

IRSN

INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Enhancing nuclear safety

Micro- and nanodosimetric calculations using the Geant4-DNA Monte Carlo code

EURADOS Winter school :
“Status and Future
Perspectives of
Computational Micro- and
Nanodosimetry”

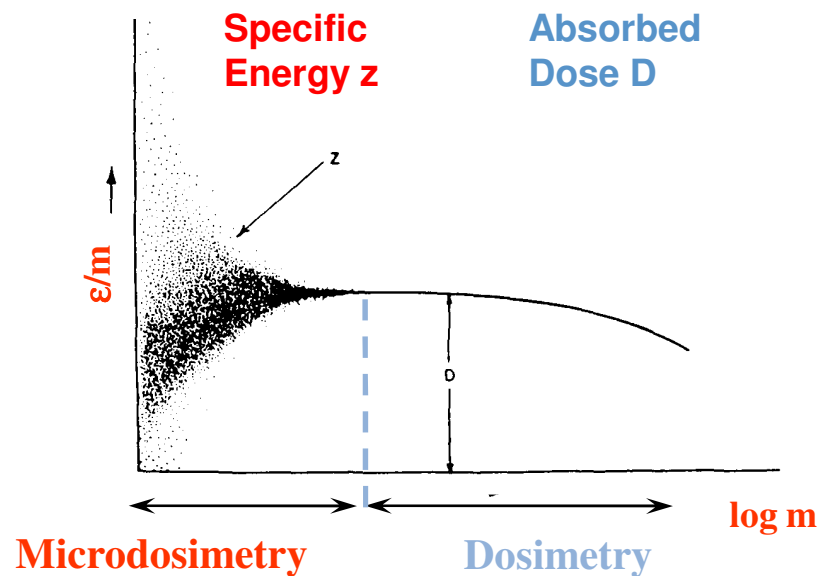
C. Villagrasa. **IRSN** (Institut de Radioprotection et de sûreté nucléaire, France). On behalf of the **Geant4-DNA collaboration**.



Introduction : Modelling Radiation Biology

Context and Motivation

Since its inception, the purpose of microdosimetry has been the study of the **stochastic character in the energy deposition** by ionizing radiation and its **consequences in the biological response** mechanism.



The stochastic character becomes more relevant when the target volume decreases

Which is the target volume relevant for studying the biological response?

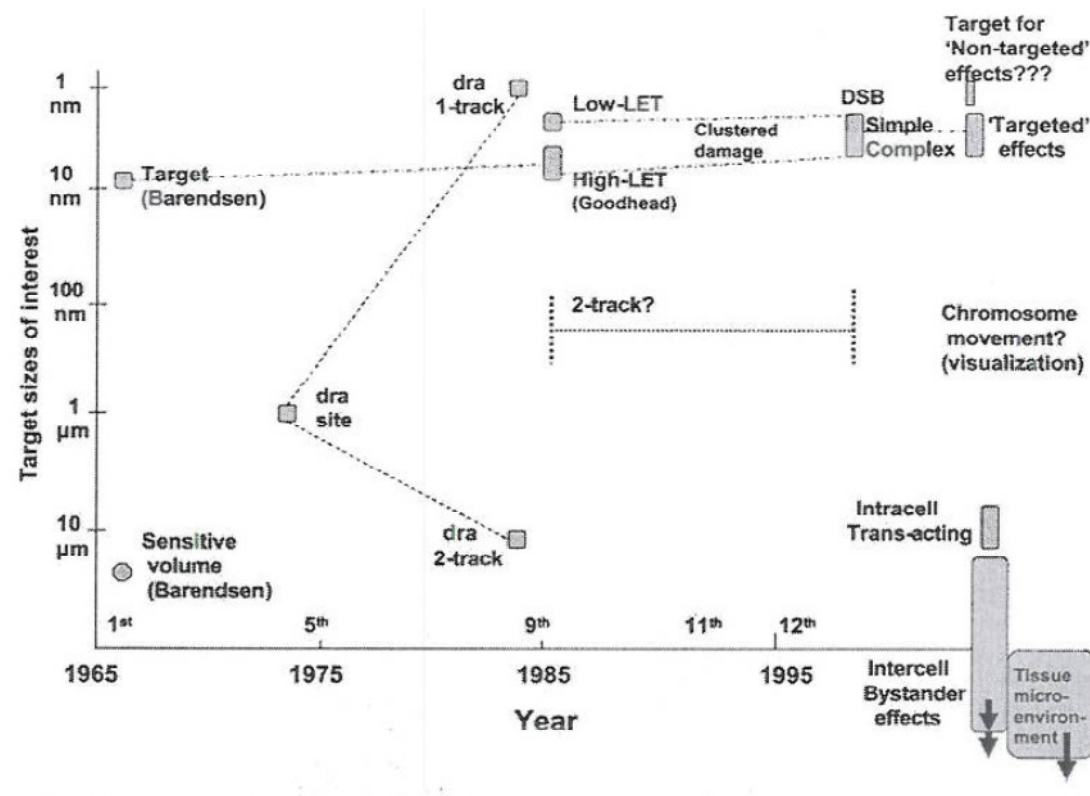
Cellular scale: micrometer

Sub-cellular scale (ex. DNA): nanometer

Introduction : Modelling Radiation Biology

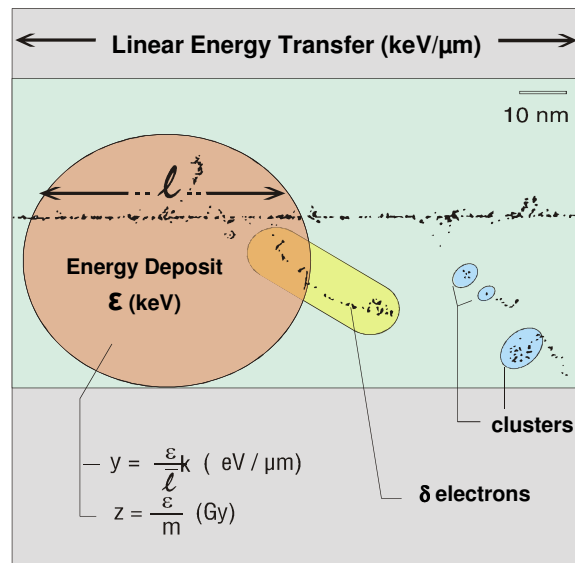
Context and Motivation

Evolution of the target size studied in the different microdosimetry symposiums
(D.T. Goodhead *Rad. Prot. Dosim.* 2006)



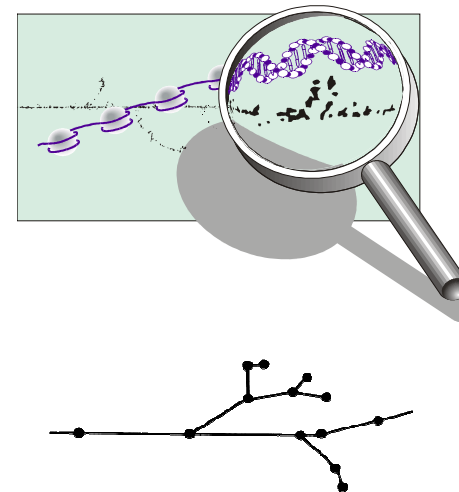
Introduction : Modelling Radiation Biology

Micro- or nanodosimetry- > Two complementary formalisms



ϵ

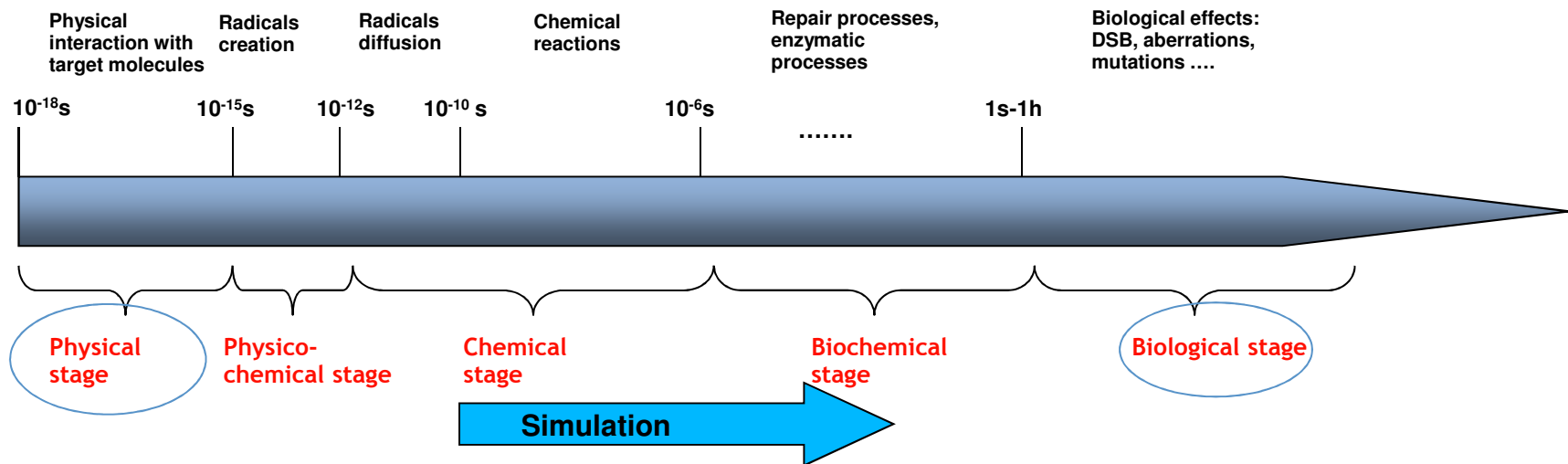
Integrated response of a critical biological site or target



ϵ_j

Track structure investigation

Introduction : Modelling Radiation Biology



Radioprotection : Describing the first steps of the interaction between ionizing radiation and biological targets would allow improving the risk evaluation of secondary effects in both low and high dose regimes.

