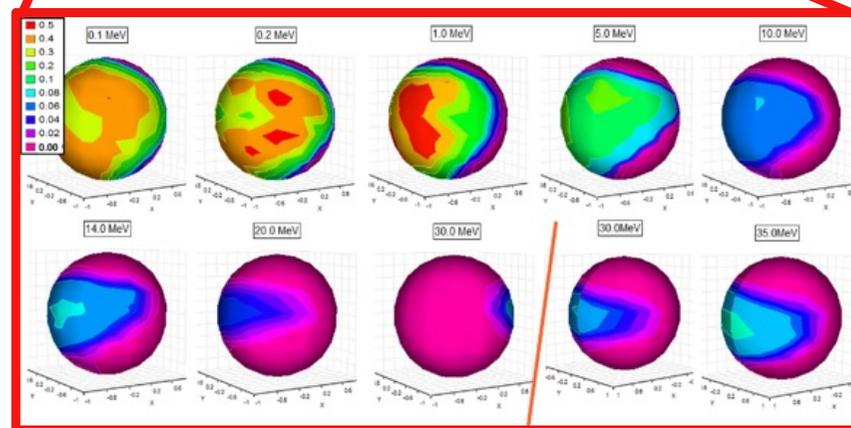
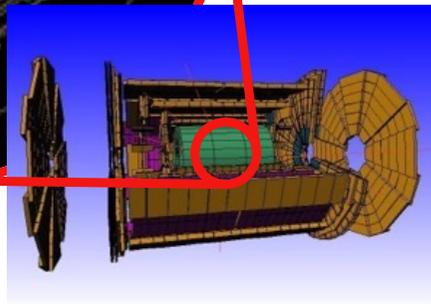
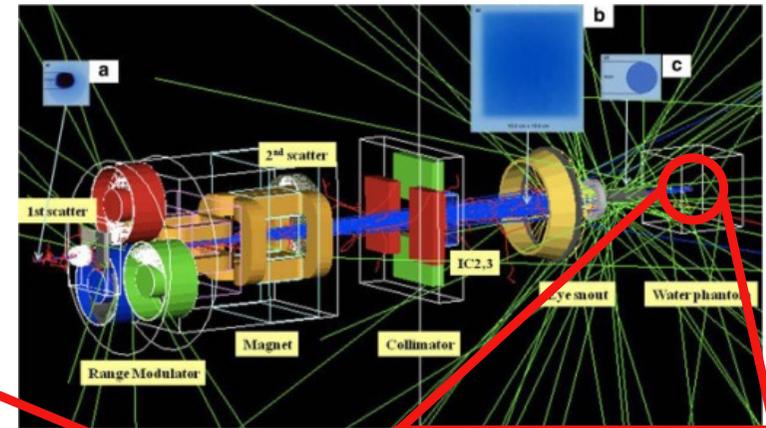
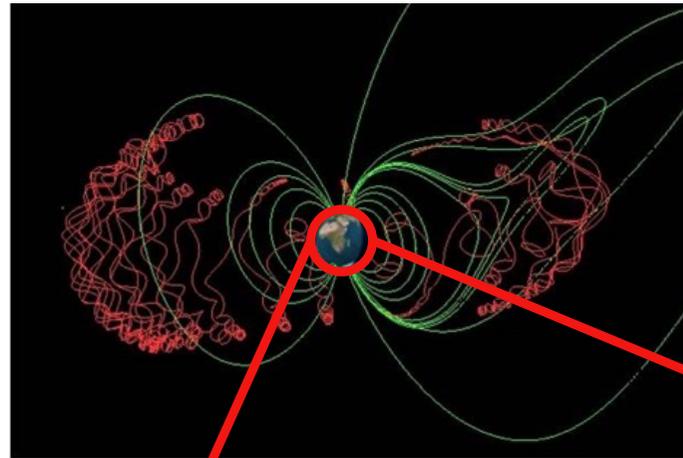
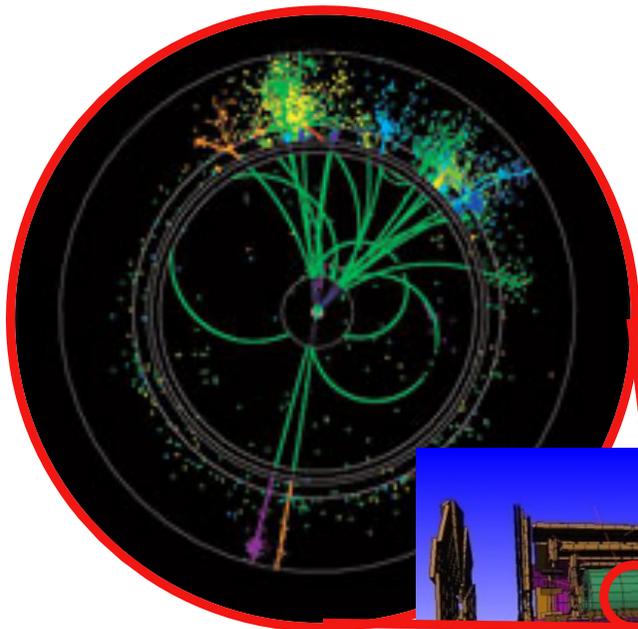


The Monte Carlo approach

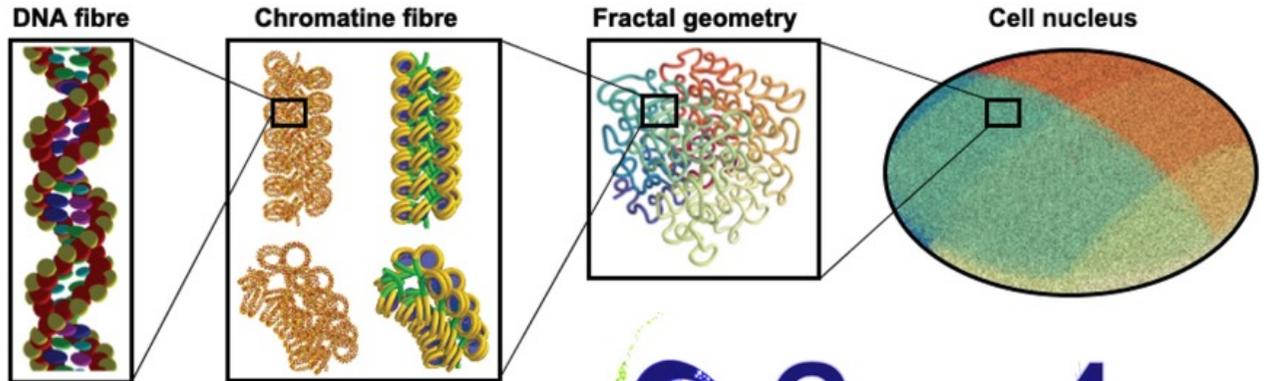
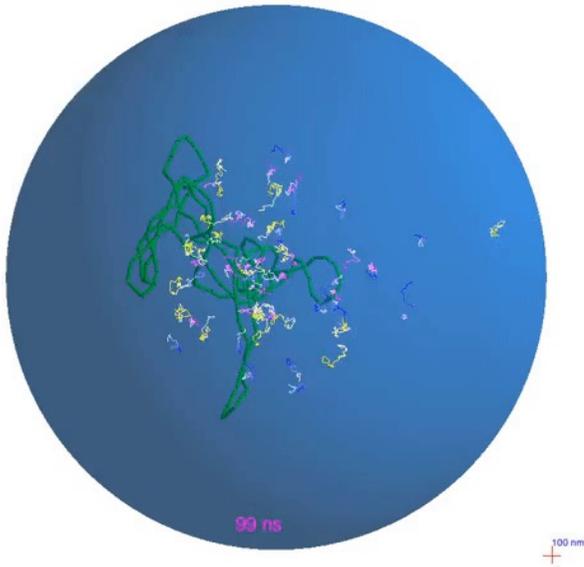
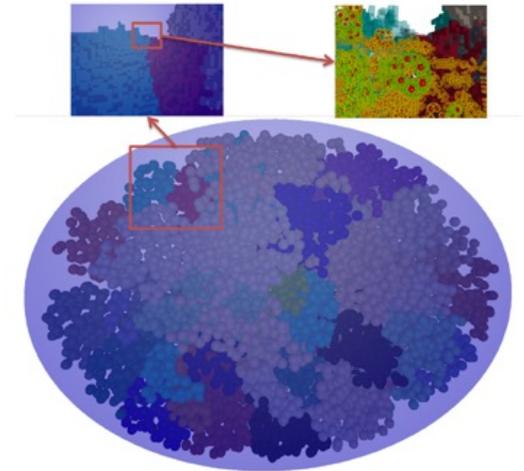
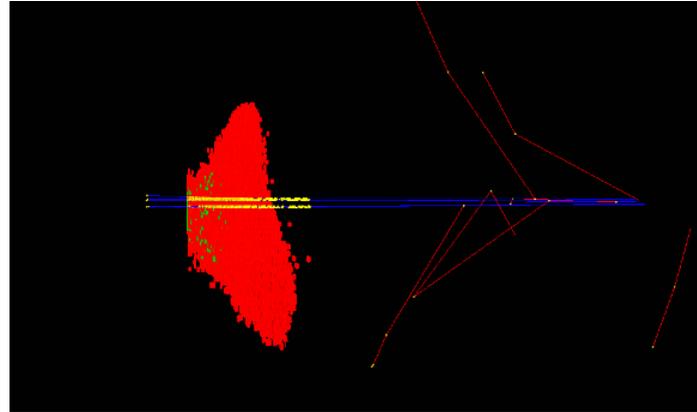
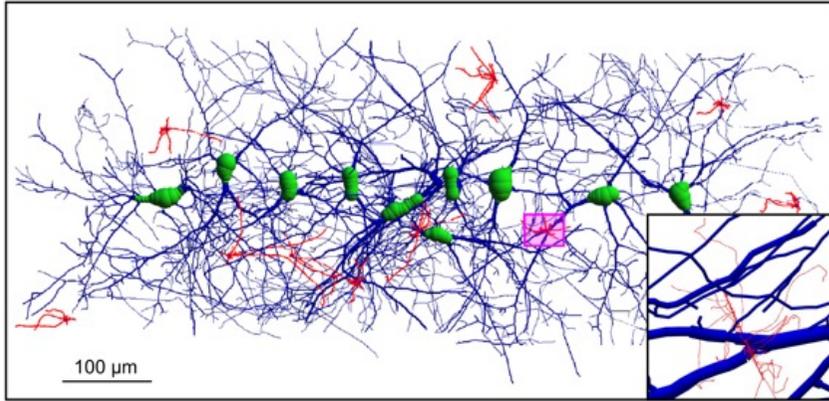
- Many **Monte Carlo codes** are already available today in radiobiology for the simulation of track structures at the molecular scale in biological medium
 - E.g. **PARTRAC**, **MC4***, **KURBUC**, **RETRACKS/RITRACKS**, **NOREC**, ...
 - Include **physics & physico-chemistry** processes, detailed **geometrical** descriptions of biological targets down to the DNA size, **DNA and chromosome damage** simulation and even **repair** mechanisms (PARTRAC)...
- Usually designed for very specific applications
- Not always easily accessible
 - Is it possible to access the source code?
 - Are they adapted to recent OSs?
 - Are they extendable by the user?

Open-source track structure MC codes
for radiobiological simulations is in high demand

What is Geant4?



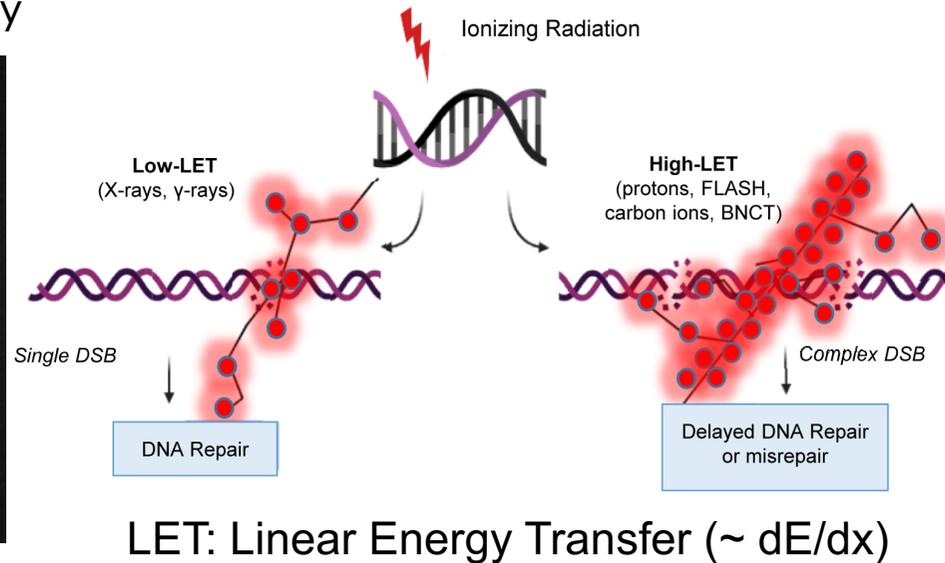
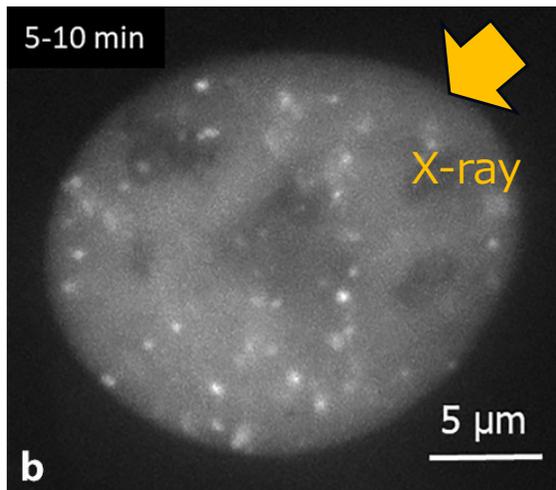
What is Geant4-DNA?



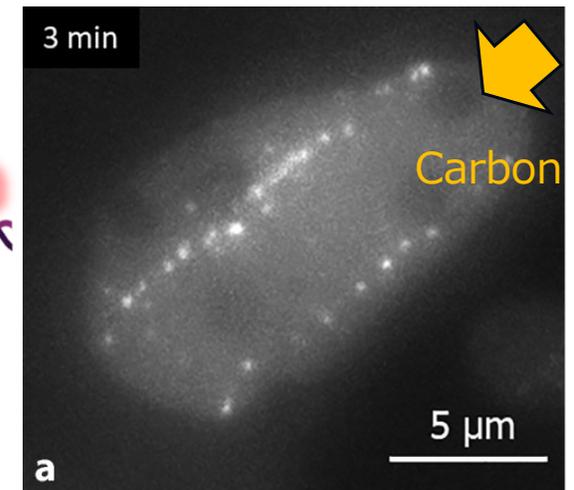
Why Geant4-DNA?

- Requirements for radiobiological simulations -

Damage distribution by X-ray



Damage distribution by ion



Low LET: Simple DNA damage
→ Easy to repair

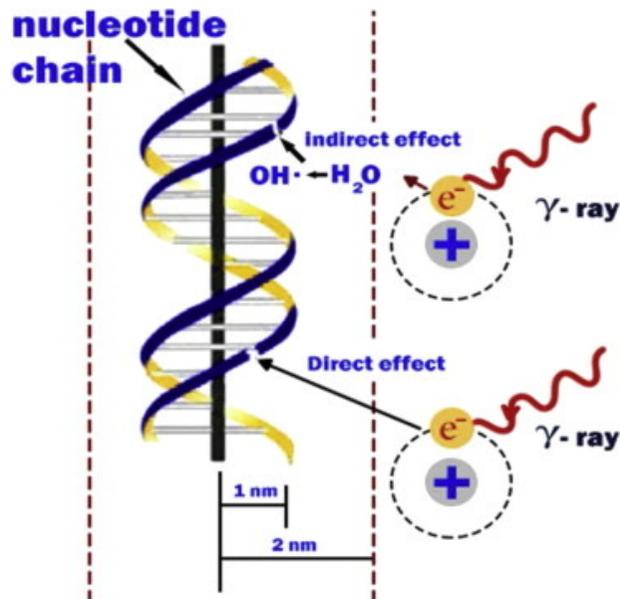
High LET: Complex DNA damage
→ Difficult to repair

High spatial resolution simulation (Geant4-DNA) allows deep investigation of DNA damage and biological response.

Why Geant4-DNA?

- Requirements for radiobiological simulations -

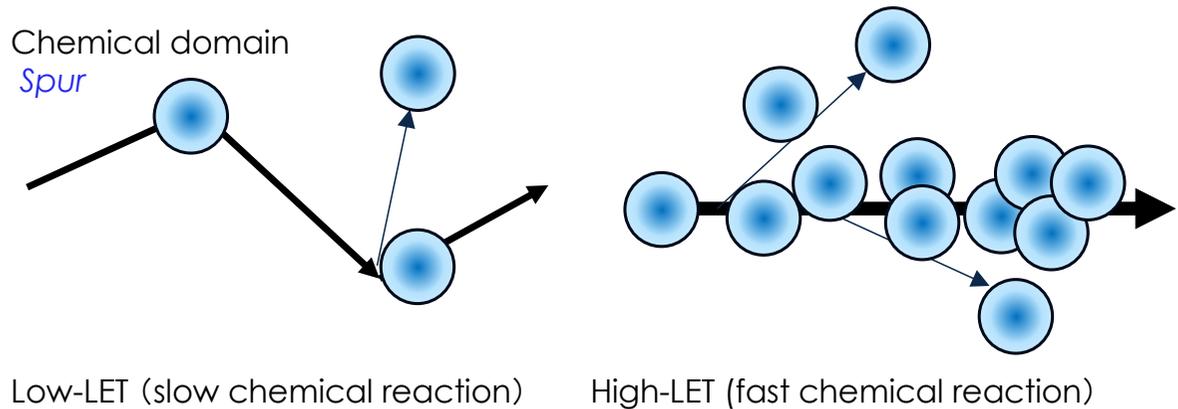
- ❑ Direct action: Damage by physical process
- ❑ Indirect action: Damage by chemical process
(reaction with chemical molecules created via water radiolysis)



- **Physical Process**
 - Interaction with water molecule
 - Interaction with bio-components
- **Chemical Process (with time evolution)**
 - Radiolysis Production
 - Diffusion of molecule
 - Interaction with molecule/bio-components

Physical processes influence radiolysis yields and subsequent chemical interactions.

Integrated implementation is necessary.



Why Geant4-DNA?

- Requirements for radiobiological simulations -

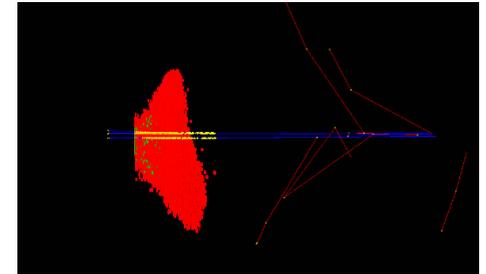
1. High spatial resolution (few μm , nm), low energy limit, reliable physics for sub-keV energies

Geant4:

Fast / Low spatial resolution, $E_{\text{limit}} \sim 250 \text{ eV}$

Geant4-DNA:

Slow / High spatial resolution, $E_{\text{limit}} \sim 10 \text{ eV}$



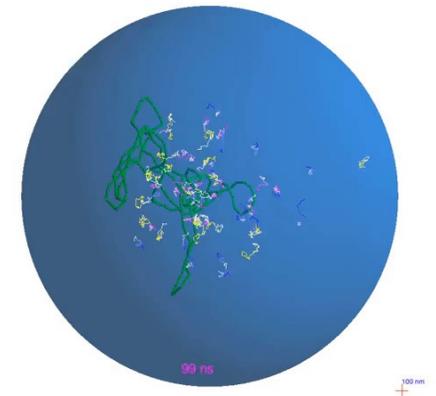
2. Interface to water radiolysis

Geant4:

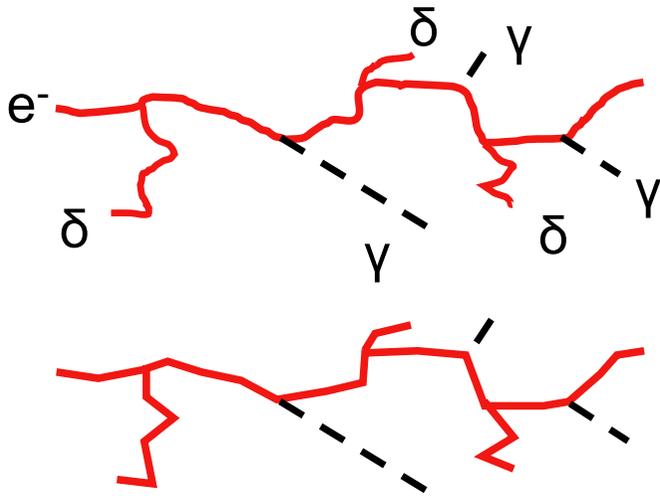
No interface

Geant4-DNA:

