GEANT4-DNA

A SIMULATION TOOLKIT

http://geant4-dna.org

OVERVIEW OF GEANT4-DNA RECENT DEVELOPMENTS

Sébastien INCERTI

CNRS / IN2P3 – France

representing the efforts of the Geant4-DNA Collaboration

4th Geant4 International User Conference at the Physics – Medicine – Biology Frontier

October 24-26, 2022 – Napoly, Italy

Int. J. Model. Simul. Sci. Comput. 1 (2010) 157 (link)

Geant4-DNA timeline

Fully included IN Geant4
2 public releases / year

Main objective

Extend the general purpose Geant4 Monte Carlo toolkit for the simulation of interactions of radiation with biological systems at the cellular and DNA level in order to predict early and late damage in the context of manned space exploration missions : a « bottom-up » approach.

C++ extension included in Geant4 designed to be developed and delivered in a FREE software spirit under the Geant4 license, "easy" to upgrade and improve.

2001
Initiated at the **European Space Agency/ESTEC** by **Petteri Nieminen**

2007
First prototypes of TS **physics models** for liquid water added to Geant4 **release 9.1**

W. Friedland
D. Emfietzoglou
M. Dingfelder

2008
Development coordinated by **CNRS/IN2P3 :** physics, **chemistry, geometries**

2014
Chemistry stage extension ready for end users in Geant4 **10.1**

2017-21
New TS models, **combination radiolysis** (SBS, IRTs) with **geometries**,
10.2 – 11

2022
Integral simulation **chains** for early DNA damage prediction
11.1

First release 15 years ago…

Int. J. Model. Simul. Sci. Comput. 1 (2010) 157 (link)

How can Geant4-DNA model early DNA damage ?

PHYSICAL STAGE
step-by-step modelling of **physical interactions** of incoming & secondary ionising radiation with biological medium
(liquid water mainly)

- Excited **water molecules**
- Ionised **water molecules**
- **Solvated electrons**

PHYSICO-CHEMICAL / CHEMICAL STAGES
- **Radical** species production
- Diffusion
- Mutual chemical interactions

GEOMETRICAL MODELS
DNA strands, chromatin fibres, chromosomes, plasmids, bacterium, cell nucleus, cells, ...

DIRECT DNA DAMAGE

INDIRECT DNA DAMAGE

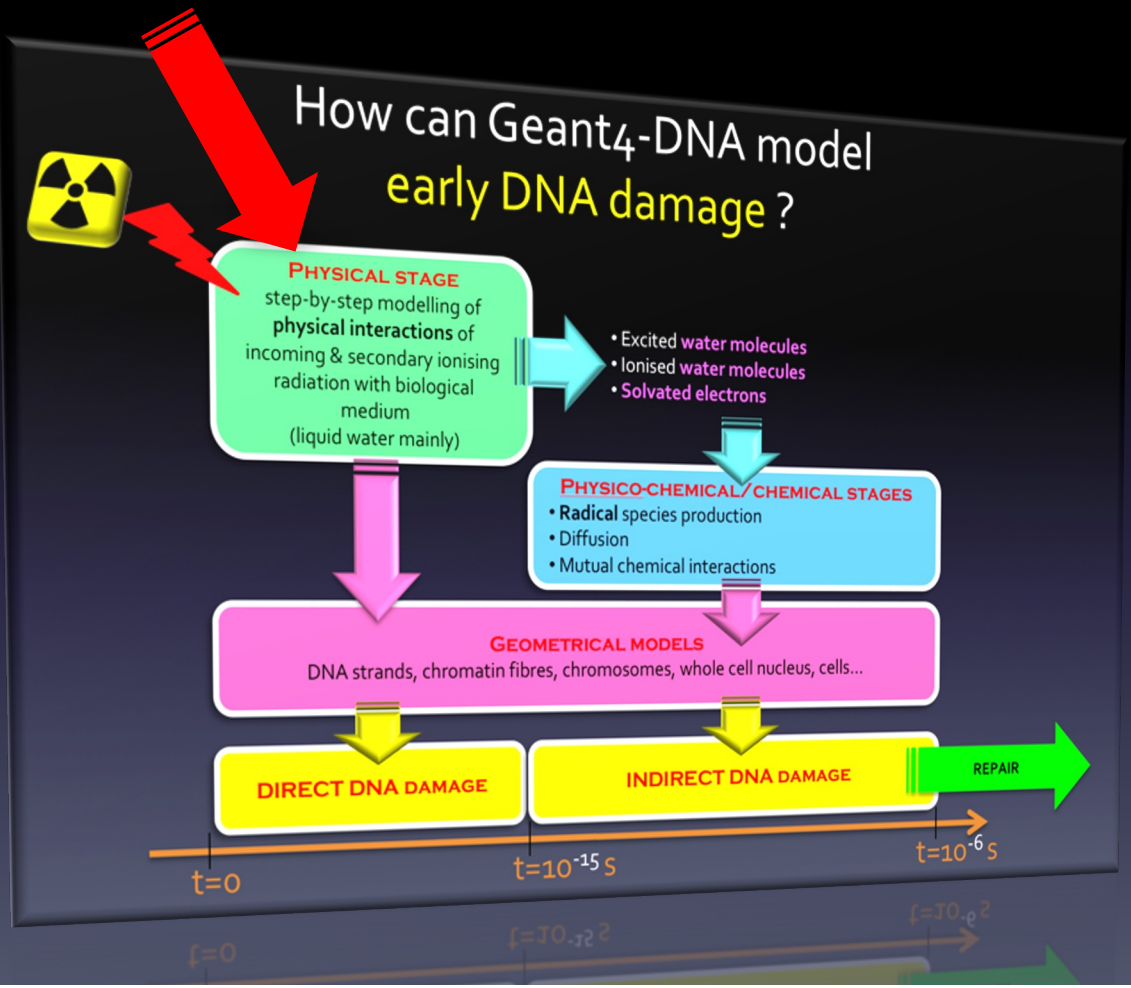
Late damage, repair, cell survival ...

t=0 | $t=10^{-15}$ s | $t=10^{-6}$ s

Last public release
Geant4 11.1 BETA
July 2022

This talk : focus only on PUBLIC developments

PHYSICAL STAGE



Overview of track structure physics models for liquid water

Geant4 11.1 BETA
July 2022

Electrons

1. **Elastic scattering**
   - Screened Rutherford and Brenner-Zaider below 200 eV
   - Updated alternative version by Uehara with vapor screening param.
   - Independent Atom Method (IAM) by Mott *et al.* & VLE data in ice from CPA100 TS code
   - Partial wave framework model by Champion *et al.*, 3 contributions to the interaction potential
   - new: ELSEPA-based for liquid water (muffin tin + rel.)
2. **Ionisation (5 shells)**
   - Dielectric formalism & FBA using Heller optical data up to 1 MeV, and low energy corrections (exchange, interference and Coulomb-field) by Emfietzoglou *et al.*
   - Improved alternative version by Emfietzoglou and Kyriakou including low energy corrections (« Ioannina U. »)
   - Relativistic Binary Encounter Bethe (RBEB) by Terrissol from CPA100 TS code
   - new: Relativistic Plane Wave Born Approximation (RPWBA) by Dominguez-Munoz *et al.* (100 – 300 MeV)
3. **Electronic excitation (5 levels) (*)**
   - Dielectric formalism & FBA using Heller optical data and semi-empirical low energy corrections, derived from the work of Emfietzoglou *et al.*
   - Improved alternative version by Emfietzoglou and Kyriakou
   - Dielectric formalism by Dingfelder from CPA100 TS code
   - new: Relativistic Plane Wave Born Approximation (RPWBA) by Dominguez-Munoz *et al.* (100 – 300 MeV)
4. **Vibrational excitation (*):** Michaud *et al.* xs measurements in amorphous ice with factor 2 to account for phase effect
5. **Dissociative attachment (*):** Melton xs measurements

Protons & H

1. **Excitation (*)**
   - Miller & Green speed scaling of e^- excitation at low energies and Born and Bethe theories above 500 keV, from Dingfelder *et al.*
2. **Ionisation**
   - Rudd semi-empirical approach by Dingfelder *et al.* and Born and Bethe theories & dielectric formalism above 500 keV (relativistic + Fermi density)
3. **Charge change (*):** Analytical parametrizations by Dingfelder *et al.*
4. **Nuclear scattering:** Classical approach by Everhart *et al.*

He^0, He^+, He^{2+}

1. **Excitation (*) and ionisation**
   - Speed and effective charge scaling from protons by Dingfelder *et al.*
2. **Charge change (*)**
   - Semi-empirical models from Dingfelder *et al.*
3. **Nuclear scattering**
   - Classical approach by Everhart *et al.*

Li, Be, B, C, N, O, Si, Fe

1. **Ionisation:** Speed scaling and global effective charge by Booth and Grant

Photons

- from Geant4 EM physics
- new: Default: « Livermore » (EPDL97) and new EPICS2017

7 PhD theses
Z. Francis (2007),
H. N. Tran (2012),
Q. T. Pham (2014),
J. Bordes (2017),
W. G. Shin (2020),
Z. Li (on-going),
D. D.-Munoz (on-going)