Monte Carlo method for the Physical Stage

➤ **Monte Carlo calculations** are a well adapted method to simulate the stochastic characteristics of the physical stage

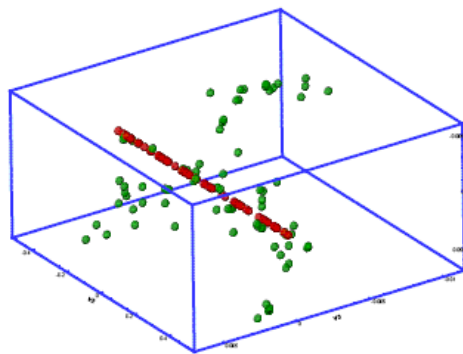
Monte Carlo Track structure simulation at nanometric level



Physical models or experimental data for **cross-section** determination of the different physical interactions **with the target material**

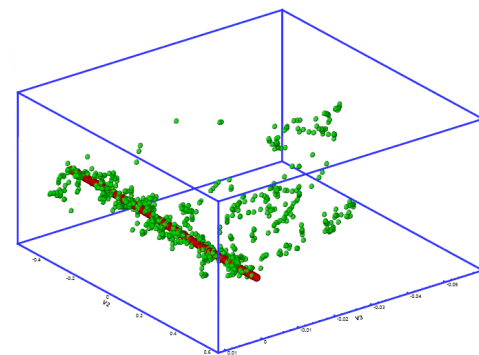
$$\sigma(Z, E, T_{cut}) = \int_{T_{cut}}^{T_{max}} \frac{d\sigma(Z, E, T)}{dT} dT$$

T_{cut} cut energy for secondary particle (electrons) creation and transportation



T_{cut} : 250 eV

T_{cut} -> some eV



T_{cut} : 15 eV

Dedicated codes for Radiobiology response modelling

Dedicated codes for nanodosimetric calculations exist fulfilling these requirements:

Code	particle	Energy range	Cross-section database	Reference
CPA100	e ⁻	≥10 eV-100 eV e ⁻	Wat. (l)	Terrissol and Beaudre, 1990
DELTA	e ⁻	≥10 eV-10 keV e ⁻	Wat. (v)	Zaider et al. (1983)
ETRACK	e ⁻ , p, α	≥ 10 eV-10 keV e ⁻	Wat. (v)	Ito (1987)
KURBUC	e ⁻	≥ 10 eV-10MeV e ⁻	Wat. (v)	Uehara et al. (1993)
LEEPS	e ⁻ , e ⁺	0.1-100 keV	Many materials	Fernandez-Varea et al. (1996)
LEPHIST	P	≥ 1 keV-1MeV	Wat. (v)	Uehara et al. (1993)
LEAHIST	α	≥ 1 keV/u-2MeV/u	Wat. (v)	Uehara and Nikjoo (2002a)
MC4	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Emfietzoglou et al. (2003)
NOTRE DAME	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Pimblott et al. (1990)
OREC	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Turner et al. (1983)
PARTRAC	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Friedland et al. (2003)
PITS04	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (l)	Wilson et al. (2004)
PITS99	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v)	Wilson and Nikjoo (1999)
SHERBROOKE	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Cobut et al. (2004)
STBRGEN	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Chatterjee and Holley (1993)
TRION	e ⁻ , ions	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Lappa et al. (1993)
TRACEL	e ⁻ , ion	≥ 10 eV e ⁻ , ions ≥ 0.3MeV/u	Wat. (v,l)	Tomita et al. (1997)

Source : "Track-structure codes in radiation research", Nikjoo et al., Rad. Meas. 41 (2006)

Here, we present the capabilities of the Geant4 Monte Carlo code for micro and nanodosimetric calculations-> the Geant4-DNA project

The Geant4-DNA project : a part of Geant4

Geant 4 GEometry ANd Tracking

Geant4 : a set of **libraries** to simulate interactions of particles with matter (not a user code)

Initiated by CERN in 1994 for **HEP (LHC)**, successor of Geant3 (20 years)

Now developed by an **international collaboration** (~100 members)

Object-Oriented technology (C++) -> Extensibility

Entirely open source and free

Constantly updated -> Two public releases / year

Geant4 : simulation of a particle physics experiment

- | Define a flexible geometry
- | Model interaction processes (electromagnetic, hadronic)
- | Generate initial particles and follow them within the geometry
- | Save physics quantities and analyze them

<http://www.geant4.org>

The Geant4-DNA project : a part of Geant4

➤ **Objective** : adapt the general purpose Geant4 Monte Carlo toolkit for the simulation of interactions of radiation with biological systems at the cellular and DNA level.

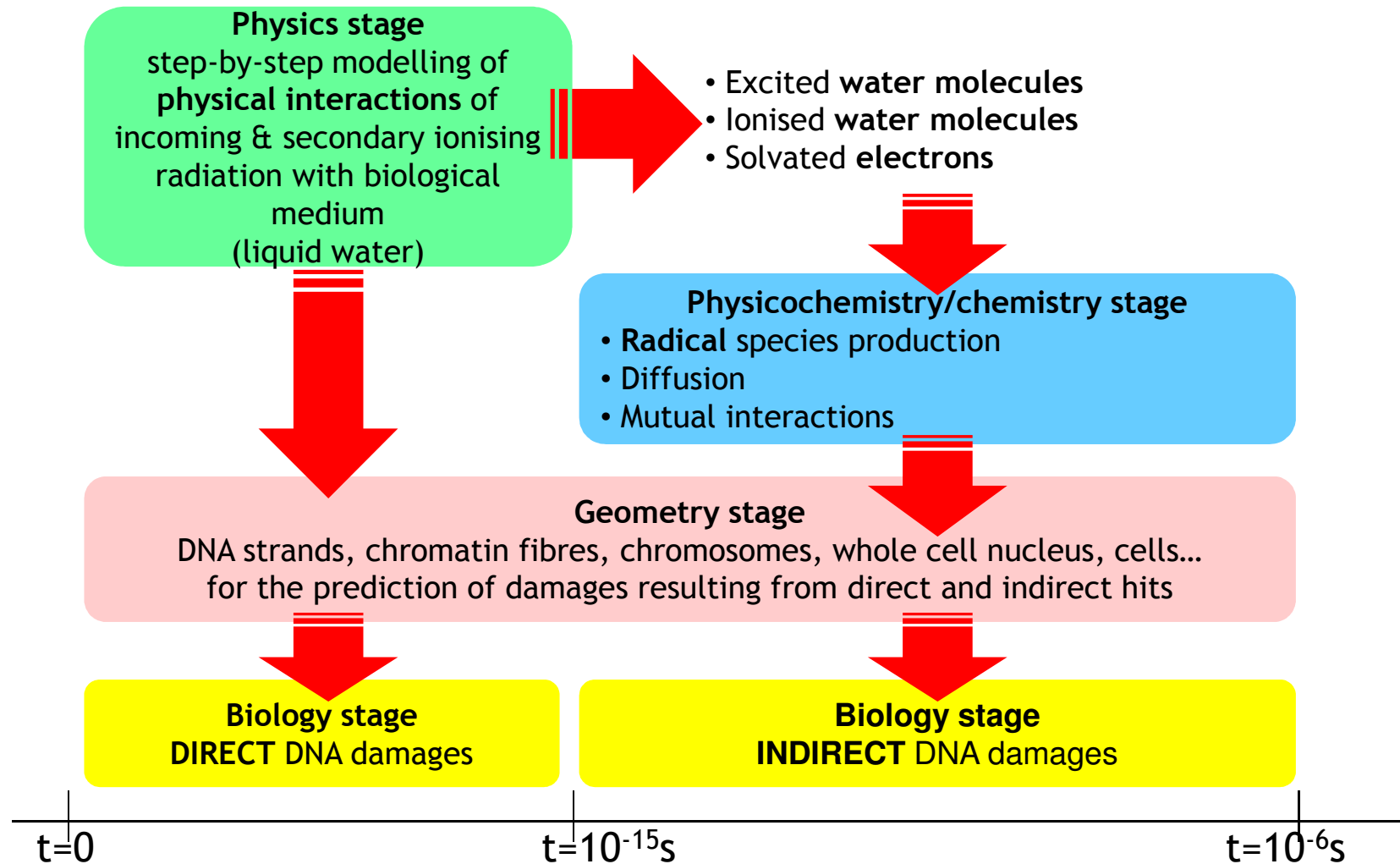
❖ Initiated in 2001 by Dr. Petteri Nieminen at the ESA (European Space Agency) with the aim of providing an open source access to the scientific community that can be easily upgraded & improved

❖ First prototypes of physics models were added to Geant4 in 2007

❖ Currently an on-going interdisciplinary activity of the Geant4 collaboration « low energy electromagnetic physics » working group -> Coordinated by S. Incerti CNRS/IN2P3 since 2008

<http://geant4-dna.org>

The Geant4-DNA project



Physical stage: Physics models available in Geant4-DNA

General features

- Electron transport can reach the **very low energy domain** down to electron thermalization
 - Sub-excitation electrons (below ~ 9 eV) can undergo vibrational excitation, attachment and elastic scattering
- Purely discrete
 - Simulate all elementary interactions on an **event-by-event** basis
 - No condensed history approximation
- Models can be purely **analytical and/or use interpolated data tables**
For eg. computation of integral cross sections
- They use the same software design as all electromagnetic models available in Geant4 (« standard » and « low energy » EM models)
Allows the combination of processes (**multi-scale design**)

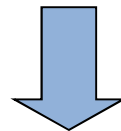
Physical stage: Physics models available in Geant4-DNA

General features

The target composition problem:

Geant4-DNA physics models are applicable currently only to **liquid water**:

- Nevertheless, liquid water is a fundamental component of biological matter and, at micrometric scale, the energy absorbed by liquid water is a good representation of that in biological matter
- Experimental data on water vapor cover a broad energy range with high accuracy but phase effects for low energy electron transport are important to take into account.
- Only few data on the liquid water dielectric function in the optical limit .
- Some experimental data on biological components (amino-bases, sugar, etc) are now available and theoretical models are being developed



In order to take into account the other components of biological matter at nanometric scale, **Geant4-DNA next releases will propose**:

- Implementation of the new **experimental cross sections for DNA constituents from PTB** (BioQuaRT project)
- Cross sections using the **classical trajectory Monte Carlo simulation (CTMC)** approach (dec. 2013 release) See **Champion et al.** PMB53, 2008, N41; PRA 79, 2009
- **Cross sections based on the CDW-EIS** (continuum-distorted wave eikonal-initial-state) **method** for interactions on DNA components

Overview of the physic models for liquid water (9.6)

Electrons

- **Elastic scattering**
 - Screened Rutherford and Brenner-Zaider below 200 eV
 - Champion's approach (partial wave framework, 3 contributions to the interaction potential)
- **Ionisation**
 - 5 levels for H₂O
 - Dielectric formalism & FBA using Heller optical data up to 1 MeV, and low energy corrections
- **Excitation**
 - 5 levels for H₂O
 - Dielectric formalism & FBA using Heller optical data and semi-empirical low energy corrections
- **Vib. Excitation**
 - Michaud *et al.* xs measurements in amorphous ice
 - Factor 2 to account for phase effect
- **Dissociative attachment**
 - Melton *et al.* xs measurements

Photons

from EM « standard » and « low energy »

Protons & H

- **Excitation**
 - Miller & Green speed scaling of e⁻ excitation at low energies and Born and Bethe theories above 500 keV
- **Ionisation**
 - Rudd semi-empirical approach by Dingfelder *et al.* and Born and Bethe theories & dielectric formalism above 500 keV (relativistic + Fermi density)
- **Charge change**
 - Analytical parametrizations by Dingfelder *et al.*

He⁰, He⁺, He²⁺

- **Excitation and ionisation**
 - Speed and effective charge scaling from protons by Dingfelder *et al.*,
- **Charge change**
 - Semi-empirical models from Dingfelder *et al.*