Production/Diffusion of chemical molecules



Requirement for physics: ① High spatial resolution



High accuracy/Slow computing



Low accuracy /Fast computing

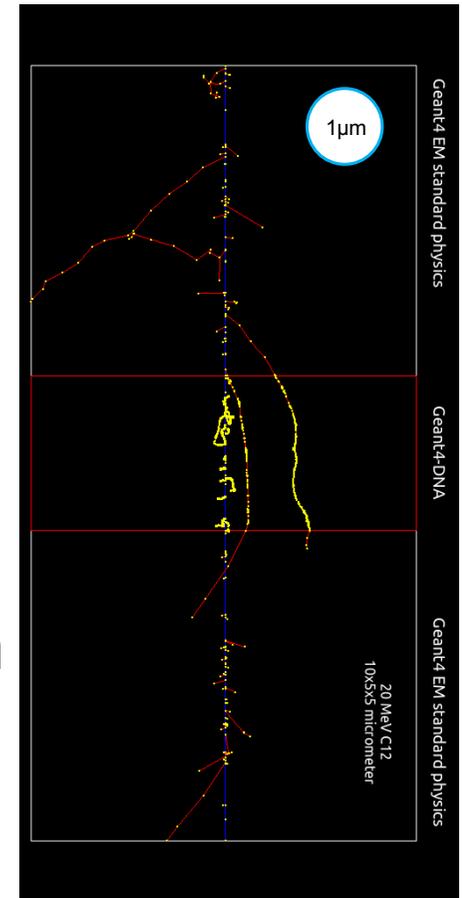
Trajectory in real world

Track-Structure approach

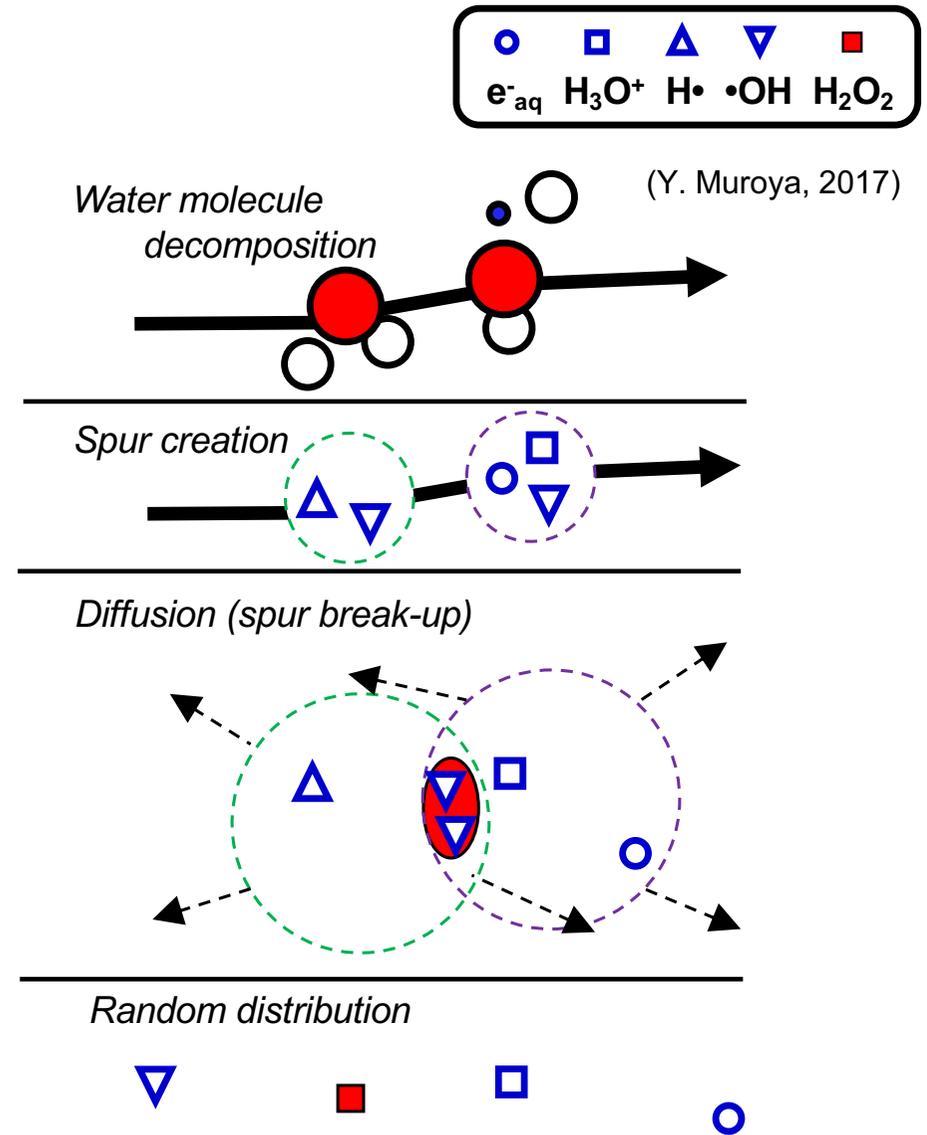
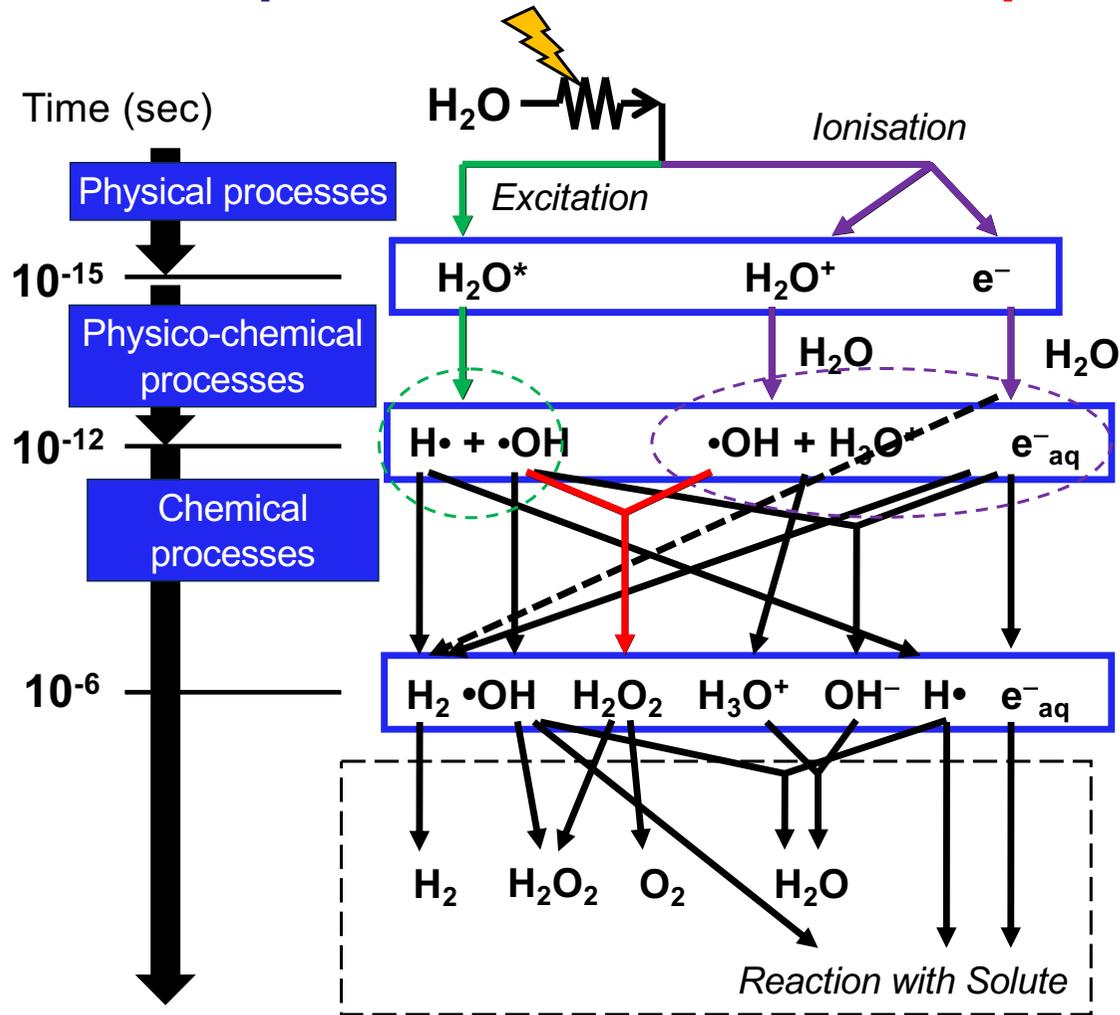
- All physical interactions are simulated individually in a sequential manner
- Example: **Geant4-DNA**, PARTRAC, RITRACKS, NOREC, KURBUC, PHITS-TS...

Condensed-History approach

- Several discrete physical interactions are “condensed” into a single transport step
- Multiple-scattering approximation
- Example: **Geant4**, PHITS, EGS, FLUKA, PENELOPE, MCNP...



Requirement: ② Water radiolysis



Geant4-DNA history

2001

Initiated by the
**European Space
Agency/ESTEC**

2007

First prototypes of
physics models
for liquid water
added to Geant4 **9.1**

2008

Re-engineered
to be coherent with
Geant4 EM physics
in Geant4 **9.3**

2014

Chemistry stage
extension
ready for end users in
Geant4 **10.1**

2014

First extended examples
applicable to "**DNA-
scale**" geometries
released in Geant4 **10.4**

dnaphysics
microdosimetry
pdb4dna
wholeNuclearDNA

2019 - 2023

Development of fully integrated
radiobiological applications
Integration of **Phys. + Chem. + Geometry** in **10.5**
Integration **with biological prediction models** in **11.1**

dnadamage1 in 10.5 (2019)
dnadamage2 in 11.1 (2022)
moleculardna in 11.1 (2022)
dsbandrepair in 11.2 (2023)

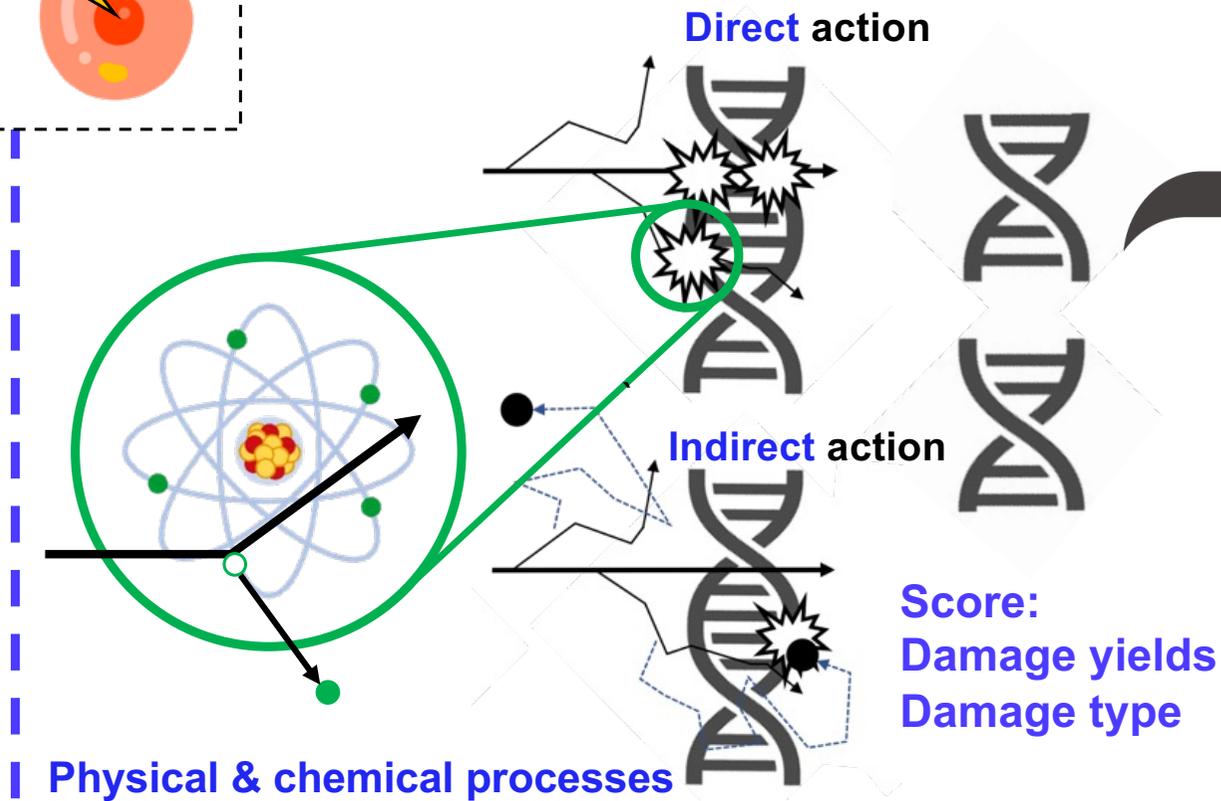
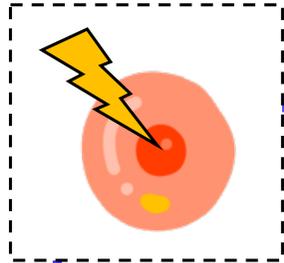
2024-2025

Extension of Physics
(energy, materials)
New approaches in
chemistry

UHDR in 11.3 (2024)

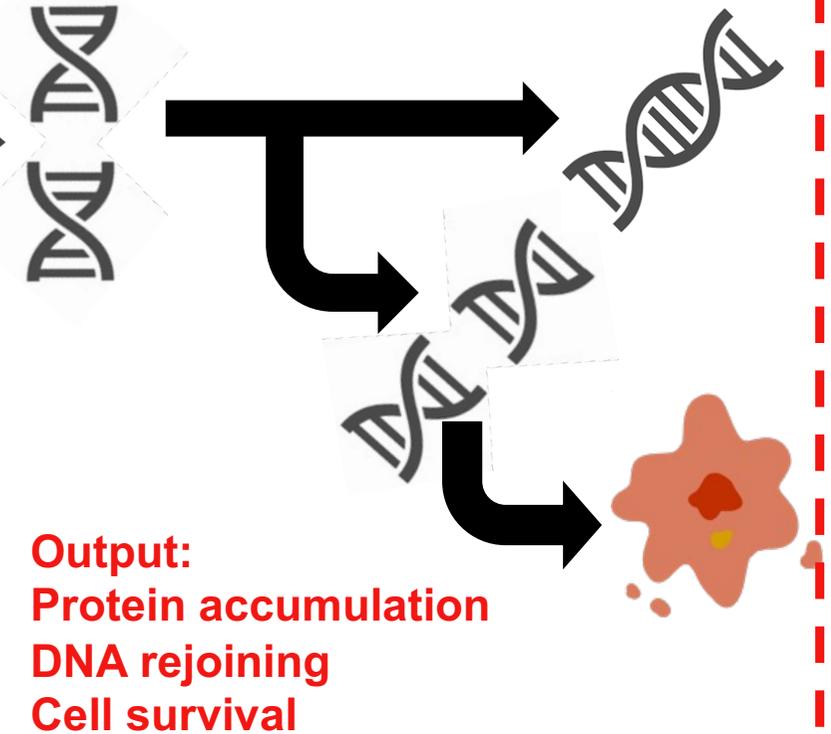
Conceptual design of the Geant4-DNA approach

Simulation Block

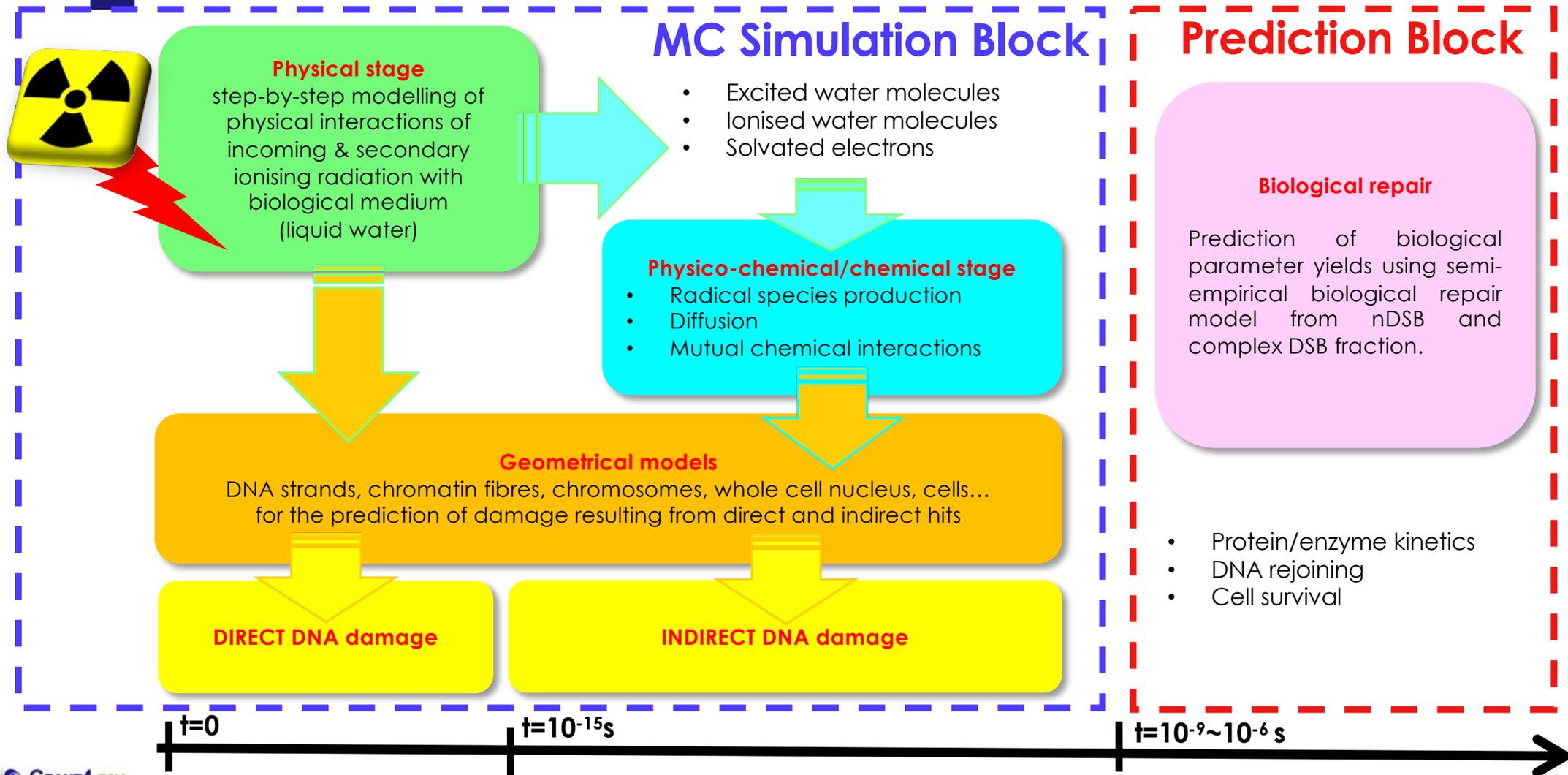


Prediction Block

Biological processes



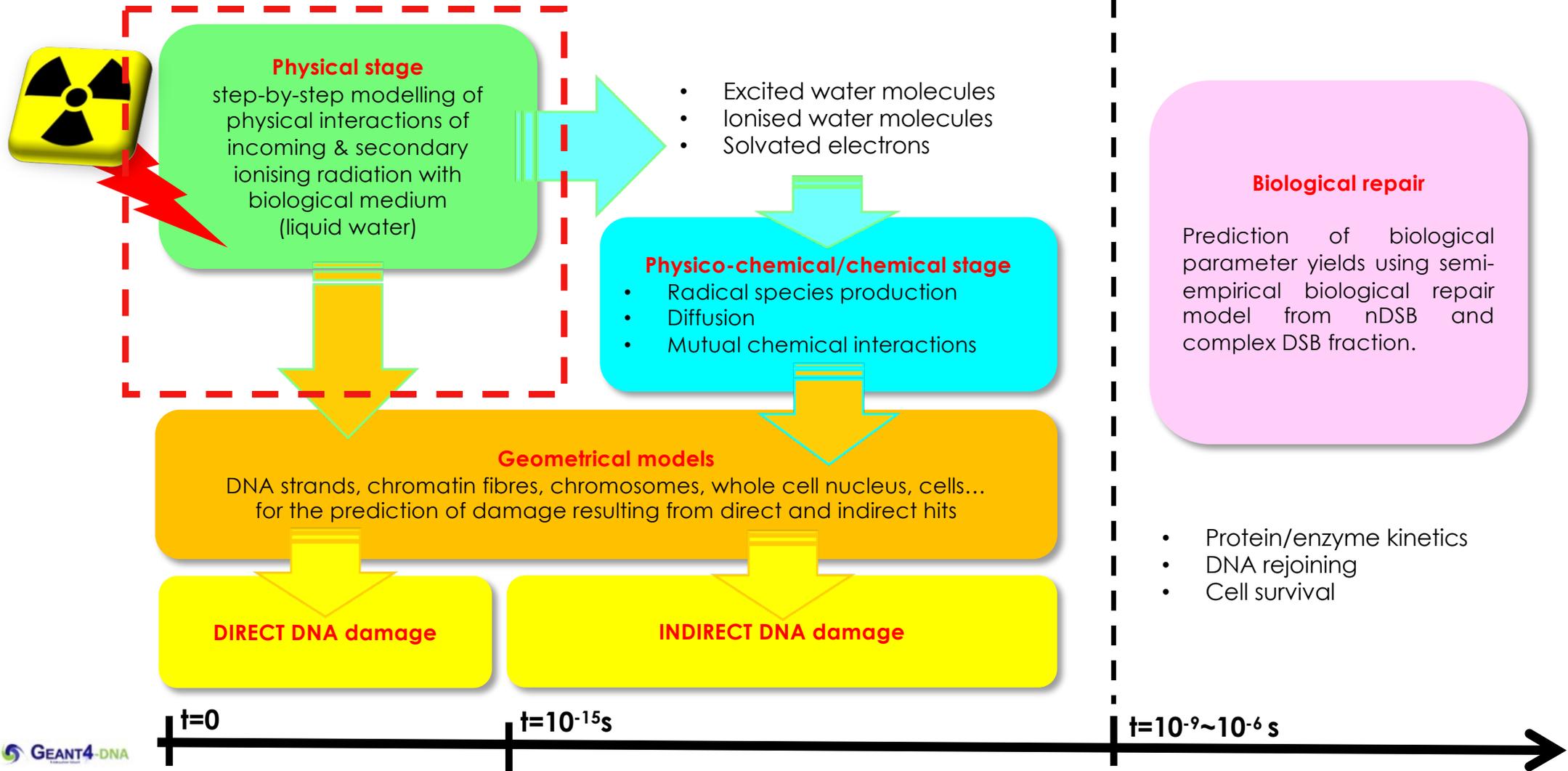
The Geant4-DNA approach



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The Geant4-DNA approach



Geant4-DNA physics for liquid water

Other materials are available:
DNA precursors, DNA bases & S-P, solid gold,...
see [Physics talkkjl](#);

