The Geant4-DNA project
Overview & Physics

http://geant4-dna.org

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representing the « Geant4-DNA » collaboration

1st Geant4-DNA tutorial

ESA/ESTEC, November 7th, 2014

Morning agenda

09:00	**Welcome**		*Einstein, European Space Research and Technology Centre (ESTEC)*	09:00 - 09:10
	Geant4-DNA Overview & Physics	*Dr. Sebastien INCERTI*	*Einstein, European Space Research and Technology Centre (ESTEC)*	09:10 - 09:30
	Geant4-DNA Chemistry	*Mr. Mathieu KARAMITROS*	*Einstein, European Space Research and Technology Centre (ESTEC)*	09:30 - 10:10
10:00	**Installation of Geant4 Virtual Machine**	*Sylvain MEYLAN*	*Einstein, European Space Research and Technology Centre (ESTEC)*	10:10 - 10:30
	Break		*Einstein, European Space Research and Technology Centre (ESTEC)*	10:30 - 11:00
11:00	**Hands-on: dnaphysics**	*Dr. Sebastien INCERTI*	*Einstein, European Space Research and Technology Centre (ESTEC)*	11:00 - 11:30
	Geant4-DNA Geometries (from molecules to cells) & hands-on: wholeNuclearDNA	*Dr. Carmen VILLAGRASA et al.*	*Einstein, European Space Research and Technology Centre (ESTEC)*	11:30 - 12:00
12:00	**Lunch at ESA**		*Einstein, European Space Research and Technology Centre (ESTEC)*	12:00 - 13:30
13:00				

Afternoon agenda

	Hands-on: chem1	*Mr. Mathieu KARAMITROS*	*Einstein, European Space Research and Technology Centre (ESTEC)*	13:30 - 14:00
14:00	**Hands-on: chem2**	*Mr. Sylvain MEYLAN*	*Einstein, European Space Research and Technology Centre (ESTEC)*	14:00 - 14:30
	Hands-on: chem3	*Dr. Vaclav STEPAN*	*Einstein, European Space Research and Technology Centre (ESTEC)*	14:30 - 15:00
15:00	**Hands-on: pdb4dna**	*Dr. Emmanuel DELAGE et al.*	*Einstein, European Space Research and Technology Centre (ESTEC)*	15:00 - 15:30
	Hands-on: microdosimetry	*Dr. Sebastien INCERTI*	*Einstein, European Space Research and Technology Centre (ESTEC)*	15:30 - 16:00
16:00	**Discussion**		*Einstein, European Space Research and Technology Centre (ESTEC)*	16:00 - 16:30

Contents

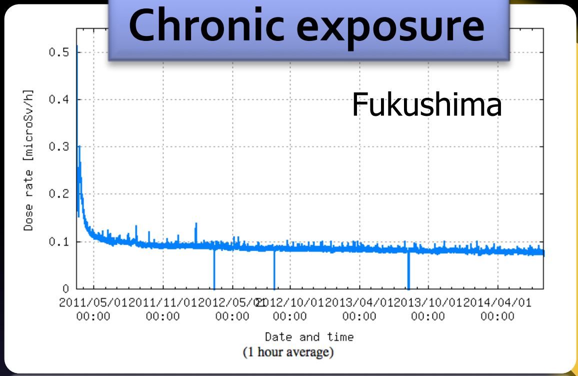
- Context of the Geant4-DNA project
- **Physical** stage
  - Overview of models
  - Recent verification & validation activities
- Where to find more information ?

See Geant4-DNA reference …(link)

1) CONTEXT

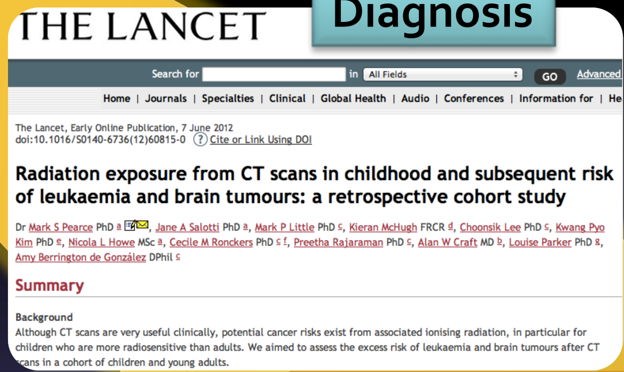
Modelling biological effects of ionising radiation remains a major scientific challenge

Chronic exposure



http://rcwww.kek.jp/norm/index-e.html

Diagnosis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The Lancet, Early Online Publication, 7 June 2012
doi:10.1016/S0140-6736(12)60815-0 Cite or Link Using DOI

Radiation exposure from CT scans in childhood and subsequent risk of leukaemia and brain tumours: a retrospective cohort study

Dr Mark S Pearce PhD, Jane A Salotti PhD, Mark P Little PhD, Kieran McHugh FRCR, Choonsik Lee PhD, Kwang Pyo Kim PhD, Nicola L Howe MSc, Cecile M Ronckers PhD, Preetha Rajaraman PhD, Alan W Craft MD, Louise Parker PhD, Amy Berrington de González DPhil

Summary

Background

Although CT scans are very useful clinically, potential cancer risks exist from associated ionising radiation, in particular for children who are more radiosensitive than adults. We aimed to assess the excess risk of leukaemia and brain tumours after CT scans in a cohort of children and young adults.

Space missions

Space exploration

Proton & hadrontherapy

« A major challenge lies in providing a sound mechanistic understanding of low-dose radiation carcinogenesis »

L. Mullenders *et al.*

Assessing cancer risks of low-dose radiation

Nature Reviews Cancer (2009)

The Monte Carlo appraoch

- Can « reproduce » with accuracy the stochastic nature of particle-matter interactions
- 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, TRIOL, PHITS, KURBUC, 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 ?

« TO EXPAND ACCESSIBILITY AND AVOID 'REINVENTING THE WHEEL', TRACK STRUCTURE CODES SHOULD BE MADE AVAILABLE TO ALL USERS VIA THE INTERNET FROM A CENTRAL DATA BANK»

H. NIKJOO, IJRB 73, 355 (1998)

Geant4 for radiobiology

- Can we try to extend Geant4 to model biological effects of radiation ?
- Limitations prevent its usage for the modelling of biological effects of ionising radiation at the sub-cellular & DNA scale
  - Condensed-history approach
    - No step-by-step transport on small distances, a key requirement for micro/nano-dosimetry
  - Low-energy limit applicability of EM physics models is limited
    - Livermore Low Energy EM models can technically go down to 10 eV but accuracy limited
    - 100 eV for Penelope 2008 Low Energy EM models
  - No description of target molecular properties
    - Liquid water, DNA nucleotides, other
  - Only physical particle-matter interactions
    - At the cellular level, physical interactions are NOT the dominant processes for DNA damage at low LET…

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

The Geant4-DNA project

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 DNA damage in the context of manned space exploration missions (« bottom-up » approach).

Designed to be developed and delivered in a free software spirit under Geant4 license, easy to upgrade and improve.

Evolution

- **2001:** Initiated in 2001 by Dr Petteri Nieminen at the European Space Agency/ESTEC
- **2007:** First prototypes of physics models added to Geant4
- **Since 2008:** Development coordinated by CNRS in Bordeaux, France
- **December 2014:** Chemistry stage extension ready for end users

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

The Geant4-DNA project

- The code is a full independent sub-category of the electromagnetic physics category of Geant4

  $G4INSTALL/source/processes/electromagnetic/dna

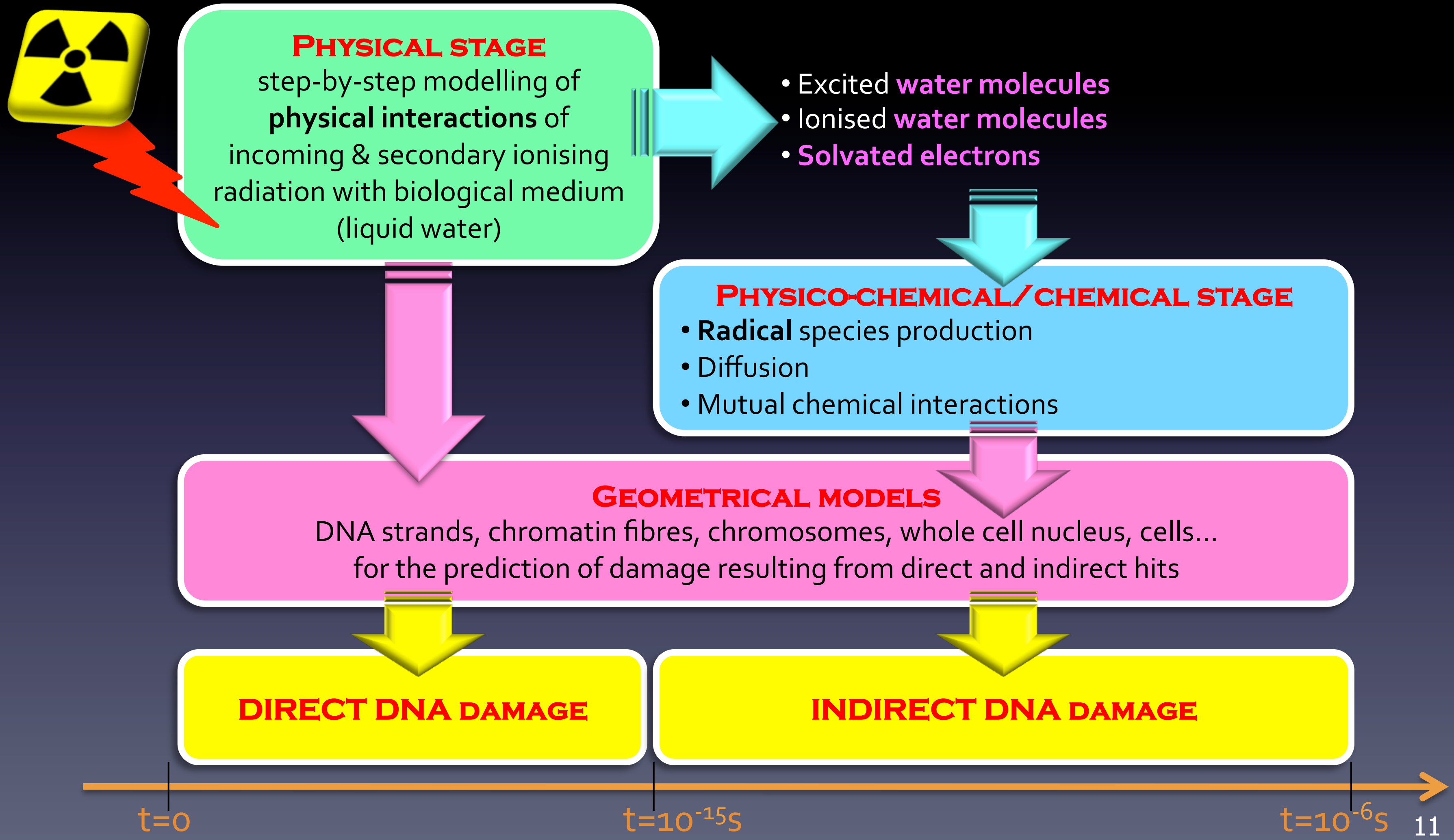
- An interdisciplinary activity of the Geant4 « low energy electromagnetic physics » working group

- Supported by several funding agencies

  ESA (AO6041, AO 7146), ANR, INSERM, IRSN…

- Integration in Geant4 enables use from inside GATE (2014), TOPAS

How can Geant4-DNA model early DNA damage ?