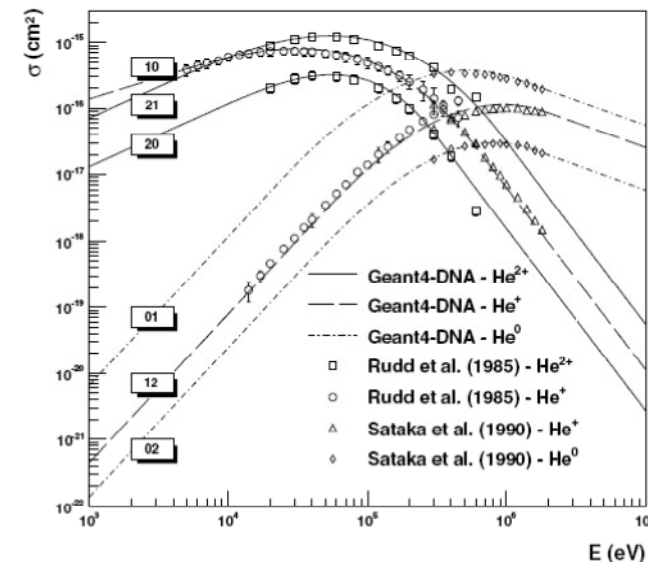
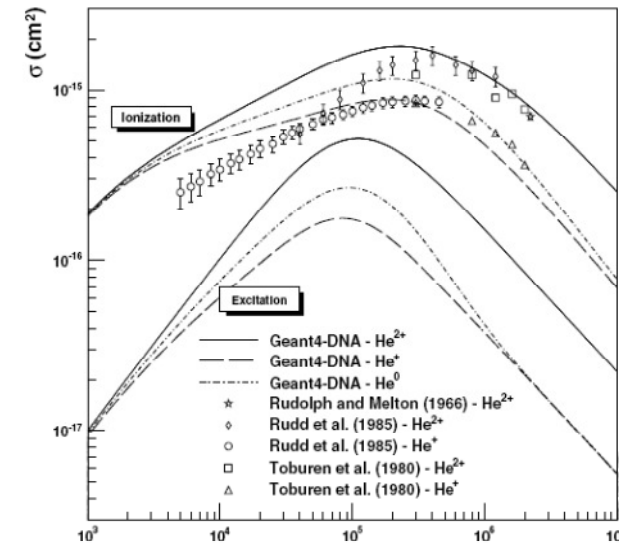
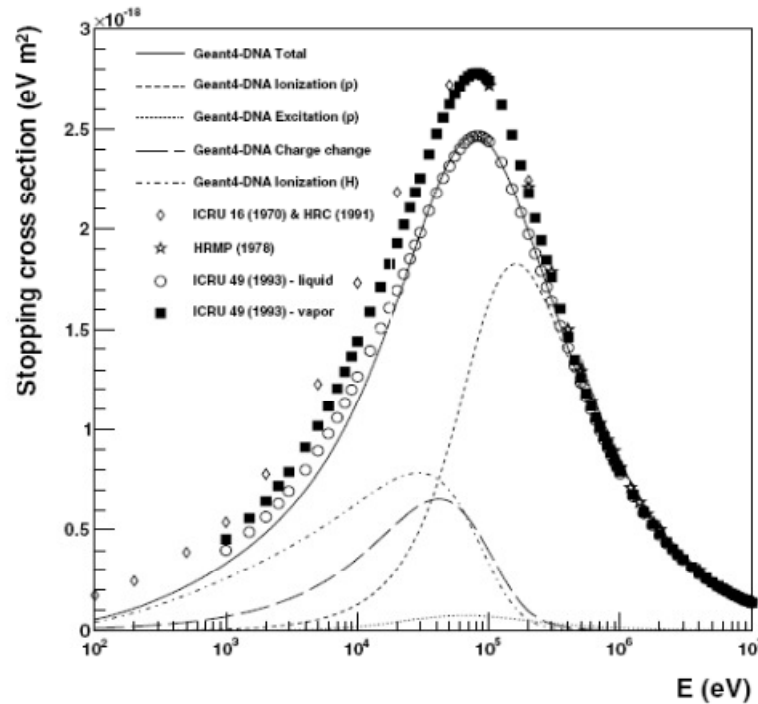
C, N, O, Fe

- **Ionisation**
 - Speed scaling and global effective charge by Booth and Grant

Overview of Geant4-DNA physics processes and models available in Geant4 9.6 for liquid water

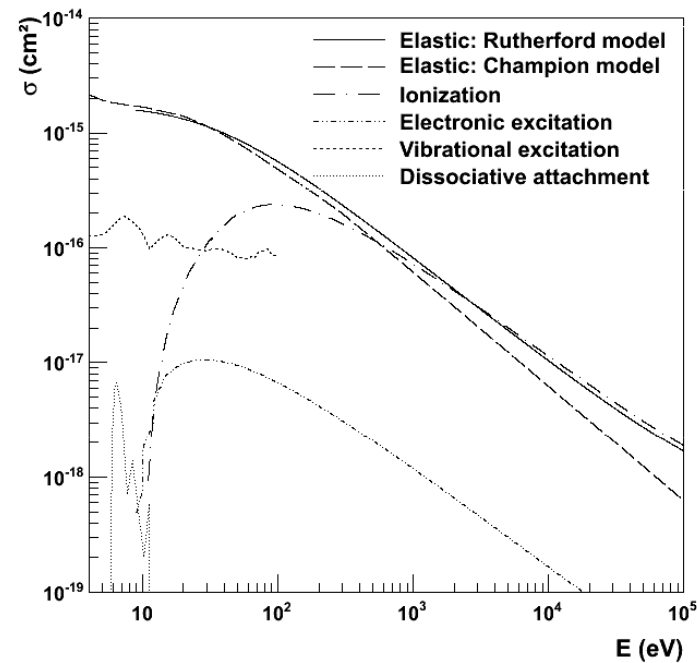
Particles	e-	p	H	He ⁺⁺ , He ⁺ , He ⁰	C, N, O, Fe,...
Elastic scattering	> 9 eV – 1 MeV Screened Rutherford >7.4 eV – 1 MeV Champion	-	-	-	-
Excitation	9 eV – 1 MeV Born	10 eV – 500 keV Miller Green 500 keV – 100 MeV Born	10 eV – 500 keV Miller Green	Effective charge scaling from same models as for proton 1 keV – 400 MeV	-
Charge Change	-	100 eV – 10 MeV Dingfelder	100 eV – 10 MeV Dingfelder		-
Ionisation	11 eV – 1 MeV Born	100 eV – 500 keV Rudd 500 keV – 100 MeV Born	100 eV – 100 MeV Rudd		Effective charge scaling 0.5 MeV/u – 10 ⁶ MeV/u
Vibrational excitation	2 – 100 eV Michaud et al.	See full details in Med. Phys. 37 (2010) 4692-4708 and Appl. Radiat. Isot. 69 (2011) 220-226			
Attachment	4 – 13 eV Melton				

Protons and alpha processes cross-sections in liquid water



- Each physics process can use one or several complementary or alternative models
- Each model provides the total cross section and a computation of the final state: kinematics, secondary particles involved

Electron processes cross-sections in liquid water



Electron process cross sections cover energy range up to 1 MeV down to either

- 7.4 eV for the Champion elastic scattering model (default model)
- or 9 eV for the Screened Rutherford elastic scattering model

The Multiscale approach

Combination of processes for different geometric regions

Particularly useful for gamma irradiations

Gammas (Livermore or Penelope(2008) models for) :

- Photoelectric effect
- Compton scattering
- Gamma conversion
- Rayleigh scattering
- + fluorescence emission or Auger electron production

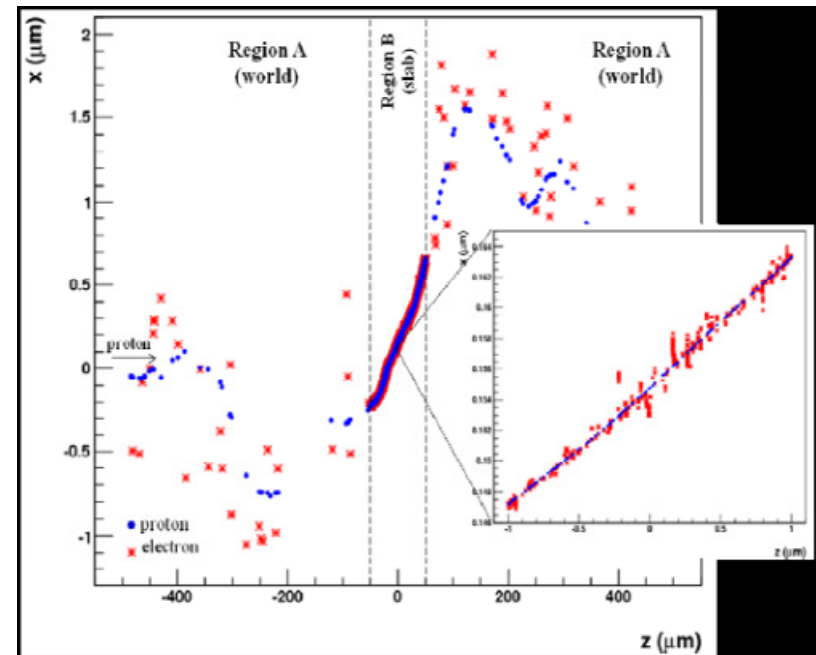
Electrons :

Outside the target volume

- Moller-Bhabha model for ionization
- Standard Bremsstrahlung model
- Standard Multiple Scattering model

Inside the target volume

- G4DNA elastic collisions (Champion Elastic Model),
- G4DNA ionization (Born Ionization model),
- G4DNA excitation (Born Excitation Model),
- electron capture $T_e < 9$ eV

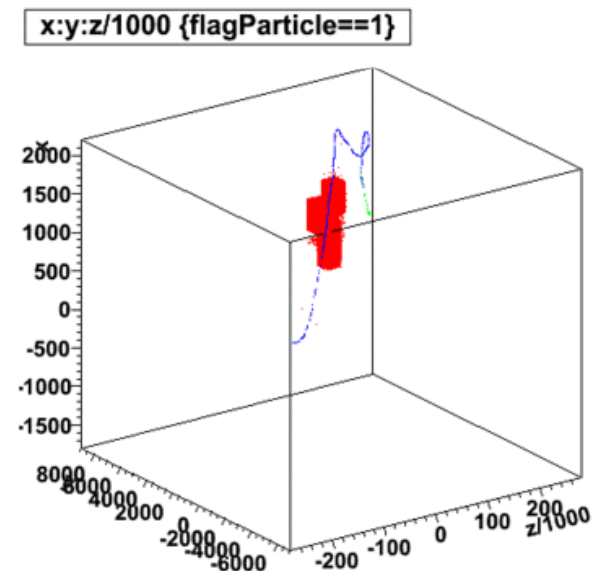
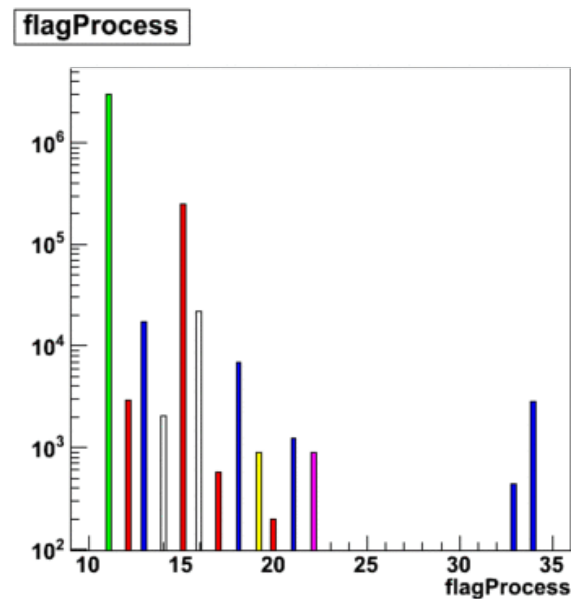