Med. Phys. 37 (2010) 4692 (link)
Appl. Radiat. Isot. 69 (2011) 220 (link)
Med. Phys. 42 (2015) 3870 (link)
Phys. Med. 31 (2015) 861 (link)
Nucl. Instrum. and Meth. B 343 (2015) 132 (link)
Phys. Med. 32 (2016) 1833 (link)
Rad. Phys. Chem (2022) (link)

(*) only available in Geant4-DNA

The 3 recommended Geant4-DNA « physics constructors » for liquid water

« option2 »
« option4 »
« option6 »

Exemple of software preservation

Process	G4EmDNAPhysics_option2	G4EmDNAPhysics_option4	G4EmDNAPhysics_option6
	Geant4-DNA physics constructors electron models		
Ionization (inelastic)	Emfietzoglou dielectric model (11 eV–1 MeV)[5]	Emfietzoglou–Kyriakou dielectric model (10 eV–10 keV)[47]	Relativistic binary encounter Bethe model from CPA100 code (11 eV–256 keV)[48]
Electronic excitation (inelastic)	Emfietzoglou dielectric model (9 eV–1 MeV)[5]	Emfietzoglou–Kyriakou dielectric model (8 eV–10 keV)[47]	Dielectric model from CPA100 code (11 eV–256 keV)[48]
Elastic scattering (elastic)	Partial wave model (7.4 eV–1 MeV)[5]	Uehara screened Rutherford model (9 eV–10 keV)[47]	Independent Atom Method model from CPA100 code (11 eV–256 keV)[48]
Vibrational excitation (inelastic subexcitation)	Sanche data (2 eV–100 eV)[49]	n/a	n/a
Attachment (inelastic subexcitation)	Melton data (4 eV–13 eV)[50]	n/a	n/a
Auger electron emission	From the EADL database[51] and the Geant4 atomic relaxation interface[52,53]		
Default tracking cut(*)	7.4 eV	10 eV	11 eV
	... up to 1 MeV	... up to 10 keV	... up to 256 keV

(identical processes & models for other particles)

Med. Phys. 45 (2018) e722-e739 (link)

Other materials already available
- DNA precursors : THF, TMP, PU, PY
- NEW : solid Gold (v1)

- Extension of option4 electron models up to 10 MeV is currently in progress : see Ioanna Kyriakou's talk (Tue.)
- Proton ionisation & excitation up to 300 MeV coming soon in all physics constructors : see Miguel Cortés-Giraldo's talk (Mon.)
- More materials to come : see Carmen Villagrasa & Francesca Nicolanti talks (Mon. & Wed.)

NEW in Geant4 10.6
December 2019

Improvement of electron elastic scattering

The default partial wave model of Geant4-DNA (in option2) shows some limitations

- Lack of relativistic correction
- Disagreement of DCSs with exp. data @ low energy and intermediate angles (RT)

New cross section data set for liquid water was calculated using the ELSEPA code (F. Salvat et al.) with muffin-tin approximation (10 eV – 1 MeV).

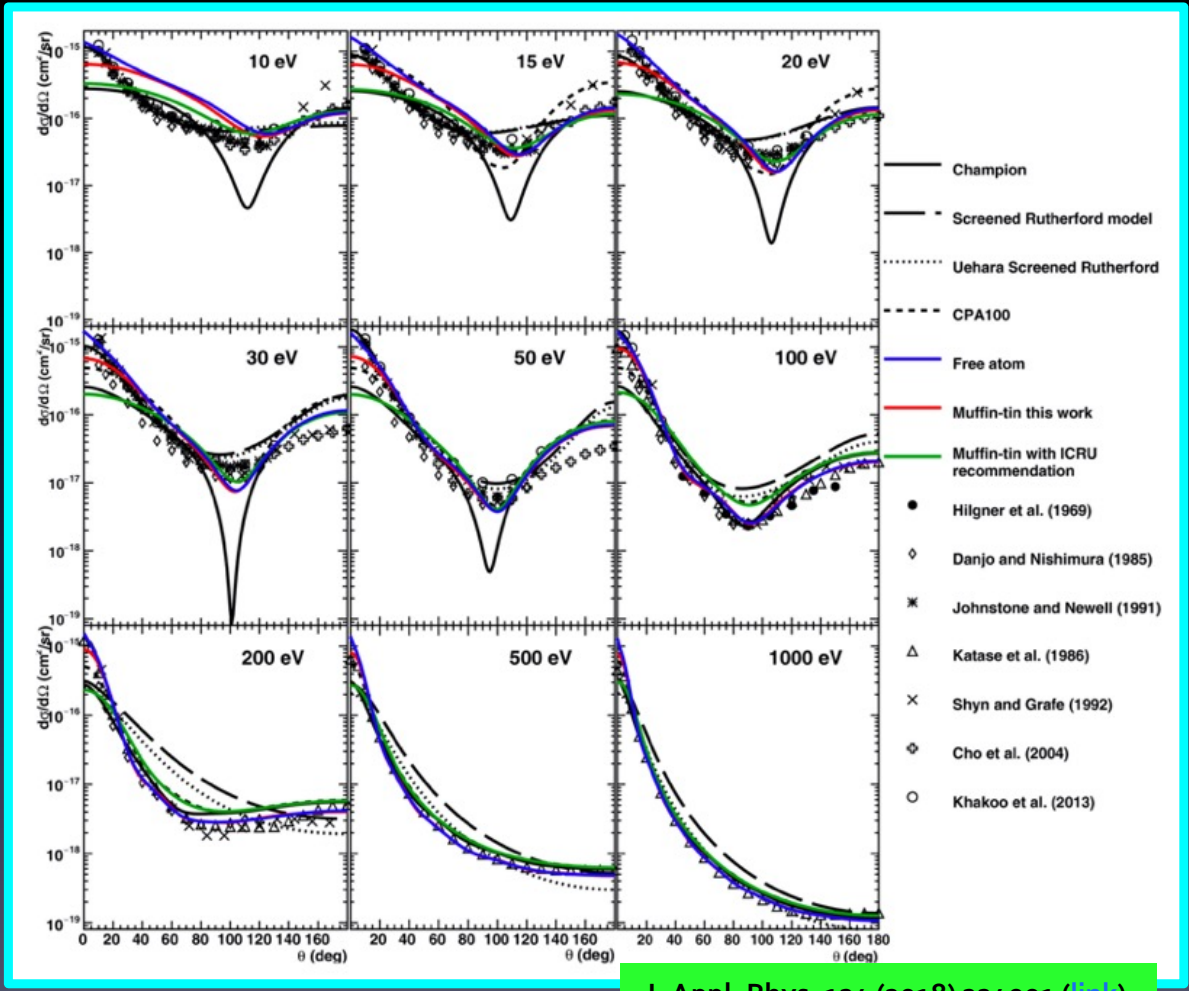
Optical parameters including correlation-polarizability potential and inelastic absorption potential have been qualitatively optimized.

$$V(r) = V_{st}(r) + V_{ex}(r) + V_{cp}(r) - iW_{abs}(r)$$

Expected to become default elastic model.

PhD thesis of W. G. Shin (Bordeaux U. & Wonju U.)