2) PHYSICAL STAGE

2) PHYSICAL STAGE

Overview

Physics models available in Geant4 10.0P03

- Geant4-DNA physics models are applicable to liquid water
  - Main component of biological matter
- They can reach the very low energy domain down to electron thermalization
  - Compatible with molecular description of interactions (5 excitation & ionisation levels of the water molecule)
  - 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 (nanometer scale geometries)
  - No condensed history approximation
- Models can be purely analytical and/or use interpolated data tables
  - For eg. computation of integral cross sections
- Can be run in MultiThreading mode from Geant4 10 since December 2013
- They use the same software design as all electromagnetic models available in Geant4 (« standard » and « low energy » EM models and processes)
  - Allows the combination & addition of models and processes
  - Allows combination of discrete/condensed models

Overview of physics models for liquid water

Overview

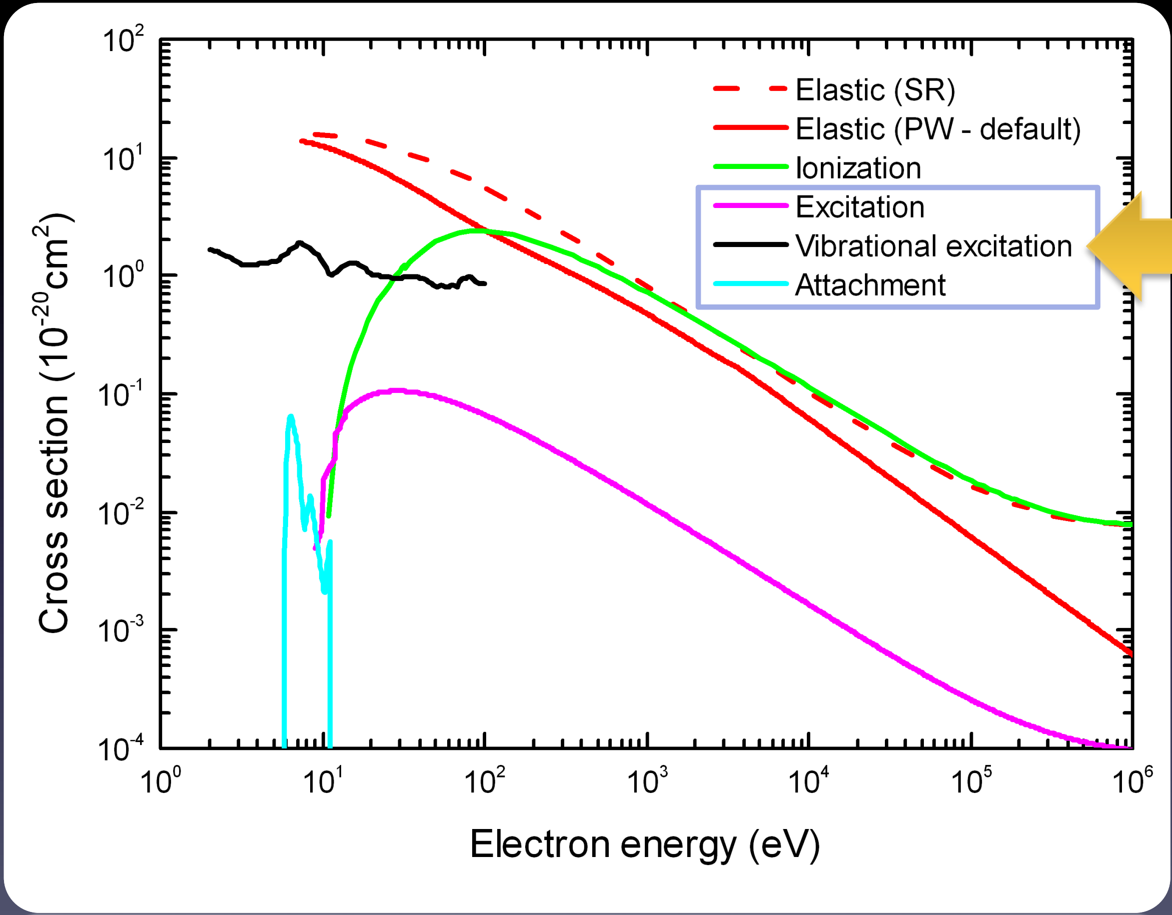
- **Electrons**
  - Elastic scattering
    - Screened Rutherford and Brenner-Zaider below 200 eV
    - Partial wave framework model, 3 contributions to the interaction potential
  - Ionisation
    - 5 levels for H_2O
    - Dielectric formalism & FBA using Heller optical data up to 1 MeV, and low energy corrections
  - Excitation (*)
    - 5 levels for H_2O
    - Dielectric formalism & FBA using Heller optical data and semi-empirical low energy corrections
  - Vibrational excitation (*)
    - Michaud *et al.* xs measurements in amorphous ice
    - Factor 2 to account for phase effect
  - Dissociative attachment (*)
    - Melton *et al.* xs measurements

(*) only available in Geant4-DNA

See Med. Phys. 37 (2010) 4692-4708 (link)
and Appl. Radiat. Isot. 69 (2011) 220-226 (link)

- **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.*
- **He^0, He^+, He^{2+}**
  - Excitation (*) and ionisation
    - Speed and effective charge scaling from protons by Dingfelder *et al.*
  - Charge change (*)
    - Semi-empirical models from Dingfelder *et al.*
- **Li, Be, B, C, N, O, Si, Fe**
  - Ionisation
    - Speed scaling and global effective charge by Booth and Grant
- **Photons**
  - from EM « standard » and « low energy »
    - Default: « Livermore »

Eg. : electron cross sections



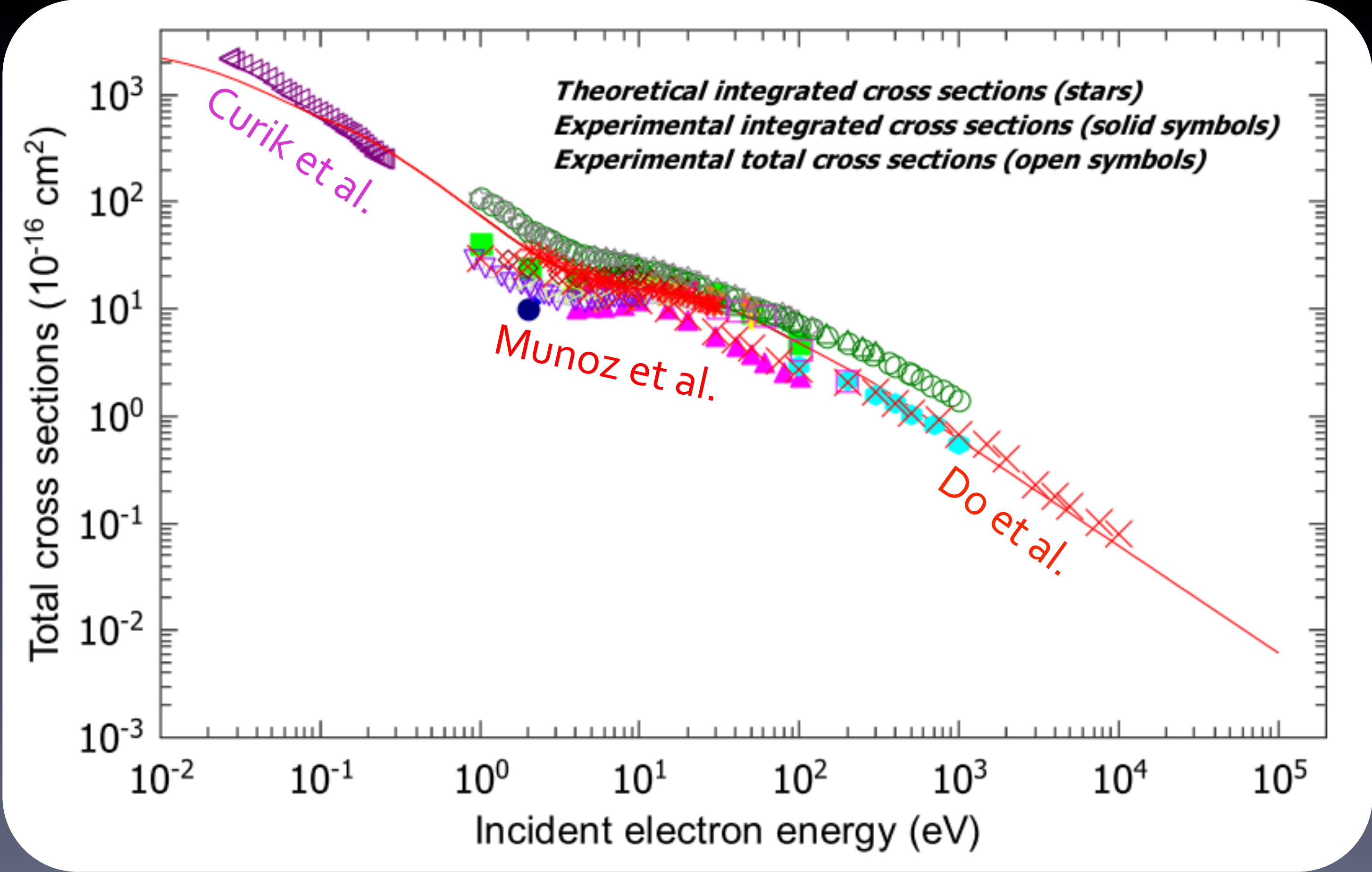
Verification and validation

ranges, stopping powers

See Med. Phys. 37 (2010) 4692-4708 (link) and NIMB 269 (2011) 2307-2311 (link)

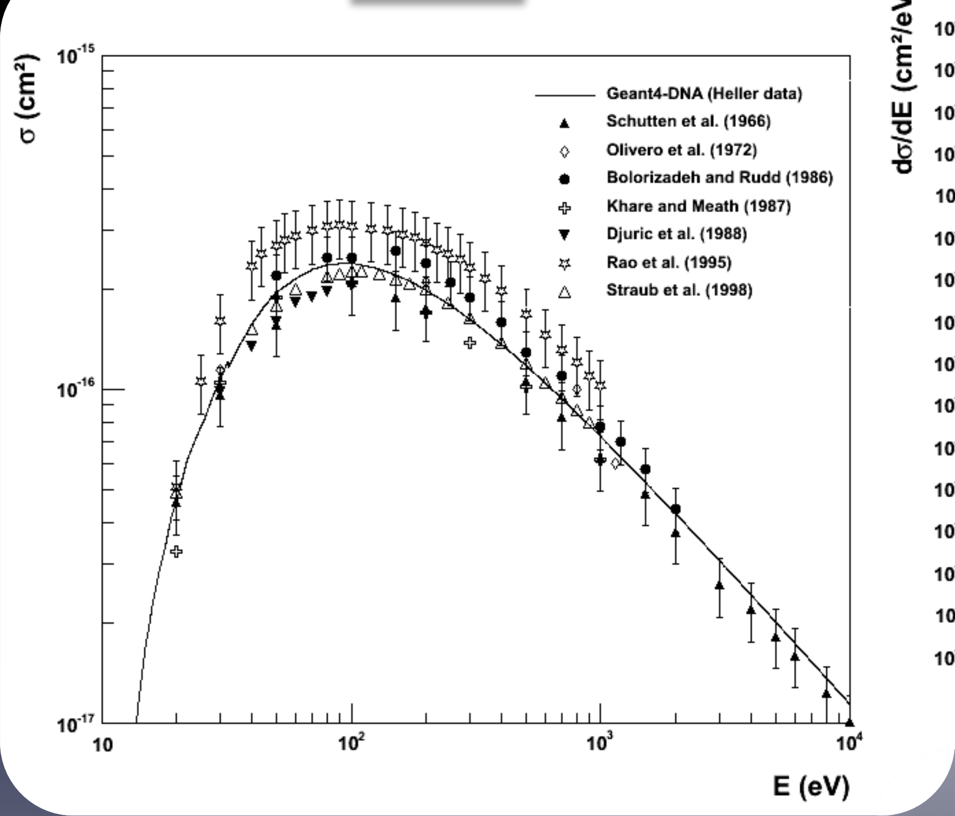
Electron elastic scattering cross section

Based on the theoretical work of C. Champion *et al*. in the partial wave framework and with a spherical potential includes three distinct terms: a **static** contribution and two fine correction terms corresponding to the **correlation-polarization** and the **exchange** interactions