See Prog. Nucl. Sci. Tec. 2 (2011) 898-903

The **microdosimetry** Geant4 “advance example”

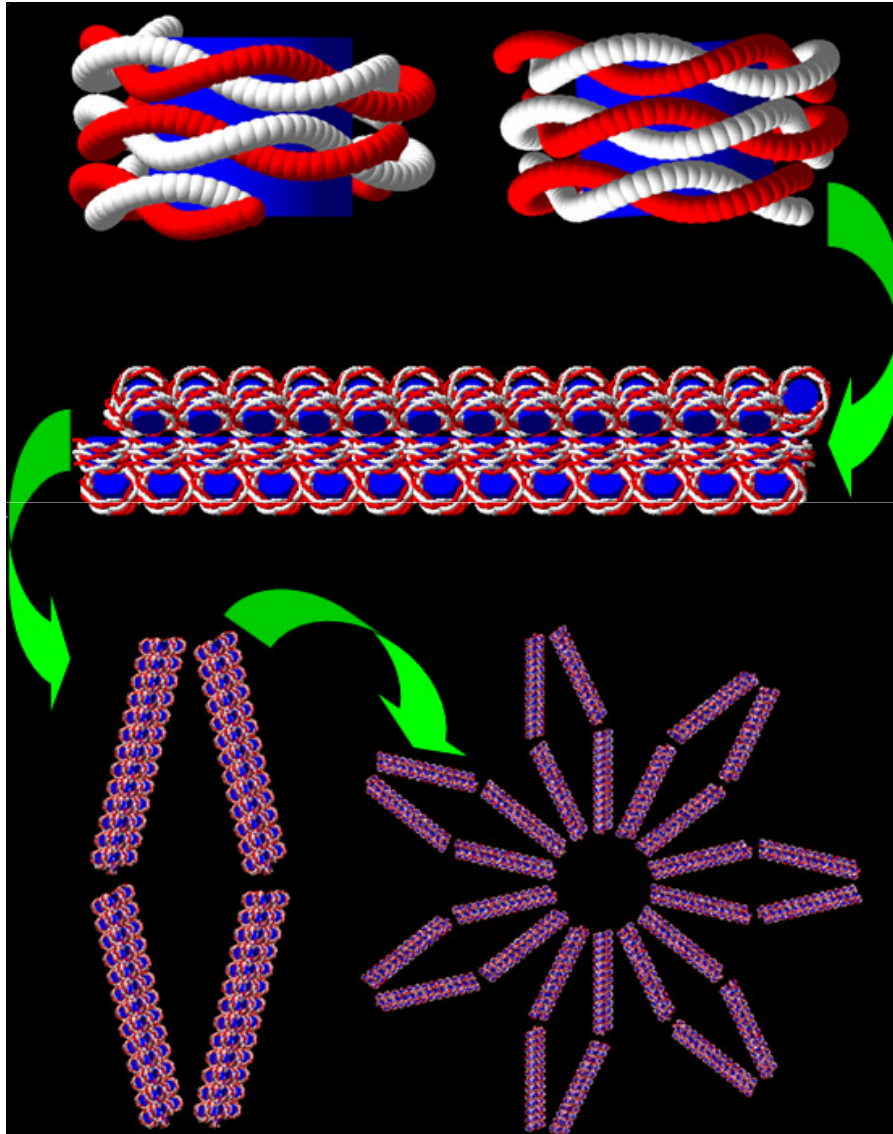
Purpose:

- Explain to users how to use Geant4 very low energy electromagnetic processes for microdosimetry
- Calculation of track structure of a He⁺ particle in liquid water, ROOT macro provided for data analysis



The target geometry

*M. Dos Santos PhD. Work
(IRSN)*



■ Nucleosome

- 200 bp / nucleosome
- DNA diameter = 2.16 nm
- Histone = cylinder of 6.5 nm in diameter and 5.7 nm in height

■ Chromatin fiber

- 90 nucleosomes / fiber
- 7 nucleosomes / turn
- $\lambda = 31$ nm
- $L = 161$ nm

■ Chromatin fiber loop

- 4 fibers / loop assembled in a diamond shape
- 7 loops to form a “flower”*

* W. Friedland & al, *Simulation of DNA damage after Proton irradiation, Radiation Research* 59 (2003), 401-410.

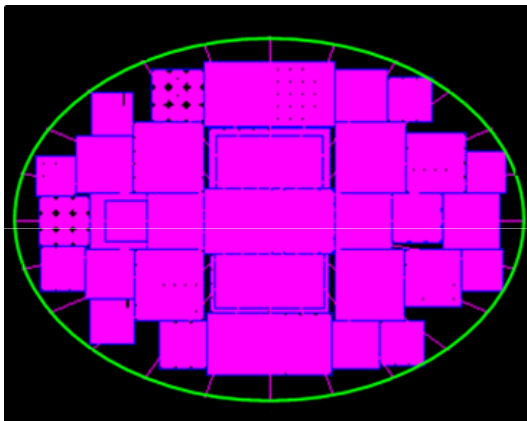
The target geometry

*M. Dos Santos PhD. Work
(IRSN)*

Implementation of two cell nuclei in GO/G1 phase (purpose: link with biological experimental data of γ -H2AX foci)

Chromatin density sensibility study

Fibroblast cell nucleus

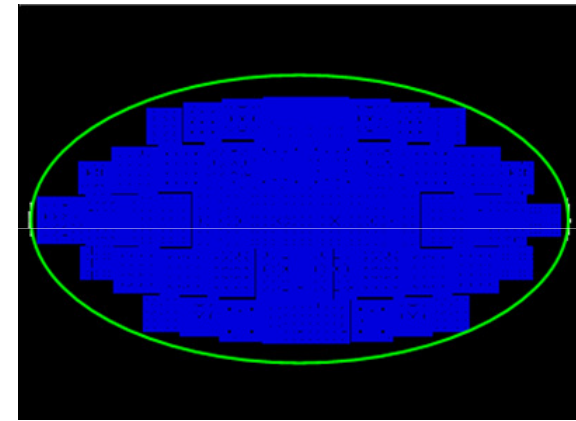


Per nucleus:

- 23 pairs of chromosomes
- 11875 flowers or 83125 loops
- 332 500 chromatin fibers
- 29 925 000 nucleosomes
- ~ 6 Gbp

- Nucleus -> ellipsoid
- Dimensions: 19.7 * 14.2 * 5 μm^3
- V = 732 μm^3
- 0.42 % of DNA / nucleus

Endothelium cell nucleus



- Nucleus -> ellipsoid
- Dimensions: 19 * 11 * 2 μm^3
- V = 219 μm^3
- 1.43 % of DNA / nucleus

Track analysis

Clustering algorithm (DBSCAN)

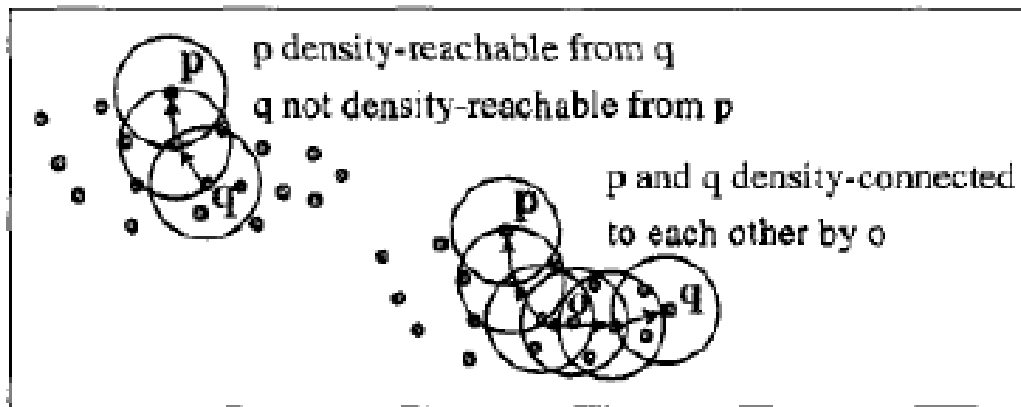
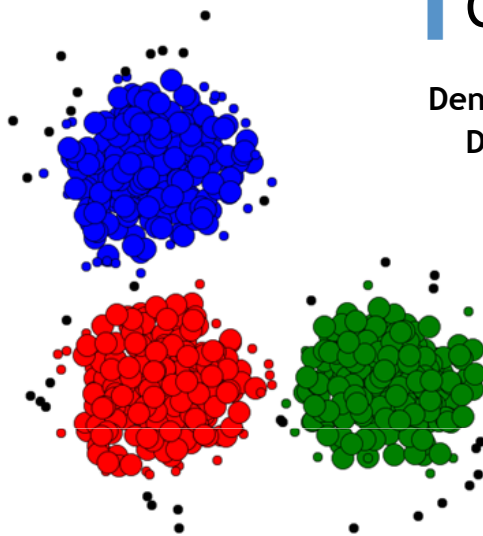
Density Based Spatial Clustering of Applications with Noise. 2nd Int. Conf. On Knowledge Discovery and Data Mining (Martin Ester et al. - 1998)

➤ Powerful method to:

- Reveal points belonging to a same group
- showing the links between them

➤ Some parameters have to be defined:

- Minimum number of points to form a cluster : 2
- Maximal radius : 3.2 nm (~ 10bp)
- Minimal Energy per point : 8 eV



- p belongs to the cluster centered in q if $\text{dist}(p, q) \leq \text{radius}$ (parameter)

- Clusters can merge if they are connected by a central cluster

Track analysis

- Currently, It is not possible to calculate the **number of SSB or DSB** as **indirect effects are missing (in progress)** and thus an **absolute normalization is not yet possible**

Type of clusters and relation to potential DAN damages

- Isolated interaction points:

» Interaction points located at more than **3.2 nm** of any other point



- Simple cluster:

» Interaction points located on the same strand and separated by less than **3.2 nm**



- Complex cluster:

» Interaction points where at least one of them is located on a different strand and separated by less than **3.2 nm**