- **Geant4-DNA processes and models allows the transport in liquid water**
 - **Electrons**: ionisation, excitation, elastic scattering, vibrational excitation, electron attachment
 - **Protons, H (0,+)**: ionisation, excitation, elastic, charge increase/decrease processes
 - **Alpha, He(0+,2+)**: ionisation, excitation, elastic, charge increase/decrease processes
 - **Generic ions**: ionisation
- **Geant4-DNA Physics constructors for simulations in liquid water**
 - **G4EmDNAPhysics_option2** (since version 9.1): accelerated default constructor, simulating electron interactions (elastic, inelastic, dissociative attachment, vibrational excitation) **up to 1 MeV**, as well as other particle interactions
 - **G4EmDNAPhysics_option4** (since version 10.2): contains electron elastic and inelastic models, **up to 10 keV**; extended up to 10 MeV (to be released)
 - **G4EmDNAPhysics_option6** (since version 10.4): contains CPA100 electron elastic and inelastic models, **up to 256 keV**

NOTE

- Protons can be tracked up to 300 MeV
- Option4 and option6 can go up to 1 MeV (beyond the default limits, Born models are used)

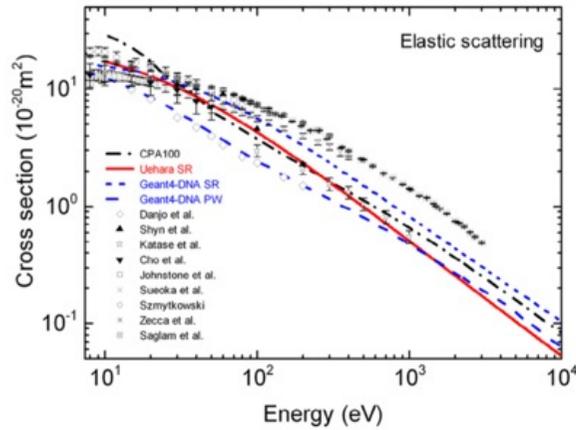
Multi-scale combination of physics processes

- Geant4-DNA is mainly dedicated to **(very) low energy charged particles**
 - Is it possible to simulate neutral particles such as photons?
 - Can we include the physics processes for high-energy particles?
- Any Geant4-DNA process can be combined with other Geant4 process such as:
 - Geant4 **photon** processes: photoelectric effect, Compton scattering, Rayleigh scattering, pair production
 - Livermore (EPDL97) included by default
 - Geant4 **alternative EM** processes for charged particles
 - E.g. bremsstrahlung
 - Geant4 **atomic de-excitation** (fluorescence + Auger emission, including cascades)
 - EADL97
 - Bearden
 - ...and also Geant4 **hadronic physics**

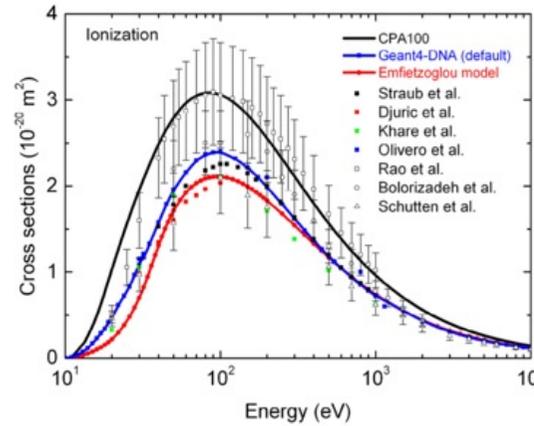
E.g. of validation and verification of Physics : total cross sections

Electron CS:

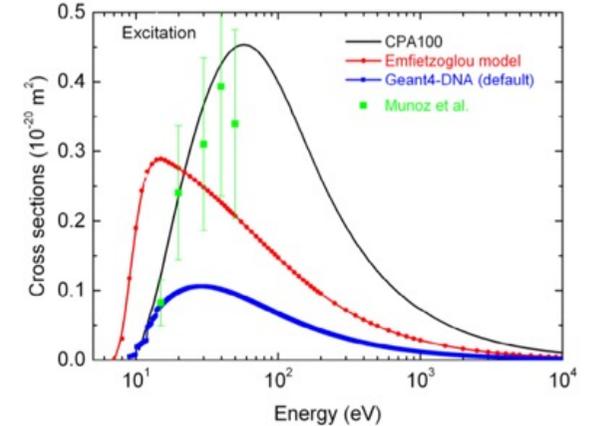
Elastic



Ionisation

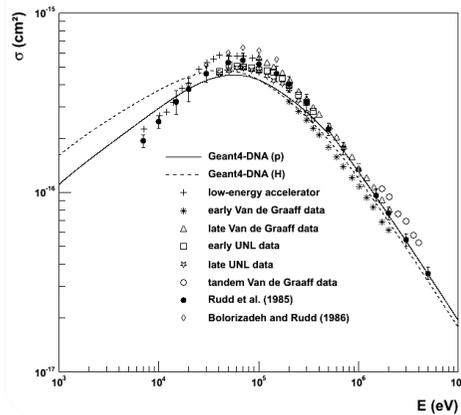


Electronic excitation

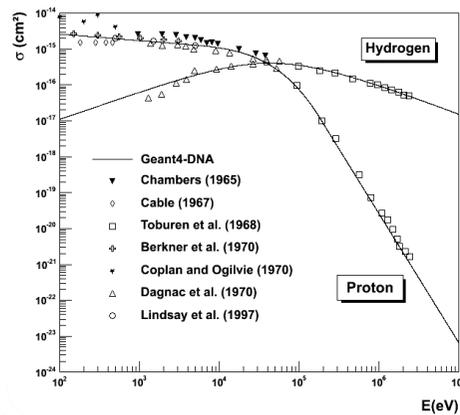


Proton CS:

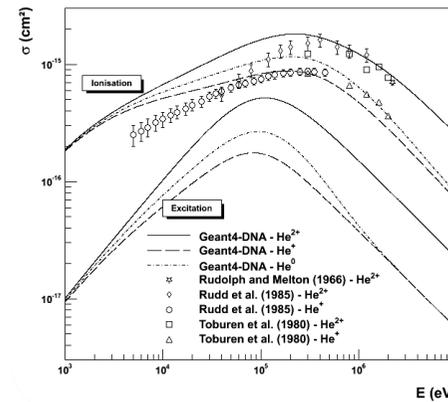
Ionisation



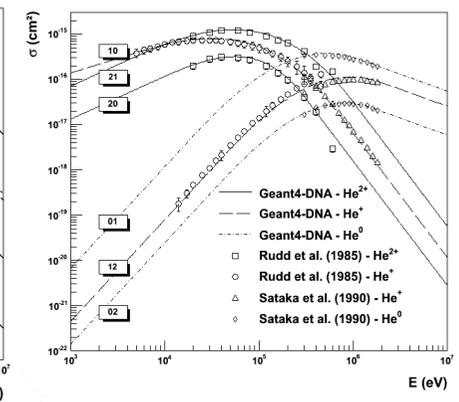
Charge exchange



Helium CS: Ionisation



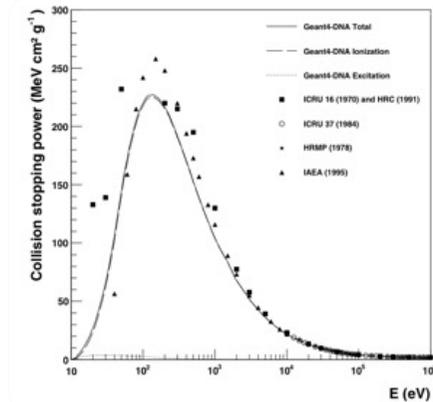
Charge exchange



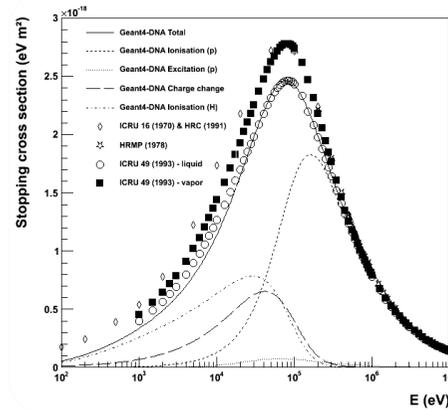
E.g. of validation and verification of Physics: **range** and **stopping power**

Stopping power:

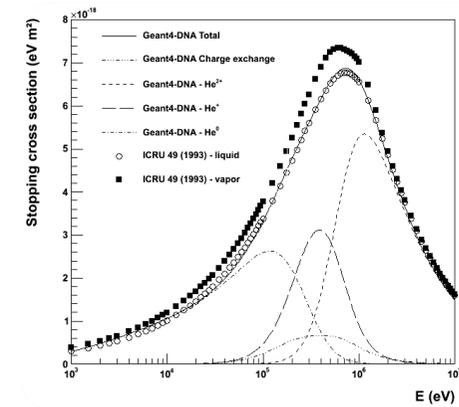
Electron



Proton

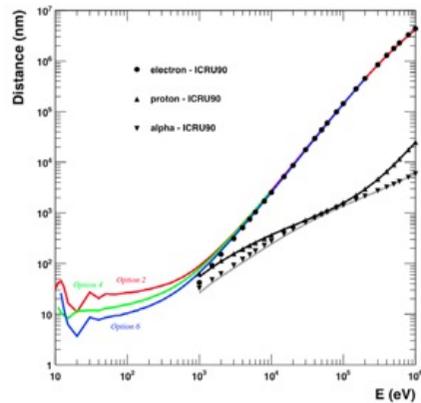


Helium

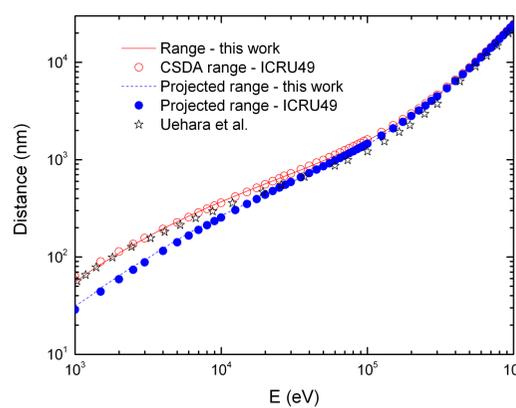


Range:

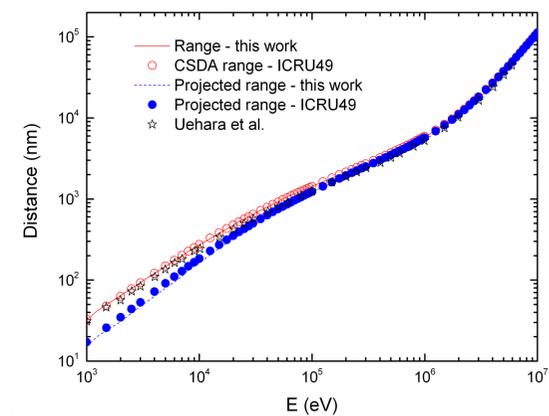
Electron



Proton



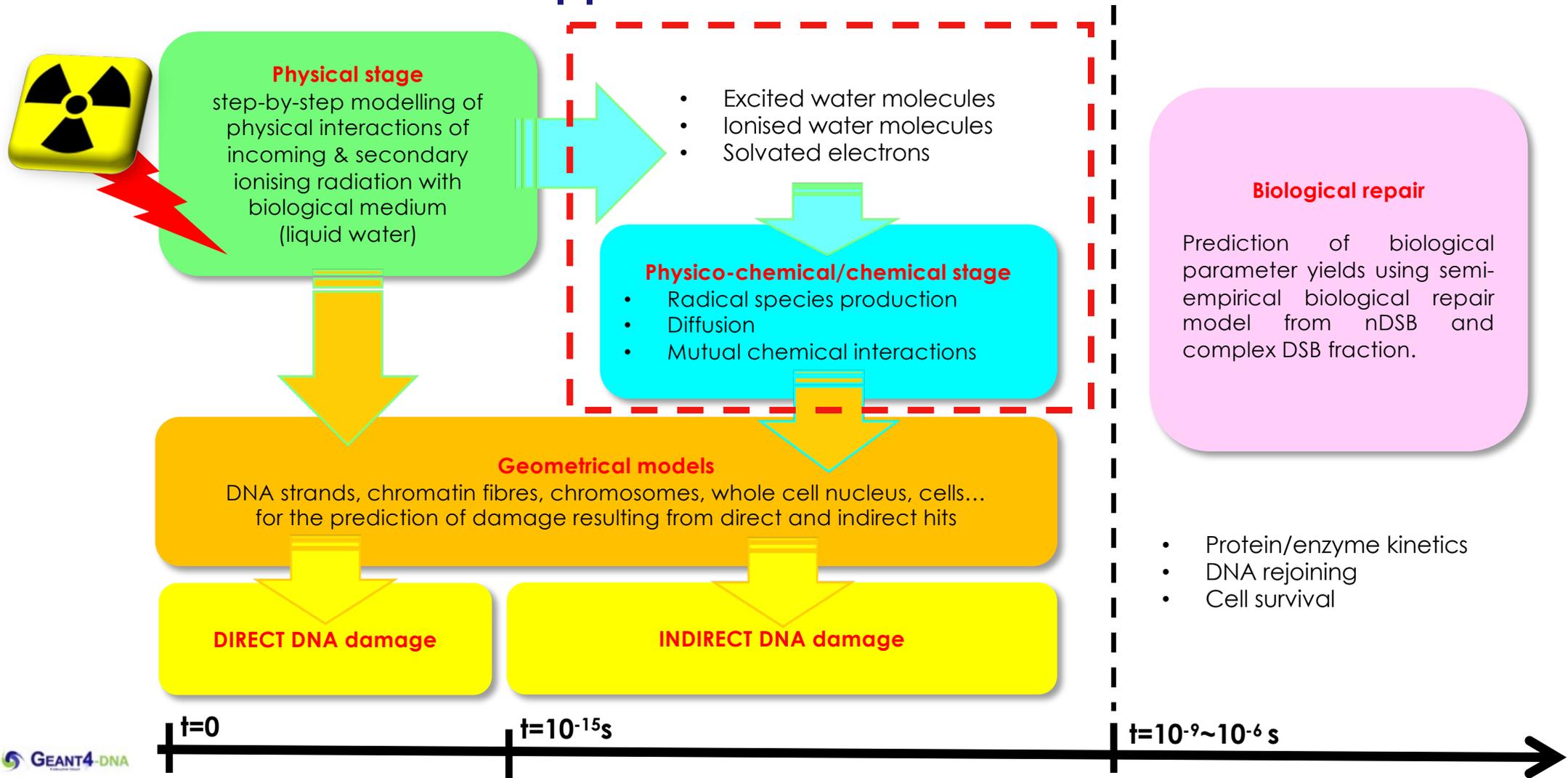
Helium



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The Geant4-DNA approach



Geant4-DNA chemistry models

- **Geant4-DNA chemistry allows the water radiolysis simulation:**
 - **Production of molecules:** e.g, place decomposed molecules at 1 ps
 - **Diffusion:** Geant4-DNA offers 3 types of diffusion algorithm
 - **Step-by-Step (SBS):** Fixed time step molecular transport method.
 - **Independent Reaction Time (IRT):** Calculates the reaction times between all possible pairs. Reactions occur one by one, starting with the pair with the shortest reaction time.
 - **IRT-sync:** IRT-sync stores all molecular positions **at each time step**, as the SBS approach.
 - **Mesoscopic:** A compartment-based representation that describes the evolution of species through their concentrations in different compartments.
 - **Reaction:** Geant4-DNA handles reactions between molecules.
- **Geant4-DNA chemistry constructors:**
 - **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)

Ref.: [Med. Phys. 51 5873–5889 \(2024\)](#)

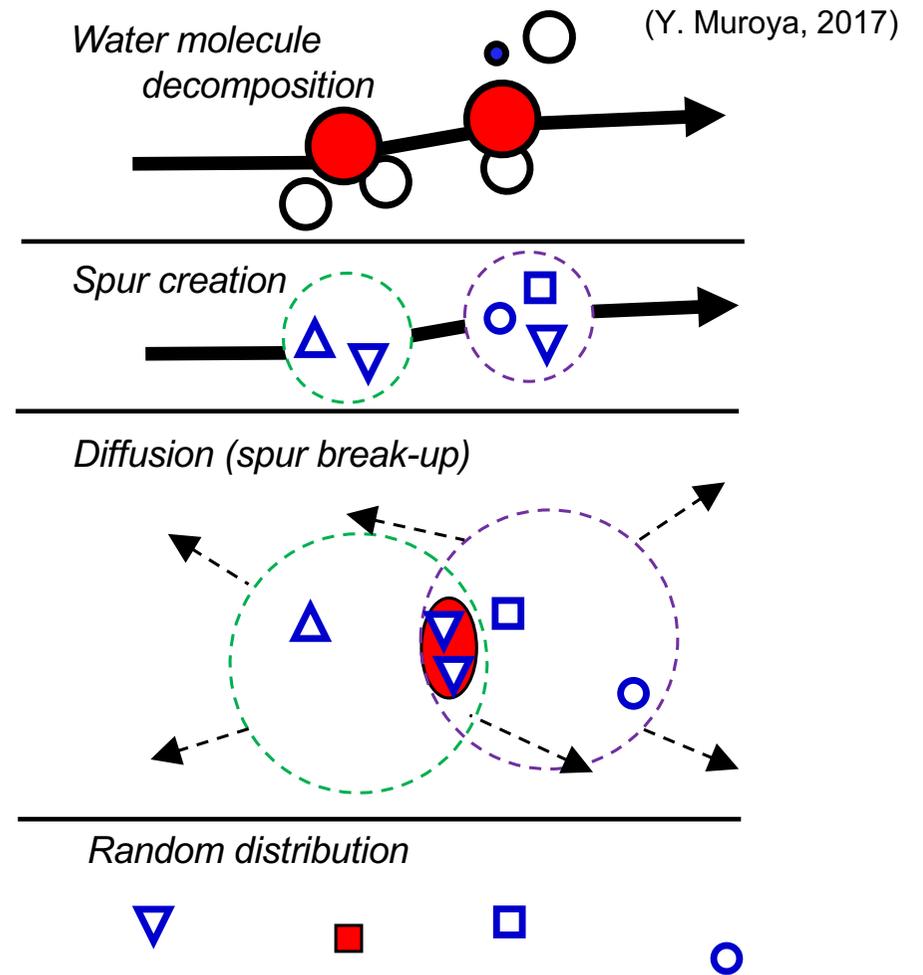
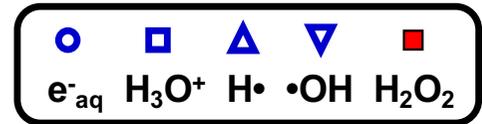
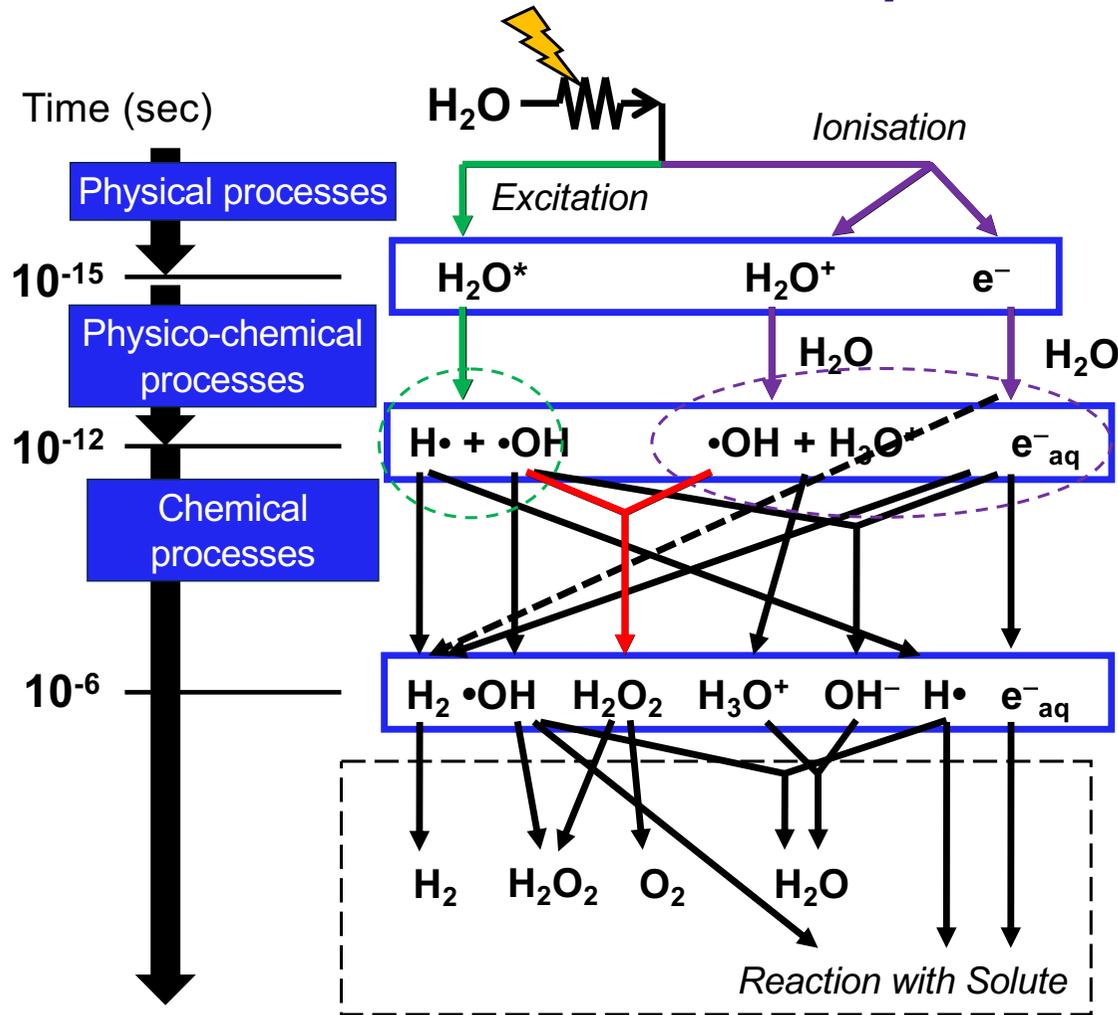
Geant4-DNA chemistry extended examples