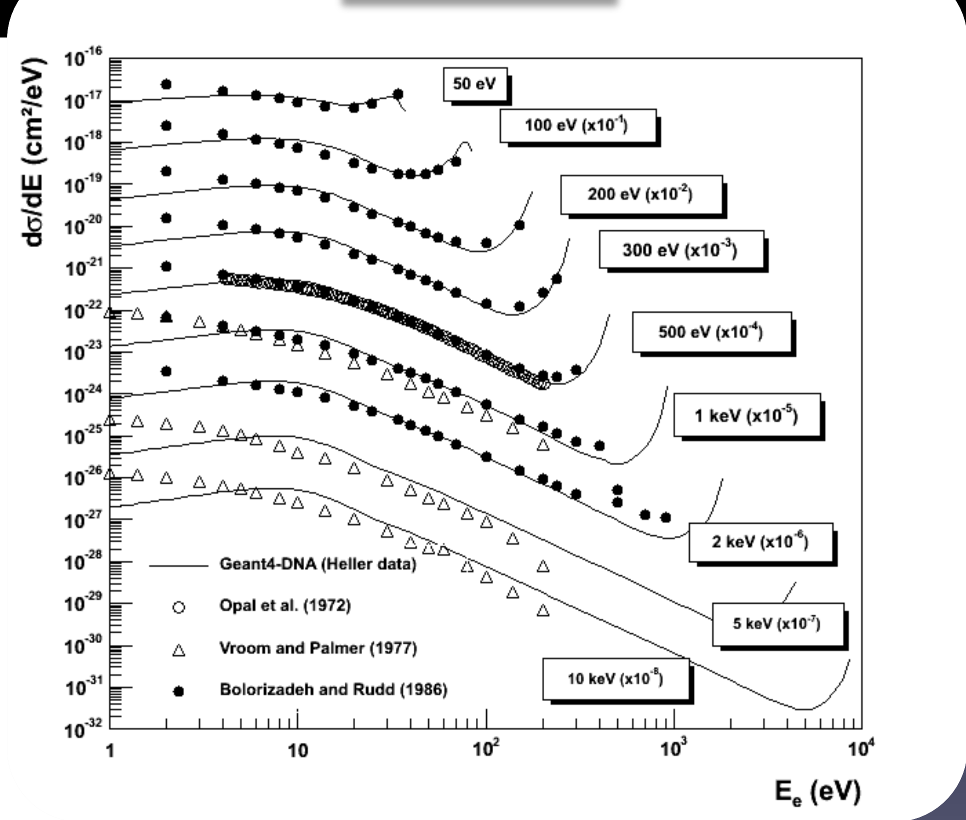


Electron ionisation

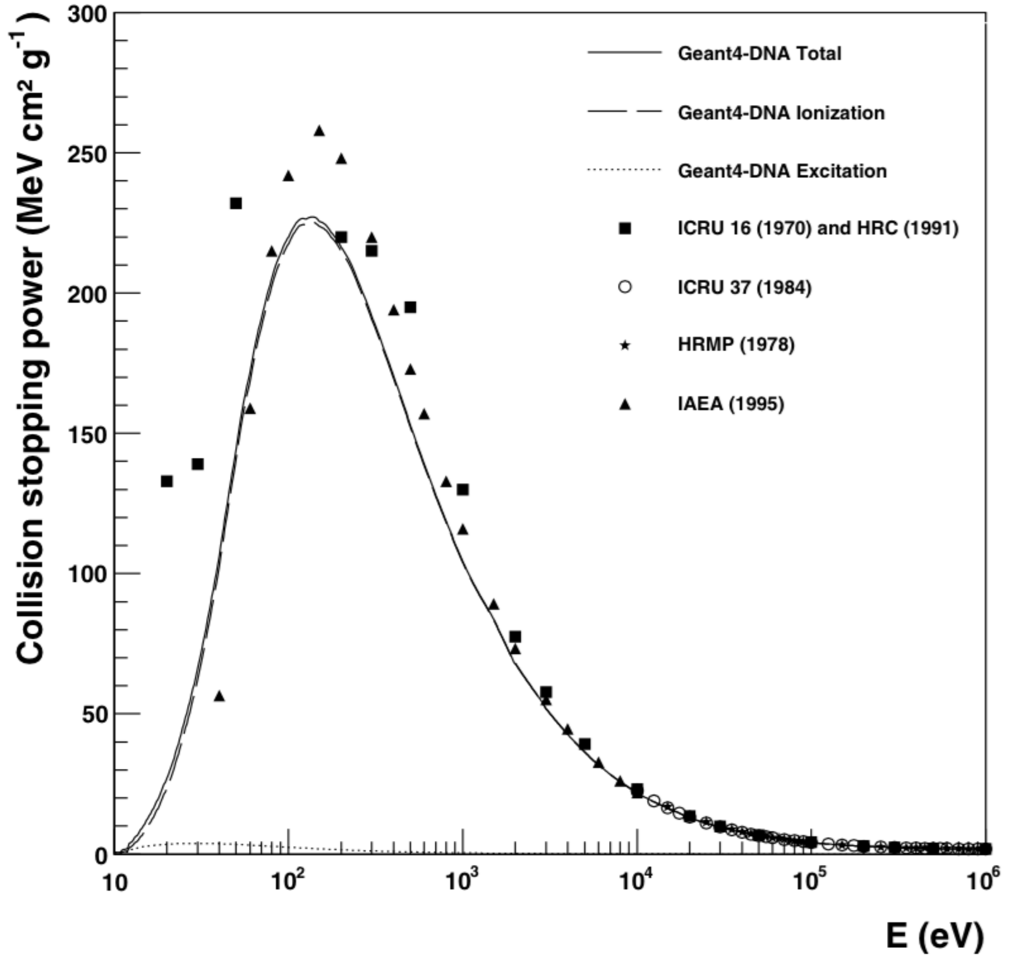
Total XS



Differential XS

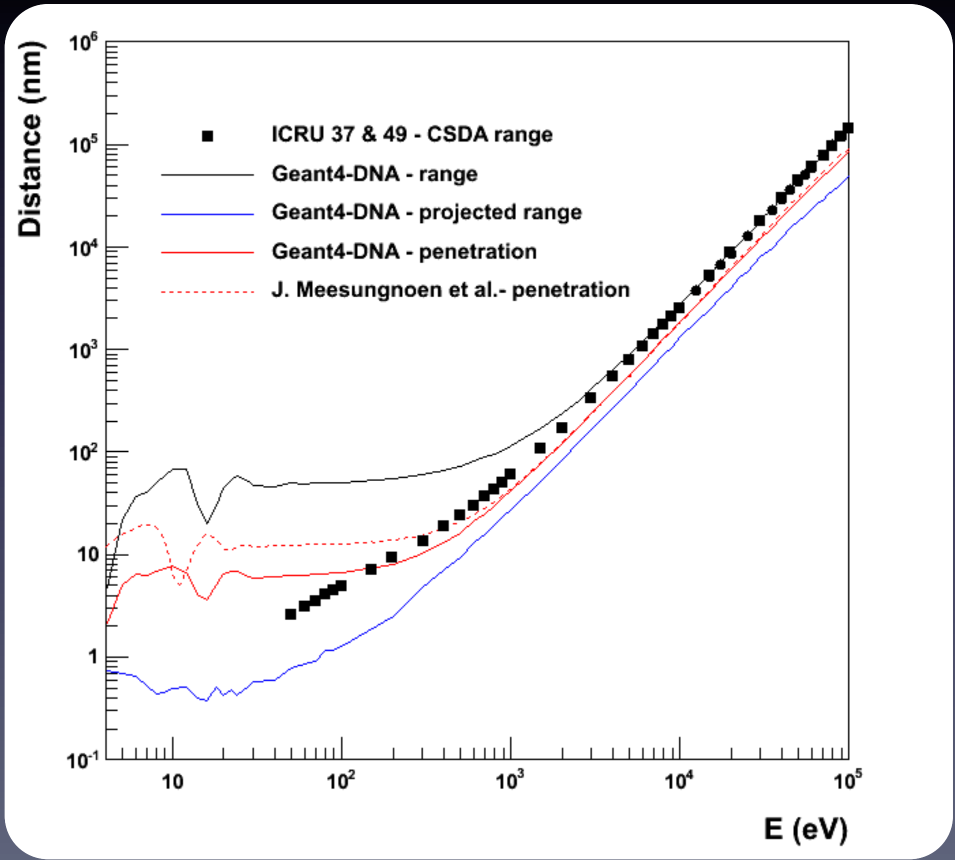


Electron stopping power



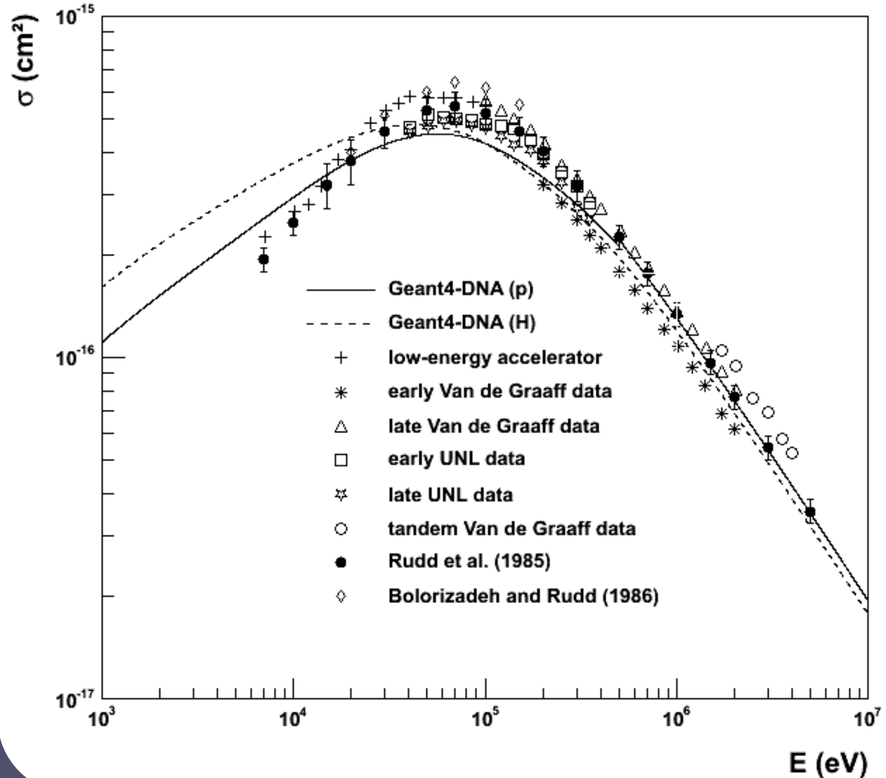
Electron range, projected range and penetration

- Obtained with the partial wave elastic scattering model
- Compared to ICRU recommendations and to penetration MC calculations by Meesungnoen *et al*. (including a 2 factor on elastic and vib. excitation cross sections measured in ice)