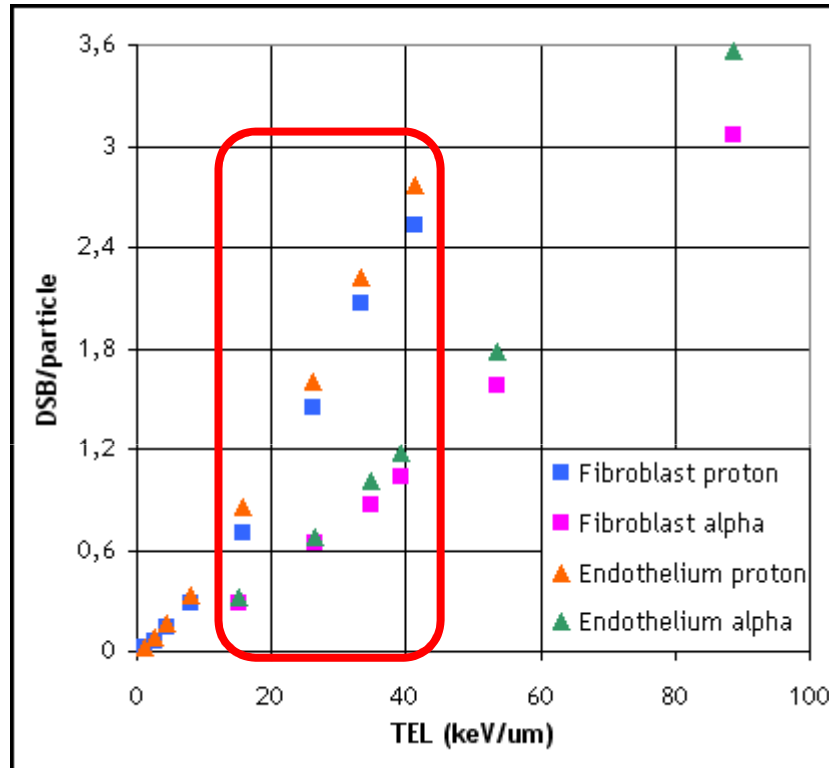


SSB_{cand}

DSB_{cand}

Some results using the target geometry and DBSCAN

*M. Dos Santos PhD. Work (IRSN)
accepted in NIM B (2013)*

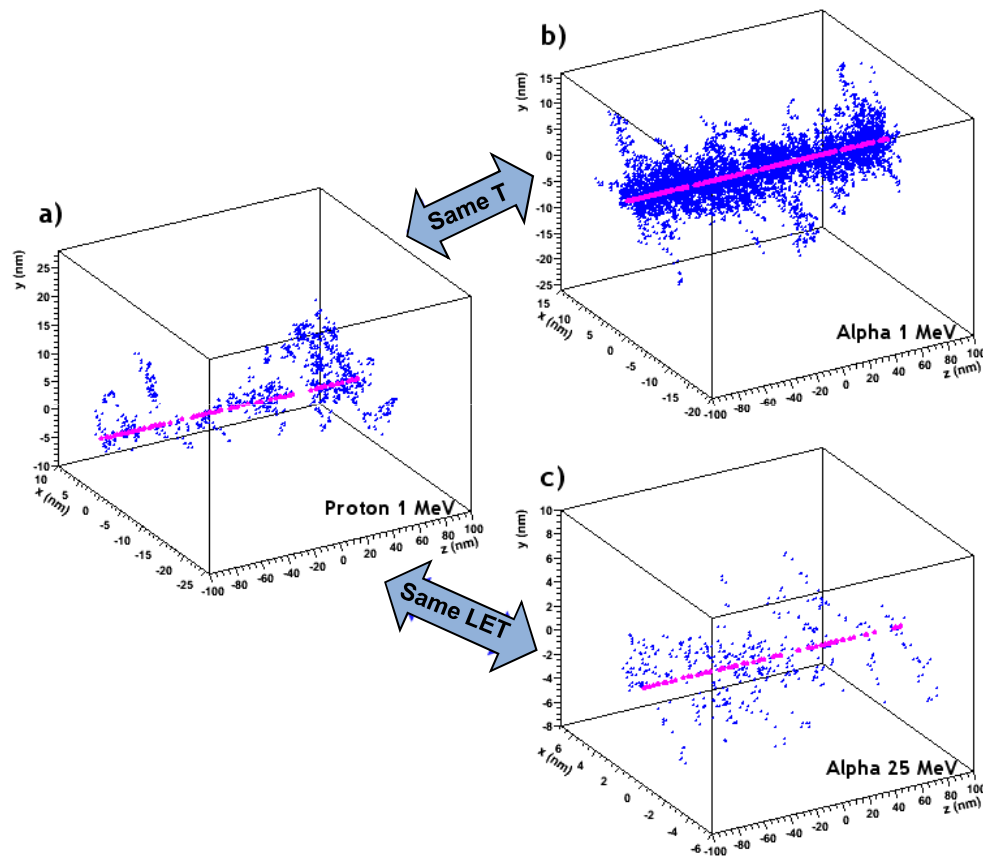
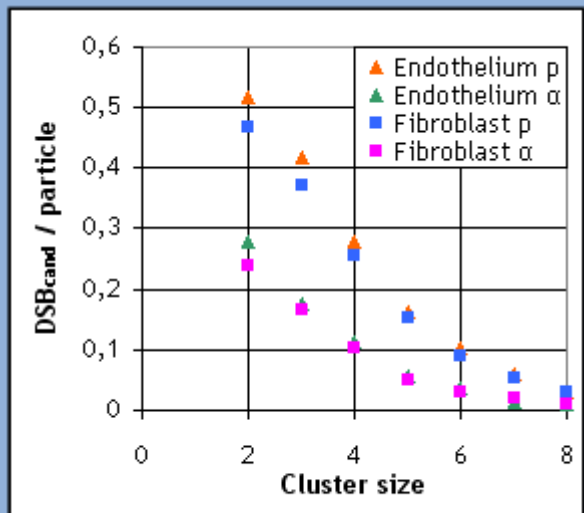


- ▮ \nearrow of DSB_{cand} with \nearrow LET
- ▮ More clusters are produced on the “endothelium” cell nuclei (more compacted DNA)
- ▮ For similar LET, more damages are created by p than alpha particles

Some results using the target geometry and DBSCAN

LET ~ 26 keV/ μ m

Cluster size	Endothelium		Fibroblast	
	Proton	Alpha	Proton	Alpha
2	0.518	0.278	0.469	0.237
3	0.419	0.175	0.373	0.165
4	0.384	0.112	0.254	0.102
5	0.260	0.058	0.151	0.051
6	0.156	0.035	0.089	0.029
7	0.095	0.0139	0.052	0.021
8	0.057	0.008	0.030	0.011



M. Dos Santos PhD. Work (IRSN)
accepted in NIM B (2013)

Micro and nanodosimetric calculations

D. Bianco post-doc (IRSN) for BioQuaRT project

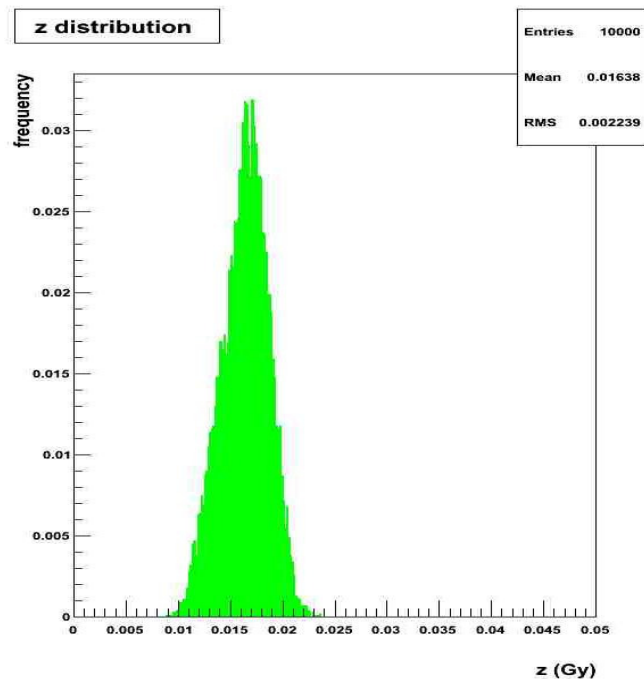
Multiscale approach

Specific energy
(stochastic variable)

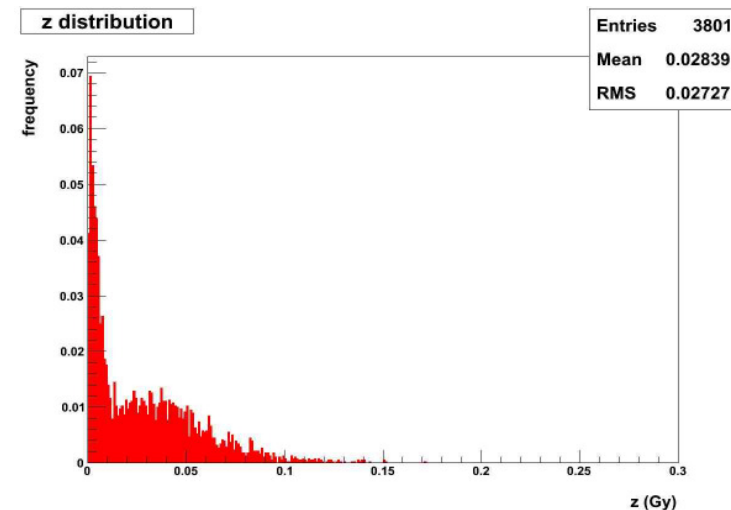
$$z = \frac{\varepsilon}{m}$$

Mean specific energy
(non stochastic)

$$\int z f(z; D) dz = \bar{z}$$



Z distribution for 1 MeV p traversing the cell nucleus ellipsoid

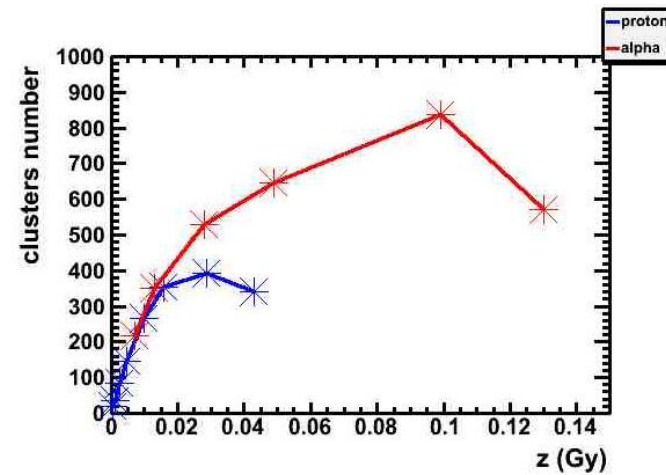
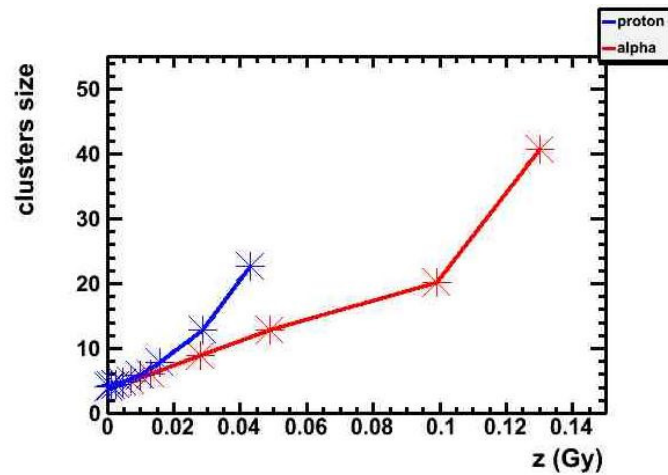


Z distribution for 1 MeV p only backbone contribution (using target geometry)-> direct effects