Singly differential angular cross section for electrons



J. Appl. Phys. 124 (2018) 224901 (link)

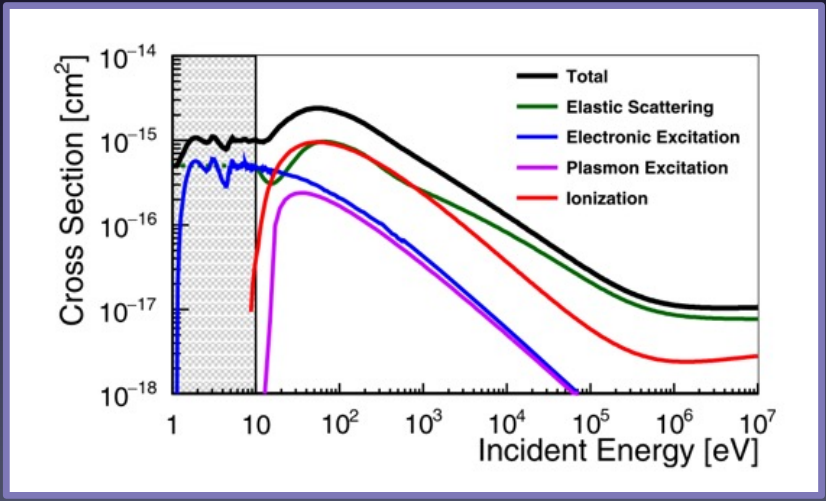
NEW in Geant4 11
December 2021

J. Appl. Phys. 120 (2016) 244901 (link)
Med. Phys. 45 (2018) 2230 (link)

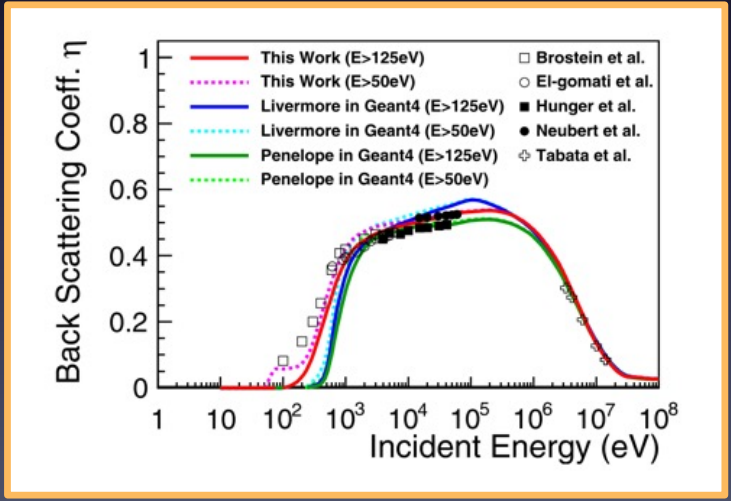
Other materials: gold

- Extension of Geant4-DNA for the modelling of radiosensitization from gold nanoparticles
- Activity initiated in 2016 by Dousatsu Sakata (Bordeaux U., France), then supported by Wollongong U. (Susanna Guatelli *et al.*), in coll. with Ioannina U.
- Discrete physics processes for electrons (10 eV – 1 GeV) were released end of 2021
  - Elastic (ELSEPA, PWA), ionisation (modified RBEBV) with full Auger cascade, electronic (4 channels, BSRM) and bulk plasmon (Quinn's) excitation (+ Seltzer & Berger for bremss.)
  - An alternative dielectric-based version will be released in the near future by Ioanna Kyriakou *et al.*

Integral cross sections for electrons



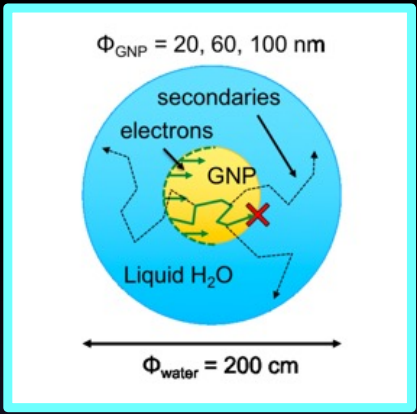
E.g. of validation: backscattering from gold plate



NEW in Geant4 11 December 2021

Application: Geant4-DNA versus Geant4 CH models for gold

Setup



- GNP irradiated with monoenergetic electrons
- Two dimensional absorbed dose in a 1 nm thick sampling plane, around the GNP
- 3 incident energies
  1 keV, 10 keV and 100 keV
- 3 sets of Physics models for gold
  Geant4-DNA, Livermore, Penelope
- A dedicated Geant4-DNA extended example:
  « AuNP », by D. Sakata (Osaka U.)

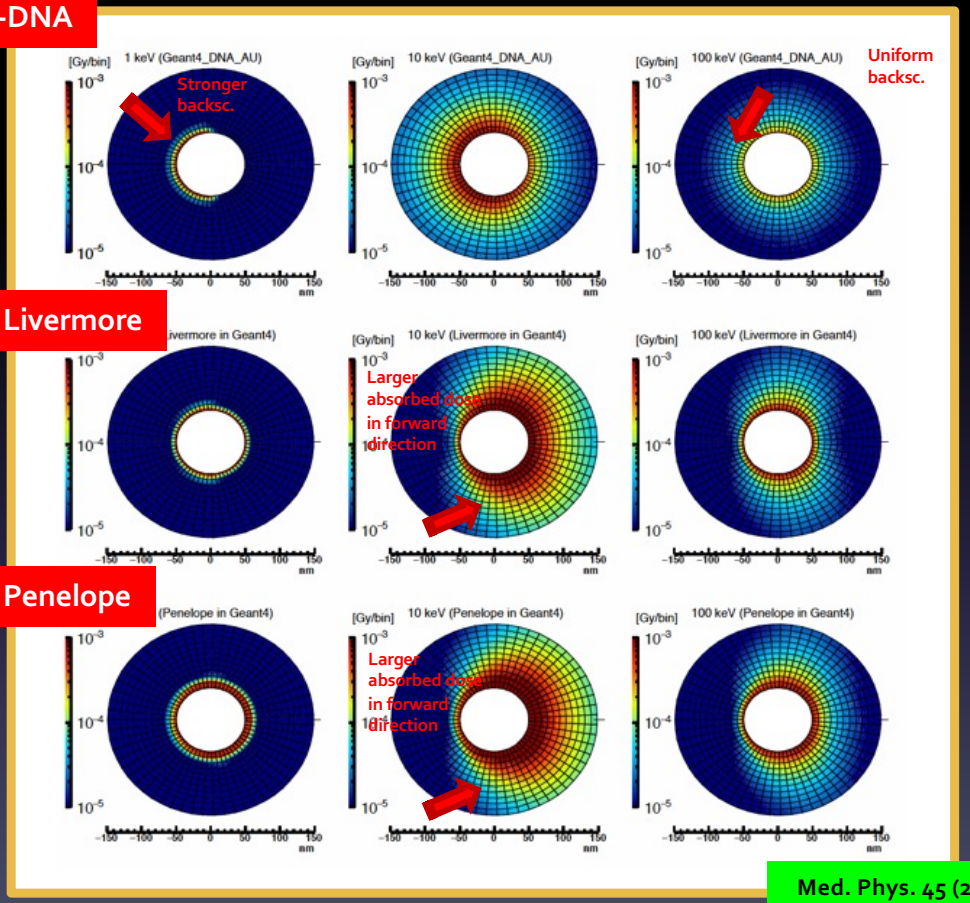
Absorbed dose

Increasing energy

Geant4-DNA

Geant4 Livermore

Geant4 Penelope



Only track structure models describe higher absorbed dose in backward direction

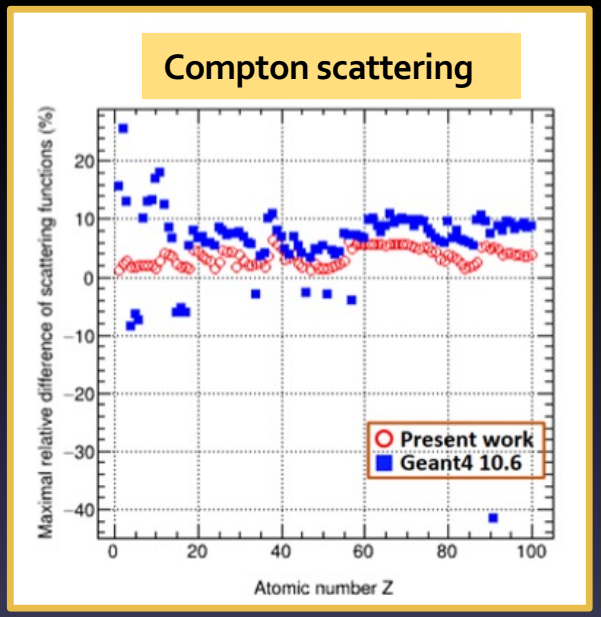
Med. Phys. 45 (2018) 2230-2242 (link)
Phys. Med. 63 (2019) 98-104 (link)
Phys. Med. Biol 65 (2020) 225017 (link)

NEW in Geant4 11 December 2021

New discrete photon models : EPICS 2017

- Database EPICS2017 (Electron Photon Interaction Cross Section library) by D. Cullen et al. contains recent physical data (cross section…) for electron and photon transport calculation
  - has been implemented for Livermore photon models
  - for both Geant4 and Geant4-DNA
- EPICS2017 database is triggered by « UI command »

  /process/em/LivermoreData epics_2017 (if G4EmLivermorePhysics is used)
- Models involved
  - G4LivermoreGammaConversionModel
  - G4LivermoreGammaConversion5DModel
  - G4LivermoreComptonModel
  - G4LivermorePhotoElectricModel
  - G4LivermoreRayleighModel