Located in \$G4EXAMPLES/extended

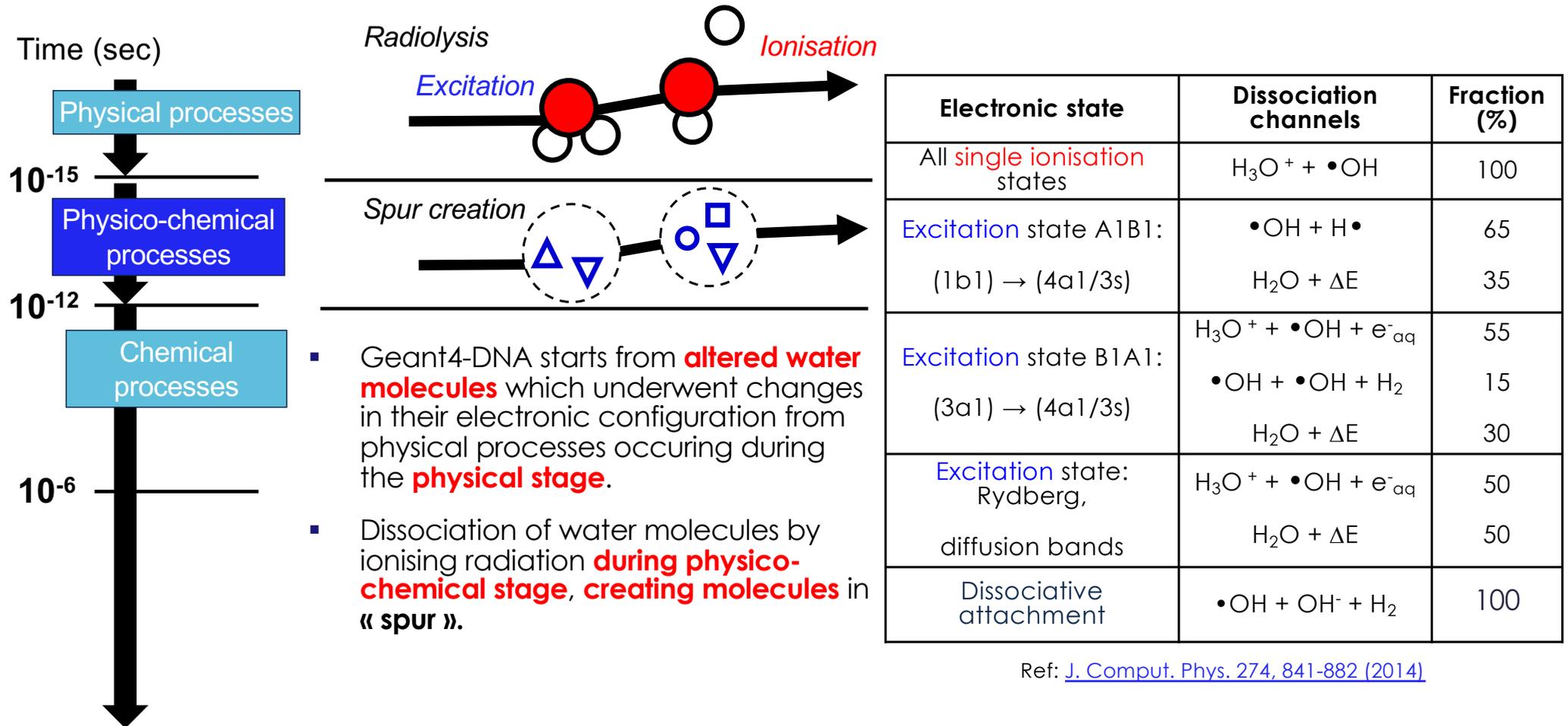
- The « **chem1** » **extended/medical/dna** example illustrates how to **activate** the simulation of water radiolysis ([step-by-step method](#)).
- The « **chem2** » **extended/medical/dna** example illustrates how to **set minimum time step** limits on water radiolysis ([step-by-step method](#)).
- The « **chem3** » **extended/medical/dna** example illustrates how to **implement user actions** in the chemistry module ([step-by-step method](#)).
- The « **chem4** » **extended/medical/dna** example illustrates how to **compute radiochemical yields ("G") versus time**, including a dedicated ROOT graphical interface ([step-by-step method](#)).
- The « **chem5** » **extended/medical/dna** example illustrates how to **compute radiochemical yields ("G") versus time**, using alternative physics and chemistry lists ([step-by-step method](#)).
- The « **chem6** » **extended/medical/dna** example illustrates how to **compute radiochemical yields ("G") versus time and LET** using [IRT method](#).
- The « **scavenger** » **extended/medical/dna** 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 μ s post-irradiation.

Towards FLASH simulations...

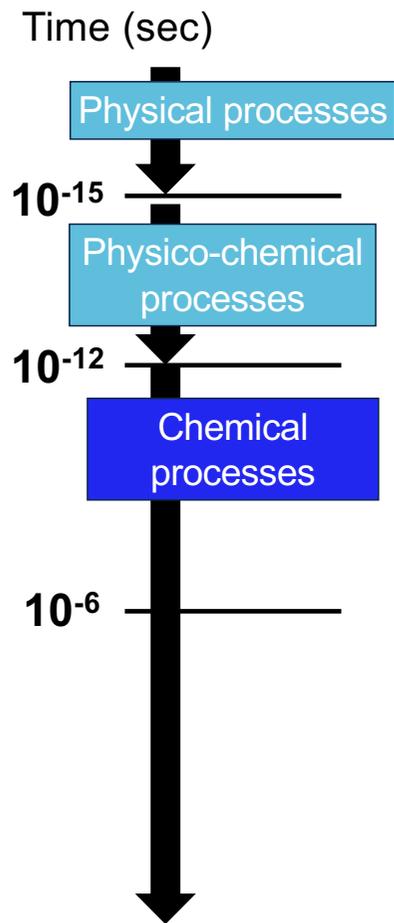
You remember, chemistry interface needed



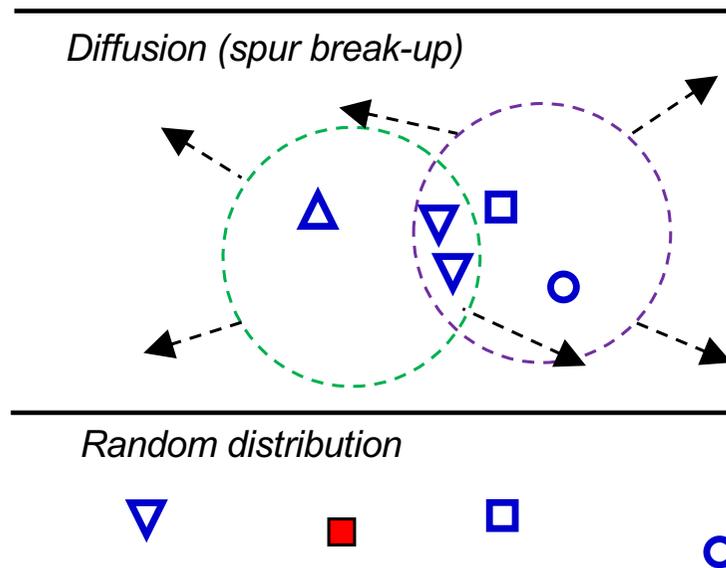
Chemistry / Physico-chemical stage: Molecule production



Chemistry / Chemical stage: Diffusion of molecules



- After the physico-chemical stage, molecules **diffuse, breaking-up spurs**.
- Finally, the molecules are distributed **homogeneously**, after 1 μs from irradiation.
- Geant4-DNA uses a table to control the diffusion speed. The user can change these values.



Species	Diffusion coefficient D ($10^{-9} \text{ m}^2 \text{ s}^{-1}$)
H_3O^+	9.0
$\text{H}\cdot$	7.0
OH^-	5.0
e^-_{aq}	4.9
H_2	5.0
$\cdot\text{OH}$	2.8
H_2O_2	1.4
H_2O	2.0

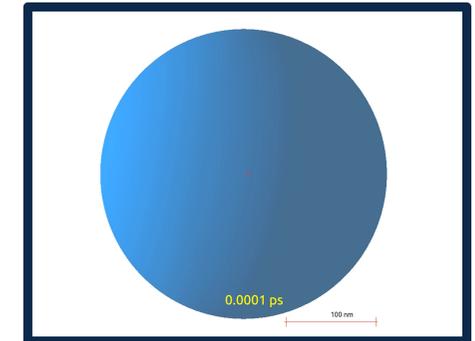
Ref: [J. Comput. Phys. 274, 841-882 \(2014\)](#)

See more details in Chemistry talk

Chemistry / Chemical stage: Diffusion of molecules

■ SBS (Step-By-Step)

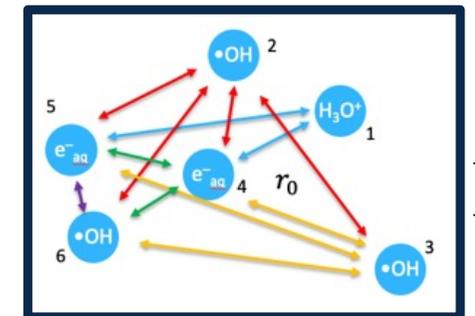
- **Brownian transport** of molecules using the Smoluchowski model
- Chemical species are represented by point objects which diffuse in the liquid medium (continuum). Chemical reactions are « **controlled by diffusion** »: two reactants interact when their separation is smaller than the reaction radius, which is calculated from the rate constant of the reaction.
- *8 species, 9 chemical reactions*



+: Tracking of species
-: Very slow & memory cons.

■ IRT (Independent Reaction Time)

- From the 1980's by Clifford, Green et al., **widely used today**.
- Iterative process where the approximation of « **independent pairs** » is assumed: calculates the reaction times between all possible pairs of reactive species, as if they were isolated. Then, reactions occur one by one, starting with the pairs having the **shortest reaction times**.
- No longer necessary to diffuse the chemical species and to calculate the possible reactions between the species at each time step.
- *15 species, 72 chemical reactions (totally & partially diff. controlled)*
- A « **synchronous** » alternative hybrid version (« IRT-sync ») which gives all spatio-temporal info. on radicals required for combination with geometries

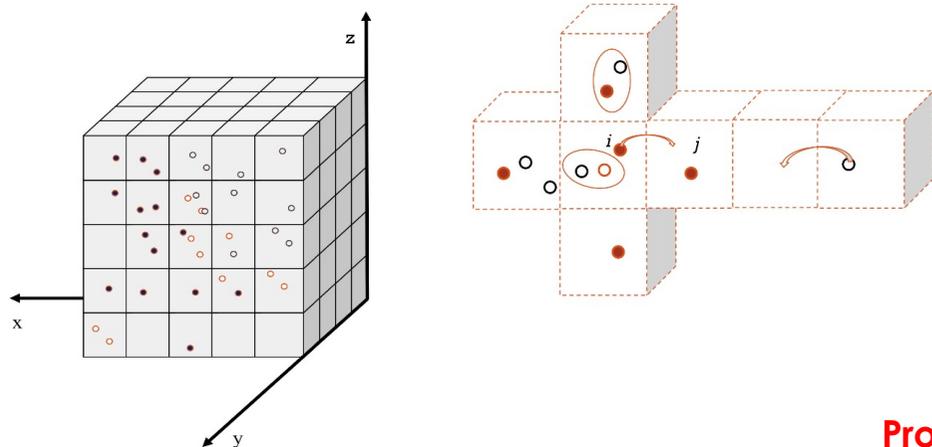
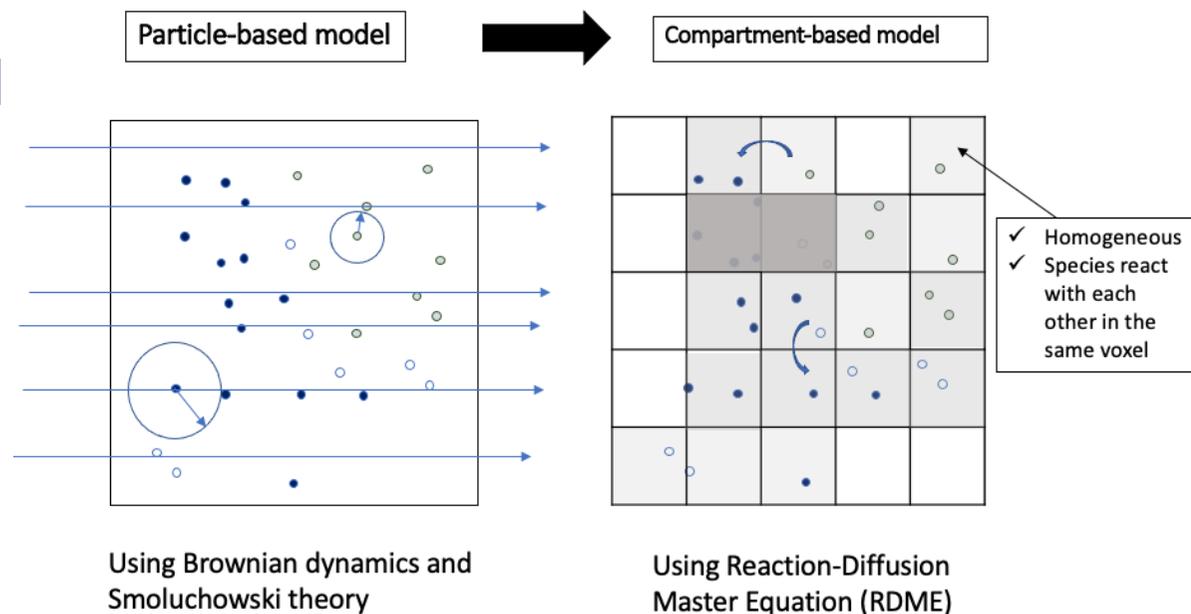


+: Very fast
-: Tracking of species

Clifford et al. (1986)

The “mesoscopic” model

- For SBS, IRT model, computation time remains the main drawback when simulations deal with a **large number of species** or **long-time scales**.
- An alternative approach has recently been implemented in Geant4-DNA using the **compartment-based** representation

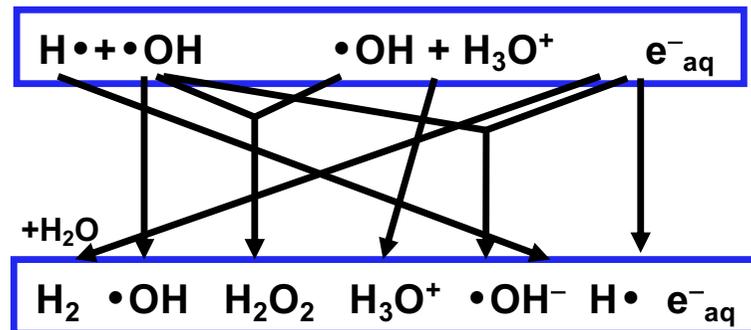
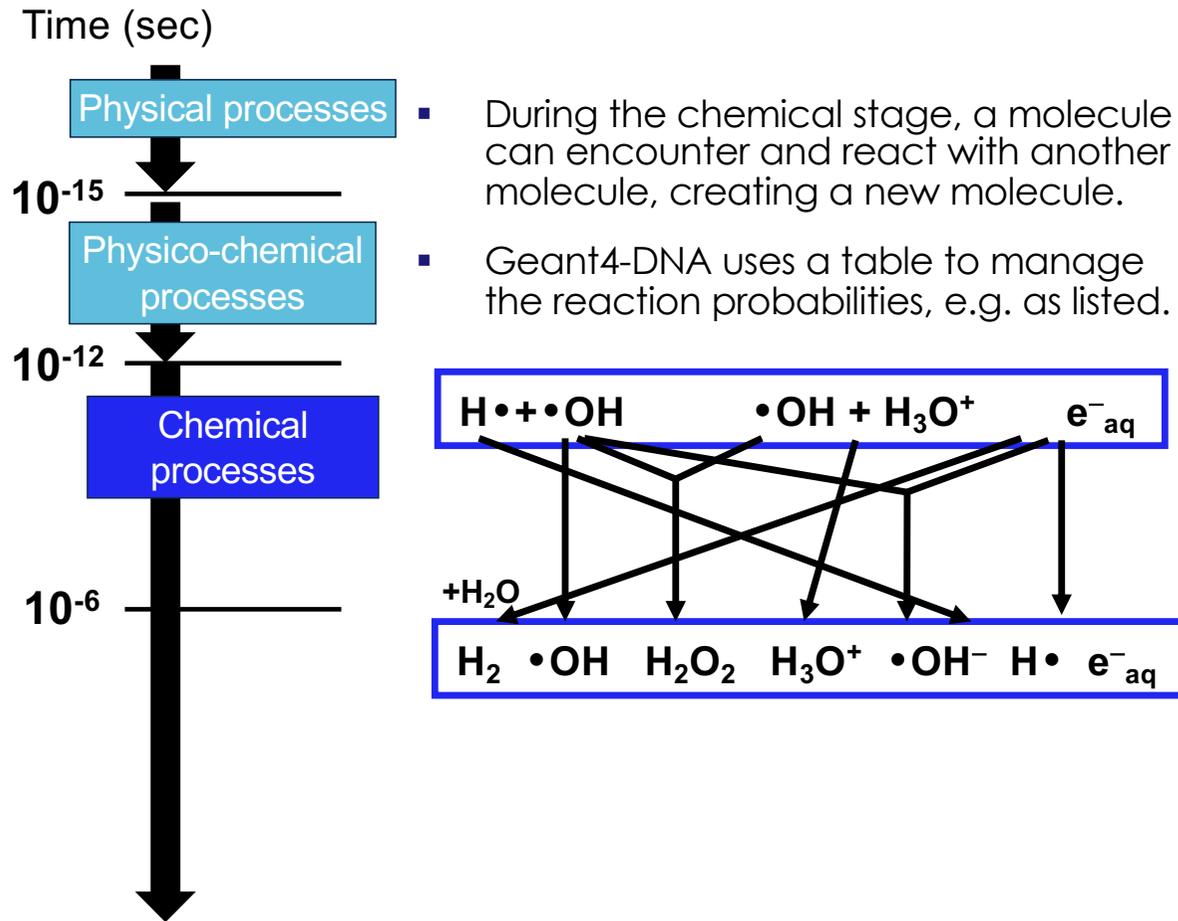


- Well-mixed species in voxels
- Species can react with each other in the voxels
- Diffusion is modelled by jumps between adjacent voxels

Promising approach for ultra-high dose rate radiolysis simulations...