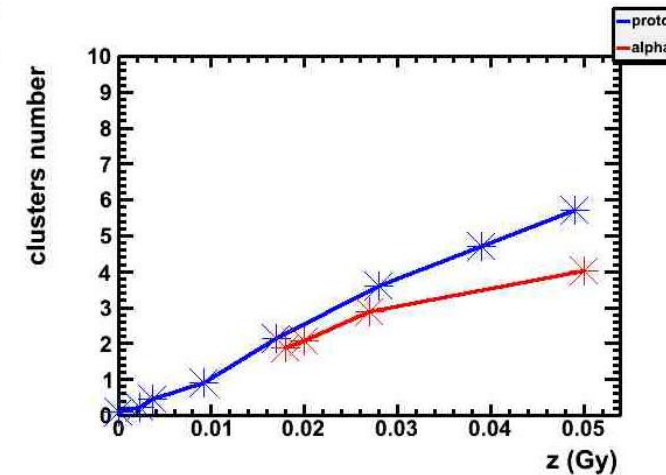
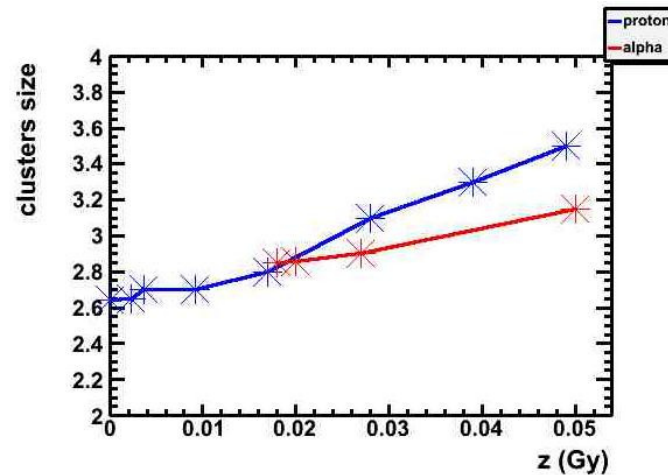
Micro and nanodosimetric calculations

D. Bianco post-doc (IRSN) for BioQuaRT project

Multiscale approach



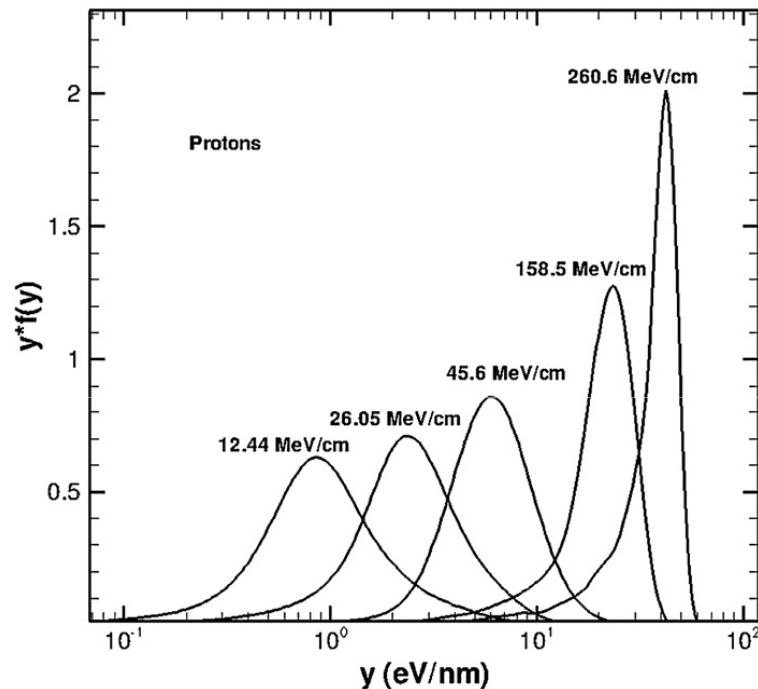
Homogeneous medium



DNA target

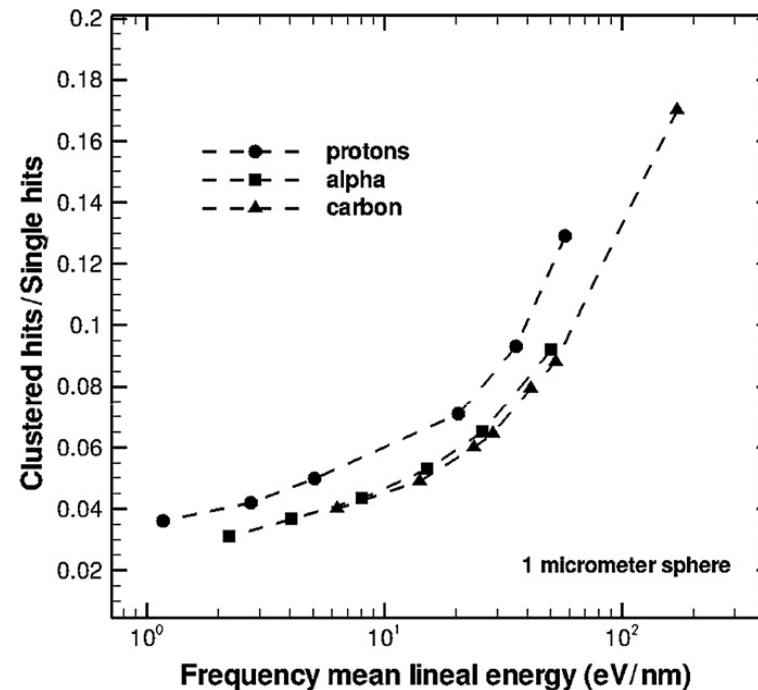
Micro and nanodosimetric calculations

Multiscale approach



Microdosimetric spectra can be calculated for p, alpha particles and light ions for different target sizes (here 1 μ m diameter sphere)

➤ See Z. Francis et al. Phys. Med. Biol. 57 (2012)



A study of the clustered energy deposits respect to the frequency mean lineal energy give us quantitative information on the different effect depending on the radiation quality

Modelling Indirect effects with Geant4-DNA

*M. Karamitros PhD. Work
(23/11/2012, CENBG)*

Physico-chemical stage

Chemical stage

$t=10^{-15}\text{s}$

$t=10^{-12}\text{s}$

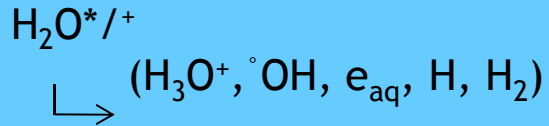
$t=10^{-6}\text{s}$

Modelling Indirect effects with Geant4-DNA

M. Karamitros PhD. Work
(23/11/2012, CENBG)

Physico-chemical stage

- **Dissociation** :



- **Thermalization** of the products down to their energy of diffusion at equilibrium.

- **Ionised** molecules **convert** into :



- **Excited** molecules **relax** or **dissociate**

	Process	Decay channel	Fraction (%)
Ionisation (H_2O^+)			
1b ₁ , 3a ₁ , 1b ₂ , 2a ₁ , K	Dissociative decay	$\text{H}_3\text{O}^+ + \text{}^\bullet\text{OH}$	100
Excitation (H_2O^*)			
A ¹ B ¹	Dissociative decay	$\text{}^\bullet\text{OH} + \text{H}^\bullet$	65
	Relaxation	$\text{H}_2\text{O} + \Delta\text{E}$	35
B ¹ A ¹	Auto-ionisation	$\text{H}_3\text{O}^+ + \text{}^\bullet\text{OH} + e_{\text{aq}}^-$	55
	Dissociative decay	$\text{H}_2 + \text{}^\bullet\text{O}^\bullet$	15
	Relaxation	$\text{H}_2\text{O} + \Delta\text{E}$	30
Ryd, diff bands	Auto-ionisation	$\text{H}_3\text{O}^+ + \text{}^\bullet\text{OH} + e_{\text{aq}}^-$	50
	Relaxation	$\text{H}_2\text{O} + \Delta\text{E}$	50

Kreipl et al, Radiat Environ Biophys, 2009

Modelling Indirect effects with Geant4-DNA

*M. Karamitros PhD. Work
(23/11/2012, CENBG)*

Physico-chemical stage

Chemical stage

Step By Step (SBS) model

- The probability of encounter is evaluated after each time step.

$t = 10^{-15}$ s

$t = 10^{-12}$ s

$t = 10^{-6}$ s

IRSN
Winter School : « micro and nanodosimetric calculations with Geant4-DNA »

Modelling Indirect effects with Geant4-DNA

*M. Karamitros PhD. Work
(23/11/2012, CENBG)*

Molecular species & diffusion

Species	Diffusion coefficient D (10 ⁻⁹ m ² s ⁻¹)
e ⁻ _{aq}	4.9
•OH	2.8
H•	7.0
H ₃ O ⁺	9.0
H ₂	4.8
OH ⁻	5.0
H ₂ O ₂	2.3

Brownian diffusion $\langle R \rangle = \sqrt{6 \cdot D \cdot \Delta t}$

Time interval (s)	Δt (ps)
Until 10 ⁻¹¹	0.1
10 ⁻¹¹ -10 ⁻¹⁰	1
10 ⁻¹⁰ -10 ⁻⁹	3
10 ⁻⁹ -10 ⁻⁸	10
Above 10 ⁻⁸	100

Chemical reactions

Reaction	Reaction rate (10 ¹⁰ M ⁻¹ s ⁻¹)
H• + e ⁻ _{aq} + H ₂ O → OH ⁻ + H ₂	2.65
H• + •OH → H ₂ O	1.44
H• + H• → H ₂	1.20
H ₂ + •OH → H• + H ₂ O	4.17 × 10 ⁻³
H ₂ O ₂ + e ⁻ _{aq} → OH ⁻ + •OH	1.41
H ₃ O ⁺ + e ⁻ _{aq} → H• + H ₂ O	2.11
H ₃ O ⁺ + OH ⁻ → 2 H ₂ O	14.3
•OH + e ⁻ _{aq} → OH ⁻	2.95
•OH + •OH → H ₂ O ₂	0.44
e ⁻ _{aq} + e ⁻ _{aq} + 2 H ₂ O → 2 OH ⁻ + H ₂	0.50

For this prototype software, we followed the set of parameters published by the authors of the **PARTRAC** software.