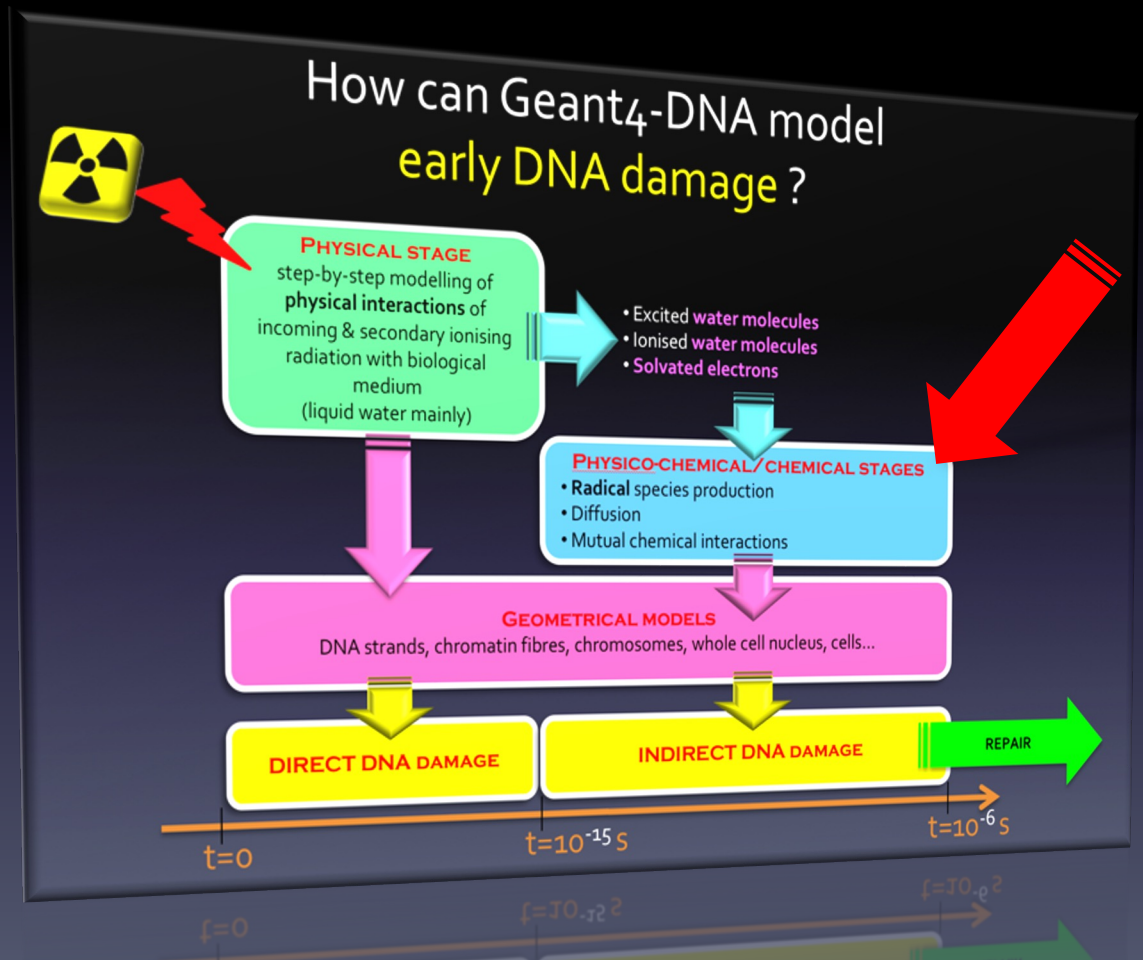
- Updated scattering functions of Compton effect, subshell cross-sections of the photoelectric effect and form factors of Rayleigh scattering.

Phys. Med. 95 (2022) 94-115 (link)

PhD thesis of Z. Lin (Bordeaux U., 2023)

Dedicated doc. : http://geant4.in2p3.fr

PHYSICO-CHEMICAL & CHEMICAL STAGES



$t=10^{-15}$s → $t=10^{-12}$s

Physico-chemical stage

PhD thesis of M. Karamitros (2012)
PhD thesis of W. G. Shin (2020)

J. Comput. Phys. 274 (2014) 841 (link)
Phys. Med. 31 (2015) 861-874 (link)
Phys. Med. 88 (2021) 86-90 (link)

During this stage, water molecules

- Dissociate if
  - Ionised
  - Electron attachment
- Relax or dissociate if
  - Excited
  - Electron-hole recombination

2 alternative sets of parameters

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

Water molecule state

		Channel	Probability (%) This work	Geant4-DNA [12]	PARTRAC [6]	TRACs [7]
Ionization	H_2O^+	$H_3O^+ + {}^{\bullet}OH$	100 #	100 @	100	100
	Auger effect H_2O^{2+}	$2H_3O^+ + H_2O_2$	*100*	–	–	100
Excitation	A^1B_1	$H^{\bullet} + {}^{\bullet}OH$	65	65	65	65
		H_2O	35	35	35	35
	B^1A_1	$H_3O^+ + {}^{\bullet}OH + e^-_{aq}$	*50*	55	55	50
		$H^{\bullet} + {}^{\bullet}OH$	*25.35*	–	–	25.35
		$H_2 + O(^1D)$[a]	*3.25*	15	15	3.25
			$H_2 + 2{}^{\bullet}OH$[c]	$H_2 + 2{}^{\bullet}OH$[c]	$H_2 + 2{}^{\bullet}OH$[c]	$H_2 + H_2O_2$[d]
		$2H^{\bullet} + O(^3P)$[b]	*3.9*	–	–	3.9
		H_2O	*17.5*	30	30	17.5
	Rydberg, Diffusion bands	$H_3O^+ + {}^{\bullet}OH + e^-_{aq}$	50	50	50	–
		$H^{\bullet} + {}^{\bullet}OH$	–	–	–	–
		H_2O	50	50	50	–
Electron capture	Electron attachment H_2O^-	$OH^- + {}^{\bullet}OH + H_2$	100	100	–	100
	Electron-hole recombination H_2O^*	$H^{\bullet} + {}^{\bullet}OH$	*35.75*	55	–	35.75
		$H_2 + O(^1D)$	*13.65*	15	–	13.65
			$H_2 + 2{}^{\bullet}OH$[c]	$H_2 + 2{}^{\bullet}OH$[c]		$H_2 + H_2O_2$[d]
		$2H^{\bullet} + O(^3P)$	*15.6*	–	–	15.6
		H_2O	*35*[e]	30	–	35[e]

- Meesungnoen *et al.* thermalization model (2002) for sub-excitation & auto-ionization electrons from excitation
  (Ritchie *et al.* or Terrissol & Beaudré models as alternatives)
- Placement of products based on PARTRAC - Kreipl (2009)

$t=10^{-15}s$ $t=10^{-12}s$ $t=10^{-6}s$

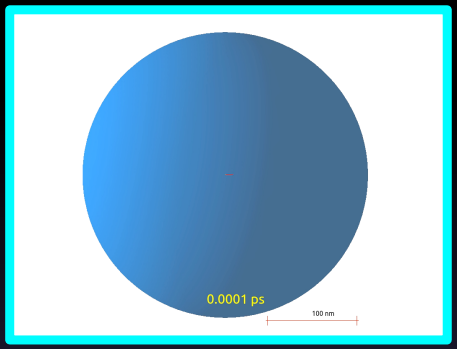
Chemical stage

A collaborative Geant4-DNA & TOPAS-nBio initiative

Geant4-DNA adopts **TWO alternative approaches**

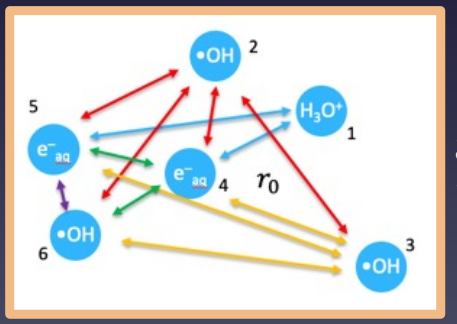
1. **STEP-BY-STEP (« SBS ») « reference » approach**
   - Brownian transport of molecules from the Smoluchowski model.
   - Chemical species are represented by point objects which diffuse in the liquid medium; the liquid medium is supposed to be continuous.
   - Chemical reactions are « controlled by diffusion »: two reactants interact when their separation is smaller than the reaction radius, which is calculated from the rate constant of the reaction.
   - 7 species, 9 chemical reactions

J. Comput. Phys. 274 (2014) 841 (link)
Phys. Med. 31 (2015) 861-874 (link)
J. Appl. Phys. 126 (2019) 114301 (link)
arXiv:2006.14225 (2020) (link)
Med. Phys. 47 (2020) 5920-5930 (link)
Phys. Med. 88 (2021) 86-90 (link)
Med. Phys. 48 (2021) 890-901 (link)



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

2. **INDEPENDENT REACTION TIMES (« IRT ») approach**
   - 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 molecular 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 ») recently released by H. Tran et al. @ IRSN, which gives all spatio-temporal info. on radicals required for combination with geometries



Clifford et al. (1986)

+: Very fast
-: Tracking of species

The 4 Geant4-DNA « chemistry constructors » for liquid water & applications

« default »
« option1 »
« option2 »
« option3 »

