Boron Neutron Capture a GEANT4 Study

Current status and development of neutron radiation for biophysical applications in Colombia

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Outline

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REVIEW

Current status and development of neutron radiation for biophysical applications in Colombia

J. Alfonso Leyva[1] · Edwin Munévar[2]

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Historical Mini-Review

Neutron Discovery

Right after the neutron discovery by Chadwick in 1932

The beginning

In 1936 Gordon Locher proposed the use of neutrons in biological applications & non-conventional cancer therapy

Brookhaven (1951-1961)

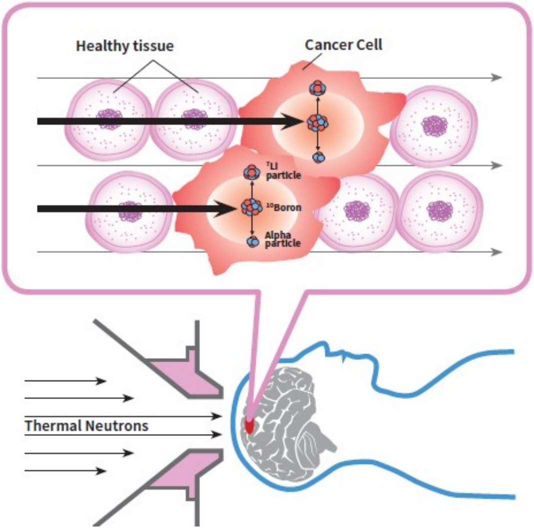
BNCT experiments

Japan (1968-1980)

Use of contrast agent (BSH) combined with radiotherapy and tumor extraction (main part)

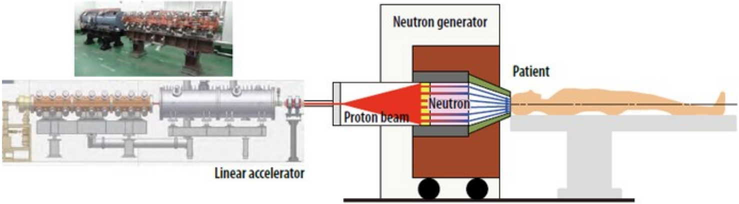
Neutron Sources

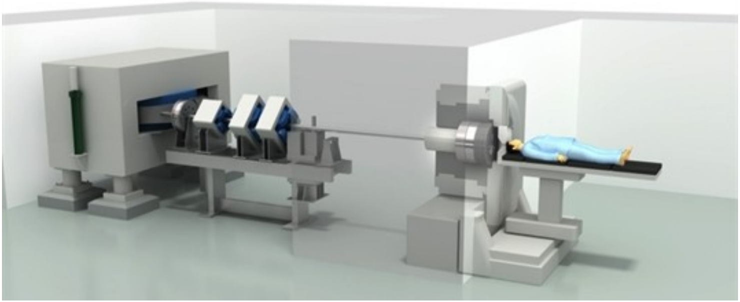
- Nuclear Reactors
- Accelerators
- Compact Generators



^{10}B Neutron Capture Reaction inside a cell

BNCT Japanese Project

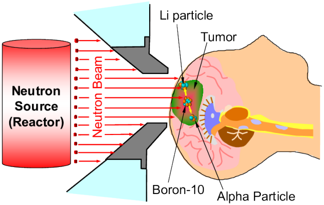




Neutron Capture Therapy (NCT)

Neutron Capture Therapy is a two-steps process

- the patient needs to take a medicament with a contrast agent (^{10}B, ^{157}Gd, ^{7}Li)
- thermal or epithermal neutron irradiation