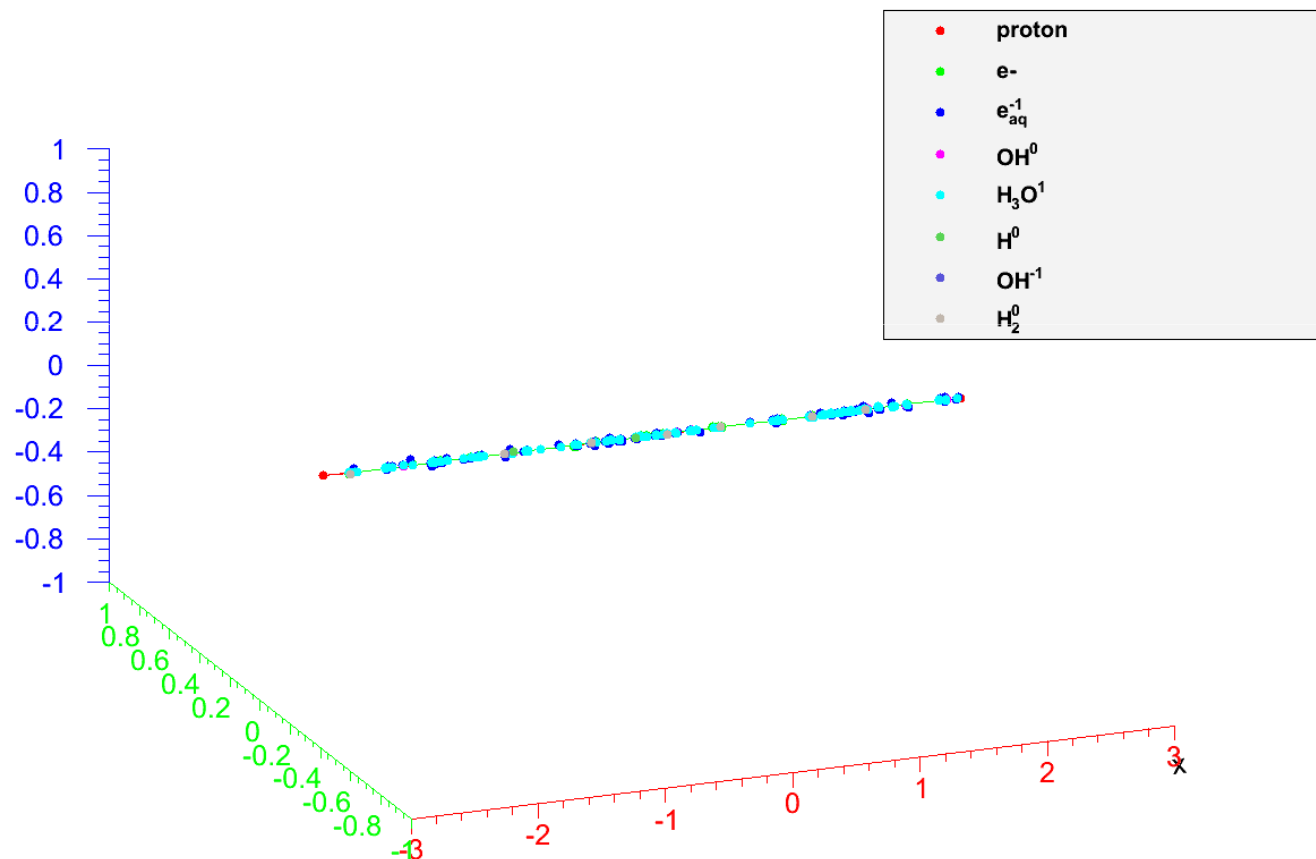
However these parameters can be **modified by the user**.

Kreipl et al, Radiat Environ Biophys, 2009

Modelling Indirect effects with Geant4-DNA

Simulation at 1 picosecond

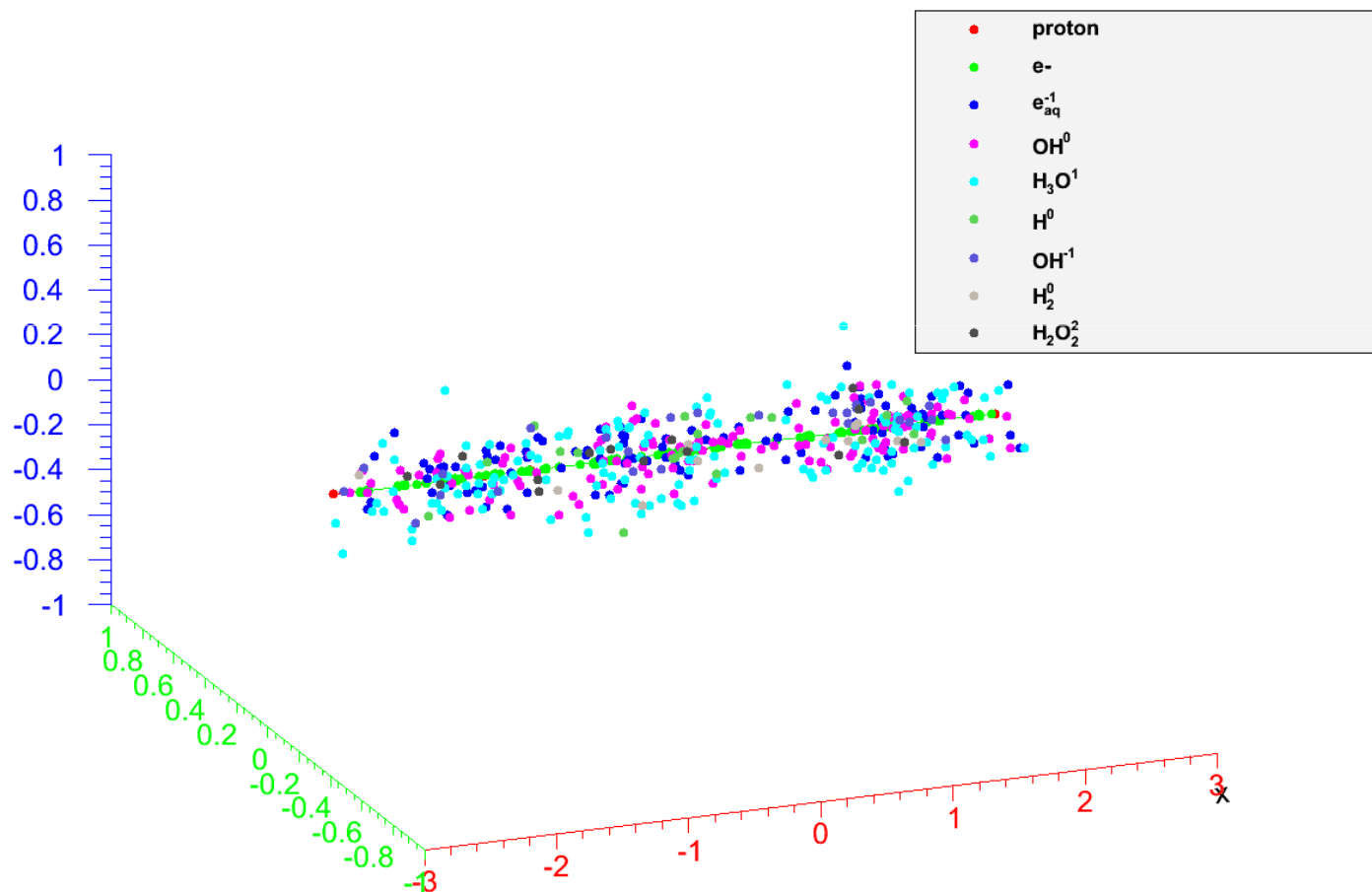
*M. Karamitros PhD. Work
(23/11/2012, CENBG)*



Modelling Indirect effects with Geant4-DNA

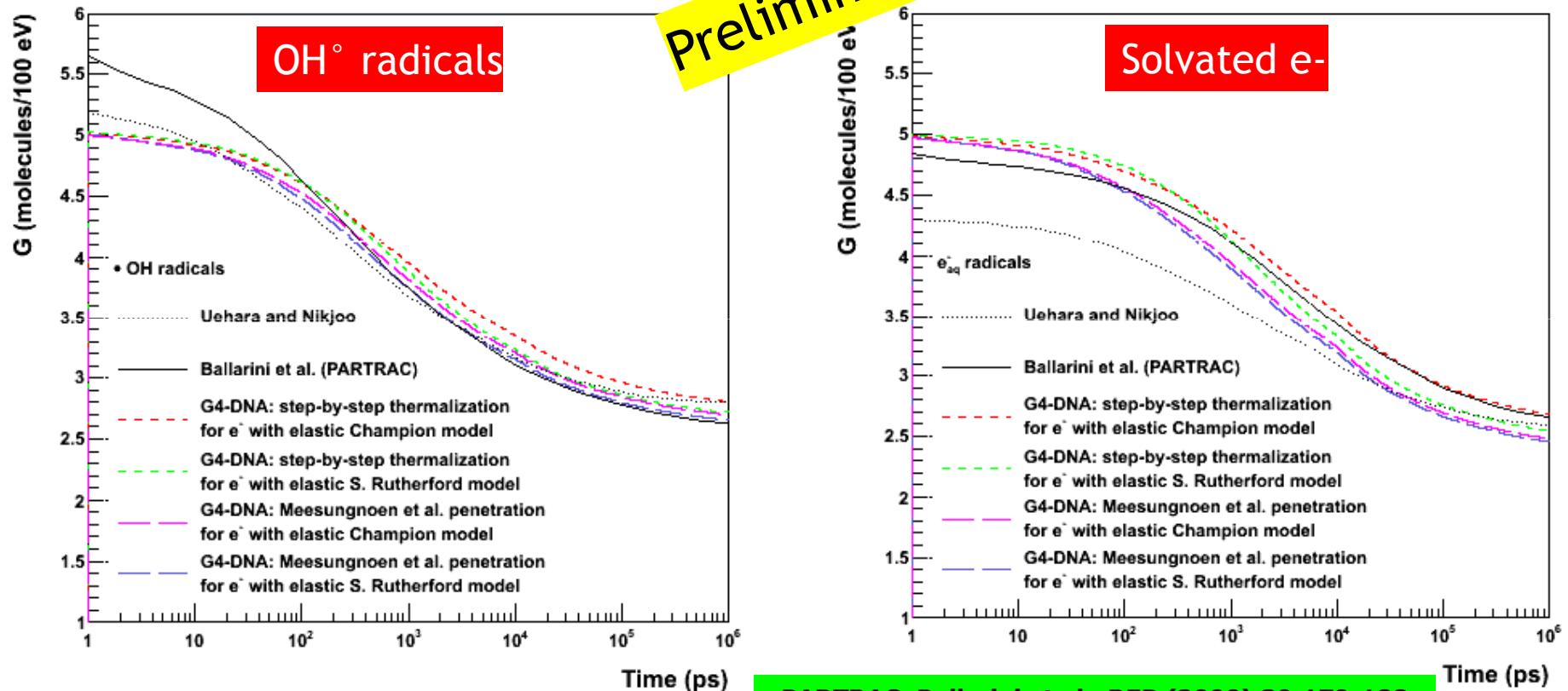
Simulation at 1 μ second

*M. Karamitros PhD. Work
(23/11/2012, CENBG)*



Modelling Indirect effects with Geant4-DNA

Radiochemical yields versus time



PARTRAC: Ballarini et al., REB (2000),39:179-188
Uehara et Nikjoo, J. Radiat. Res. (2006),47:69-81

- Effect of the two **alternative** electron elastic scattering models
- Results are obtained in **30 minutes** on a cluster of 80 CPUs (Physics + Chemistry)

Geant4-DNA from the internet

A unique web site for Geant4-DNA: <http://geant4-dna.org>

The Geant4-DNA project

Extending the Geant4 Monte Carlo simulation toolkit for radiobiology

[Geant4-DNA](#)

[Software](#)

[Physics](#)

[Chemistry](#)

[User examples](#)

[Publications](#)

[Collaboration](#)

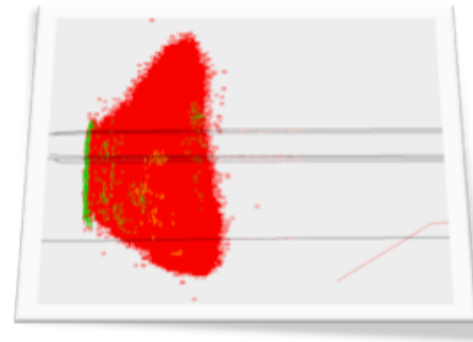
[Funding](#)

Welcome to the Internet page of the **Geant4-DNA project**.