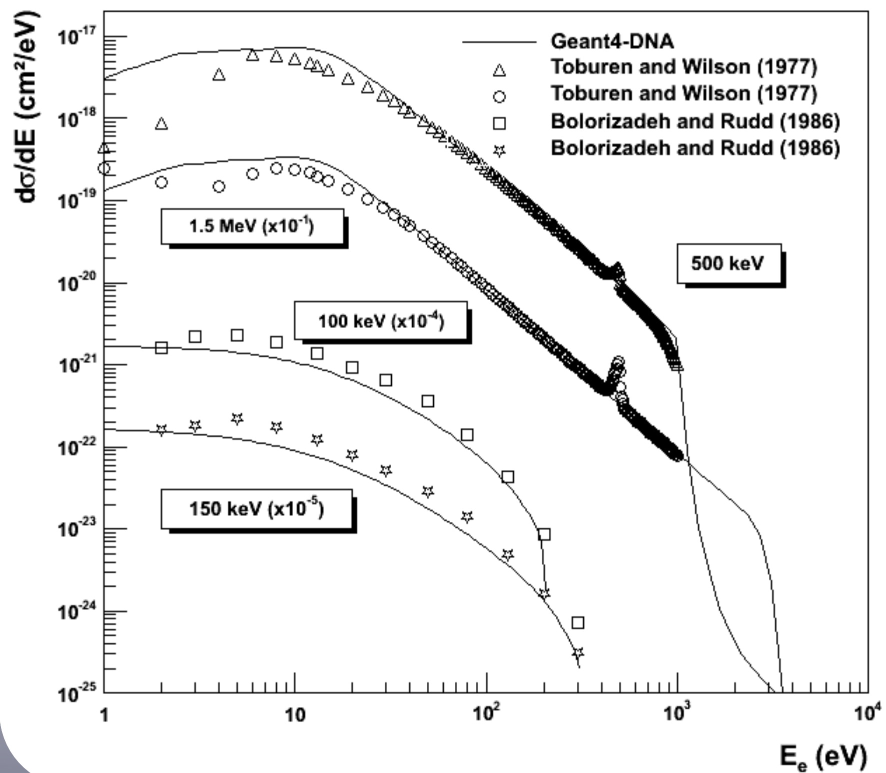


Proton & Hydrogen ionisation

Total XS



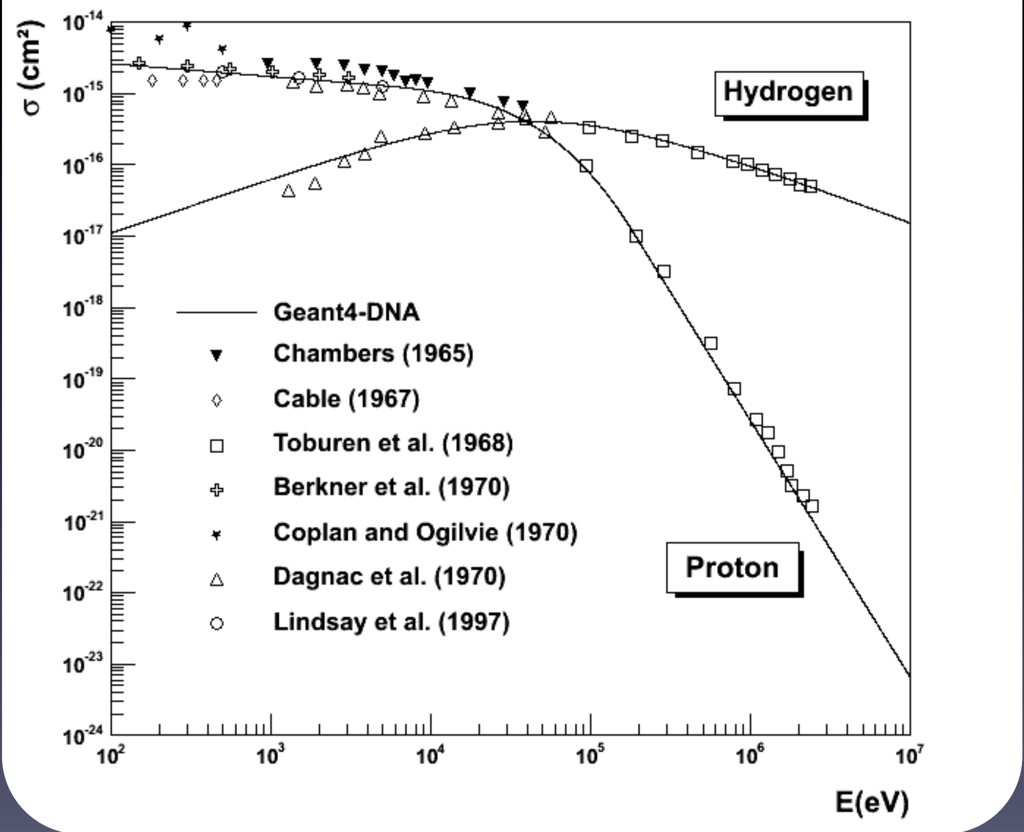
Differential XS



Overview

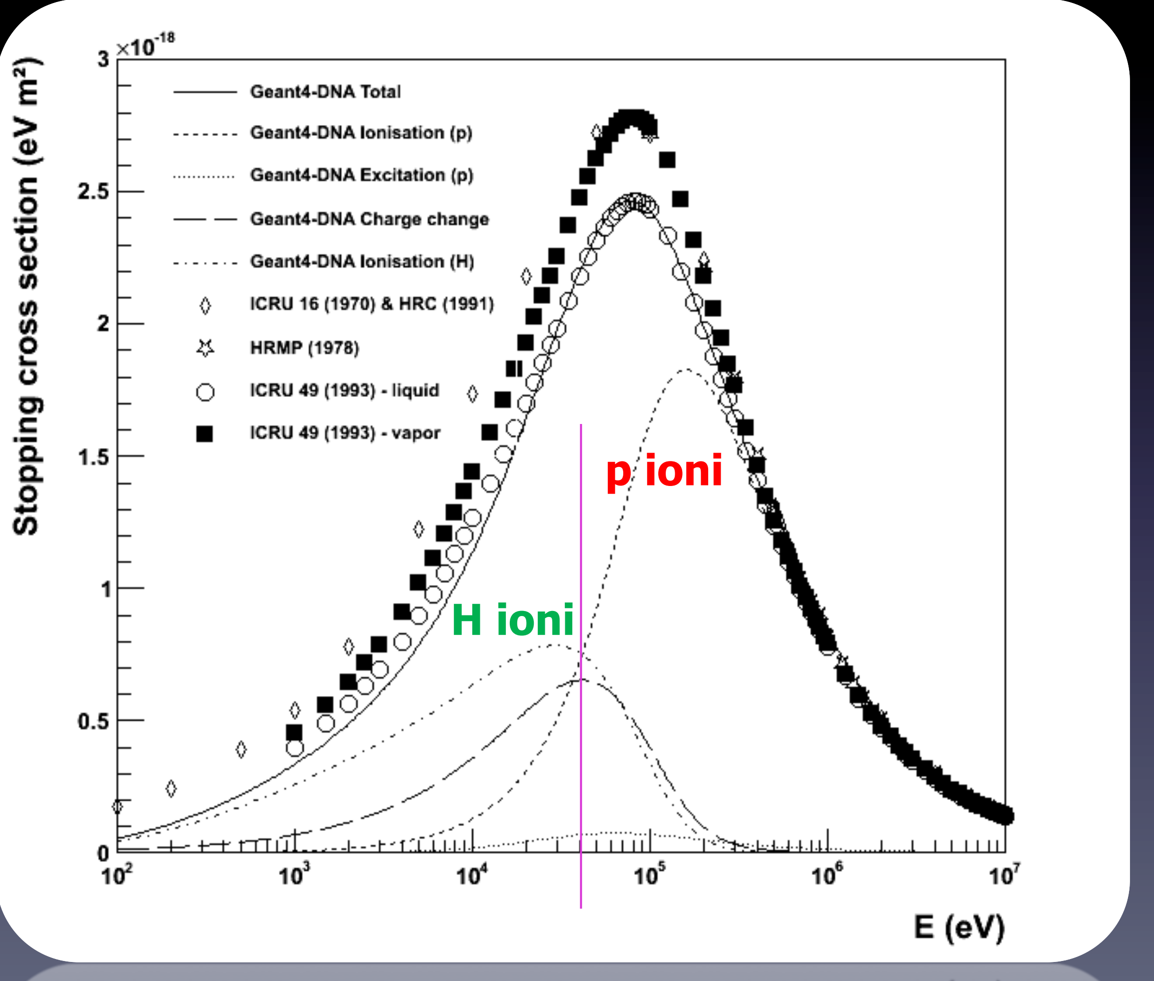
Proton and Hydrogen charge exchange

Total XS



Proton stopping cross section in liquid water

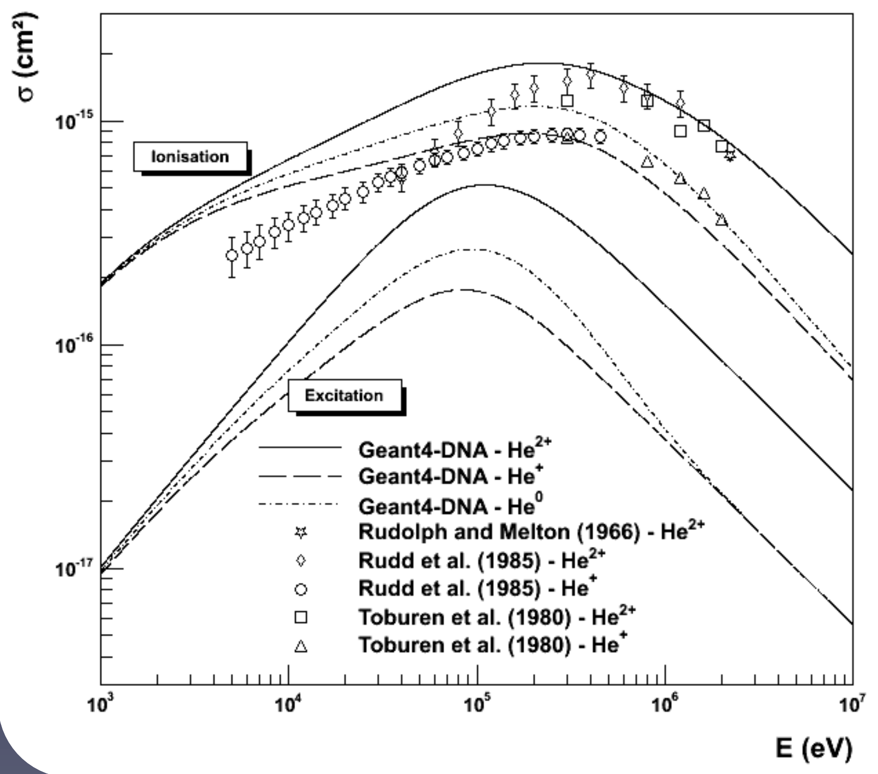
- Contributions of **ionisation** (p, H), **excitation** (p) and **charge change**
- Comparison to recommendations (ICRU, HRMP) for **liquid** and **vapour** water