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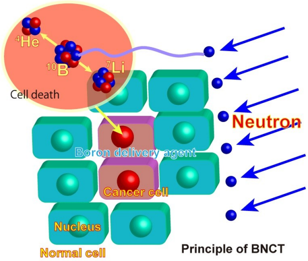
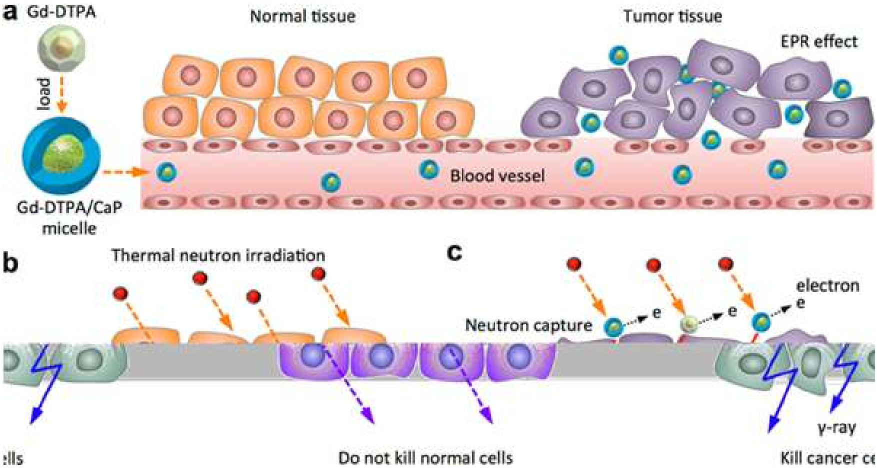
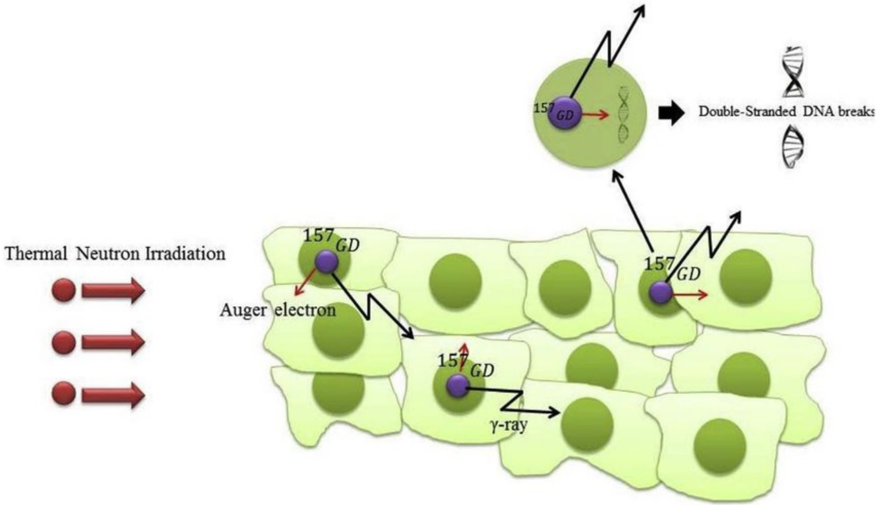


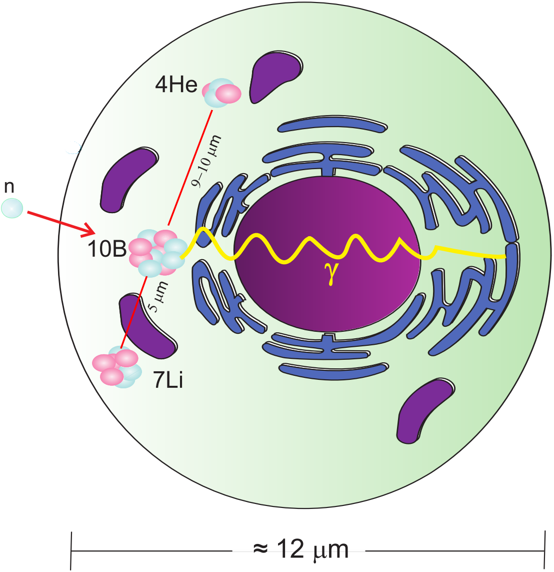
Contrast Agent Transport



GdNCT Reaction at Celular level



BNC Reaction inside the Cell



Most common used contrast agents

- Boron
  - BSH: sodium mercaptoundecahydro-closo-dodecaborate $Na_2B_{12}H_{11}SH$, commonly known as sodium borocaptate
  - BPA: amino acid (L)-4-dihydroxy-borylphenylalanine, known as boronophenylalanine
- Gadolinium
  - Gd-DTPA: Gadopentetic acid $C_{14}H_{18}GdN_3O_{10}$
  - DOTA-Gd: is an organic compound with the formula $(CH_2CH_2NCH_2CO_2H)_4$

Neutron Energy Distribution Ranges

In terms of their kinetic energy E_K, neutrons are classified into several groups:

Energy Range	**Kinetic Energy**
Ultracold Neutrons	$E_K < 2 \times 10^{-7}$ eV
Very Cold Neutrons	2×10^{-7} eV $\leq E_K \leq 5 \times 10^{-5}$ eV
Cold Neutrons	5×10^{-5} eV $\leq E_K \leq 0.025$ eV
Thermal Neutrons	$E_K \approx 0.025$ eV
Epithermal Neutrons	1 eV $< E_K <$ 1keV
Intermediate Neutrons	1 keV $< E_K <$ 0.1 MeV
Fast Neutrons	$E_K > 0.1$ MeV

Table: Neutrons clasifications in terms of their kinetic energy E_K.
Source: Ervin B. Podgorša, Radiation Physicists Medical Physics, Springer International Publishing Switzerland 2006, 2010, 2016 [?]

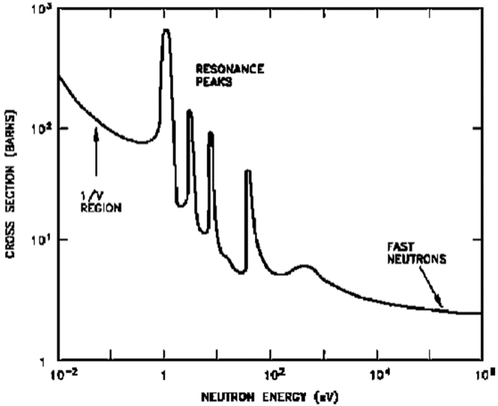
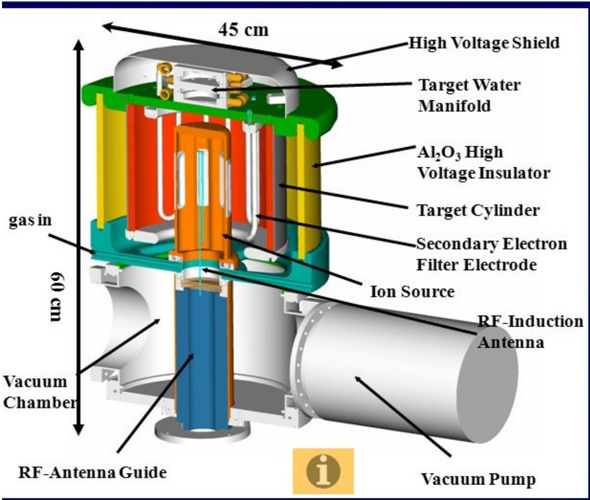


Figure: Neutron capture cross section as a function of the neutron energy. Source: Narayan S Hosmane et all ,Boron and Gadolinium Neutron Capture Therapy for Cancer Treatment. 2012 by World Scientific Publishing Co. Pte. Ltd,



- A 13.56 MHz radio frequency (RF) discharge is used to produce deuterium ions.
- The ion beam is accelerated to energy of 120 kV.
- The beam impinges on a titanium coated aluminum target where neutrons are generated through D-D fusion reaction:

$$D + D \rightarrow {}^{3}He + n\ (2.45\ MeV)$$

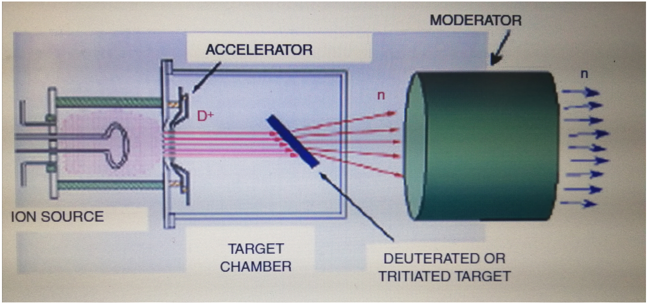
LBNL Prototype

Primary Working Team

From left to right: J. Alfonso Leyva, Andrea Garcia, Ka-Ngo Leung, José A. Sarta, Edwin Munévar.

From left to right: Kevin Alexis Luna, Marcela Cruz, Jorge Cifuentes y Lida Velasquez.