The [Geant4](#) Monte Carlo simulation toolkit is being extended with processes for the **modeling of early biological damages induced by ionising radiation at the DNA scale**. Such developments are on-going in the framework of the Geant4-DNA project, initiated in 2000 by the [European Space Agency/ESTEC](#).

On-going developments include

- **Physics** processes in liquid water and other biological materials
- **Chemistry** and **physico-chemistry** processes
- Molecular **geometries**
- Quantification of **damages** (single-strand, double-strand breaks, ...)



Recent posts

The last Geant4 release (9.5) is available for download, see our **Software** section.

Acknowledgments

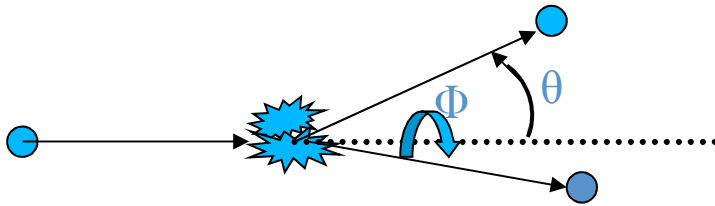
- The Geant4-DNA collaboration thanks **all theoreticians** who are helping us for the development of this extension in the Geant4 toolkit, in particular:
 - **Dr M. Dingfelder** (East Carolina U., NC, US)
 - **Dr D. Emfietzoglou** (Ioannina U., Greece)
 - **Dr B. Grosswendt** (PTB, Germany)

- We also thank **Dr W. Friedland** (Helmholz Zentrum, Munich, Germany), developer of **PARTRAC**, for his guidance and constant support, since the early days of Geant4-DNA

Thank you for your attention

Diffusions angulaires

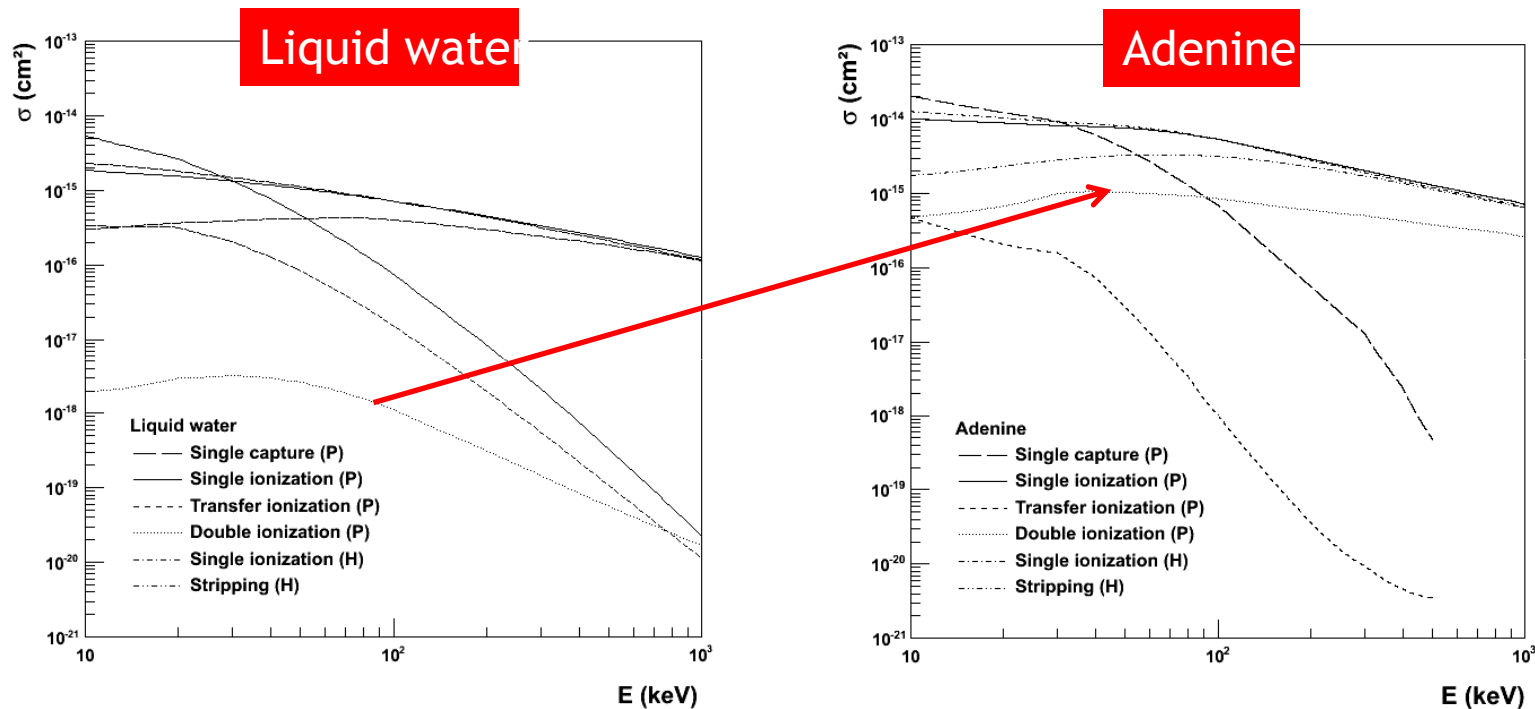
- Procédure de Grosswendt pour les interactions des électrons
- Conservation de la quantité de mouvement pour les protons



- Tirage aléatoire entre les processus d'interaction possibles tenant compte des valeurs des sections efficaces totales
- La longueur du parcours avant la collision est déduite du libre parcours moyen du processus choisis
- Un tirage aléatoire suivant les sections efficaces relatives à chaque couche du cortège électronique permet de choisir la couche interagissant avec la particule incidente
- Si nécessaire (ionisation), un tirage aléatoire suivant la section efficace différentielle permet de déduire l'énergie de la particule secondaire générée
- La direction de la particule secondaire est déduite suivant le modèle adapté (Grosswendt pour les électrons, conservation de la quantité de mouvement pour les protons...)

Comparison for DNA -liquid water cross sections

Classical trajectory Monte Carlo approach (CTMC-COB)



Protons : single capture, single ionization, transfer ionization (**new process**), double ionization (**new process**)

Neutral hydrogen : single ionization, stripping

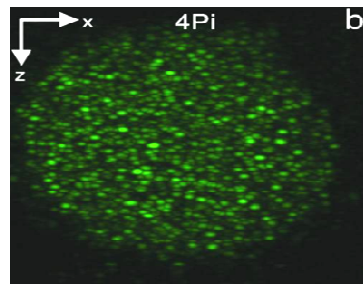
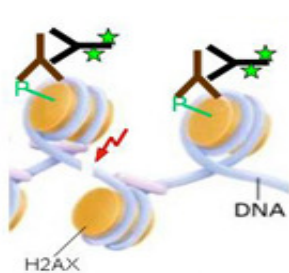
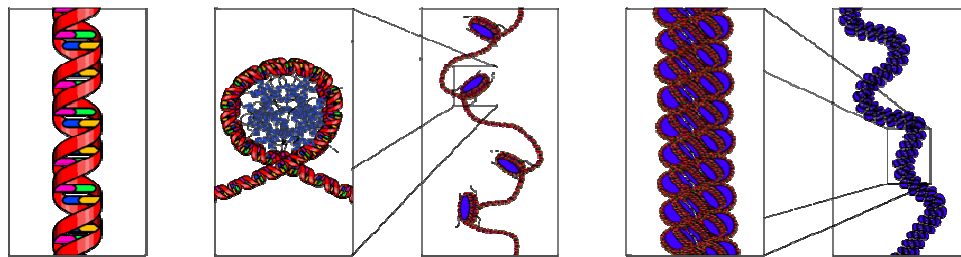
Adenine cross sections are of about **one order of magnitude greater** than their homologous in liquid water for all the ionizing processes (double ionization shows a 2 orders of magnitude ratio) (but, density is different for both materials->

The target geometry

- “Realistic” relative position of the nanometric volumes of interest at micrometric scale for track intersection analysis
- G0/G1 phase -> DNA almost homogeneously distributed within the cell nucleus

γ -H2AX foci data obtained in this cell cycle phase

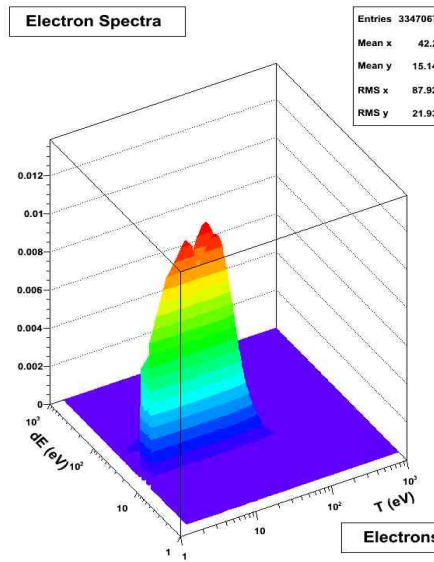
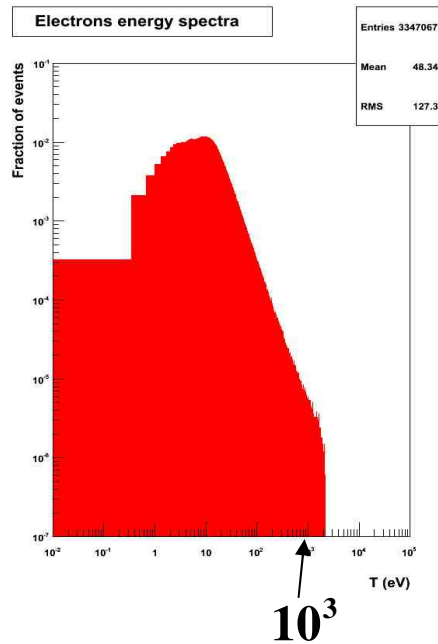
γ H2AX foci
=> signalization of DSB



- The target geometry is included in the Monte Carlo simulation-> Detector Construction.cc
- First selection of interesting points for direct effects
- Purpose: available as an example in next releases of Geant4
- In progress-> Hetero-Euchromatin influence study

Electron spectra calculated with Geant4-DNA

D. Bianco post-doc (IRSN) for BioQuaRT project



➤ First secondary electron spectra from 1 MeV proton tracks traversing the cell nuclei ellipsoid

➤ First secondary electron spectra from 25 MeV alpha tracks traversing the cell nuclei ellipsoid. One can also see the production shell of the electrons