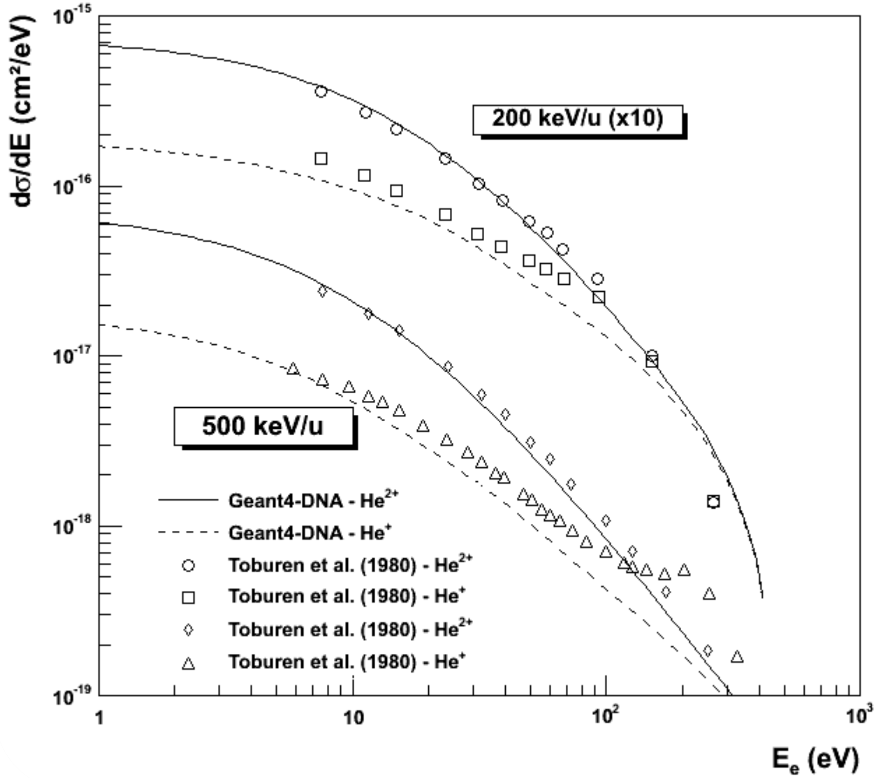
Overview

Helium ionisation

Total XS

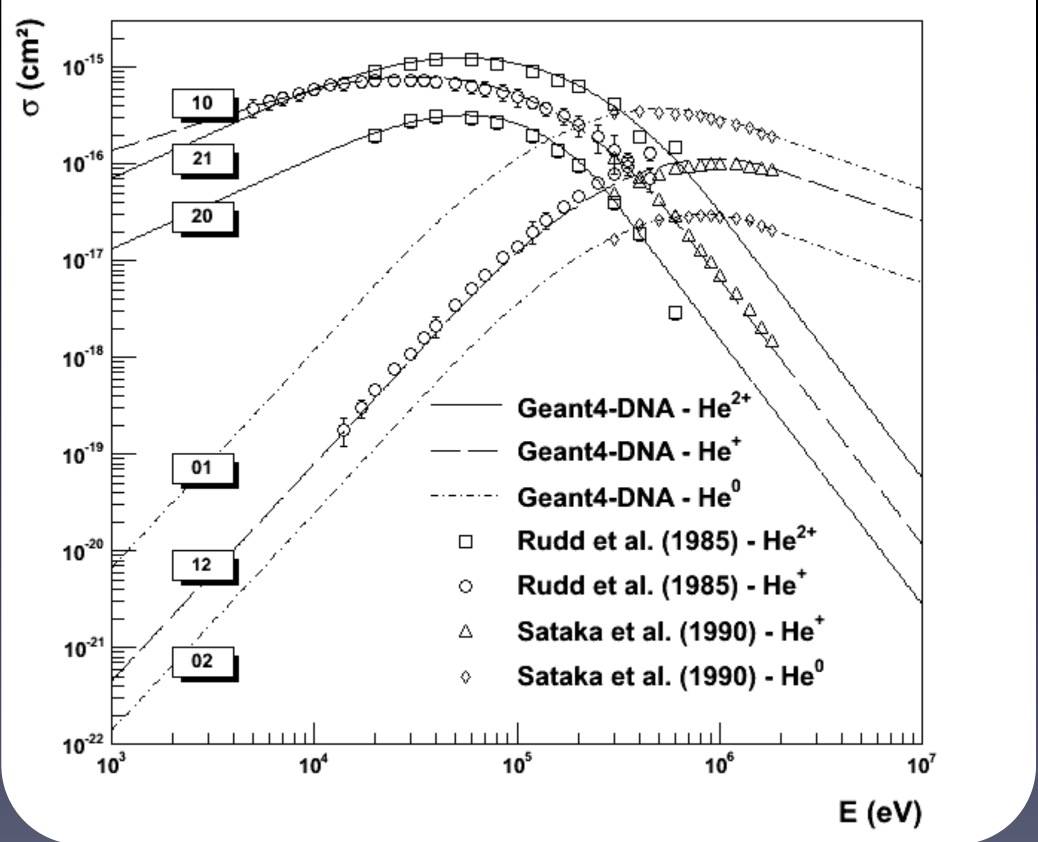


Differential XS



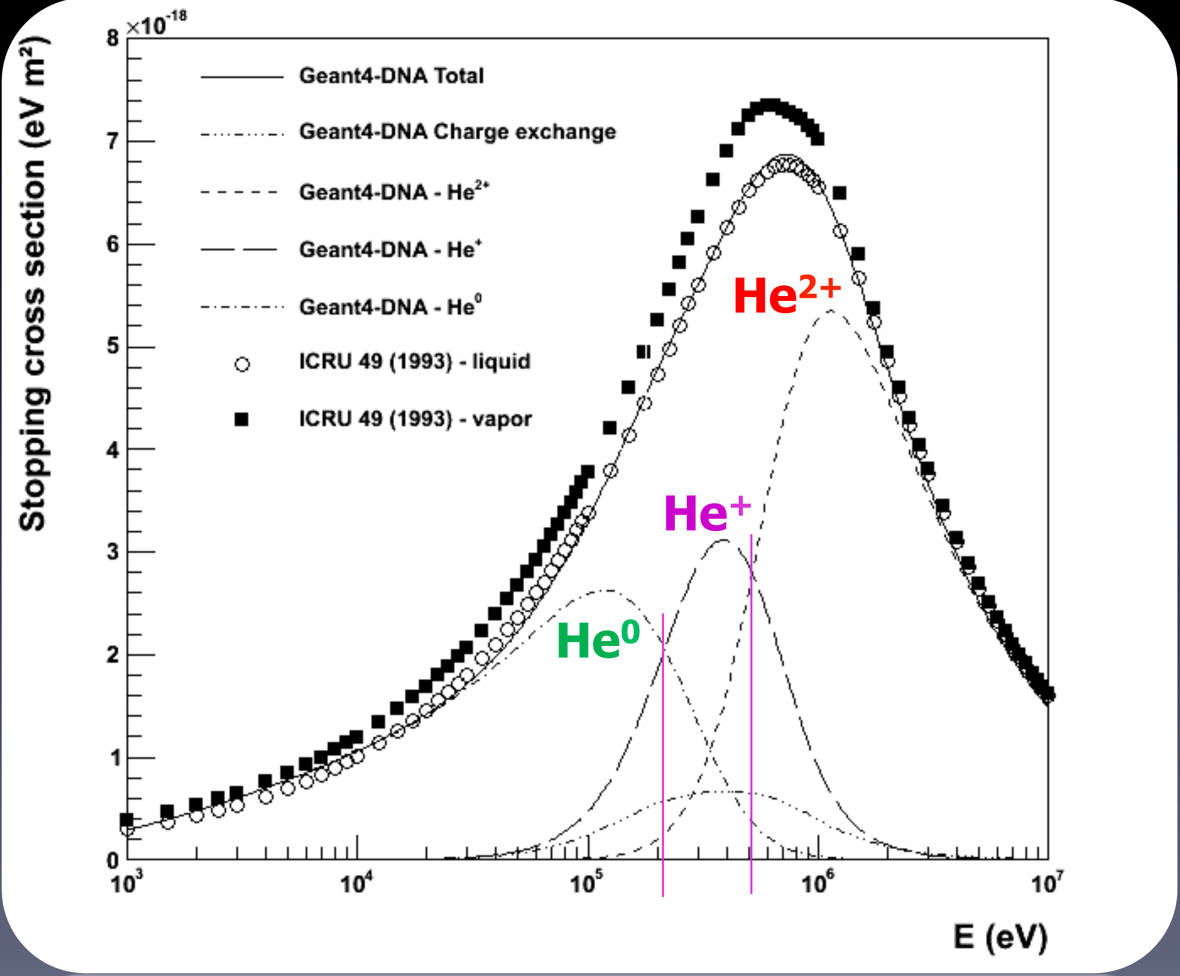
Helium charge exchange

Total XS



Helium stopping cross section

- Contributions of **3 charged states** of Helium
- Comparison to recommendations (ICRU) for **liquid** and **vapour** water



http://geant4-dna.org
in Physics…Processes

Overview

1) Electrons

- **Electron interactions**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill	Type
elastic scattering	G4DNAElastic	G4DNAChampionElasticModel	0 eV	1 MeV	7.4 eV	interpolated
elastic scattering	G4DNAElastic	G4DNAScreenedRutherfordElasticModel (**)	0 eV	1 MeV	9 eV (*)	analytical
electronic excitation	G4DNAExcitation	G4DNABornExcitationModel	9 eV	1 MeV	-	interpolated
ionisation	G4DNAIonisation	G4DNABornIonisationModel	11 eV	1 MeV	-	interpolated
vibrational excitation	G4DNAVibExcitation	G4DNASancheExcitationModel	2 eV (*)	100 eV	-	intepolated
attachment	G4DNAAttachment	G4DNAMeltonAttachmentModel	4 eV	13 eV	-	interpolated

(*) indicates that the low energy limit applicability of the model can be **further decreased** in an energy regime where it has not been validated, see **FAQ** section.

(**) the G4DNAScreenRutherfordElasticModel is an **alternative** model for the simulation of elastic scattering. The G4DNAChampionElasticModel is the default model used in the G4EmDNAPhysics constructor.

Overview

2) Protons and hydrogen

- **Proton interactions**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill	Type
electronic excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	10 eV	500 keV	-	analytical
electronic excitation	G4DNAExcitation	G4DNABornExcitationModel	500 keV	100 MeV	-	interpolated
ionisation	G4DNAIonisation	G4DNARuddIonisationModel	0 eV	500 keV	100 eV	interpolated
ionisation	G4DNAIonisation	G4DNABornIonisationModel	500 keV	100 MeV	-	interpolated
electron capture	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	100 eV	100 MeV	-	analytical

- **Hydrogen interactions**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill	Type
electronic excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	10 eV	500 keV	-	analytical
ionisation	G4DNAIonisation	G4DNARuddIonisationModel	0 keV	100 MeV	100 eV	interpolated
charge increase	G4DNAChargeIncrease	G4DNADingfelderChargeIncreaseModel	100 eV	100 MeV	-	analytical

Overview

3) Helium and charge states

- **Neutral Helium ionised twice (« alpha ») interactions**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill	Type
electronic excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	1 keV	400 MeV	-	analytical
ionisation	G4DNAIonisation	G4DNARuddIonisationModel	0 keV	400 MeV	1 keV	interpolated
charge decrease	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	1 keV	400 MeV	-	analytical

- **Neutral Helium ionised once (« alpha+ ») interactions**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill	Type
electronic excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	1 keV	400 MeV	-	analytical
ionisation	G4DNAIonisation	G4DNARuddIonisationModel	0 keV	400 MeV	1 keV	interpolated
charge decrease	G4DNAChargeDecrease	G4DNADingfelderChargeDecreaseModel	1 keV	400 MeV	-	analytical
charge increase	G4DNAChargeIncrease	G4DNADingfelderChargeIncreaseModel	1 keV	400 MeV	-	analytical

- **Neutral Helium (« helium ») interactions**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill	Type
electronic excitation	G4DNAExcitation	G4DNAMillerGreenExcitationModel	1 keV	400 MeV	-	analytical
ionisation	G4DNAIonisation	G4DNARuddIonisationModel	0 keV	400 MeV	1 keV	interpolated
charge increase	G4DNAChargeIncrease	G4DNADingfelderChargeIncreaseModel	1 keV	400 MeV	-	analytical

Overview

4) Other particles

- **Li, Be, B, C, N, O, Si, Fe interactions**

Interaction	Process class	Model class	Min. energy	Max. energy	Kill	Type
ionisation	G4DNAIonisation	G4DNARuddIonisationExtendedModel	0.5 MeV/u	1e6 MeV/u	0.5 MeV/u	interpolated

- **Gamma interactions**

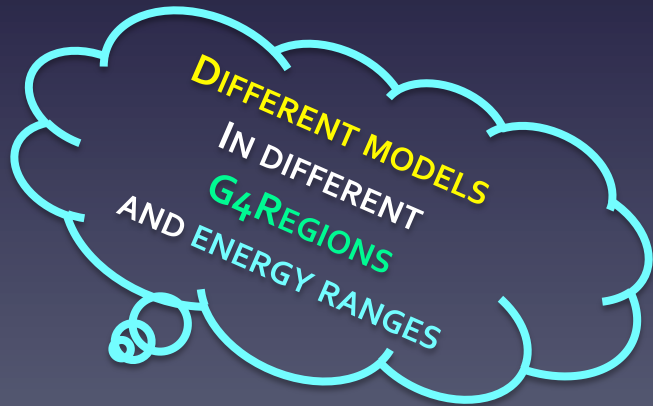
Gamma interactions are based on the Geant4 Livermore models and they are included by default in the **G4EmDNAPhysics constructor**. Please see more on Physics List.