- **Jorge Cifuentes:** *“Evaluación Preliminar de la Aceleración de D en un generador de neutrones D-D compacto de alto flujo”*
- **Lida Velasquez:** *”Evaluación preliminar de la moderación de neutrones en un generador compacto D-D de alto flujo”*
- **Yuly Cruz:** *“Cálculo preliminar de dosis en la terapia por captura neutrónica empleando teoría de difusión y remoción”*
- **Kevin Luna:** *“Algoritmo preliminar de cálculo de flujo de neutrones para terapia por captura neutrónica mediante la implementación del método de lattice Boltzmann”*



Geant4 "GEometry ANd Tracking" Monte Carlo Simulation Toolkit

GEANT4
A SIMULATION TOOLKIT

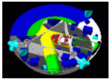
Overview

Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. The three main reference papers for Geant4 are published in Nuclear Instruments and Methods in Physics Research A 506 (2003) 250-303, IEEE Transactions on Nuclear Science 53 No. 1 (2006) 270-278 and Nuclear Instruments and Methods in Physics Research A 835 (2016) 186-225.

Applications

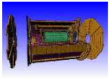
A sampling of applications, technology transfer and other uses of Geant4

User Support



Getting started, guides and information for users and developers

Publications



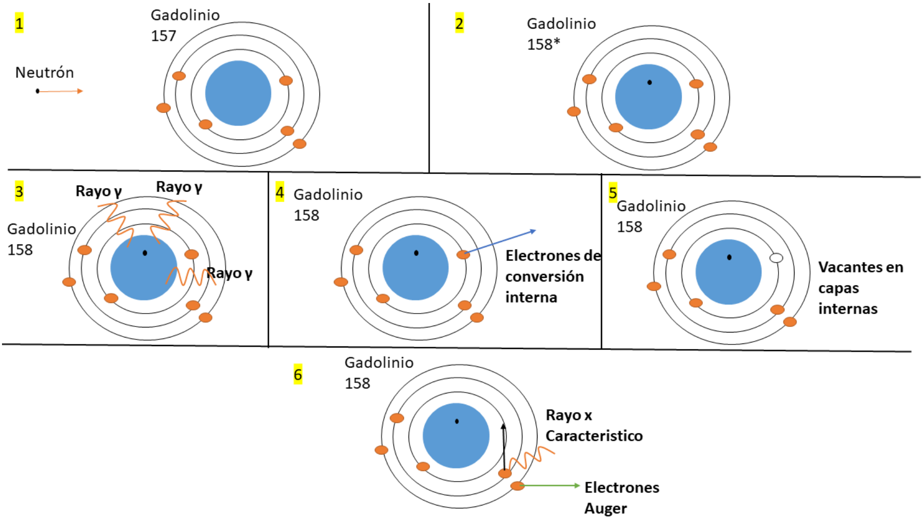
Validation of Geant4, results from experiments and publications

Collaboration

Who we are: collaborating institutions, members, organization and legal information

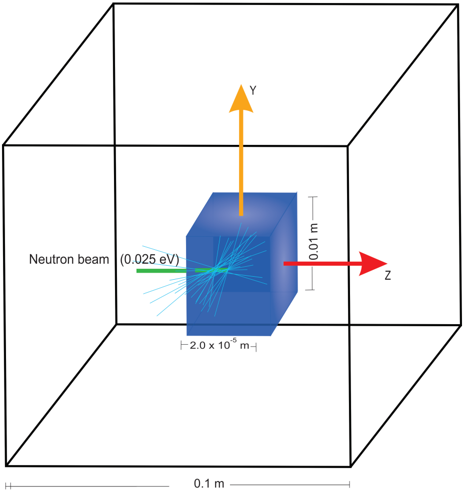
printer-friendly version

From left to right: Diego Tellez, Angie Hernandez, Brayan Villalobos and Steven Medina.