See more details in Chemistry talk

Chemistry / Chemical stage: Reactions

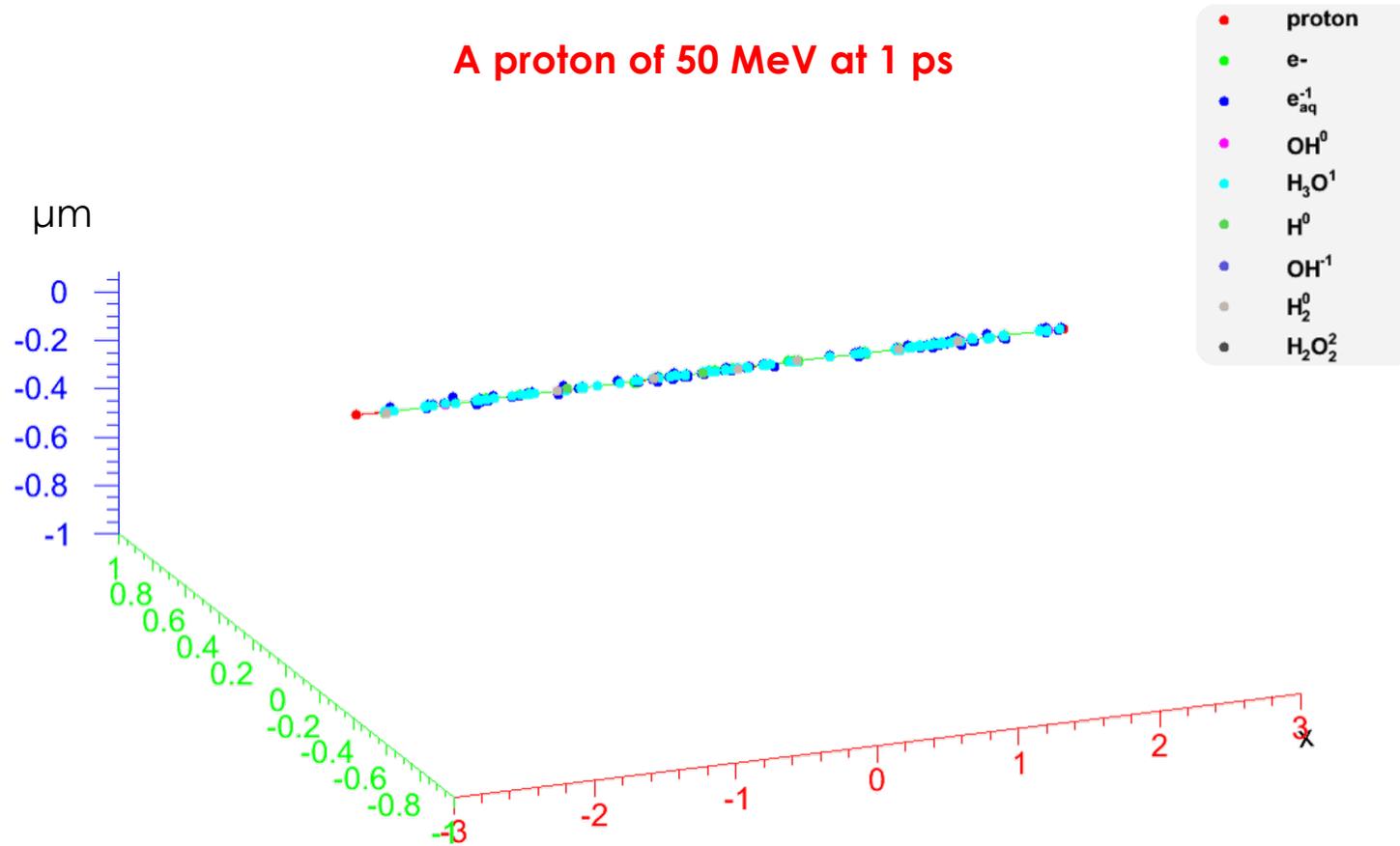


Reaction	Reaction rate (10 ⁷ m ³ mol ⁻¹ s ⁻¹)
$H_3O^+ + OH^- \rightarrow 2 H_2O$	14.3
$\bullet OH + e^-_{aq} \rightarrow OH^-$	2.95
$H\bullet + e^-_{aq} + H_2O \rightarrow OH^- + H_2$	2.65
$H_3O^+ + e^-_{aq} \rightarrow H\bullet + H_2O$	2.11
$H\bullet + \bullet OH \rightarrow H_2O$	1.44
$H_2O_2 + e^-_{aq} \rightarrow OH^- + \bullet OH$	1.41
$H\bullet + H\bullet \rightarrow H_2$	1.20
$e^-_{aq} + e^-_{aq} + 2 H_2O \rightarrow 2 OH^- + H_2$	0.50
$\bullet OH + \bullet OH \rightarrow H_2O_2$	0.44

Ref: [J. Comput. Phys. 274, 841-882 \(2014\)](#)

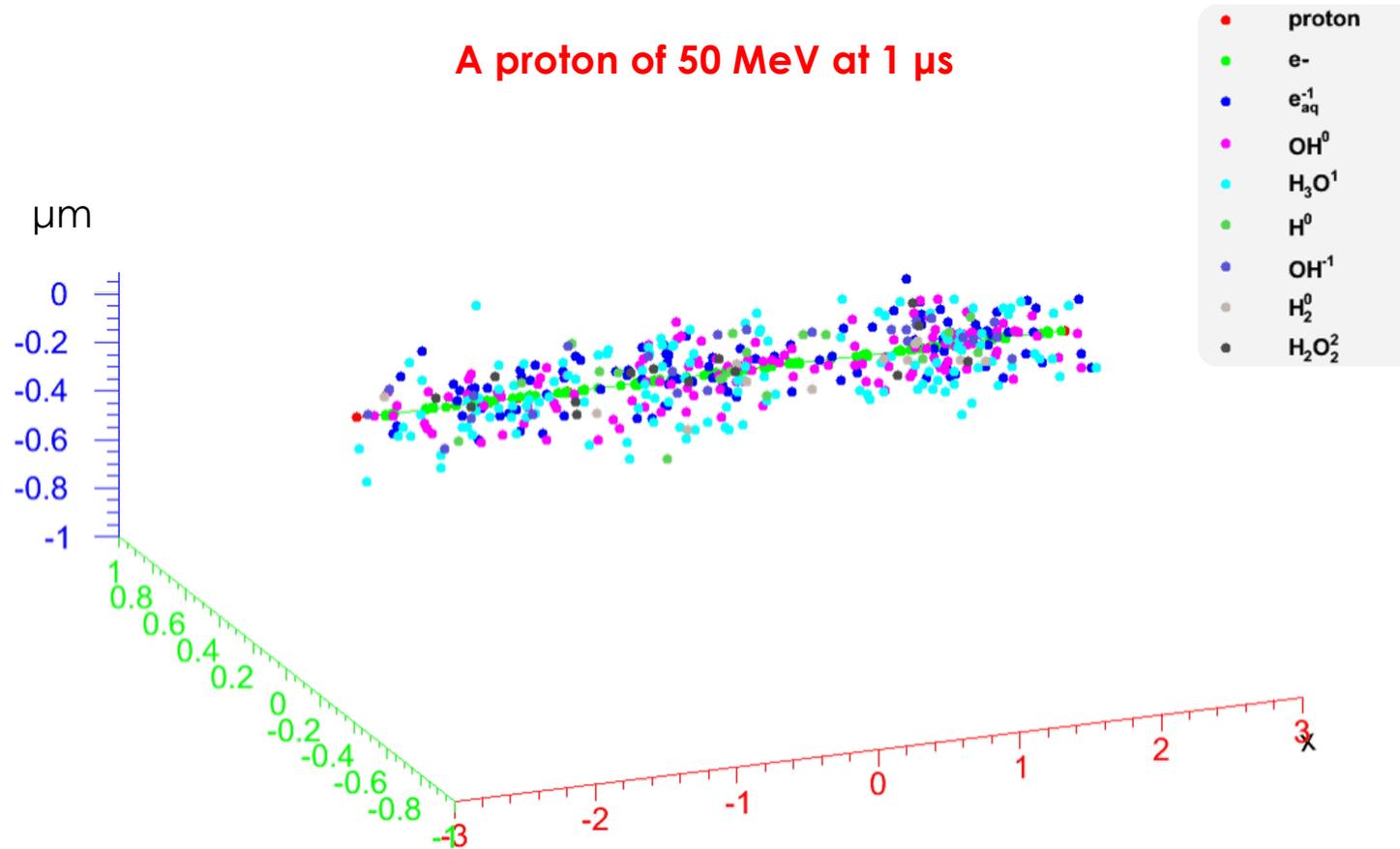
Distribution of chemical molecules using Geant4-DNA

A proton of 50 MeV at 1 ps

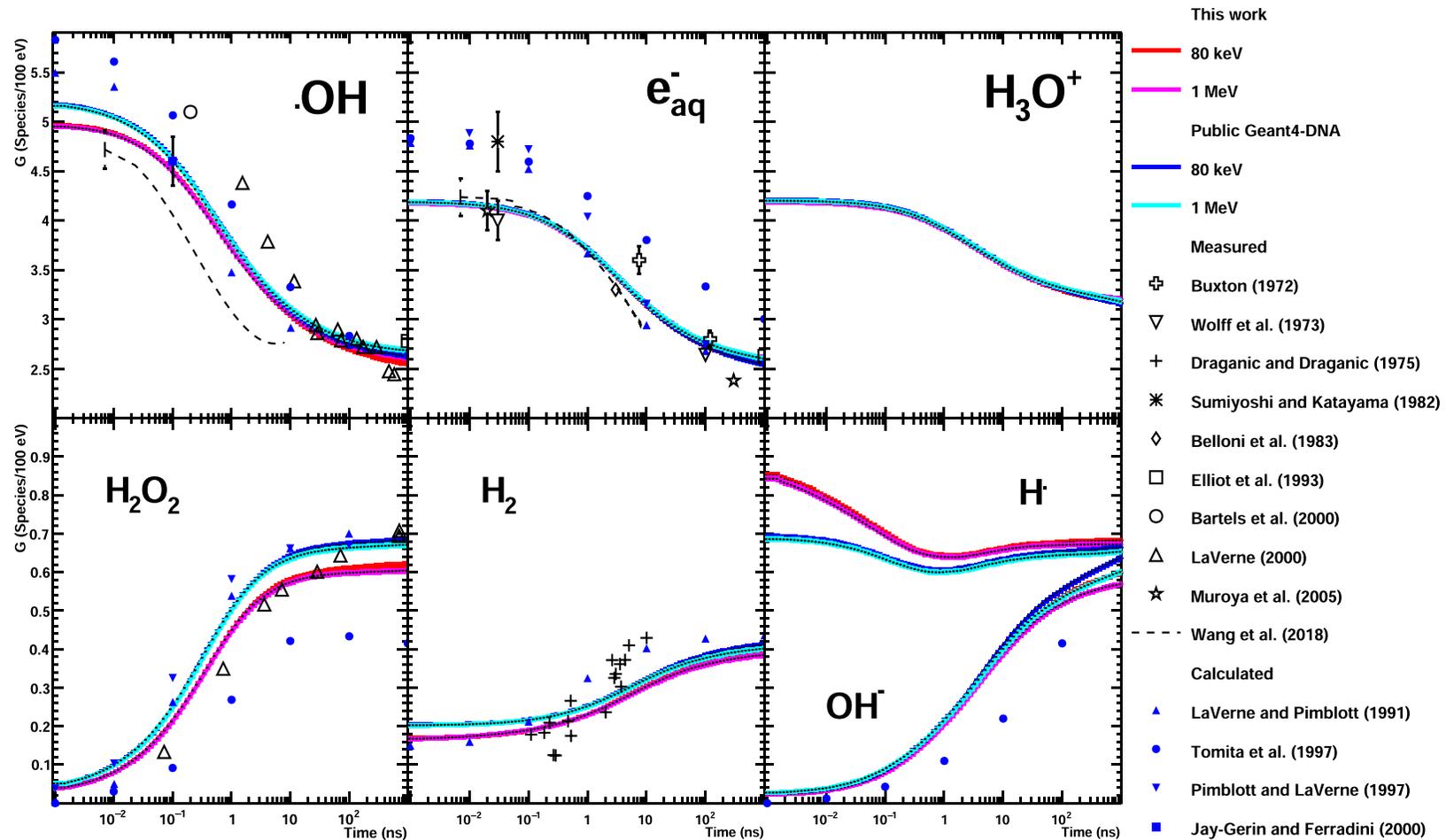


Distribution of chemical molecules using Geant4-DNA

A proton of 50 MeV at 1 μs

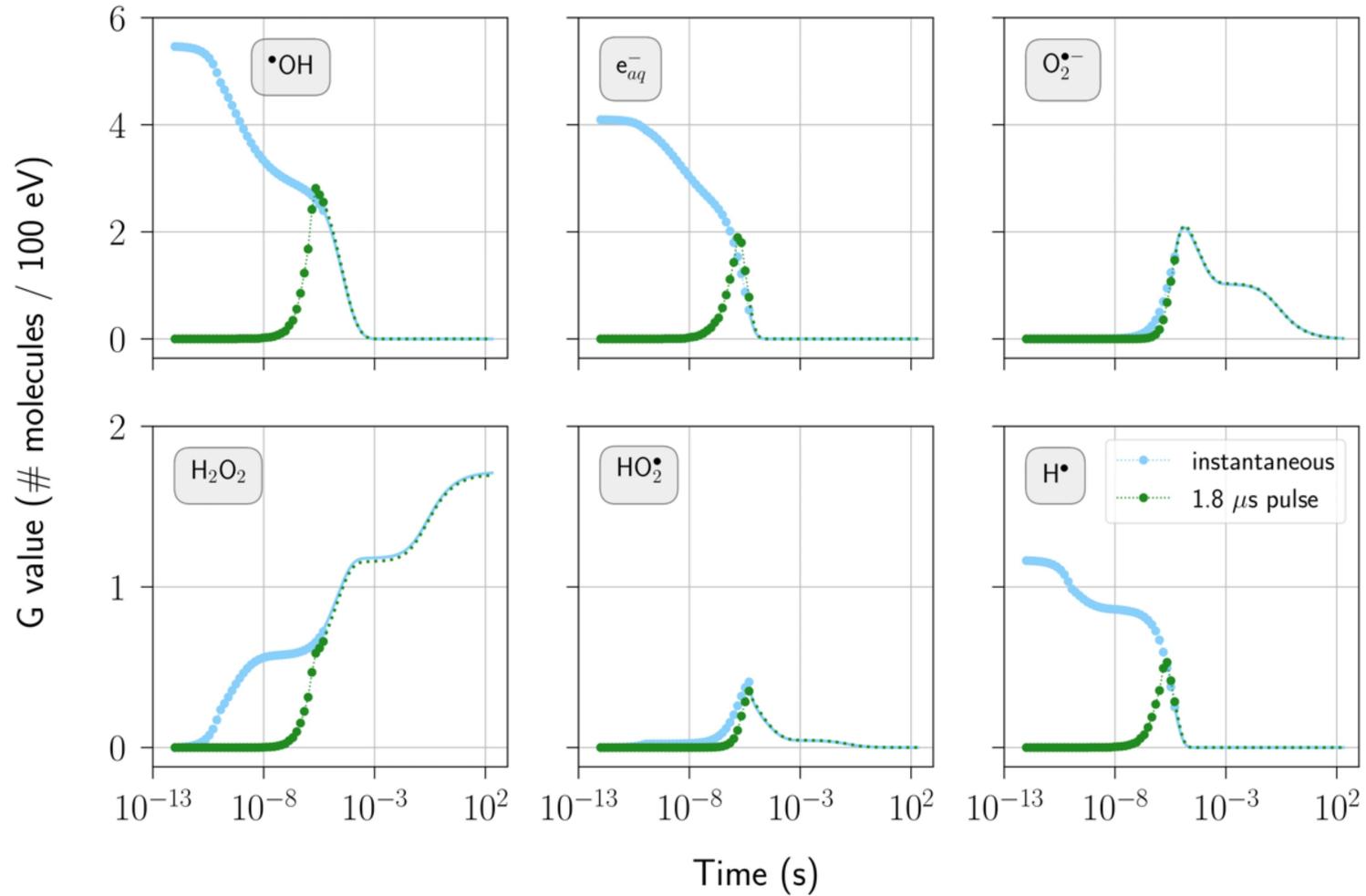


Validation and verification of chemistry: G-value vs time

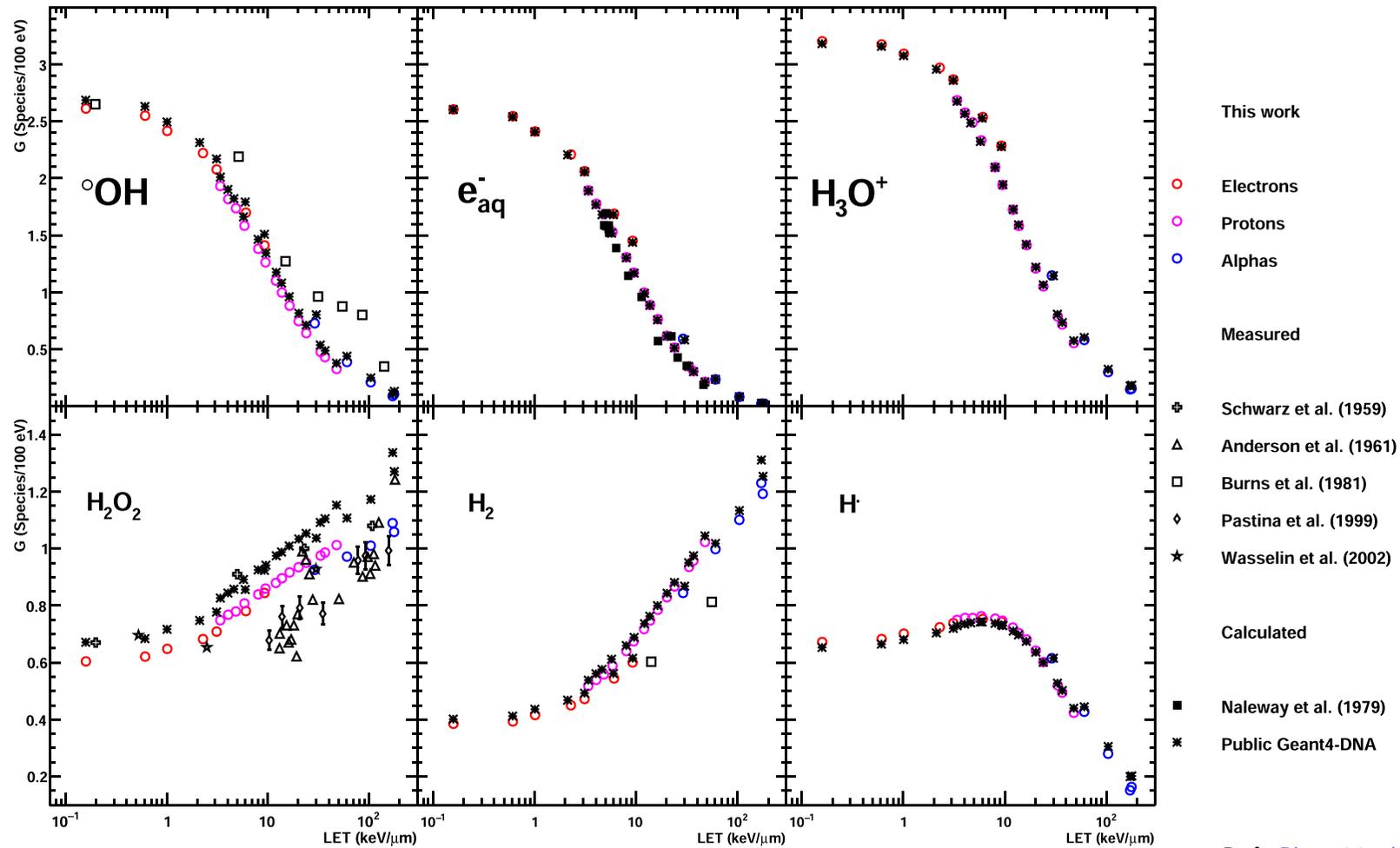


Ref.: [Phys. Med. 88, 86-90 \(2021\)](#)

Validation and verification of chemistry: G-value vs time for FLASH



Validation and verification of chemistry: G-value vs LET

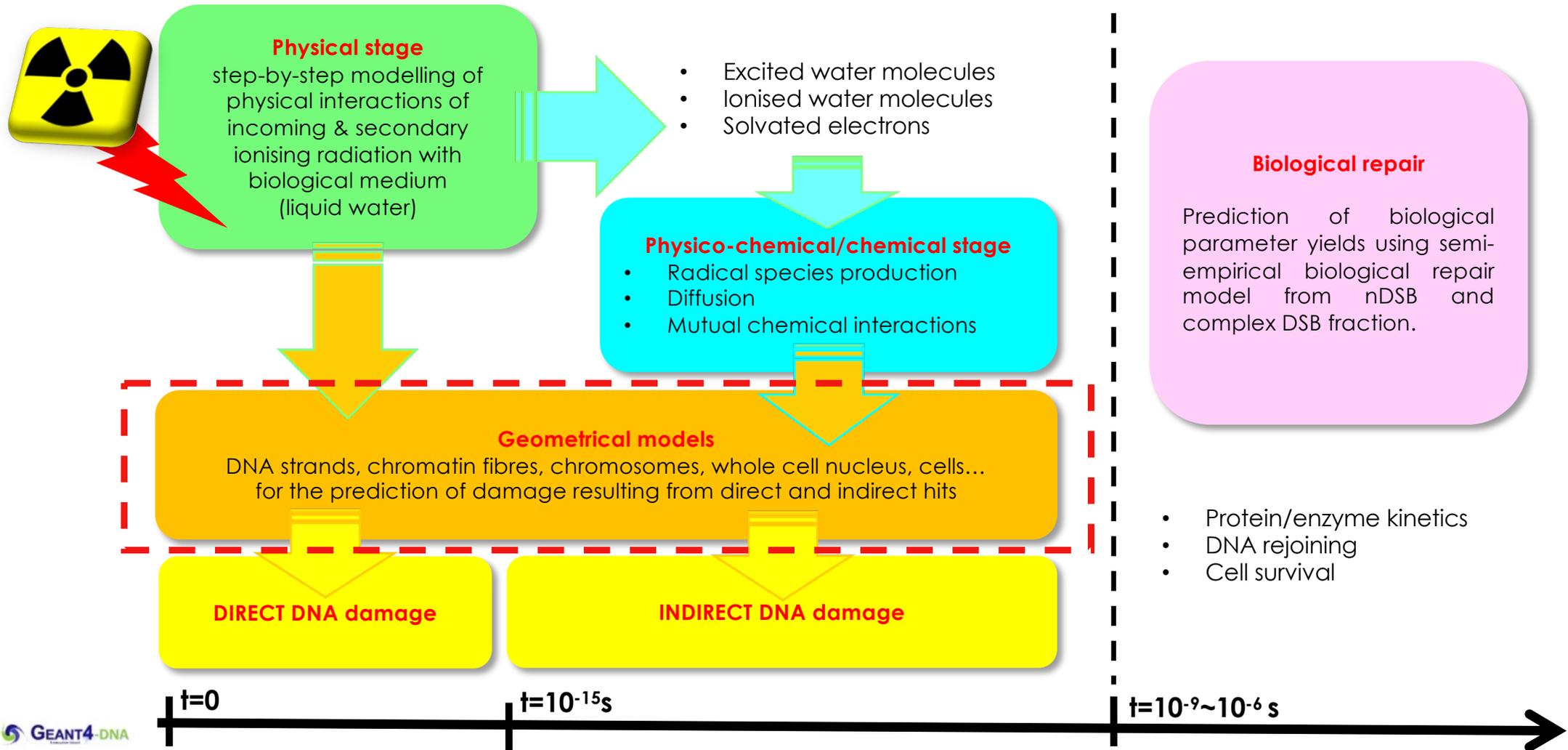


Ref.: [Phys. Med. 88, 86-90 \(2021\)](#)

Contents of this talk

- Context of the Geant4-DNA project
- Physical stage
- Physico-chemical & chemical stage
- **Geometrical models**
- DNA damage and biological models
- More...