Physics constructor

- For any application based on the Geant4-DNA extension, we recommend the implementation of a **Geant4-DNA Physics list based on the G4EmDNAPhysics** Physics constructor, which is regularly tested.
- The source code of this G4EmDNAPhysics Physics contructor may be found in the **$G4INSTALL/source/physics_lists/constructors/electromagnetic** directory.
- This is described in the « **dnaphysics** » extended example
  - see hands-ons

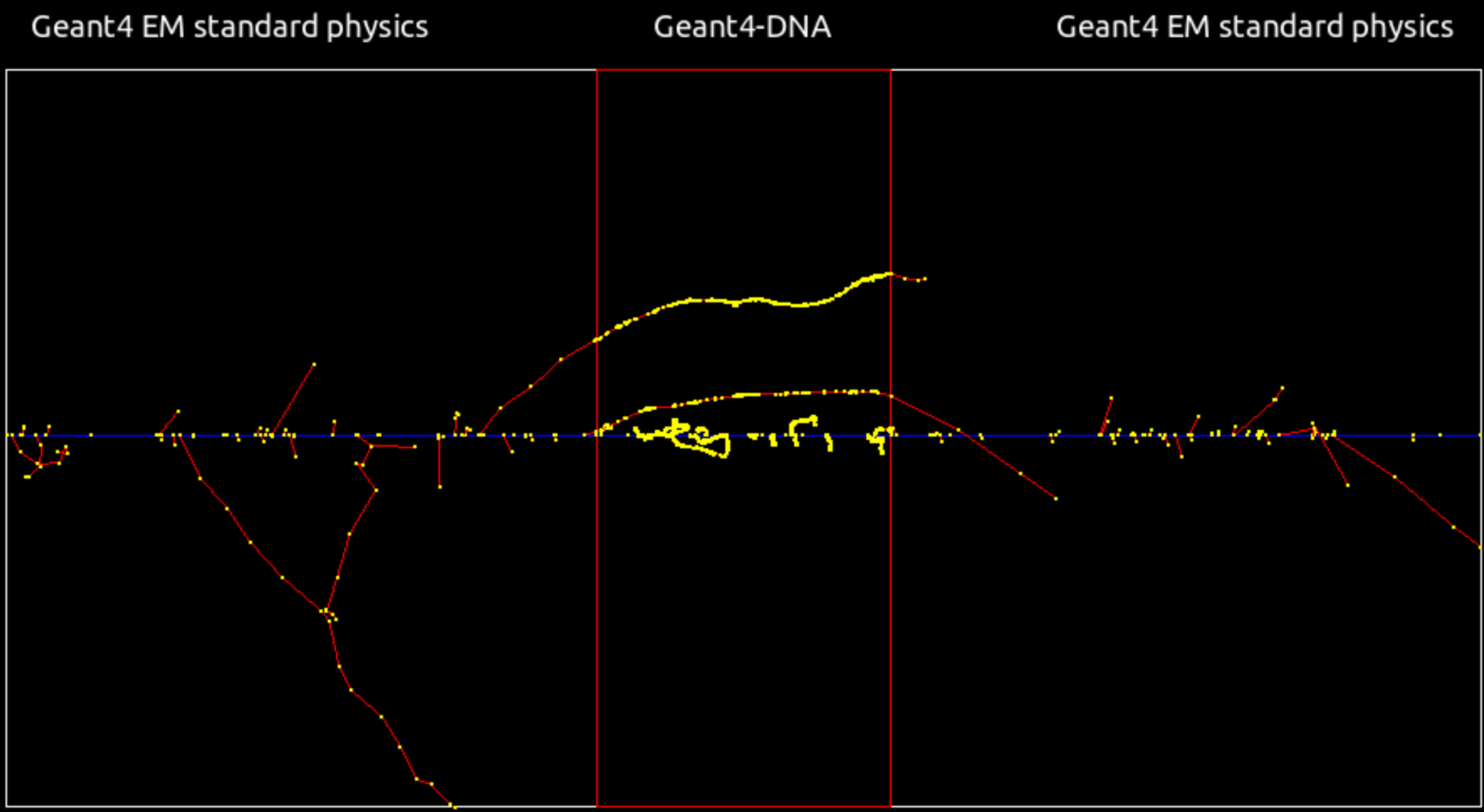
Multiscale combination of EM processes

- In Geant4-DNA and Geant4 electromagnetic (EM) categories
  - A physical interaction is described by a process class
    - Eg. G4DNAIonisation
  - A process class uses a model class in order to calculate the interaction cross section and final state, according to a selected theoretical / semi-empirical / empirical model
    - Eg. G4DNABornIonisationModel
- Thanks to this unified software design, users can easily combine Geant4-DNA processes and models with
  - Geant4 photon processes and models
    - Photoelectric effect, Compton sc., Rayleigh sc., pair production
    - Livermore (EPDL97) included by default
  - Geant4 alternative EM processes and models for charged particles
    - Ionisation, bremmstrahlung, elastic scattering, etc…
    - Electrons, positrons, photons, ions, etc…
  - Geant4 atomic deexcitation (fluorescence + Auger emission)
    - EADL97



Mixed physics lists in space regions: the « microdosimetry » example

Overview



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Courtesy of V. Stepan (CENBG)

See NIMB 273 (2012) 95-97 (link)
Prog. Nucl. Sci. Tec. 2 (2011) 898-903 (link)

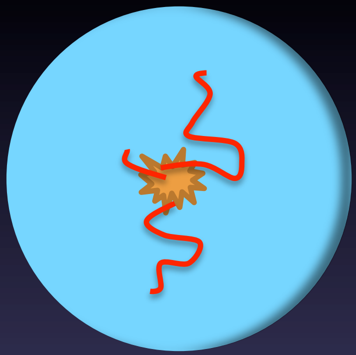
2) PHYSICAL STAGE

Verification

Verification

Dose Point Kernel simulations

- Accurate test of electron transport in small scale geometries
- We compared Geant4-DNA electron Dose Point Kernels (DPK) in liquid water with several MC codes
  - CPA100
  - EGSnrc
  - FLUKA 2011.2.15
  - MCNPX 2.7.0
  - PENELOPE 2006



- 4 electron energies : 10 keV, 30 keV, 50 keV and 100 keV and 120 bins (r/r_{CSDA})
- Geant4-DNA partial wave elastic scattering model
- Kolmogorov-Smirnov test used to compare Geant4-DNA with the other Monte Carlo codes

See Appl. Radiat. Isot. 83 (2014) 137-141 (link)

Verification

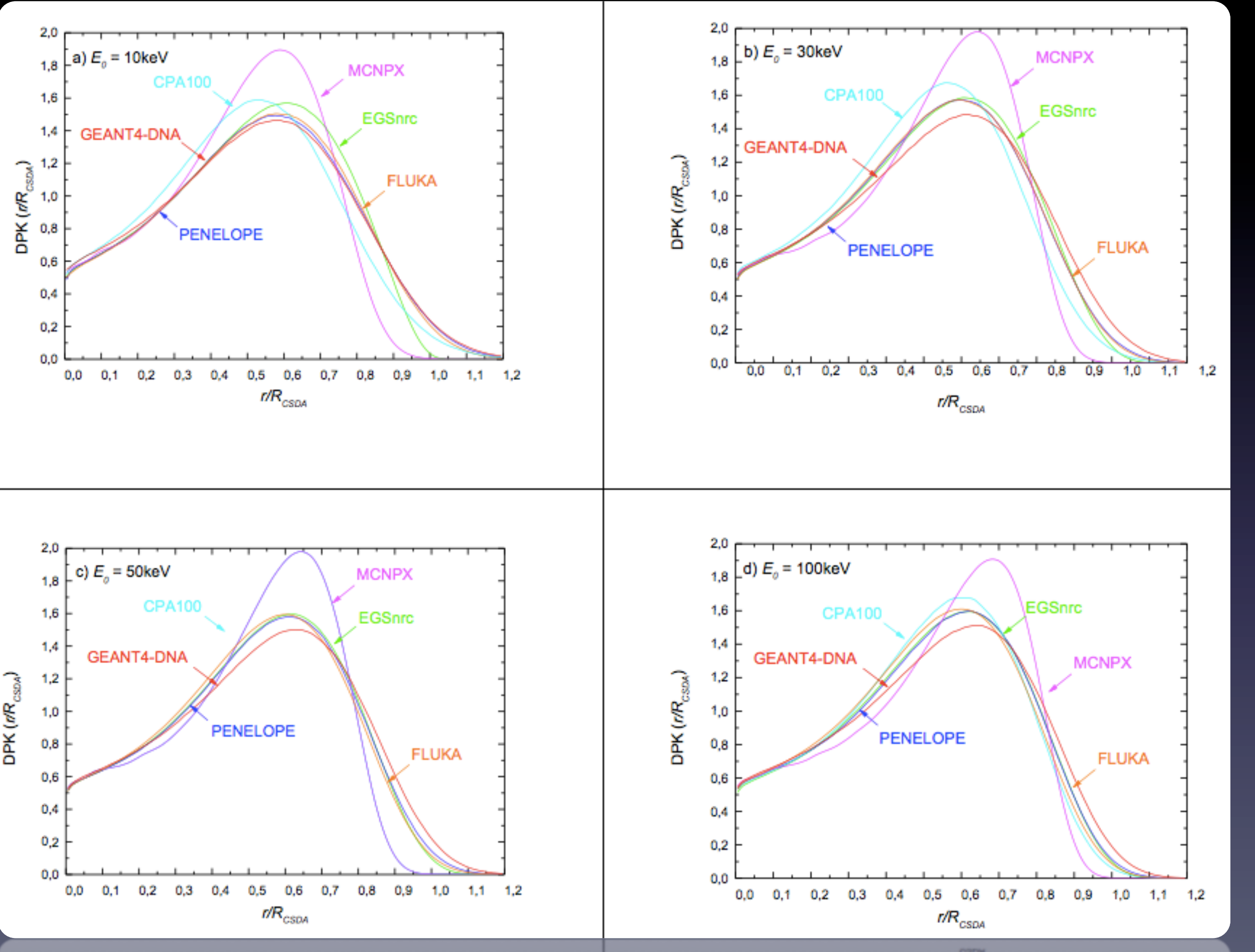
DPK simulations in liquid water

- Geant4-DNA is compatible with EGSnrc, PENELOPE and FLUKA

- But not compatible with CPA100 (30 keV and 50 keV) and with MCNPX* (all energies)

*

- v2.7.0
- F8 tally
- EFAC=0.917
- transport cutoff of 1 keV
- ITS option
- ESTEP = 10 or 100



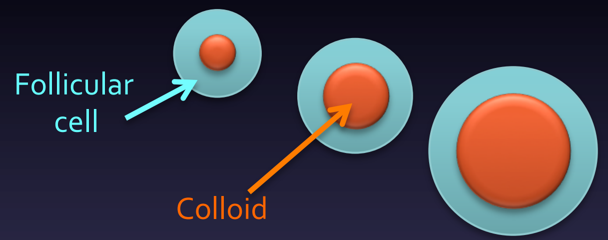
The geometrical granularity used in this study might be too large to get accurate DPK profiles using MCNPX

See Appl. Radiat. Isot. 83 (2014) 137-141 (link)

Verification

S-values simulations in liquid water

- Alternative accurate test of electron transport in small scale geometries
- We compared Geant4-DNA electron S-values in liquid water with several MC codes
  - CPA100
  - EGSnrc
  - EPOTRAN/CELLDOSE
  - MC4V
  - MCNP
  - PENELOPE



$$\overline{D}(r_T \leftarrow r_S) = \tilde{A}_{r_S} S(r_T \leftarrow r_S),$$

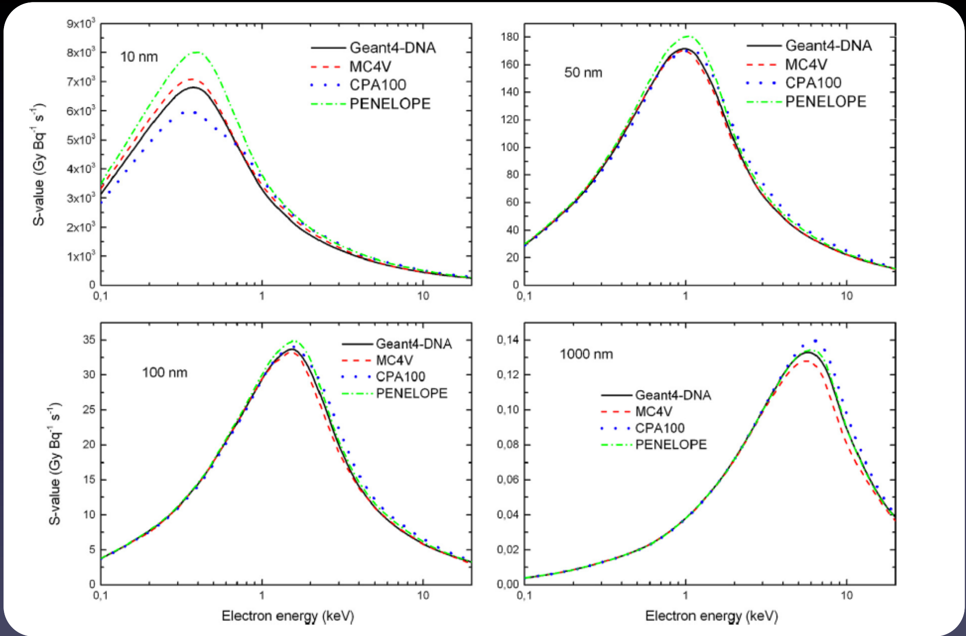
See NIMB 319 (2014) 87-94 (link)