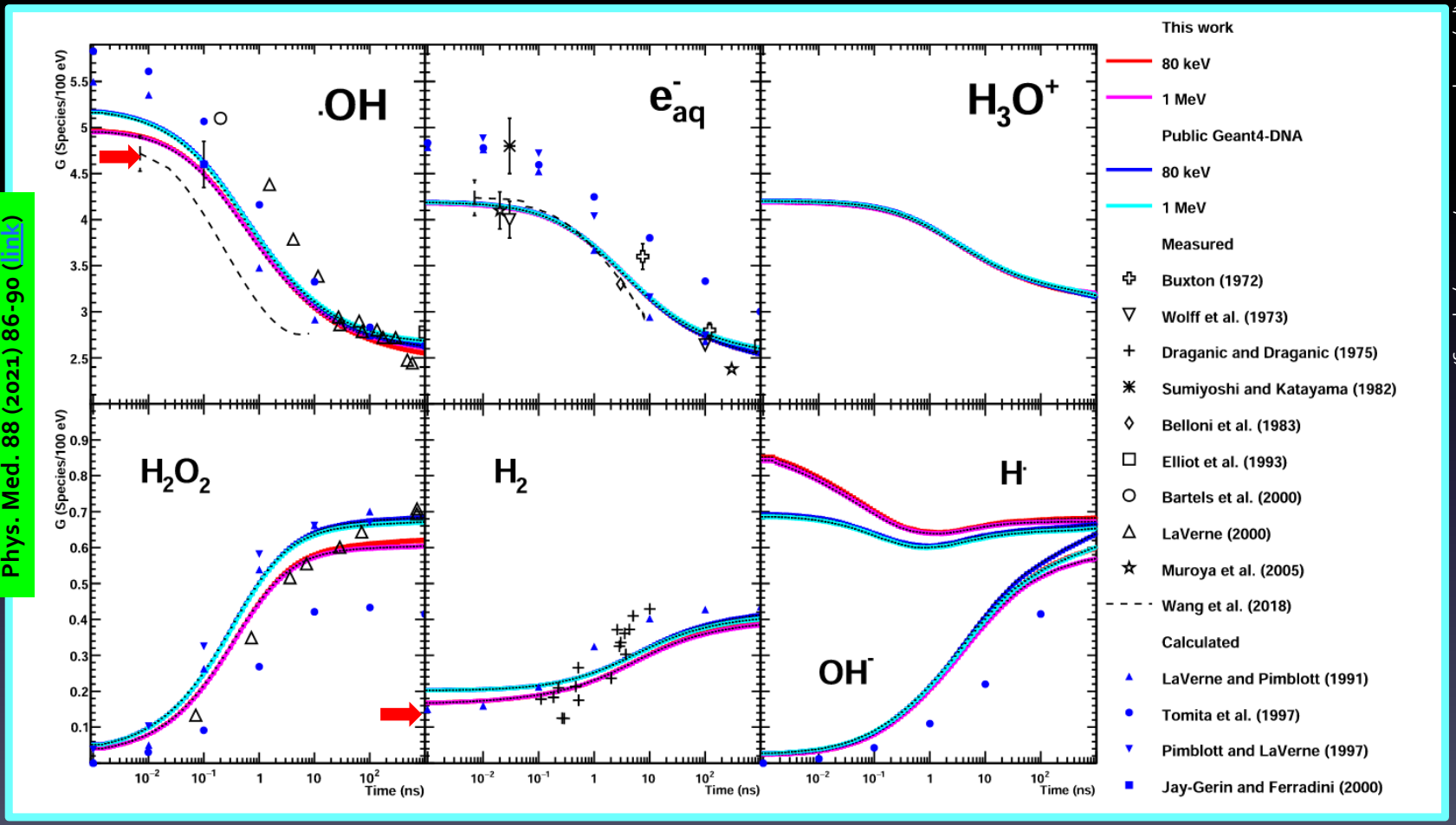
Chemistry constructor	Description	Approach
G4EmDNAChemistry	**First constructor** implemented in Geant4-DNA for the chemistry processes with parameter values from Karamitros et al. (2014) – from PARTRAC	SBS
G4EmDNAChemistry_option1	Implements a **revisited set of chemistry parameters** from Shin et al. (2019) – from TRACs + Burns et al. (1981) + Rowe et al. (1988)	SBS
G4EmDNAChemistry_option2	Includes chemistry parameters for simulating **reactions with DNA components** – from Buxton et al. (1988)	SBS
G4EmDNAChemistry_option3	Implements the **IRT approach** from Ramos-Mendez et al. (2020) – from RITRACKS & Elliot et al. (1994)	**IRT**

Phys. Med. 88 (2021) 86-90 (link)
Med. Phys. 47 (2020) 5920-5930 (link)

- Review currently under preparation
- Toward a recommended chemistry constructor?

Chemistry constructors: radiochemical yields vs time

Impact of the pre-chemical stage settings for electrons



0.186 - 0.314 keV/µm

From the new « chem6 » Geant4-DNA extended example

Number of molecules at time *t*

$$G(t) = \frac{N(t)}{E_{dep}}$$

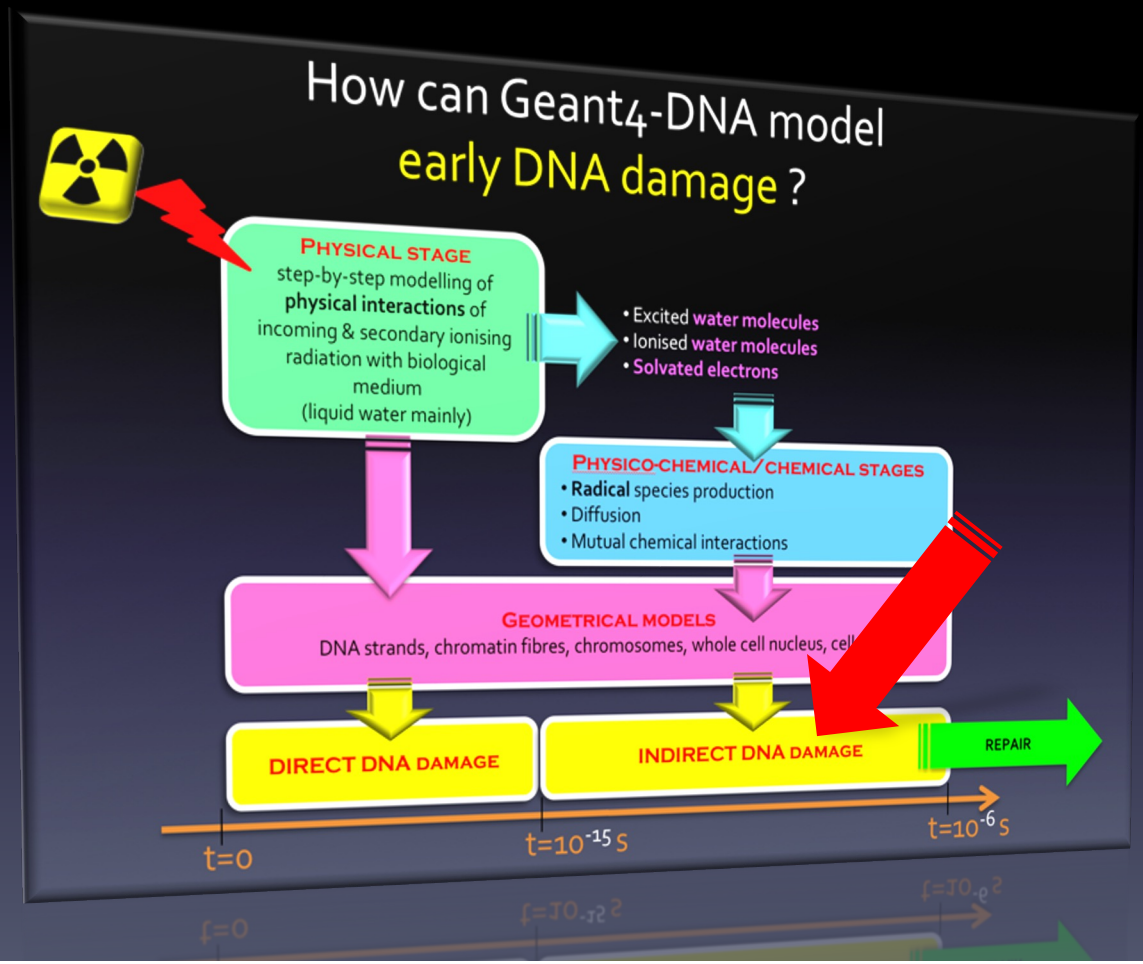
Time-dependent radiochemical yield

Deposited energy scaling to 100 eV

Possibility to handle scavengers, new « scavenger » extended example by Flore Chapuis *et al.*

See talk by Laurent Desorgher (Tue.)

EARLY DAMAGE

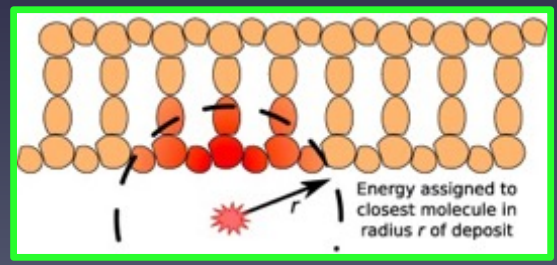


Phys. Med. 48 (2018) 135-145 (link)

Simulation parameters for damage induction

DIRECT damage induction

1. Choice of G4DNA physics constructor
2. Volume for energy scoring
3. Probability of Single Strand Break induction on DNA backbone (D+P)
   - Threshold, linear…



E.g. 6 A° for ~3 hydration sh.