Neutron Capture Reaction by ^{157}Gd

Geometry of the Simulation



Physics List and Primary Source

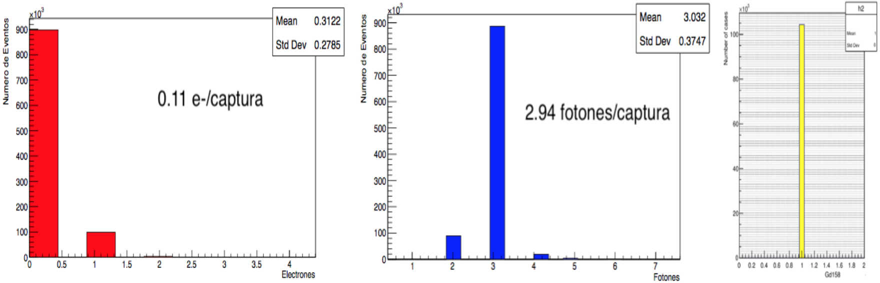
Physics List

- G4EmStandardPhysics
- G4HadronPhysicsQGPS_BIC_HP

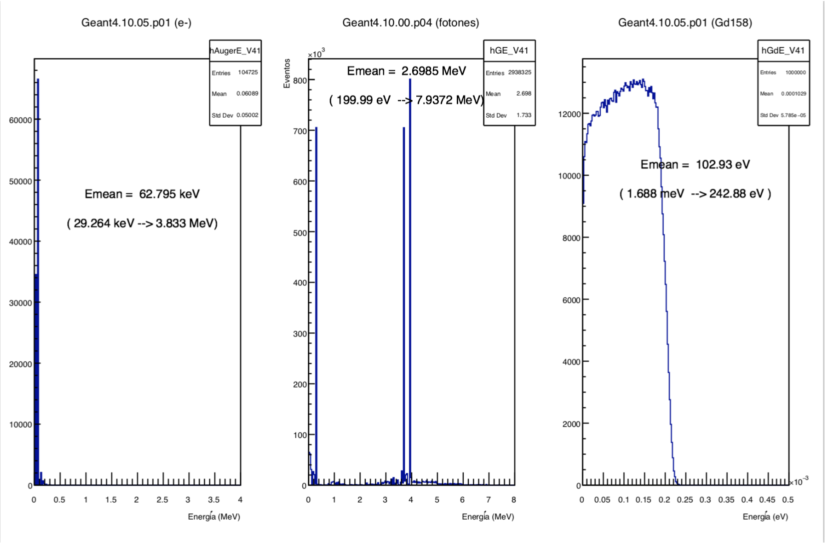
QGPS_BIC_HP: high precision (HP) neutron model used for neutrons below 20 MeV. Recommended for radiation protection, shielding and medical aplications[?] and Dennis Wright (SLAC) & Vladimir Ivantchenko (CERN) lectures

Primary source

Neutron thermal monoenergetic beam located at (0, 0, -4.5) cm respect to the center of the world volume

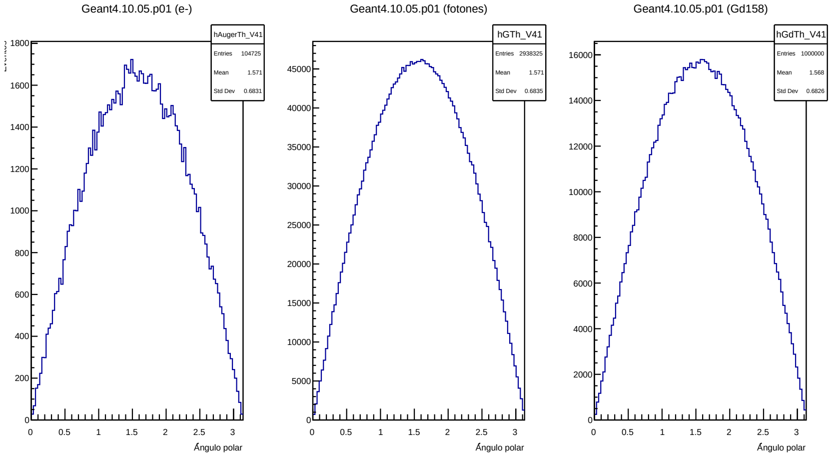


Counting of electrons, photons and 158-Gd.