- Electron energies
  - monoenergetic case in a sphere of liquid water
  - 5 iodine isotopes: 131, 132, 133, 134, 135 in context of thyroid targeted immunotherapy
    - Two concentric spheres of liquid water separated by 10 microns :
      inner sphere with varying radius (colloid) and outer sphere with 10 micron thickness (follicular cell)

Verification

S-values simulations in liquid water

Monoenergetic electrons

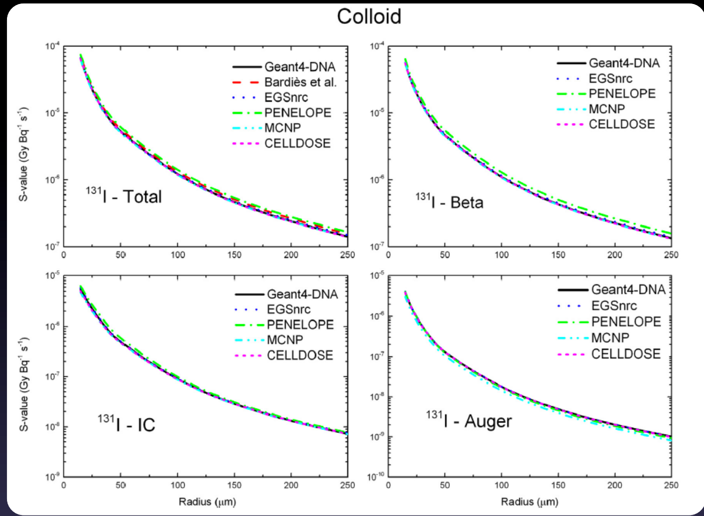


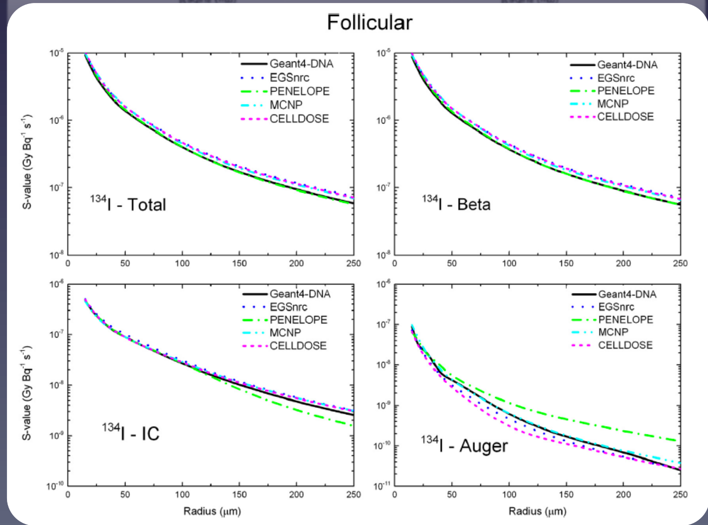
Best agreement with MC4V

See NIMB 319 (2014) 87-94 (link)

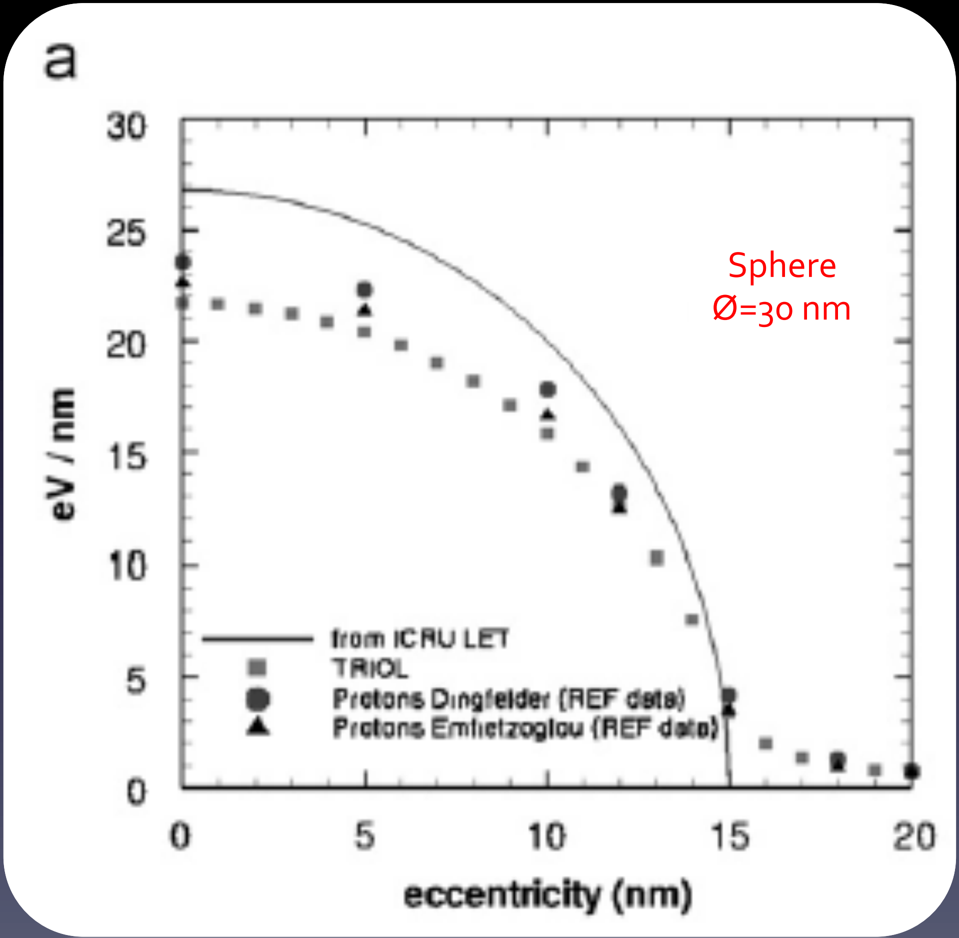
Iodine : colloid and follicular

Best agreement with CELLDOSE

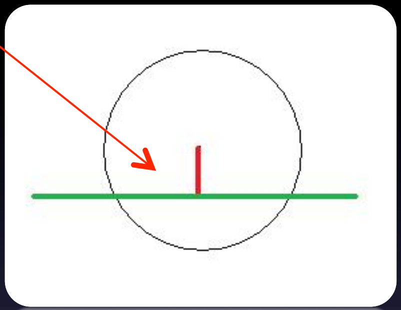




Mean energy deposition of protons



eccentricity



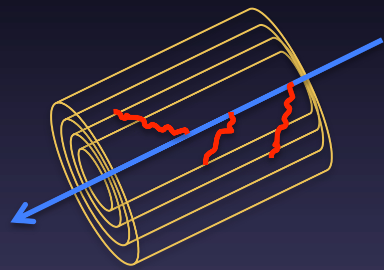
Mean energy deposit per event for 1 MeV proton tracks going through spherical volume of water with 30 nm of diameter. The source was placed at 100 nm from the target. The full line represents the energy deposit calculated using the LET values published in the ICRU report 49

Appl. Radiat. Isot. 69 (2011) 220-226

Verification

Radial doses

- Investigation of Geant4-DNA performance for radial dose distribution around ion tracks
  - Protons, alphas, C, O, Fe
  - MeV–GeV range



- Comparison to published data
  - Analytical calculations
  - Monte Carlo simulations
  - Experimental data in tissue equivalent gas

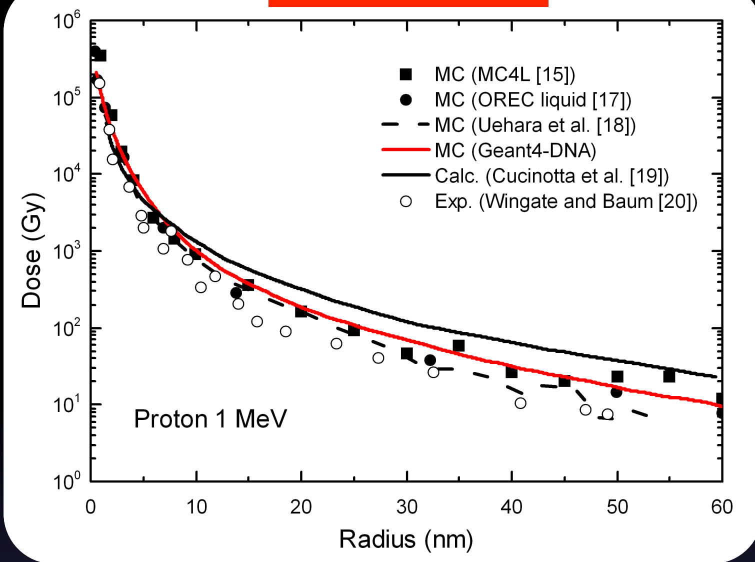
See NIMB 333 (2014) 92-98 (link)

Verification

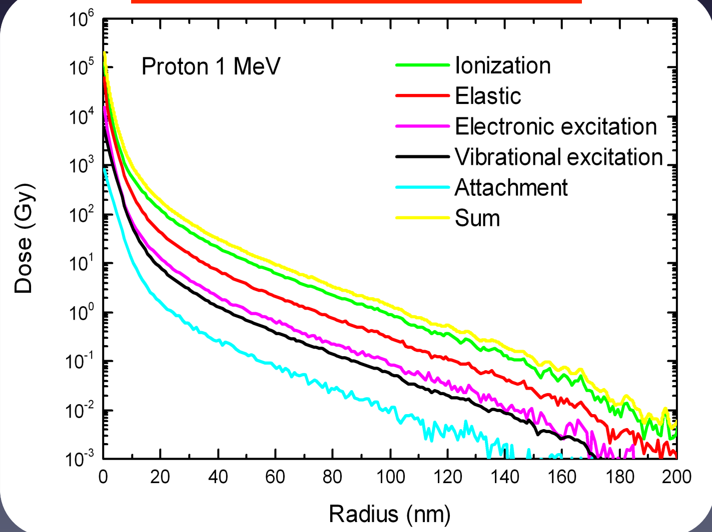
Radial doses

- General good agreement of dose profiles with a variety of literature data
- Selection of results for 1 MeV protons
  - Dose profile
  - Geometrically restricted LET
  - Individual process contribution to absorbed dose