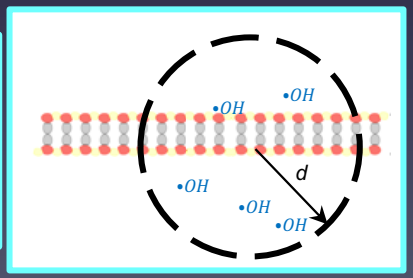
1 DSB = 2 SSB on opposite strands, less then 10 bp apart

NON-DIRECT damage induction

1. Choice of G4DNA chemistry constructor
   - Including reactions with DNA components
2. Probability of non-direct SSB induction
   - •OH on DNA backbone
3. Distance from DNA to kill radicals (scavenging in cells)
4. Histones considered as full scavengers (in cells)
5. Radiolysis maximum time steps
6. Chemical stage end time

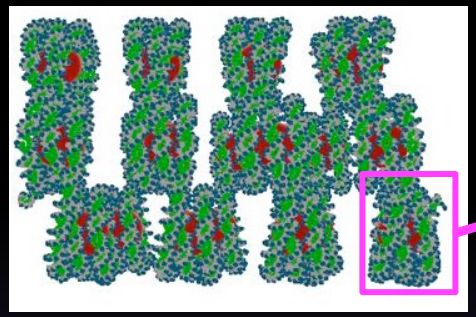
Reaction rates used between radicals and DNA components ($\times 10^9$ L mol^{-1} s^{-1}), from Buxton et al. [65].

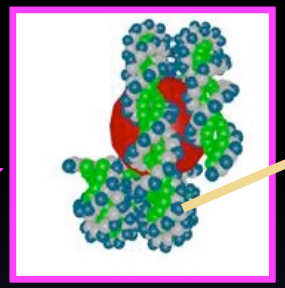
	$^{\cdot}OH$	$H^{\cdot}$	e^-_{aq}
$C_6H_5O_8P$	1.8	0.029	0.01
Adenine	6.1	0.10	9.0
Thymine	6.4	0.57	18.0
Guanine	9.2	–	14.0
Cytosine	6.1	0.092	13.0

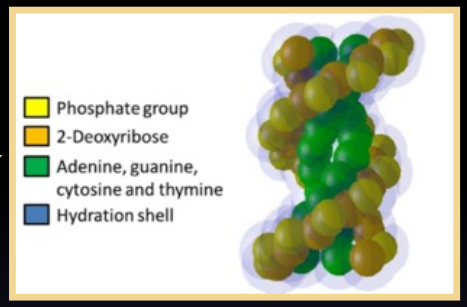


New « dnadamage1 » extended example : simulation chain on a chromatin fiber

« dnadamage1 » example







1 voxel = **18 nucleosomes + 19 linkers** = **3640 nucleotide pairs**

Reaction	Reaction rate ($10^9 M^{-1}.s^{-1}$)
2-deoxyribose + $OH^•$	2.5
Adenine + $OH^•$	6.10
Guanine + $OH^•$	9.20
Thymine + $OH^•$	6.40
Cytosine + $OH^•$	6.10
Histone + molecule → $histone_{modified}$	—

Buxton et al., J. Phys. Chem. Ref. Data. 17 (1988) 513–886

- Physical and chemical stages are both simulated
  - Step-by-step approch for radiolysis
- A voxel of 40 nm heterochromatin straight fiber generated using the "DNAFabric" tool by S. Meylan et al.
- Basis for a full simulation chain in cell nuclei

Parameters
- Geant4-DNA Physics: option2
- R_{direct}: 0.2 nm
- E_{direct}: 17.5 eV
- Geant4-DNA Chemistry: option2
- P_{OH}: 0.4
- Histone as absorber
- d_{kill}: 0 nm
- Δt_{chem}: 0 ns
- t_{chem}: 5 ns
- **Output: SDD**

Public version will soon provide cell. geometries

See Yann Perrot's & Yann Thibault's talks (Wed.)

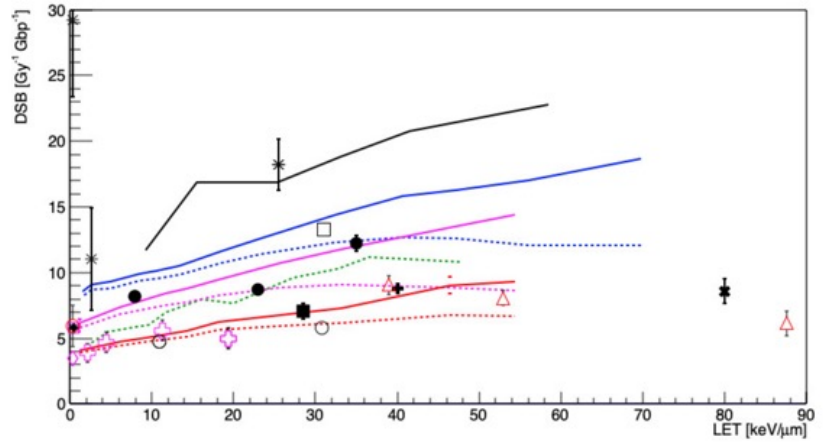
Comput. Phys. Commun. 204 (2016) 159-169 (link)
Sc. Rep. 7 (2017) 11923 (link)
Med. Phys. 48 (2021) 890-901 (link)

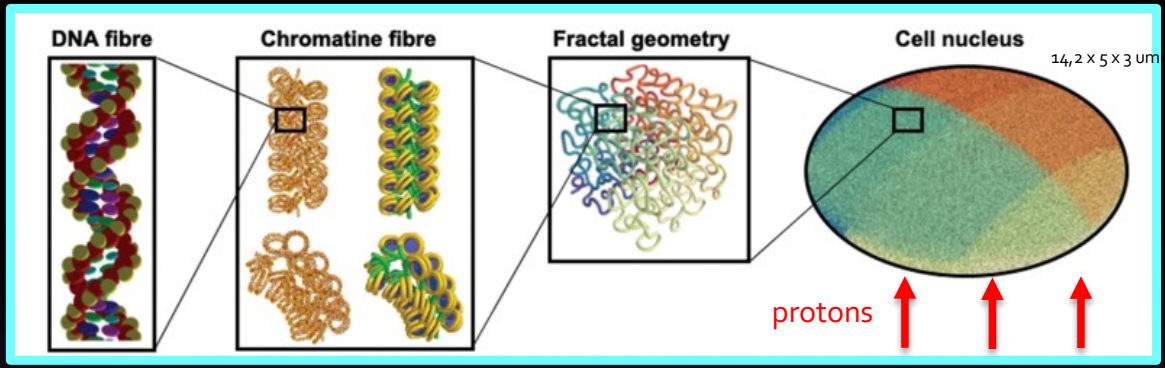
PhD thesis of S. Meylan (2016)
PhD thesis of N. Tang (2019)
PhD thesis of Y. Thibaut (2023)
Hoang Tran et al.

DNAFabric : https://bitbucket.org/sylMeylan/opendnafabric

New « molecularDNA » extended example : simulation chain on a fractal cell nucleus model

« molecularDNA » example





- A full fractal geometrical model of a cell has been developed from realistic pieces of chromatin fibers (0.012 bp/nm^3) – straight, turned and turned-twisted segments (75 nm, 38 histones)
- The simulation of physics, physico-chemistry and chemistry (IRT) are combined with such a geometry in a single Geant4-DNA application fully controlled by macro files
- Early DNA damage can be simulated reasonable agreement with simulations and experiments (protons)

Parameters

- Geant4-DNA Physics: option2 + ELSEPA
- R_{direct}: 3,5 A°
- E_{direct}: 5 eV – 37,5 eV
- Geant4-DNA Chemistry: option3
- P_{OH}: 0.405
- Histone as absorber
- d_{kill}: 9 nm
- Δt_{chem}: 0.5 ns
- t_{chem}: 5 ns
- **Output: Nikjoo (Nikjoo, 1997), SDD**

Phys. Med. 62 (2019) 152-157 (link)
Cancers 2021, 13 (2021) 4940 (link)

PhD thesis of N. Lampe (2017)
PhD thesis of W. G. Shin (2020)
D. Sakata et al.
K. Chatzipapas et al.
M. Dordevic et al.
Hoang Tran et al.

New « molecularDNA » extended example

NEW in Geant4 11.1 BETA July 2022

- Released in Geant4 11.1 BETA, July 2022 : a "BETA" version
- Full integral simulation chain (physics + chemistry + geometries + early DNA damage) as a Geant4 example
- 3 geometries are included in this BETA version
  - DNA cylinders
  - *E. coli*
  - Fibroblast nucleus
  - Constructed using the "FractalDNA" Python tool by N. Lampe et al.