The Geant4-DNA approach

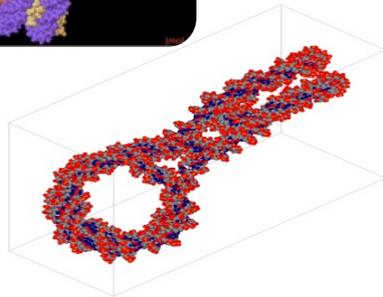
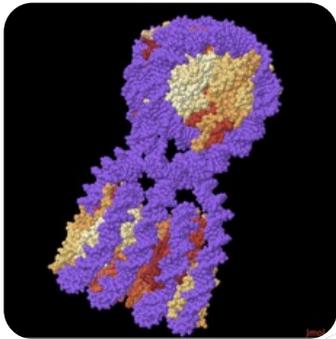


Geant4-DNA geometry models (in examples)



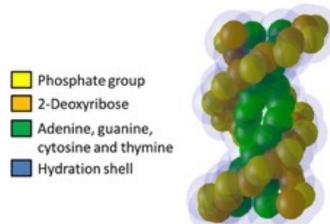
Atomic scale

- `pdb4dna`

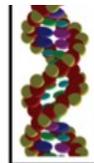


Molecular scale

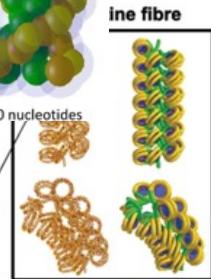
- `wholeNuclearDNA`
- `dnadamage1,2`
- `dsbandrepair`
- `molecularDNA`



- Phosphate group
- 2-Deoxyribose
- Adenine, guanine, cytosine and thymine
- Hydration shell



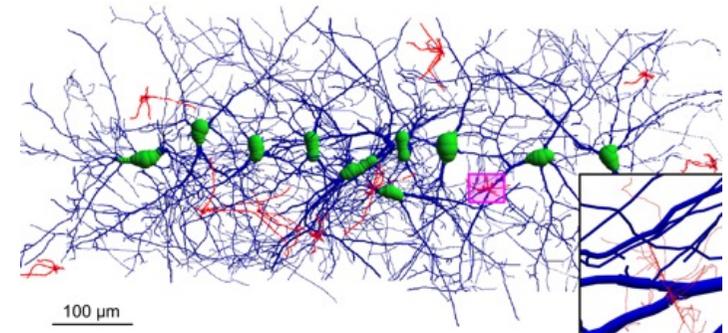
20 nucleotides



line fibre

Fractal geometry

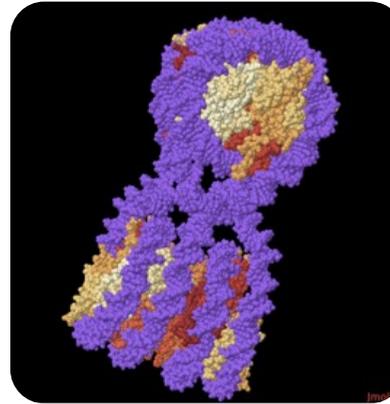
Cell nucleus



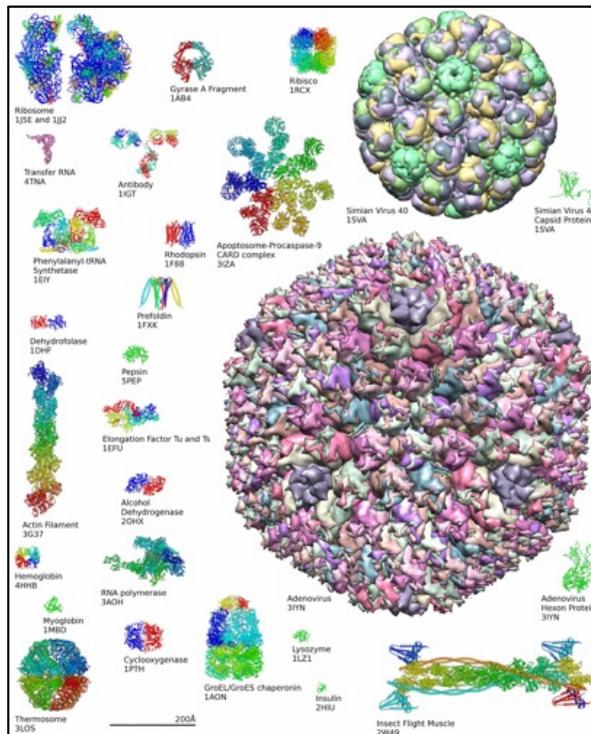
Geometry: Atomic scale pdb4dna example

- Protein Data Bank (PDB)
<http://www.rcsb.org/pdb/>
 - 3D structure of molecules
 - Proteins
 - Nucleic acids

Ref.: [Comput. Phys. Commun. 192, 282-288 \(2015\)](#)



- E.g.: **1ZBB.pdb**
- Tetranucleosome
 - 2 nucleosomes: 347 pairs of bases
 - (9,5 x 15,0 x 25,1 nm³)



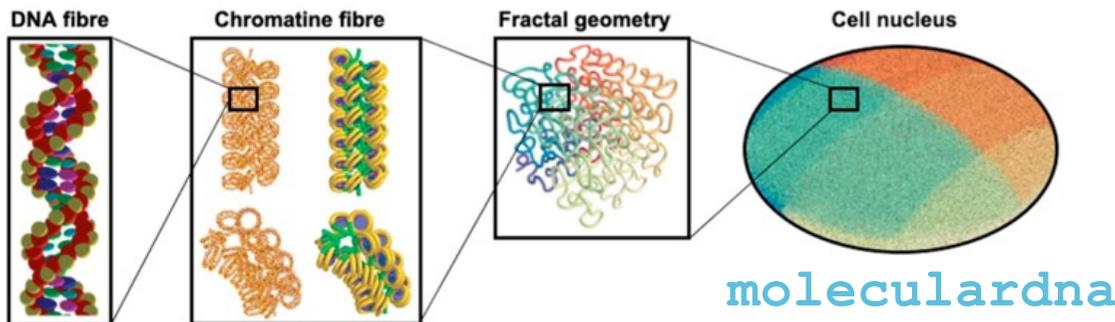
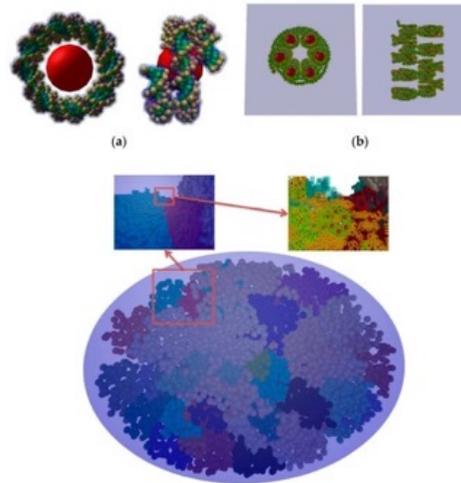
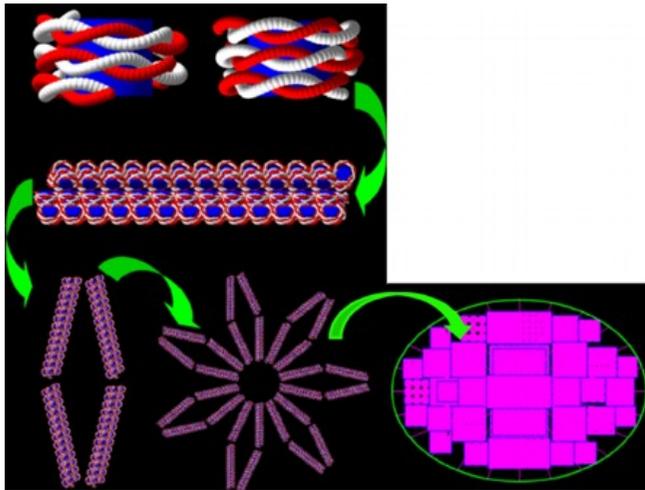
HEADER	STRUCTURAL PROTEIN/DNA						08-APR-05	1ZBB		
TITLE	STRUCTURE OF THE 4_601_167 TETRANUCLEOSOME									
...										
ATOM	1	O5'	DA	I	1	70.094	16.969	123.433	0.50238.00	O
ATOM	2	C5'	DA	I	1	70.682	18.216	123.054	0.50238.00	C
ATOM	3	C4'	DA	I	1	69.655	19.289	122.776	0.50238.00	C
...										
TER	14223				DT J 347					
...										
HELIX	1	1	GLY A	44	SER A	57	1			14
HELIX	2	2	ARG A	63	ASP A	77	1			15
...										
SHEET	1	A	2	ARG A	83	PHE A	84	0		
SHEET	2	A	2	THR B	80	VAL B	81	1	O	VAL B 81 N ARG A 83

See implementation in
geant4/examples/extended/medical/dna/pdb4dna

See <http://geant4-dna.org> → Examples

Geometry: Molecular scale

wholeNuclearDNA



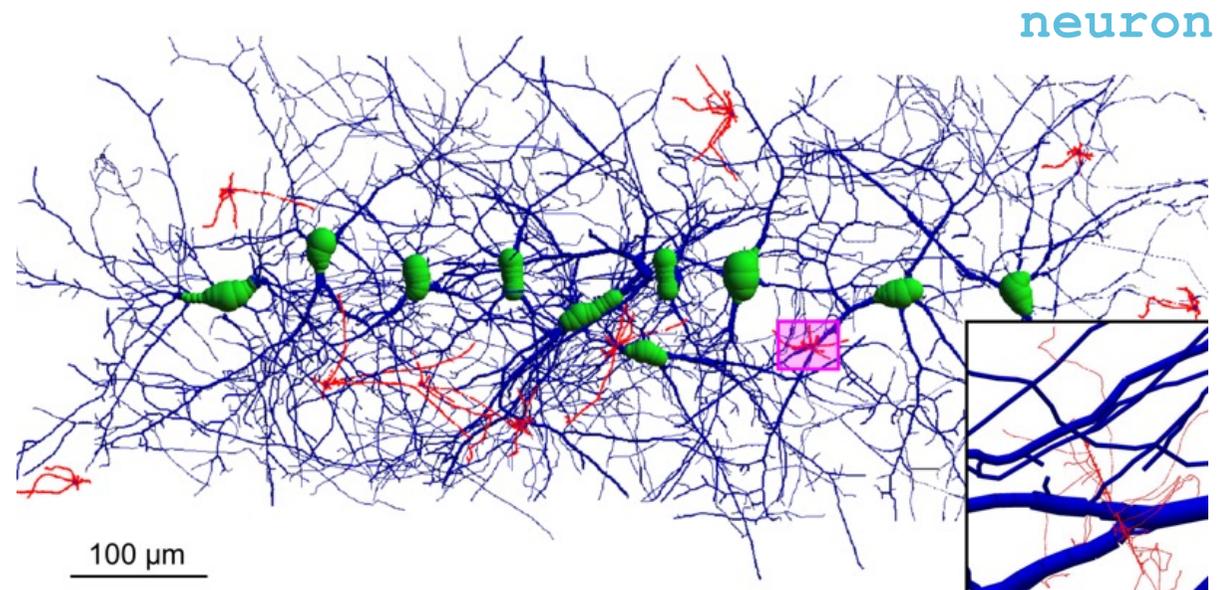
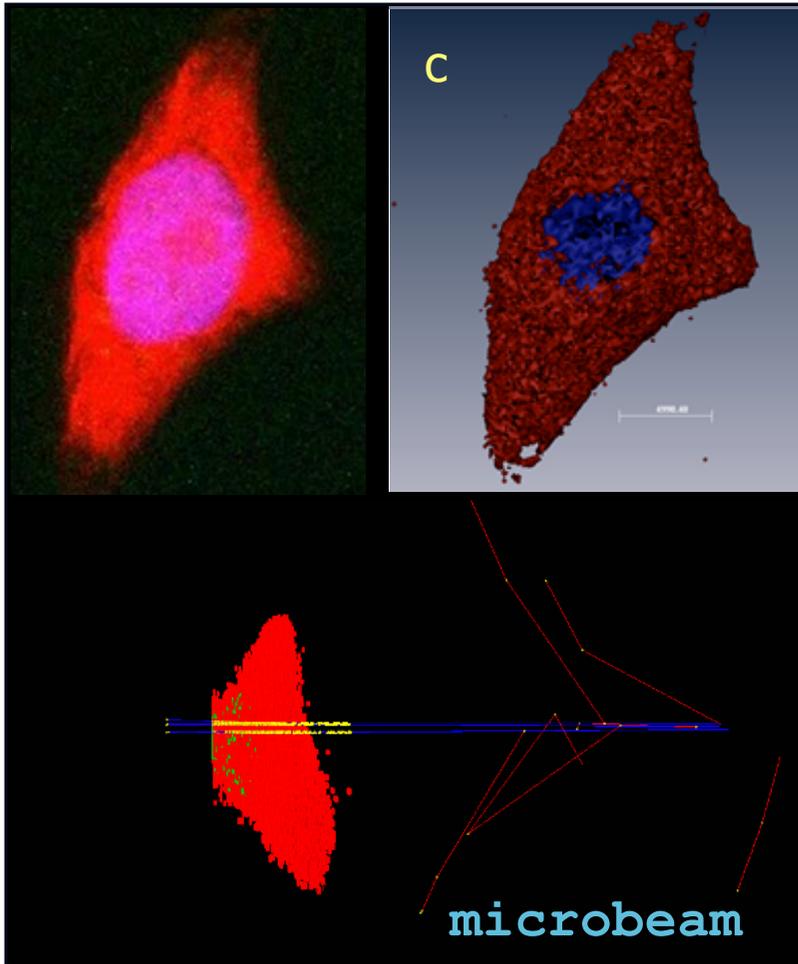
- Geant4-DNA offers **5 examples** of cell nucleus models, which consist of molecular-based DNA geometry models

- `wholeNuclearDNA*`
- `dnadamage1,2`
- `dsbandrepair`
- `moleculardna`

- These examples offer the possibility of simulating the **water radiolysis*** as well as the **energy deposition** of ionizing radiation at a nanometric scale within a geometrical representation of the **whole DNA molecule contained in a cell nucleus.**

See <http://geant4-dna.org> → Examples

Geometry: Cellular scale or Larger



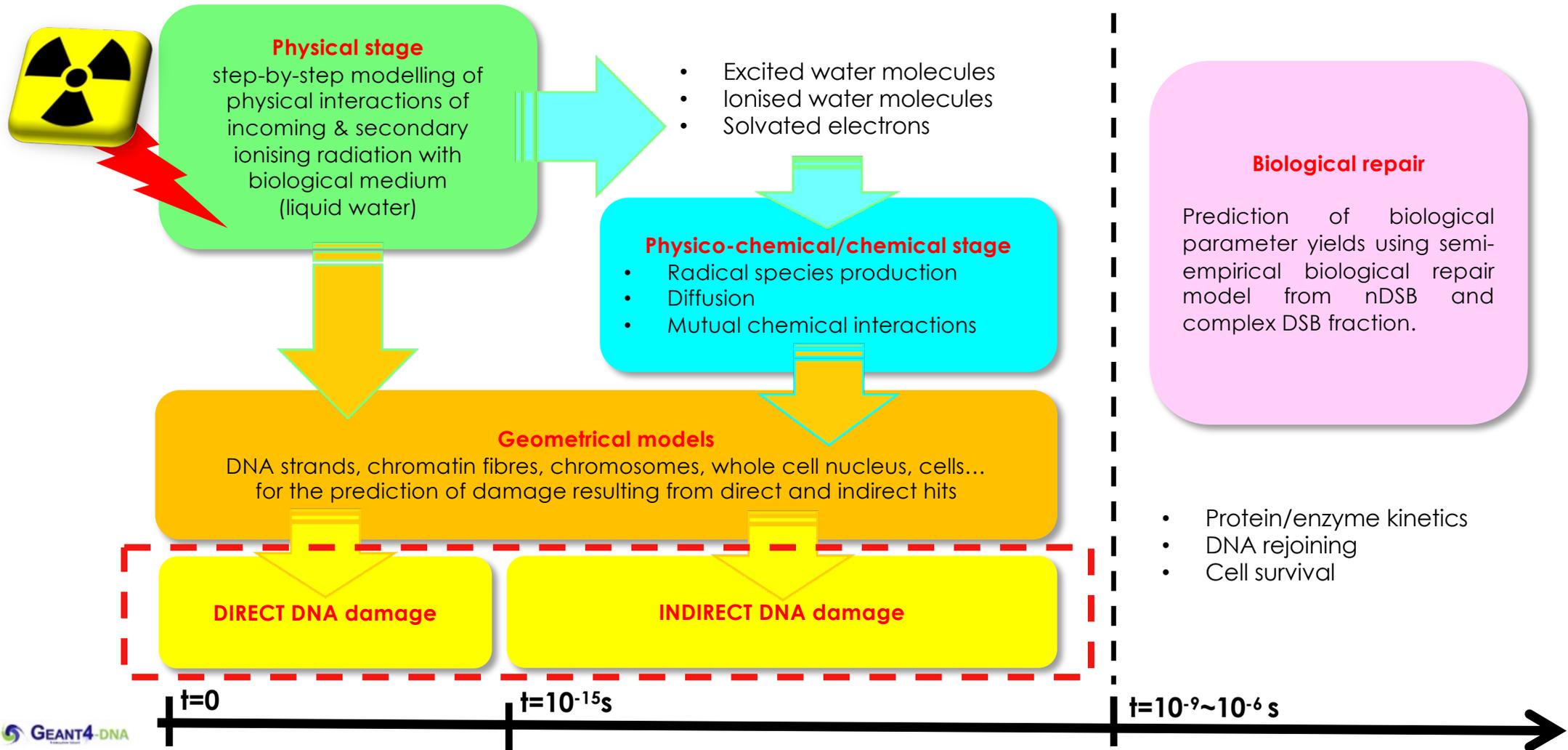
- Geant4-DNA also offers 2 examples that provide realistic geometry of a cell and neurons:
 - **microbeam**
 - **neuron**

See <http://geant4-dna.org> → Examples

Contents of this talk

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- More...

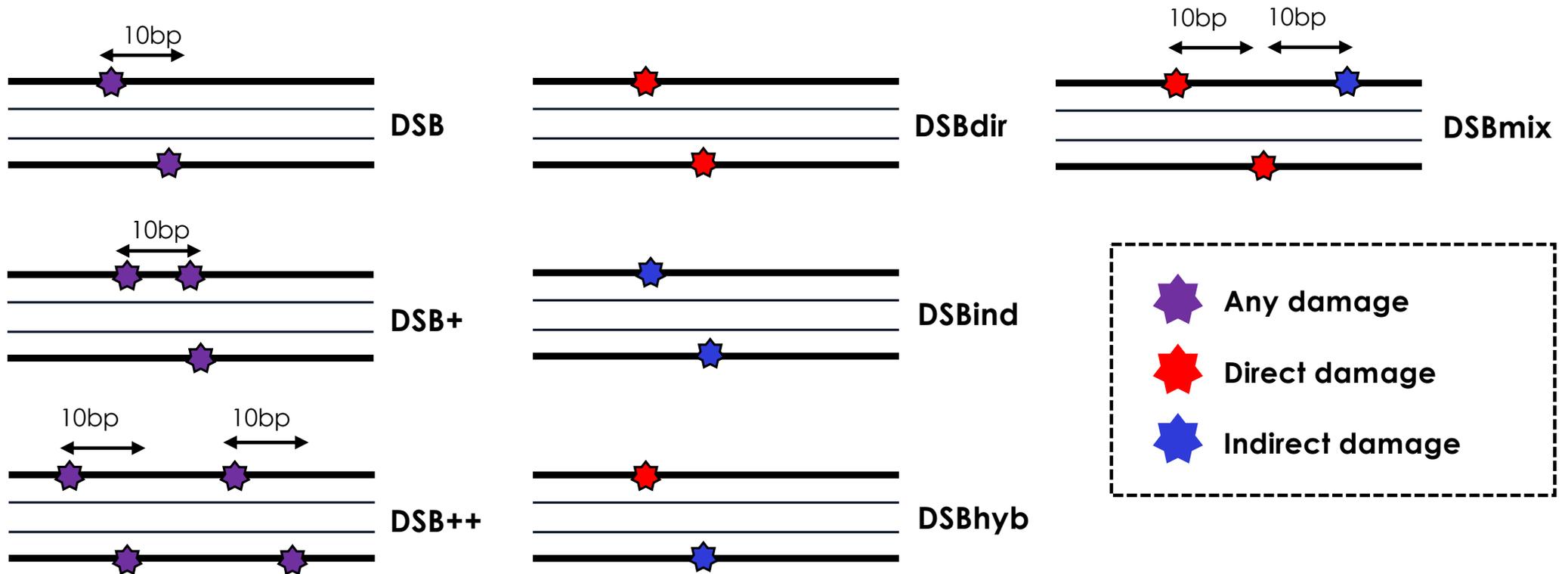
The Geant4-DNA approach



DNA damage and biological models

- Geant4-DNA follows a **standard** DNA damage calculation approach:
 - **Direct action: Structural damage to DNA molecules induced by excitation/ionisation processes**
 - Score local energy deposition in a nanoscopic domain: nanodosimetric approach
 - Two damage probability models are commonly used:
 - **Threshold** model (KURBUC model)
 - **Proportional** model (PARTRAC model)
 - **Indirect action: Structural damage to DNA molecules induced by a chemical process**, typically interaction with reactive oxygen species
 - A **constant probability** model can be used (the probability should be adjusted)
- **DNA damage classification:**
 - The complexity of the DNA damage structure affects the subsequent biological repair process and its endpoint. In particular, two strand breaks within a short distance (leading to physical disconnection of the DNA fiber), so-called **Double Strand Break (DSB)**, induce crucial radiobiological effects such as cell death.
 - Thus, the classification of DNA damage is one of the most important issues in evaluating the radiobiological effects.
 - So far, two classification models are proposed: **Nikjoo's** model and the **Standard DNA Damage (SDD)** model.