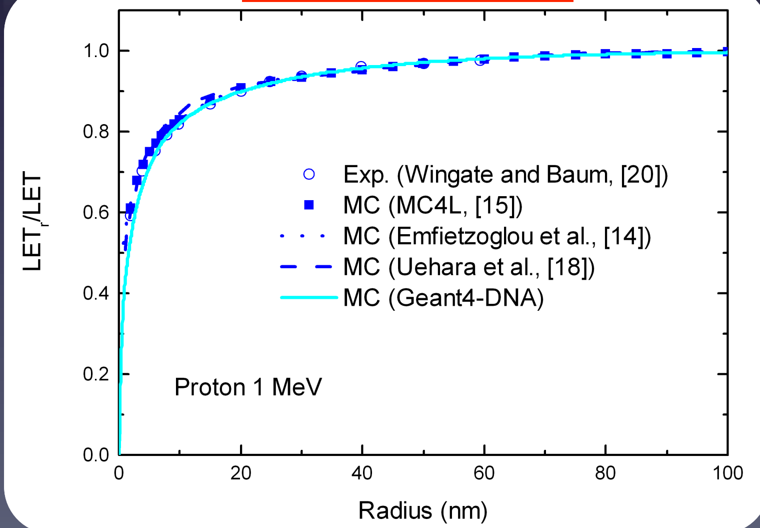
Dose profile



Process contribution



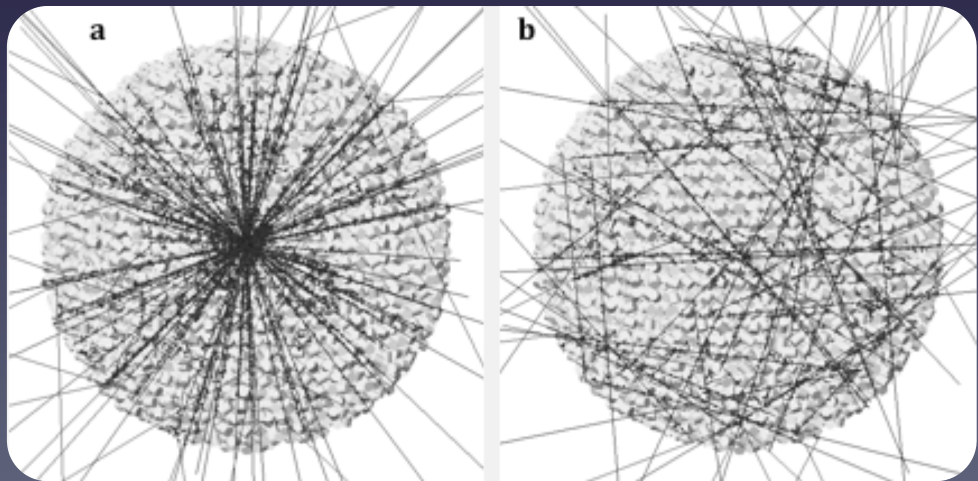
Restricted LET



See NIMB 333 (2014) 92-98 (link)

Energy deposition in nanometer size targets

- We have recently evaluated performances of Geant4-DNA physics models in very small size targets
- Simulate frequencies of energy deposition in cylindrical targets of biological interest : 2 nm x 5 nm (DNA bases), 10 nm x 5 nm (nucleosome), 25 nm x 25 nm (chromatine fiber)
- Comparison with literature simulations (MOCAX series of MC codes)
- Geometry implemented from a voxellized phantom containing randomly oriented cylindrical targets
- Two shooting methods : centred or random



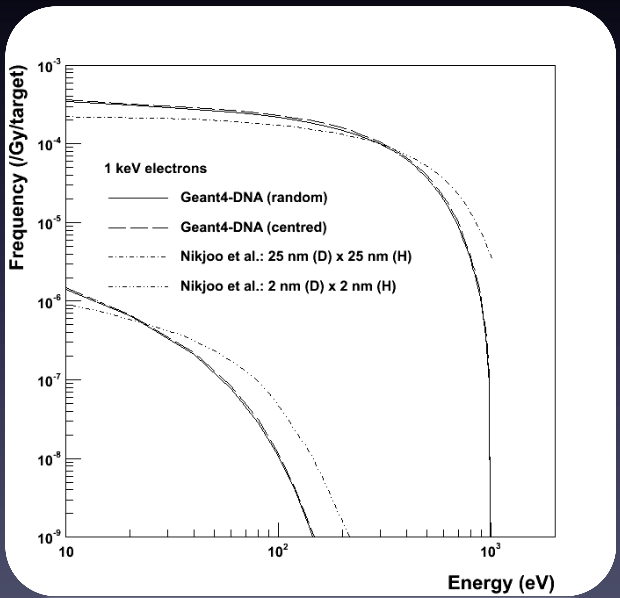
Verification

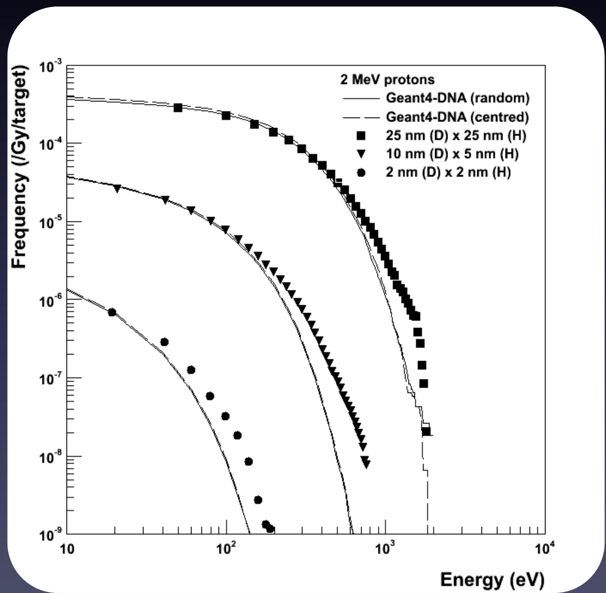
Frequency of energy deposition: comparison with MOCAX series

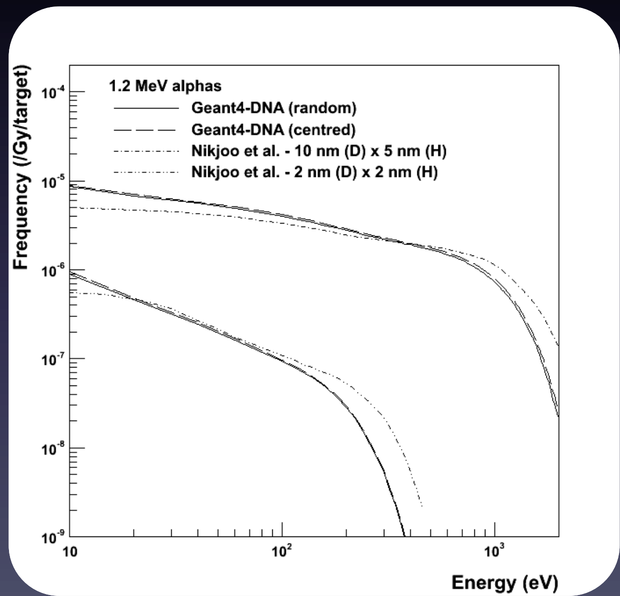
1 keV electrons

2 MeV protons

1.2 MeV alphas







See NIMB 306 (2013) 158-164

3) PHYSICO-CHEMICAL & CHEMICAL STAGE

See talks and hands-ons by Mathieu, Sylvain and Vaclav

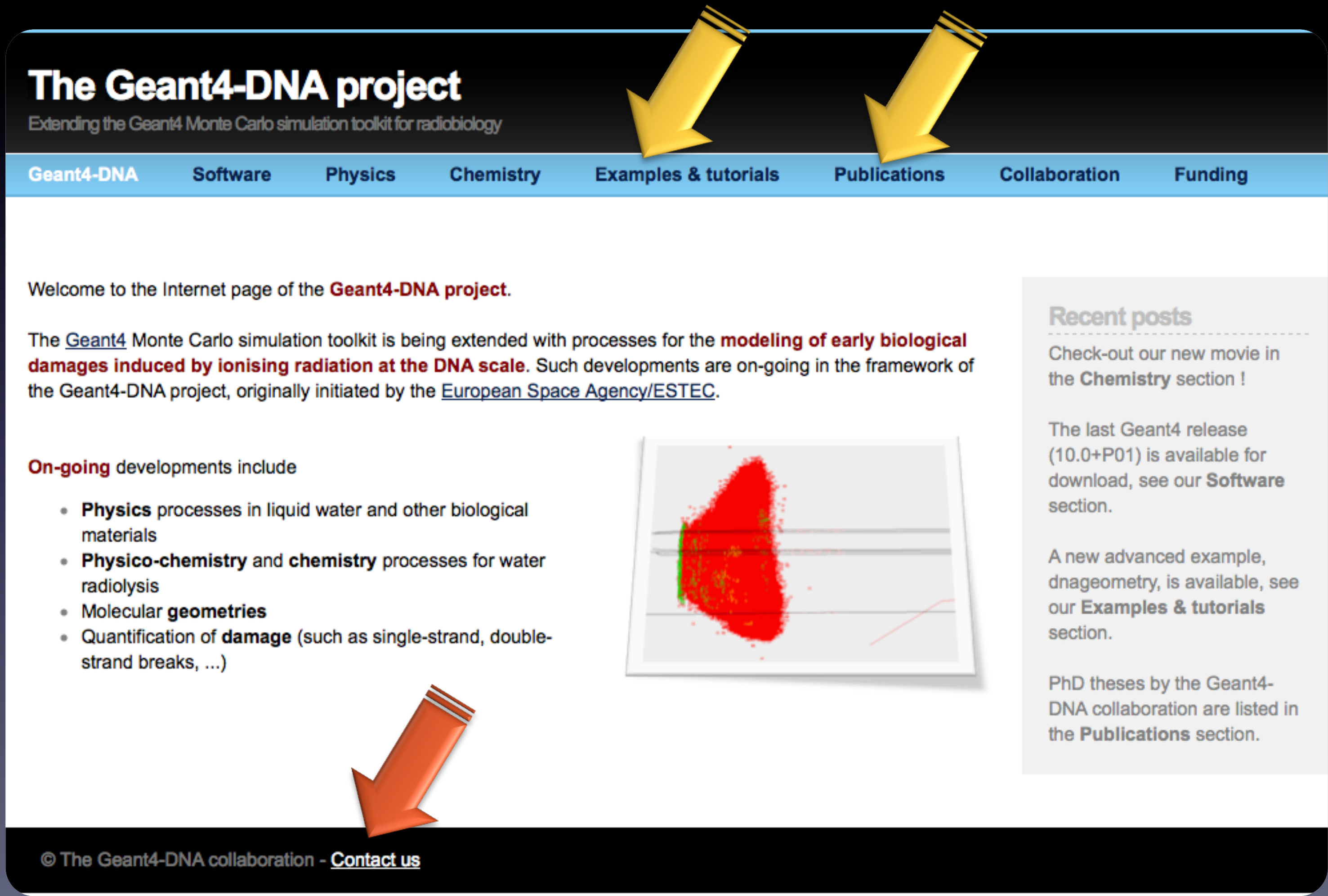
4) GEOMETRICAL MODELS

See talks and hands-ons by Carmen, Emmanuel, Yann

5) WHERE TO FIND MORE INFORMATION ?

Geant4-DNA website

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



Geant4-DNA examples included in Geant4

Example code name	Purpose	Location	Availability
dnaphysics	• Usage of Geant4-DNA Physics processes • variable density	$G4INSTALL/examples/extended/medical/dna	from Geant4 9.5 BETA
microdosimetry	Combination of Standard EM or Low Energy EM processes with Geant4-DNA Physics processes	$G4INSTALL/examples/extended/medical/dna	from Geant4 9.5 BETA
chem1, chem2, chem3	Usage of Geant4-DNA chemistry	$G4INSTALL/examples/extended/medical/dna	***Geant4 10.1***
wholeNuclearDNA	Cell nucleus	$G4INSTALL/examples/extended/medical/dna	from Geant4 10.0
PDB4DNA	Interface to PDB database	$G4INSTALL/examples/extended/medical/dna	***Geant4 10.1***
microbeam	3D cellular phantom	$G4INSTALL/examples/advanced	From 2009
TestEm12	DPK	$G4INSTALL/examples/extended	from Geant4 9.5 BETA
(TestEm2)	Usage of Physics constructors	$G4INSTALL/examples/extended	from Geant4 9.4
(TestEm14)	Extraction of cross sections	$G4INSTALL/examples/extended	from Geant4 9.4

PERSPECTIVES

Perspectives

- **PHYSICS**
  - Inclusion of cross section models for electrons and ions
    - Liquid water & DNA material & gas for nanodosimeters
    - BioQuart project (Dr Hans Rabus @ PTB – see Carmen's talk), Ioannina U. team, LAPLACE team
- **PHYSICO-CHEMISTRY/CHEMISTRY**
  - Addition of scavenger species and reactions
  - Combination of geometry & chemistry - composite material approach
- **BIOLOGY**
  - Prediction of direct and non-direct DNA simple & complex damages

  in plasmids and realistic cells, time evolution
  - Verification (with other codes) and validation (with experimental data)

All this takes time to implement and publish before the software is publicly released in Geant4… thank you for your patience

You are kindly invited to contact us if you are interested in contributing to Geant4-DNA

Thank you for your attention
...and a special thank you to

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