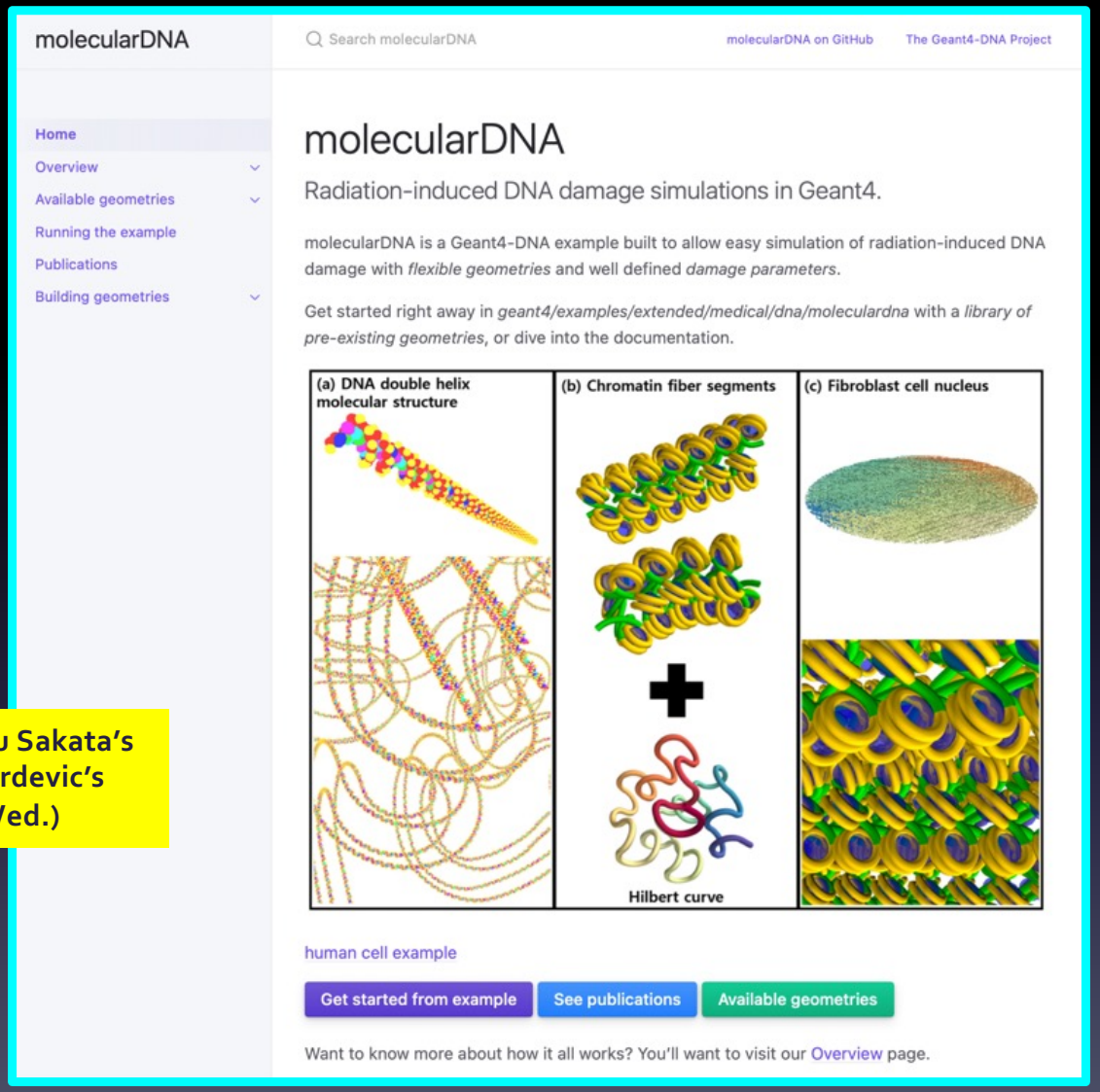
FractalDNA : https://natl.github.io/fractaldna/

- Can simulate
  - Molecular species hits on backbone & bases
  - Damage yields and their complexity
  - Breaks yields
  - Distribution of fragments
- See detailed documentation on dedicated web site

https://geant4-dna.github.io/molecular-docs/

- Don't hesitate to try it and give us your feedback (bugs, usability…)
  - a multi-core machine is recommended !

See Dousatsu Sakata's & Milos Dordevic's talks (Wed.)



Our main perspectives

- **PHYSICS**
  - Inclusion of alternative or improved cross section models for electrons, photons and ions and new materials
    - Liquid water + biological materials + gas materials for nanodosimeters (N_2, propane, …) / atmospheres (O_2, CO, CO_2, NO, NO_2…) + metals (Au v2, …)
  - Toward a unique « recommended » physics constructor
- **PHYSICO-CHEMISTRY/CHEMISTRY**
  - Mesoscopic example (e.g. Fricke dosimetry, Flash - UHDR…)
  - Toward a unique « recommended » chemistry constructor
- **GEOMETRIES**
  - Library of multi-scale geometrical models of biological targets
    - E.g. plasmids, bacteria, realistic cells, cell assemblies, multi-cell organisms…
- **BIOLOGY**
  - Optimization of simulation parameters for the prediction of direct and non-direct DNA simple & complex damage
  - Time evolution of damage: repair processes for the simulation of late damage, cell survival, … toward risk assessment ?
- **VERIFICATION (WITH OTHER CODES) AND VALIDATION (WITH EXPERIMENTAL DATA)**

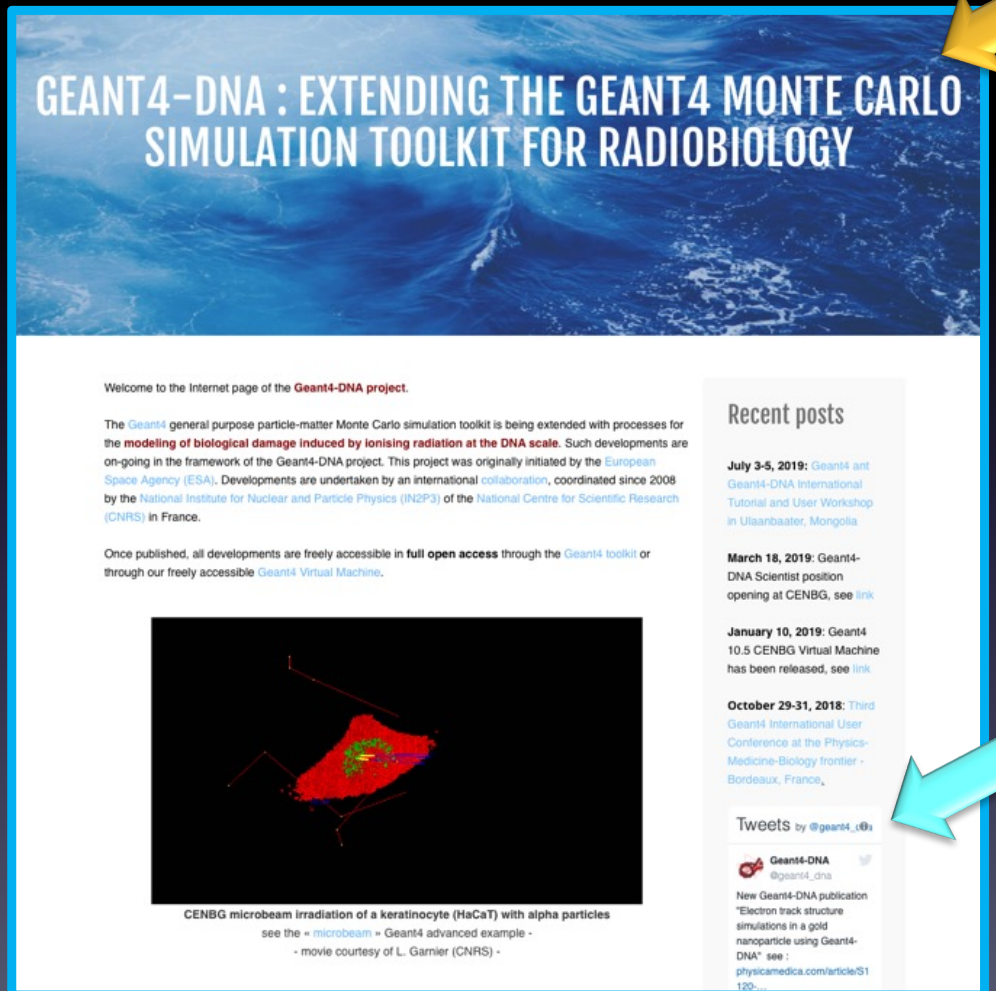
What's coming next in or with Geant4-DNA ?