Damage classification: Nikjoo's classification





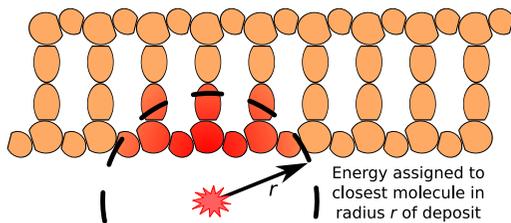
Important:
parameter choice
– e.g. molecular dna

Physics

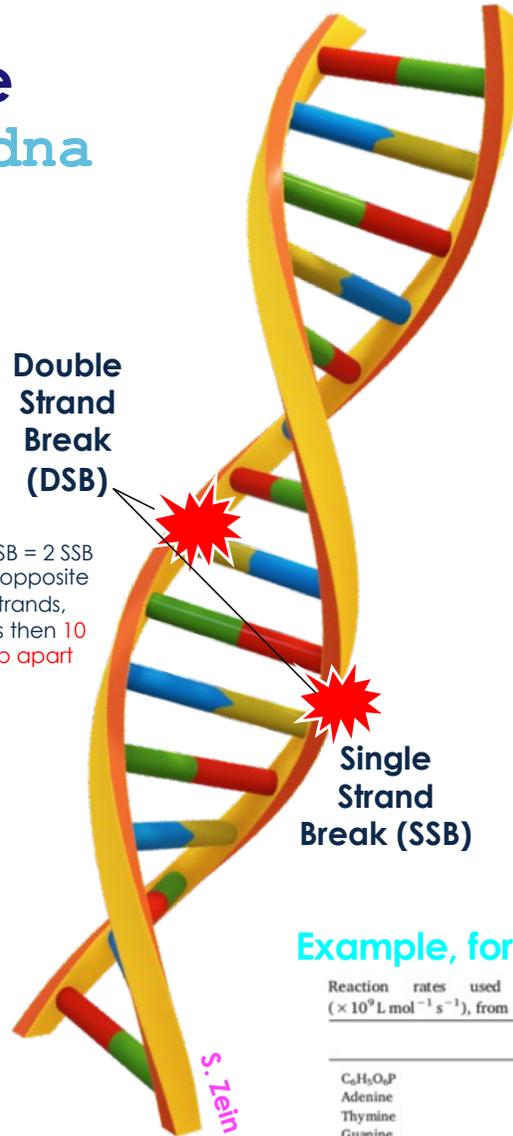
DIRECT damage induction

- Choice of G4DNA physics constructor
- Volume for energy deposition scoring in DNA backbone (S or P molecule)
 - Threshold, linear...
- Probability of Single Strand Break induction in DNA backbone

Example, for item 2:



E.g. 2 Å for ~1 hydration layer



NON-DIRECT damage induction

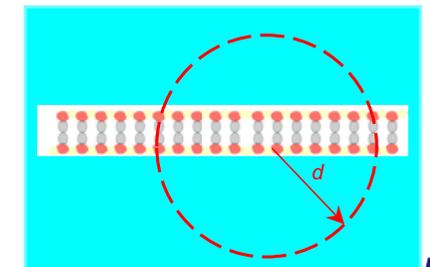
- Choice of G4DNA chemistry constructor
 - Including reactions with DNA components
- Probability of non-direct SSB induction
 - OH on DNA backbone : e.g. 40.5 %
- Distance from DNA to kill radicals (mimic scavenging in cells)
- Histones considered as full scavengers (in cells)
- Radiolysis maximum time steps
- Chemical stage end time

Example, for item 1:

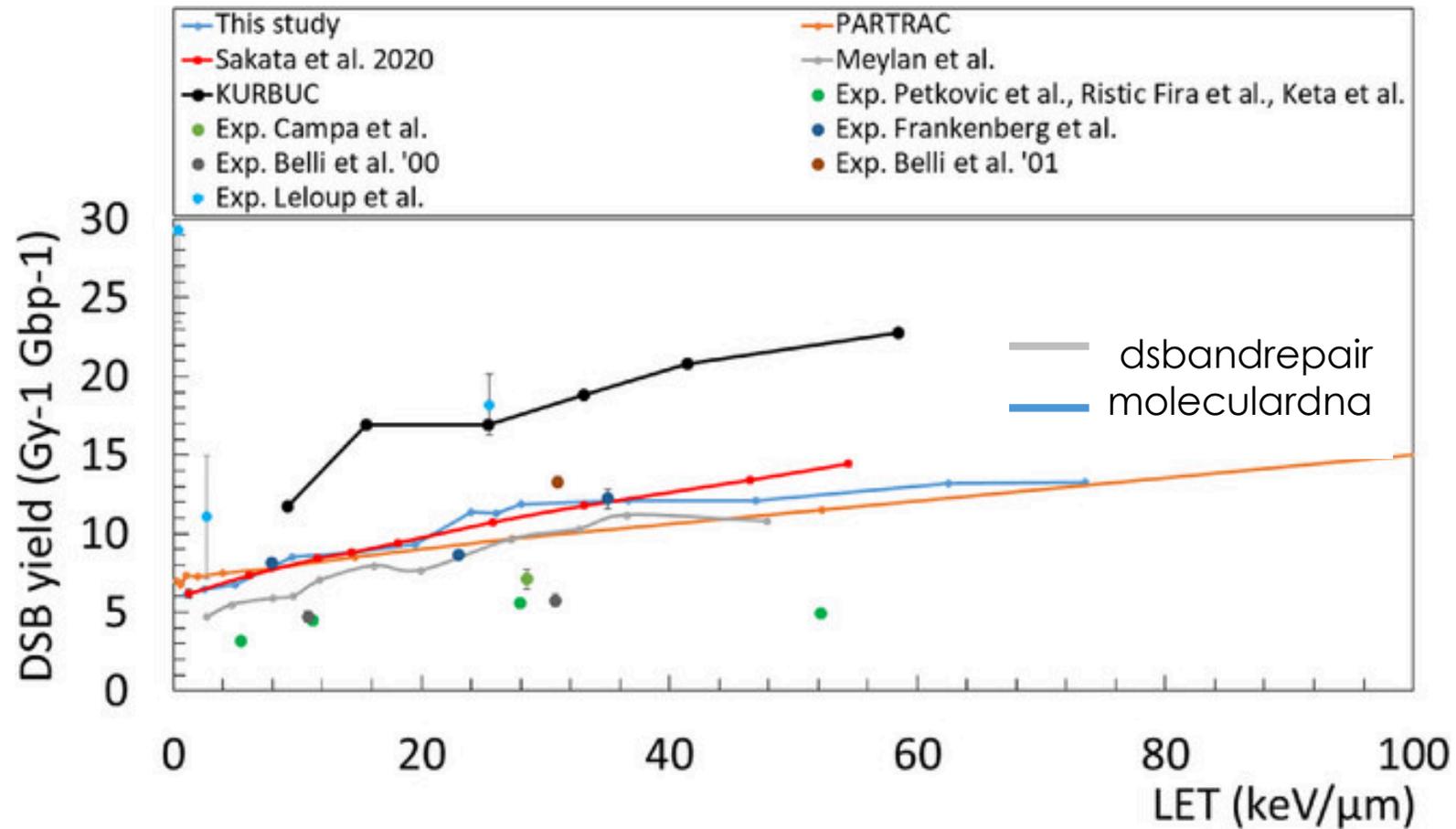
Reaction rates used between radicals and DNA components ($\times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$), from Buxton et al. [65].

	•OH	H•	e_{aq}^-
$C_6H_5O_6P$	1.8	0.029	0.01
Adenine	6.1	0.10	9.0
Thymine	6.4	0.57	18.0
Guanine	9.2	-	14.0
Cytosine	6.1	0.092	13.0

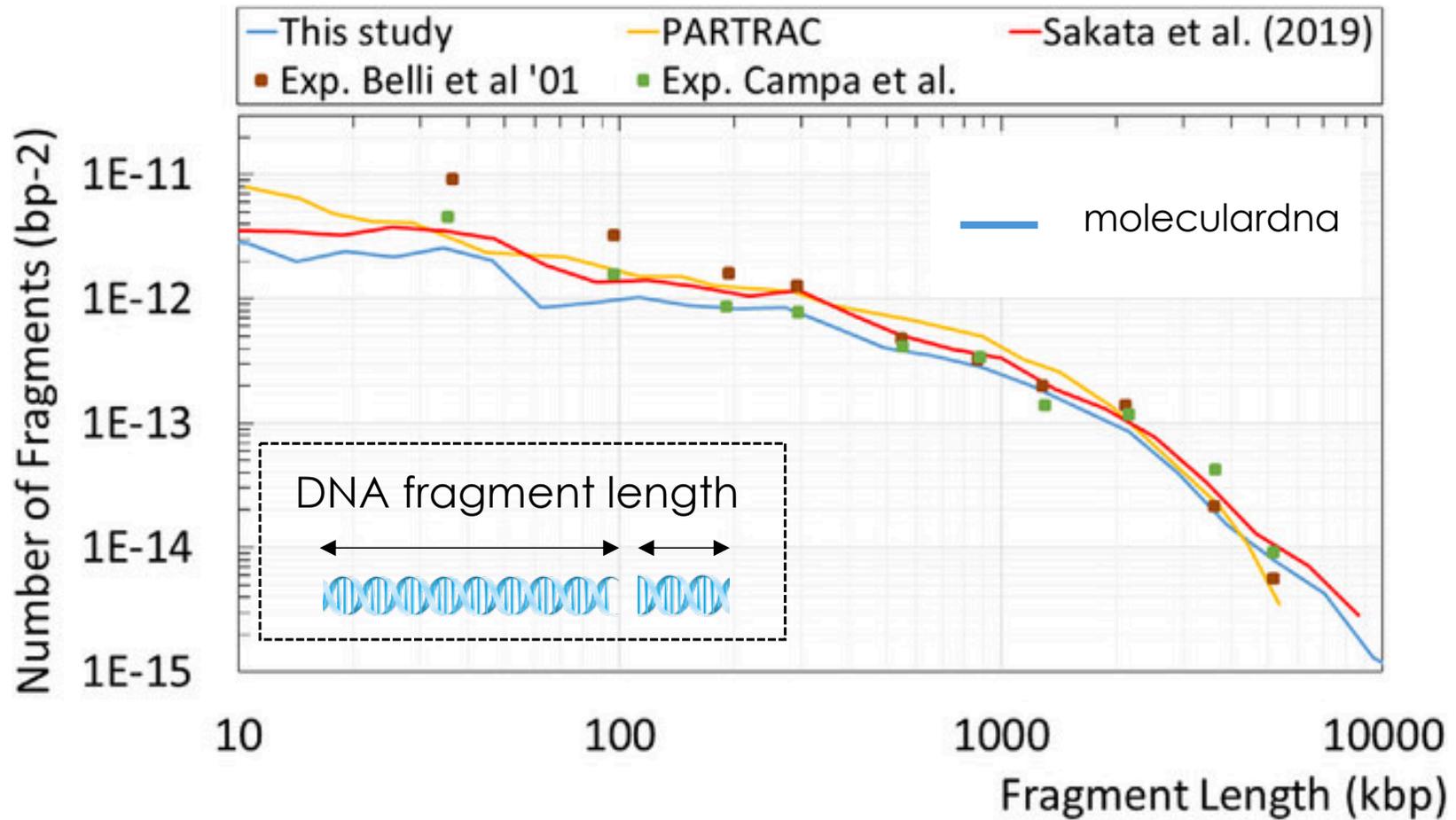
Example, for item 3:



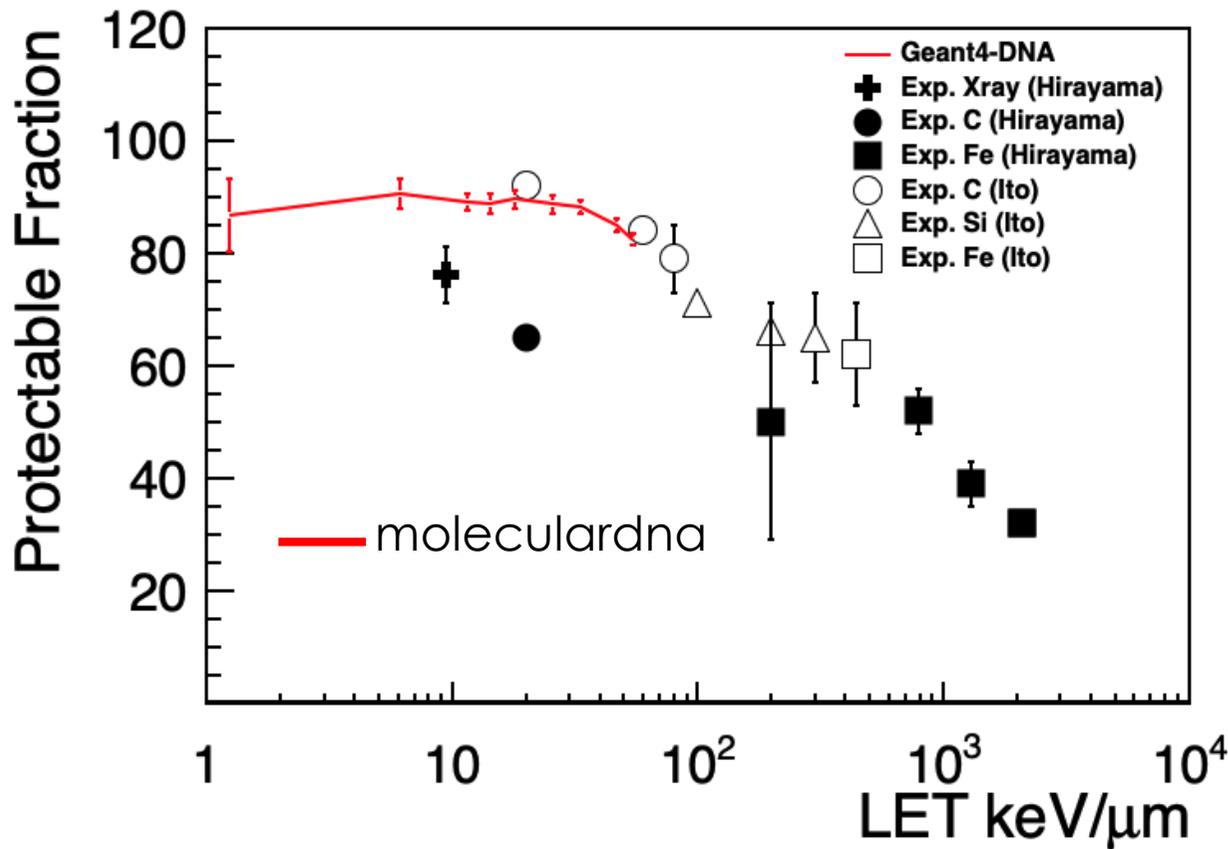
Validation and verification: **Damage** yield from protons



Validation and verification: **Fragment** yield

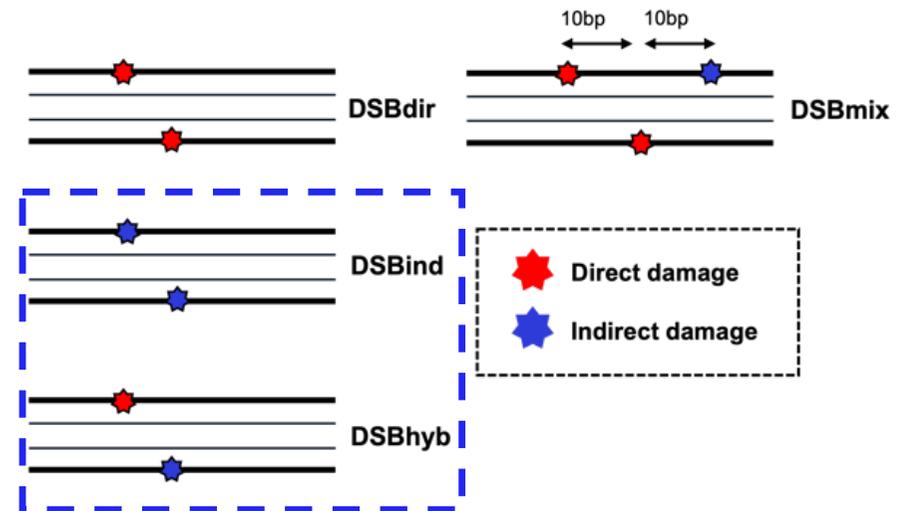


Validation and Verification: Indirect damage fraction

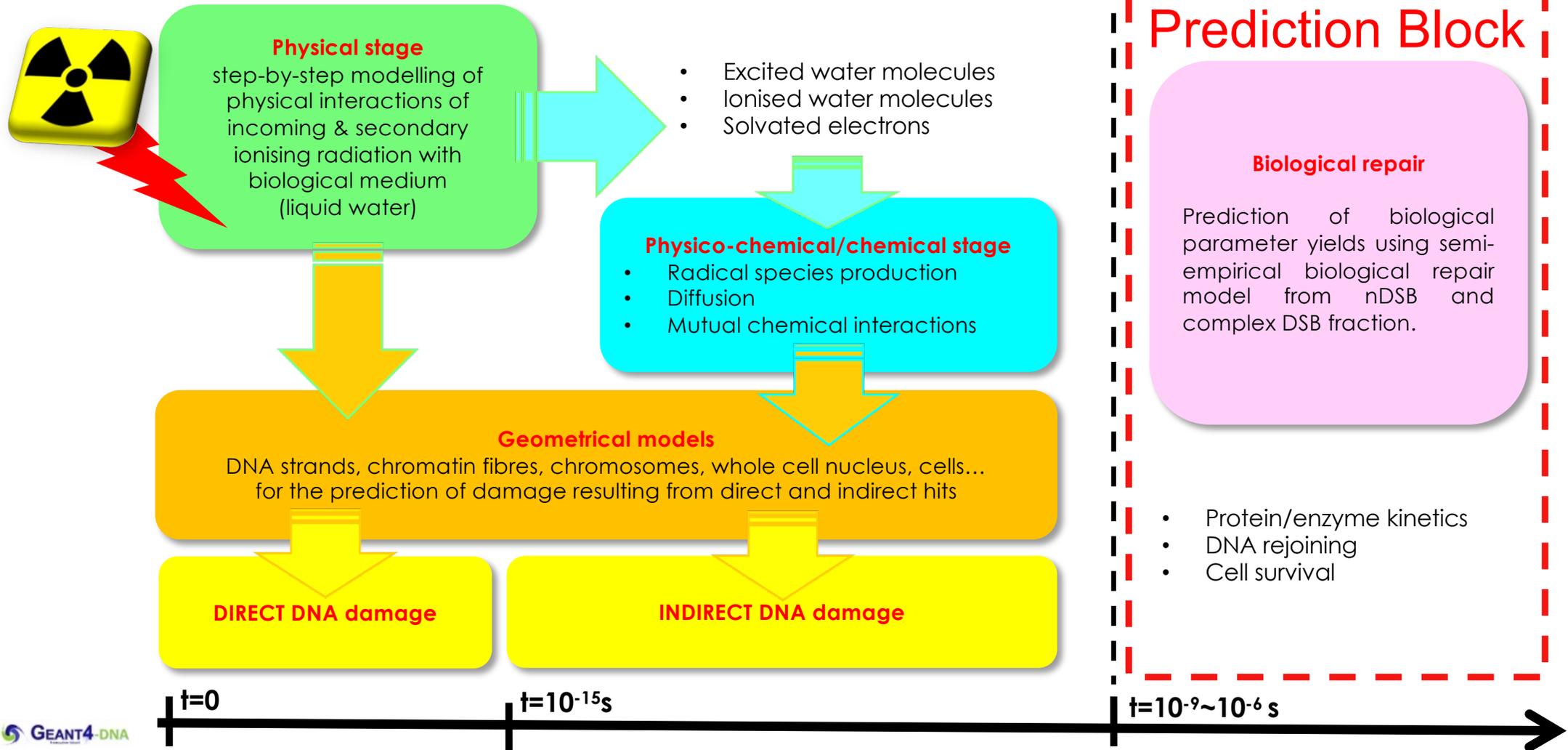


Protectable fraction
(damage type based)

$$\frac{N_{\text{DSB}_{ind}} + N_{\text{DSB}_{hyb}}}{N_{\text{DSB}_{dir}} + N_{\text{DSB}_{mix}} + N_{\text{DSB}_{ind}} + N_{\text{DSB}_{hyb}}}$$