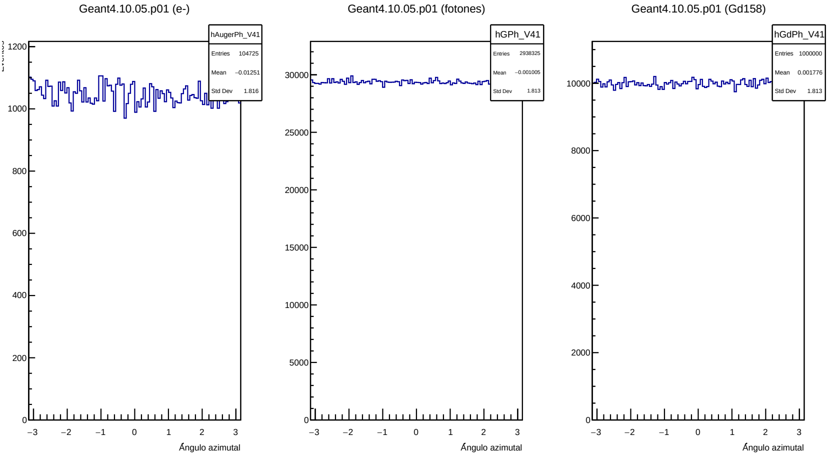


e-, gammas y 158-Gd Energy Distributions

Results - Angular Distribution of the Gd-NCR



Angular Distribution for e-, γ and 158-Gd



Angular Distribution for e-, γ and 158-Gd

Team @ Universidad Distrital Francisco Jose de Caldas

from left to right : Jaiver Salazar, Mariana Paez y Miguel Rubio.