Please see these 17 talks From Geant4 11.1 December 2022 & beyond

- **PHYSICS**
  - « Extension of the discrete electron transport capabilities of the Geant4-DNA toolkit to the radiotherapeutic regime » by Ioanna Kyriakou (TUE)
  - « The new "RPWBA" implemented model for proton ionization and excitation of liquid water above 100 MeV» by Miguel Cortes-Giraldo (MON)
  - « Implementation of nitrogen cross-sections in Geant4-DNA » by Carmen Villagrasa (WED)
  - « Development of interaction models in Geant4- DNA to simulate cosmic rays' effects on ion-molecules reaction in the atmosphere » by Francesca Nicolanti (MON)
- **CHEMISTRY**
  - « Geant4 for Flash radiotherapy: status and challenges » by Laurent Desorgher (TUE)
  - « Calculation of chemical species yields in liquid water after high energy electron irradiation up to 10 MeV using Geant4-DNA » by Sara Zein (TUE)
  - « Monte Carlo simulations of microdosimetry and radiolytic species production for preclinical proton beam using GATE and Geant4-DNA as part of the FLASHMOD project » by Lydia Maigne (WED)
  - « Evaluation of the effect of oxygen in Flash irradiation through Geant4-DNA » by Fateme Farokhi (TUE)
- **BIOLOGICAL DAMAGE**
  - « DNA damage simulation and prediction of biological endpoints using Geant4-DNA : development of molecularDNA » by Dousatsu Sakata (WED)
  - « A Geant4-DNA simulation of human cancer cells irradiated with helium ion beams » by Milos Dordevic (WED)
  - « Simulation of radio-induced DNA damages and their repair by means of Geant4-DNA Monte Carlo Track Structure code » by Yann Perrot (WED)
  - « MINAS TIRITH: a Geant4-DNA-based tool for modeling damage at the cell population scale » by Yann Thibaut (WED)
  - « Simulation and validation of plasmid DNA irradiation by electrons using Geant4-DNA » by Sara Zein (WED)
  - « A new genome geometrical model with atomic resolution based on HiC-maps. » by Mario Bernal (WED)
- **APPLICATIONS**
  - « In-silico calculations of DNA damage induced by DaRT for a better understanding of the radiobiological effectiveness of this treatment » by Laura Ballisat (WED)
  - « Calculation of organ-specific radiation quality factors for the radioprotection of astronauts on the Moon: a microdosimetric approach » by Matthew Large (MON)
  - « Nanodosimetric Study of Radiation in the Brain and Eyes of Astronauts on the Lunar Surface » by Jay Archer (MON)

http://geant4-dna.org

Geant4-DNA website



Publications, examples, PhD theses, tutorials, virtual machine…

Twitter

@geant4_dna

Geant4-DNA examples included in Geant4 (29)

Geant4 11.1 BETA
July 2022

	Example code name	Purpose	Location
Track structure physics	dnaphysics	• Usage of Geant4-DNA Physics processes • Automatic combination of Standard EM with Geant4-DNA Physics processes • variable density	$G4INSTALL/examples/extended/medical/
	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
	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	new Gold NP	$G4INSTALL/examples/extended/medical/dna
Radiolysis	chem1, chem2, chem3, chem4, chem5, chem6	new Usage of Geant4-DNA chemistry (SBS & IRT)	$G4INSTALL/examples/extended/medical/dna
	scavenger	new New UI for IRT	$G4INSTALL/examples/extended/medical/dna
Geometries & damage	wholeNuclearDNA	Cell nucleus	$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	new DNA damage induction a a chromatin fiber	$G4INSTALL/examples/extended/medical/dna
	moleculardna	new DNA damage induction in E. coli & human cell	$G4INSTALL/examples/extended/medical/dna
	microbeam	3D cellular phantom	$G4INSTALL/examples/advanced
TS & CH physics	TestEm5	Atomic deexcitation tagging	$G4INSTALL/examples/extended
	TestEm12	DPK	$G4INSTALL/examples/extended
	TestEm14	Extraction of cross sections	$G4INSTALL/examples/extended

ROOT Data Analysis Framework
https://root.cern

https://geant4.lp2ib.in2p3.fr

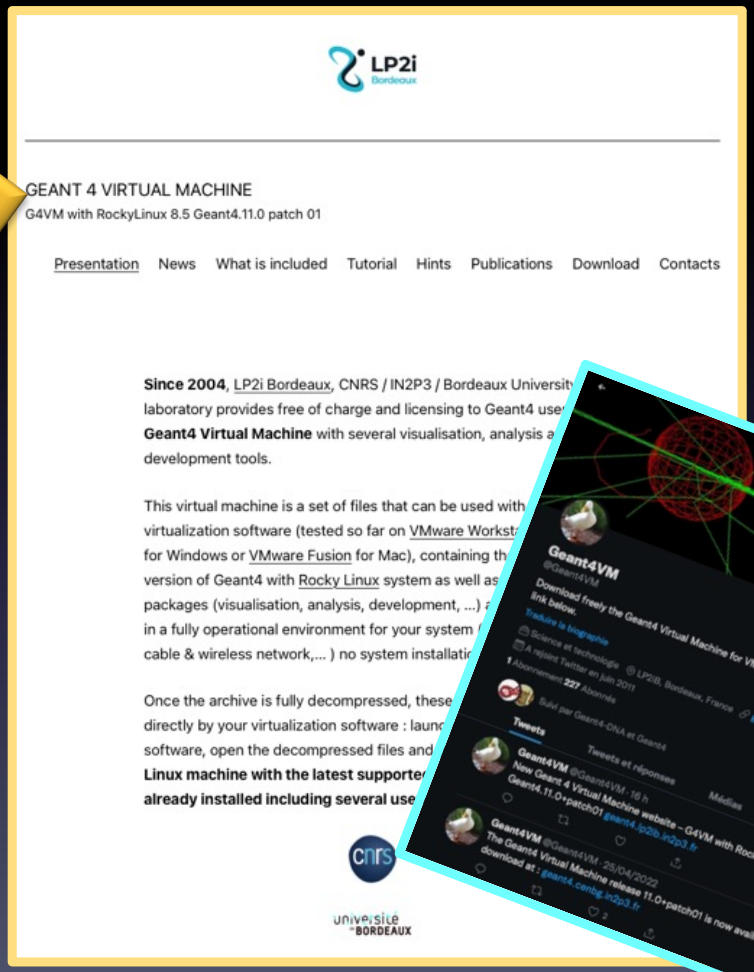
http://geant4-dna.org

https://geant4.in2p3.fr

Int. J. Model. Simul. Sci. Comput. 1 (2010) 157–178 (link)

Geant4 « Virtual Machine »

Regularly updated



Note: for Apple M1 machines, see instructions http://geant4-dna.org)

A virtual RockyLinux PC with Geant4 and tools fully installed (e.g. ROOT)

Works with
Windows™
Mac™ (except M1)
Linux™

Twitter

@Geant4VM

The Geant4-DNA collaboration in 2022

- 62 collaborators, 22 institutions worldwide
- 2 year mandate
- 1 collaboration meeting / year
- *ad hoc* topic meetings
- GATE & TOPAS / TOPAS-nBio are collaboration members *

An international collaboration

- **62 collaborators** & 22 institutions in 2022
  - Radiation physics
  - Radiation chemistry
  - Radiobiology
  - Computing
- including **23 in France**
  - CNRS / IN2P3 (15)
  - IRSN (4)
  - CEA (1)
  - Other (3)

Our main core contributors

Mario Bernal (UNICAMP, Brazil)
Marie-Claude Bordage (CNRS & Inserm, France)
Jeremy Brown (Swinburne U., Australia)
Flore Chappuis (CHUV, Switzerland)
Konstantinos Chatzipapas (CNRS, France)
Marie Davidkova (NPI/CAS, Czech Rep.)
Laurent Desorgher (CHUV, Switzerland)
Jorge Naoki Dominguez Kondo (UCSF, USA)
Milos Dordevic (Vinca I. & Belgrade U., Serbia)
Ziad Francis (London, UK)
Susanna Guatelli (Wollongong U., Australia)
Sébastien Incerti (CNRS, France)
Vladimir Ivantchenko (G4AI Ltd, UK)
Mathieu Karamitros (Bordeaux, France)
Ioanna Kyriakou (Ioannina U., Greece)
Nathanael Lampe (Melbourne, Australia)
Tuan Anh Le (IRSN, France)
Zhuxin Li (Bordeaux U., France)
Sylvain Meylan (Paris, France)
Claire Michelet (Bordeaux U., France)
Shogo Okada (Kobe U., Japan)
Yann Perrot (IRSN, France)
Ivan Petrovic (Vinca I. & Belgrade U., Serbia)
Jose Ramos-Mendez (UCSF, USA)
Alexandra Ristic-Fira (Vinca I. & Belgrade U., Serbia)
Dousatsu Sakata (NIRS, Japan)
Takashi Sasaki (KEK, Japan)
Wook-Geun Shin (MGH, USA)
Vaclav Stepan (NPI/CAS, Czech Rep.)
Yann Thibaut (IRSN, France)
Hoang N. Tran (CNRS, France)
Carmen Villagrasa (IRSN, France)
Sara Zein (CNRS, France)

Alumni

J. Bordes (CRCT/Inserm/UPS, Toulouse, France)
M. Bug (PTB, Germany)
E. Delage (LPC/IN2P3/CNRS, France)
M. Dos Santos (IRSN, France)
A. Ivantchenko (G4AI Ltd., UK)
A. Mantero (SwHaRD srl, Italy)
H. Payno (LPC/IN2P3/CNRS, France)
N. Tang (IRSN, France)

Thank you for your attention

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Werner Friedland (Helmholtz Z., Germany)
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http://geant4-dna.org
Fully incuded IN Geant4

GEANT4-DNA
A SIMULATION TOOLKIT

If you use Geant4-DNA, please be kind to cite in your work our 4 collaboration papers
Med. Phys. 45 (2018) e722-e739
Phys. Med. 31 (2015) 861-874
Med. Phys. 37 (2010) 4692-4708
Int. J. Model. Simul. Sci. Comput. 1 (2010) 157–178

Our users !