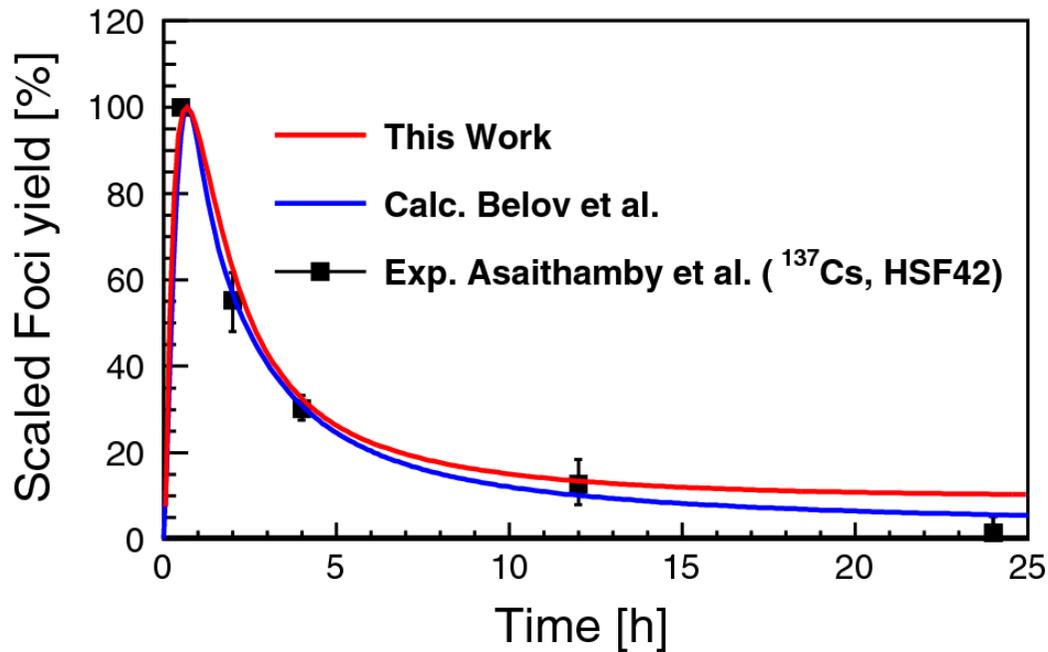
The Geant4-DNA approach



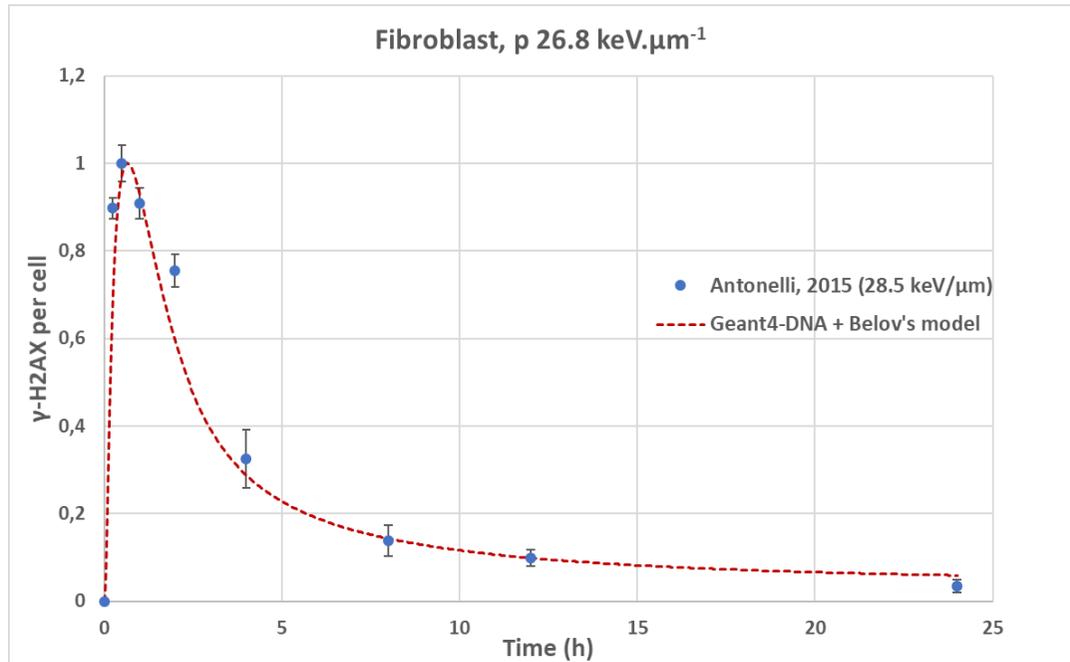
DNA damage and biological models

- Prediction models are able to **link DNA damage to biological endpoints**:
 - **Belov model**: Prediction model of **protein/enzyme accumulation yield** from the number of DSBs and **irreparable fraction**. In Geant4-DNA applications, the irreparable fraction is assumed to be the fraction of complex DSBs w.r.t the total number of DSBs.
 - **Two-Lesion kinetic (TLK)** model: The TLK model links the number of simple-/complex-DSBs and **cell survival**, considering the rejoining of DSBs and lethality of the residual DNA damage.
 - **Local Effect Model (LEM)-IV**: The LEM-IV calculates **cell survival** from a number of lethal damage that considers the induction of DSBs and their spatial distribution and fast-/slow-rejoining of DSBs.
- Geant4-DNA examples offer such biological prediction models:
 - **wholeNuclearDNA**: No biological prediction model provided (Physics only)
 - **dsbandrepair**: Belov model, TLK model and LEM-IV model
 - **moleculardna**: Belov model, TLK model

Validation and verification: time evolution of foci yields



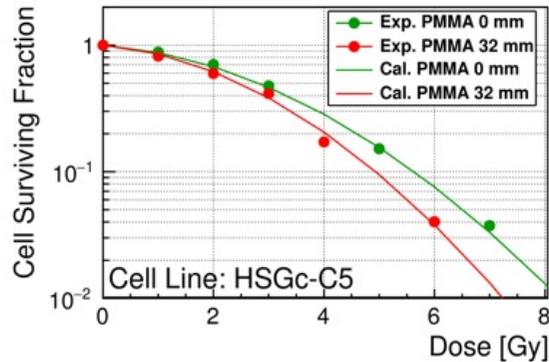
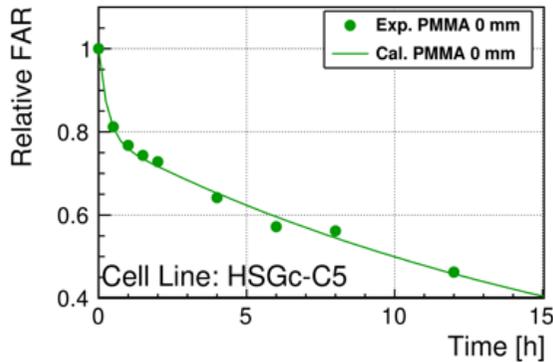
`moleculardna`: for gamma-ray (^{137}Cs)



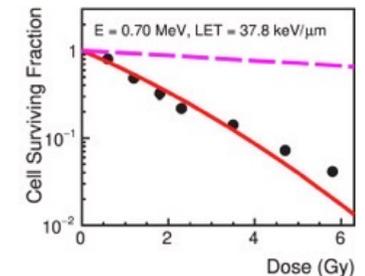
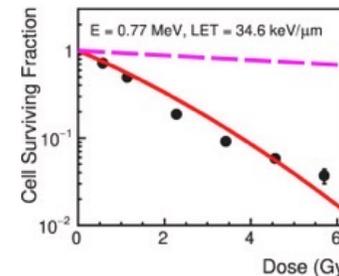
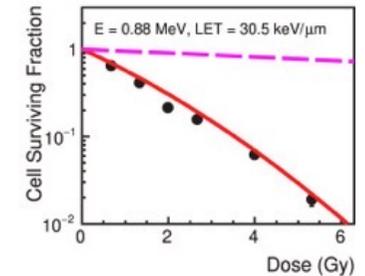
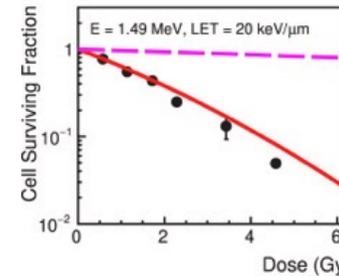
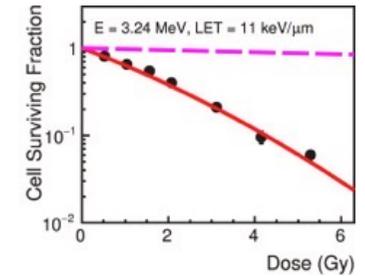
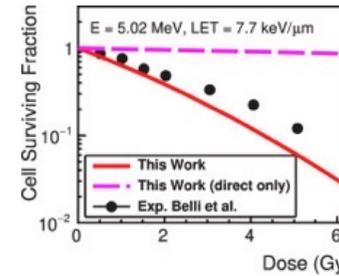
`dsbandrepair`: for proton

Validation and verification: DNA rejoining & cell survival

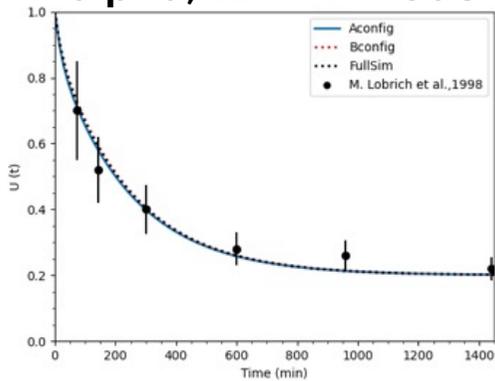
moleculardna: proton, TLK model, HSGc-G5 cell



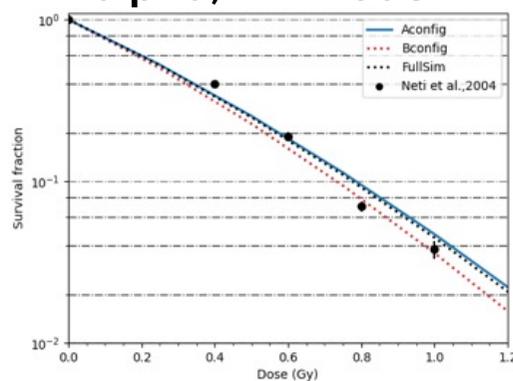
moleculardna: proton, TLK model, V79 cell



dsbandrepair: alpha, LEM-IV model



dsbandrepair: alpha, TLK model



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Geant4-DNA examples available in Geant4

Track structure physics

Radiolysis chemistry

Geometries & damage

TS & CH physics

Example code name	Purpose	Location
dnaphysics	<ul style="list-style-type: none"> Usage of Geant4-DNA Physics processes Automatic combination of Standard EM with Geant4-DNA Physics processes variable density 	\$G4INSTALL/examples/extended/medical/dna
microdosimetry	"Hand" combination of Standard EM or Low Energy EM processes with Geant4-DNA Physics processes	\$G4INSTALL/examples/extended/medical/dna
range	Range simulation	\$G4INSTALL/examples/extended/medical/dna
spower	Calculation of stopping power	\$G4INSTALL/examples/extended/medical/dna
mfp	Mean Free Path	\$G4INSTALL/examples/extended/medical/dna
wvalue	W values	\$G4INSTALL/examples/extended/medical/dna
svalue	S values	\$G4INSTALL/examples/extended/medical/dna
microyz	Microdosimetry spectra (y, z)	\$G4INSTALL/examples/extended/medical/dna
microprox	Microdosimetry proximity functions	\$G4INSTALL/examples/extended/medical/dna
slowing	Electron slowing down spectra	\$G4INSTALL/examples/extended/medical/dna
clustering	Clustering code	\$G4INSTALL/examples/extended/medical/dna
icsd	Usage of alternative bio-materials	\$G4INSTALL/examples/extended/medical/dna
splitting	Acceleration of processes	\$G4INSTALL/examples/extended/medical/dna
AuNP	Gold NP	\$G4INSTALL/examples/extended/medical/dna
jetcounter	ICSD in a Jet Counter nanodosimeter	\$G4INSTALL/examples/extended/medical/dna
chem1, chem2, chem3, chem4, chem5, chem6	Usage of Geant4-DNA chemistry (SBS & IRT)	\$G4INSTALL/examples/extended/medical/dna
scavenger	UI for IRT & scavengers	\$G4INSTALL/examples/extended/medical/dna
UHDR	Mesoscopic chemistry	\$G4INSTALL/examples/extended/medical/dna
wholeNuclearDNA	Cell nucleus (physics only)	\$G4INSTALL/examples/extended/medical/dna
pdb4dna	Interface to PDB database	\$G4INSTALL/examples/extended/medical/dna
neuron	3D neural network	\$G4INSTALL/examples/extended/medical/dna
dnadamage1	DNA damage induction in a chromatin fiber	\$G4INSTALL/examples/extended/medical/dna
dnadamage2	DNA damage induction in plasmids	\$G4INSTALL/examples/extended/medical/dna
dsbandrepair	DNA damage induction in various biological models	\$G4INSTALL/examples/advanced/dna
moleculardna	DNA damage induction in various biological models	\$G4INSTALL/examples/advanced/dna
microbeam	3D cellular phantom	\$G4INSTALL/examples/advanced
TestEm5	Atomic deexcitation tagging	\$G4INSTALL/examples/extended
TestEm12	DPK	\$G4INSTALL/examples/extended
TestEm14	Extraction of cross sections	\$G4INSTALL/examples/extended

Where to find more information ?

<https://geant4-dna.org/>

Our publications are also announced on X



@geant4_dna

GEANT4-DNA : EXTENDING THE GEANT4 MONTE CARLO SIMULATION TOOLKIT FOR RADIATION BIOPHYSICS & RADIOBIOLOGY

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 **Geant4 Virtual Machine**.

Geant4 Virtual Machine

Examples, publications

Documentation

Contact us

Last posts

- Dec. 20, 2024:** Geant4-DNA in the Winter 2024 issue of the EFOMP European Medical Physics News.
- Dec. 17, 2024:** The Geant4 11.3.0 LP2i Virtual Machine with AlmaLinux 9 has been released, see [link](#).

You may follow us on [X](#) and [Bluesky](#).

On-going **developments** include

- **Physics** processes in liquid water and other materials
- **Physico-chemistry** and **chemistry** processes for water radiolysis
- **Molecular geometries**
- **Quantification of biological damage** (e.g. DNA strand, double-strand breaks, base oxidation...)

Dedicated **example applications** are provided as well.

Please refer to our list of **publications** and **theses** for more information.

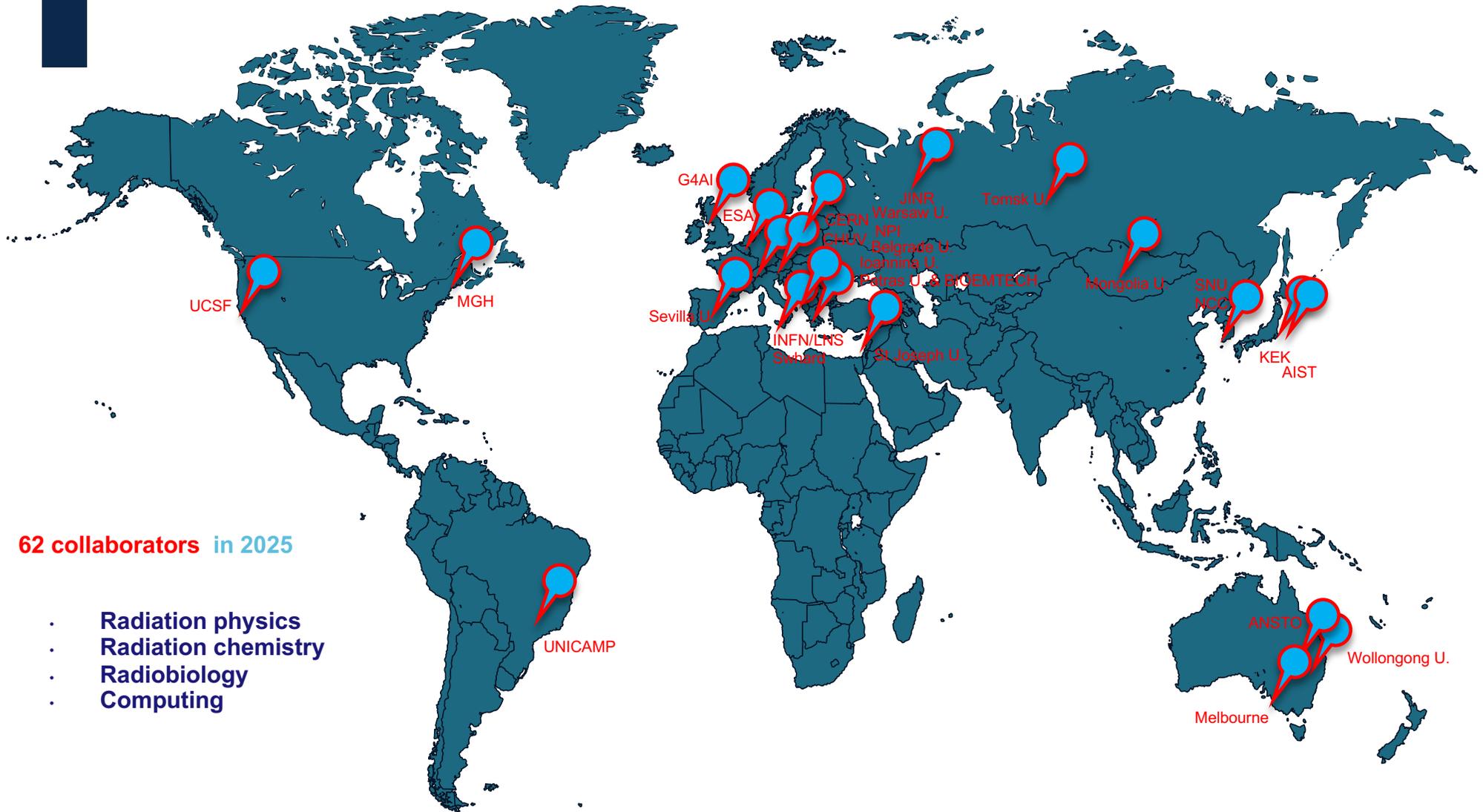
Dedicated **documentation** is also provided in the Geant4 **Book For Application Developers**.

Our current **job listing** is available [here](#).

You may follow us on [X](#) and [Bluesky](#).

© THE GEANT4-DNA COLLABORATION [CONTACT US](#)

An international collaboration



62 collaborators in 2025

- Radiation physics
- Radiation chemistry
- Radiobiology
- Computing



Thank you for your attention!

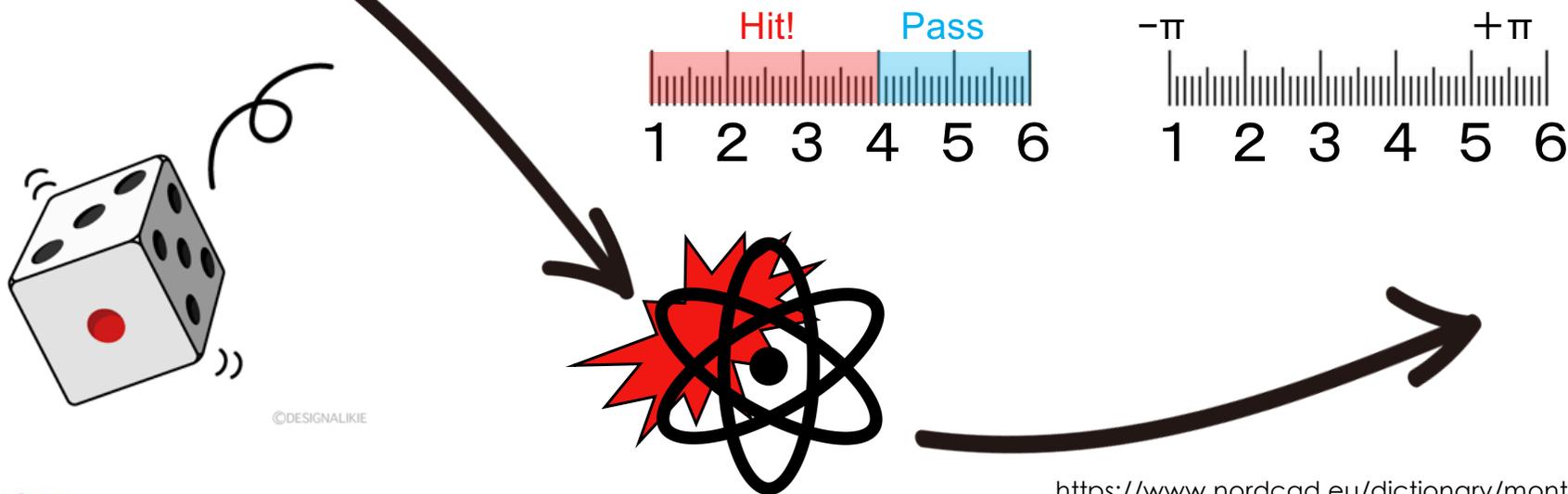


Backup

Monte Carlo methods in particle & molecule transport

“Monte Carlo simulation is a model used to predict the probability of various events when the potential for random variable is present”

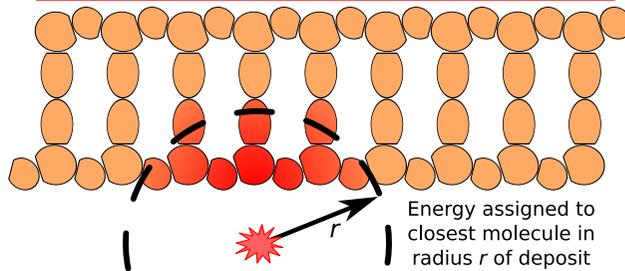
We can use the MC method to simulate particle transport (such as particle hits, scattering, etc).



How can we score DNA damage?

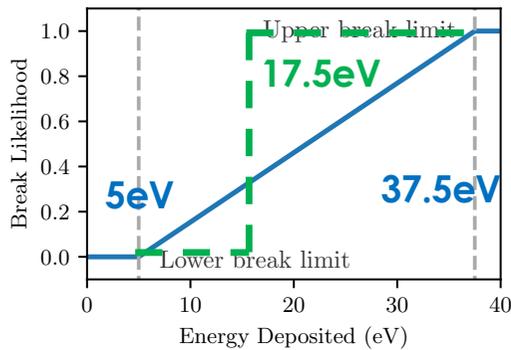
- **DNA damage model** – (e.g. `molecular dna`)

Direct action model



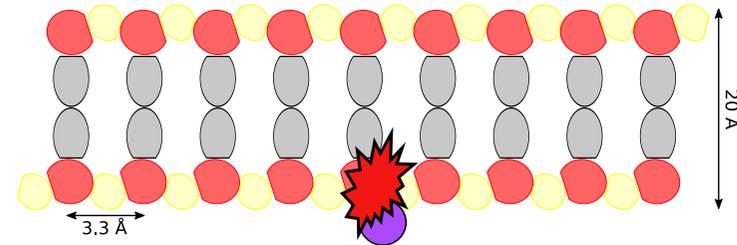
R_{direct} (R of nucleotides: 2.3~2.6 Å)

E_{dep} assigned to closest strand molecule



KURBUC model
PARTRAC model

Indirect action model



P_{OH} : possible range (measured) 40 – 80%

Each single damage is regarded as a **strand break**.

Extensions of Geant4-DNA

- **GATE**
(<http://www.opengatecollaboration.org/>)
 - GATE is a particle transport simulation toolkit based on Geant4 and dedicated to numerical simulations in medical imaging and radiotherapy. GATE can perform Geant4-DNA physics and chemistry simulations, directly in the platform which proposes a Python interface.
- **TOPAS-nBio**
(<https://github.com/topas-nbio/TOPAS-nBio>)
 - TOPAS-nBio is based on Geant4-DNA. The goal is to provide user friendly interface, making Monte Carlo simulations easy-to-use with focus on radiation biology at sub-cellular scales.
- **MPEXS-DNA**
(<https://wiki.kek.jp/display/mpexs/MPEXS+Project>)
 - MPEXS-DNA is a newly developed MC code based on Geant4-DNA physics/chemistry models that offer high computing performance by using a GPU.