Eukaryote Céll

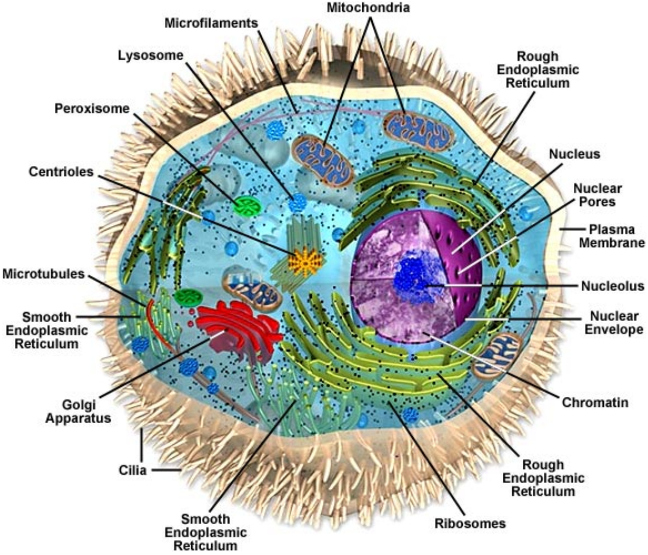


Figure: Célula Animal, 1 a 100 μm

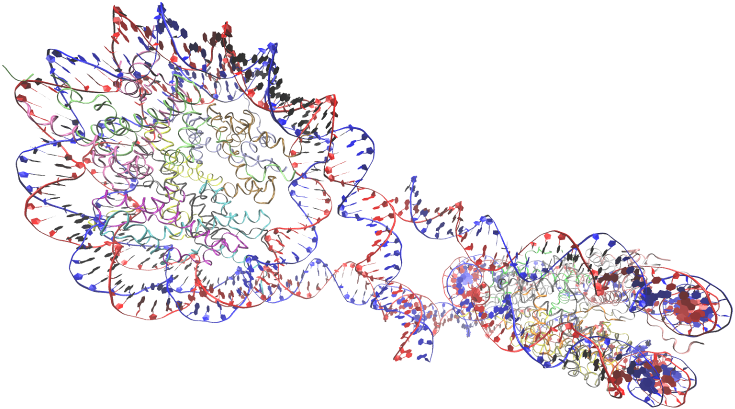


Figure: 1ZBB

DNA Fragment

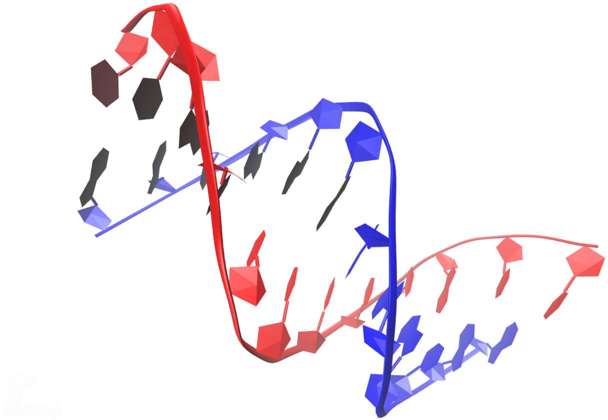


Figure: 1FZX

Bond Modification

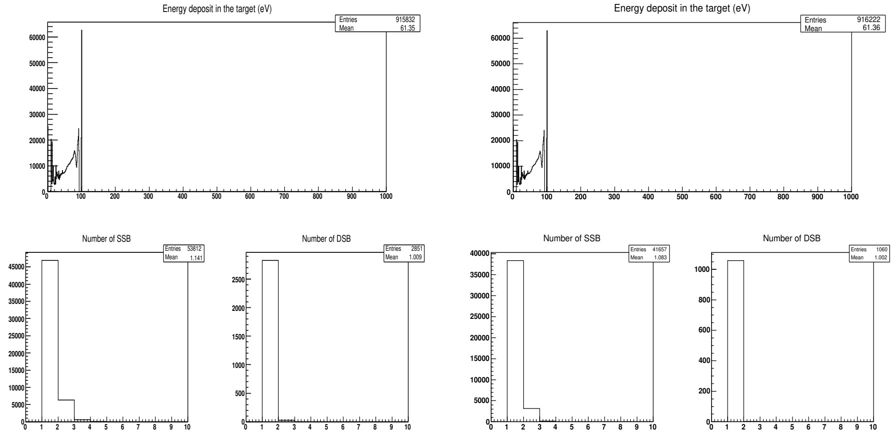


Figure: 1ZBB,Sugar-Base(left), Phosphate-Sugar(right), Electron ($e-$),1000000 events @ 100eV, breaking @ 8.22eV

Bond Modification

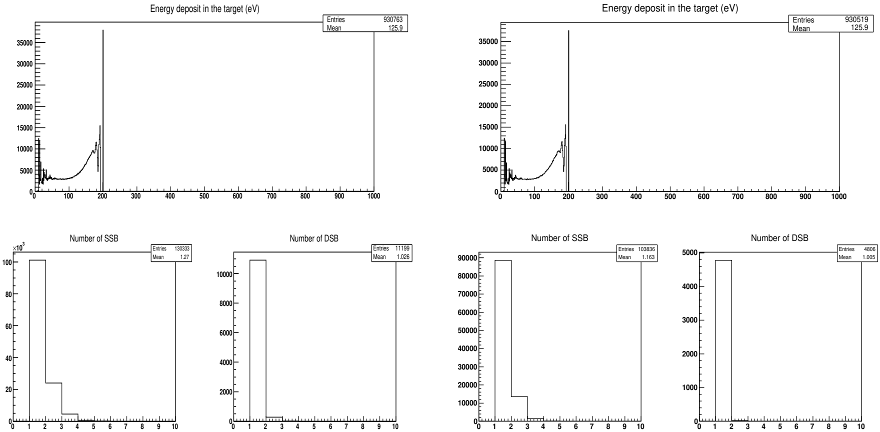
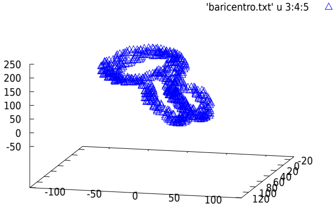
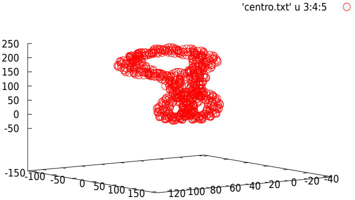


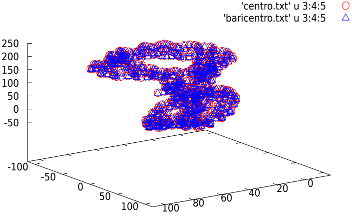
Figure: 1ZBB,Sugar-Base(left), Phosphate-Sugar(right), Electron ($e-$),1000000 events @ 200eV, breaking @ 8.22eV



'baricentro.txt' u 3:4:5
250
200
150
100
50
0
-50
-100 -50 0 50 100
120 100 80 60 40 20 0 -20



'centro.txt' u 3:4:5
250
200
150
100
50
0
-50
-150 -100 -50 0 50 100 150
120 100 80 60 40 20 0 -20 -40



'centro.txt' u 3:4:5
'baricentro.txt' u 3:4:5
250
200
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100
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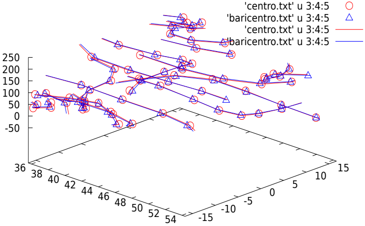
-50
-100 -50 0 50 100
100 80 60 40 20 0



'centro.txt' u 3:4:5
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'baricentro.txt' u 3:4:5
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36 38 40 42 44 46 48 50 52 54
-15 -10 -5 0 5 10 15

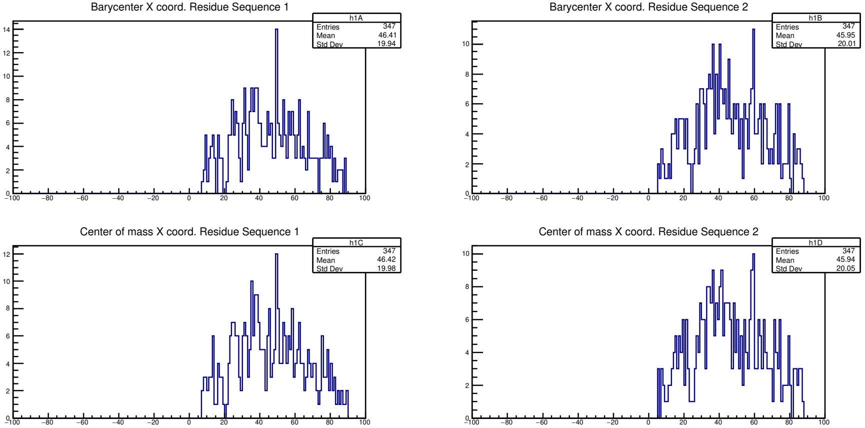
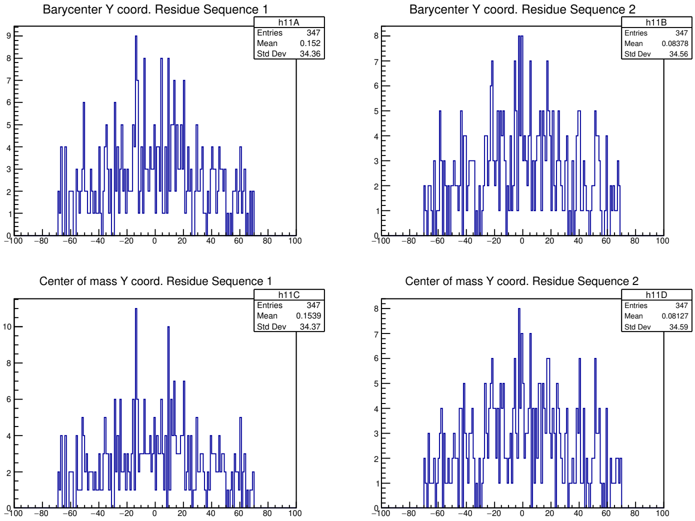


Figure: Baricenters en x vs centers of mass x-component 1ZBB

Baricenters vs Centers of Mass

1ZBB Y-Axis component



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Baricenters vs Centers of Mass

1ZBB Z-Axis component

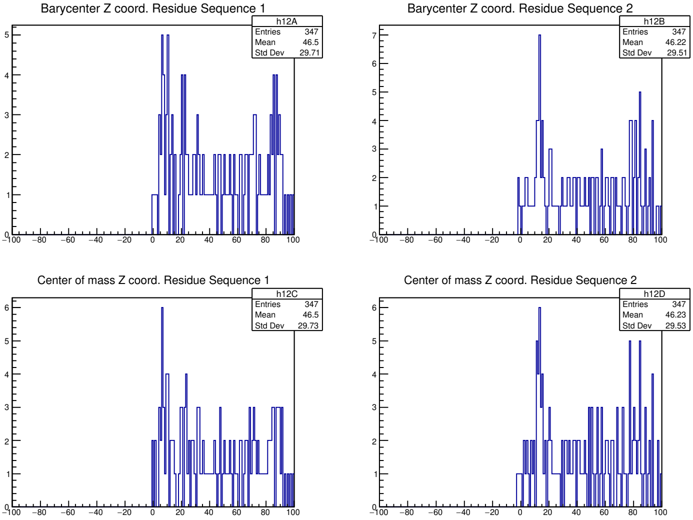


Figure: Baricenters en z vs centers of mass z-component 1ZBB

Counting for baricenters and centers of mass

Energy deposition and Double and single breaking bonds

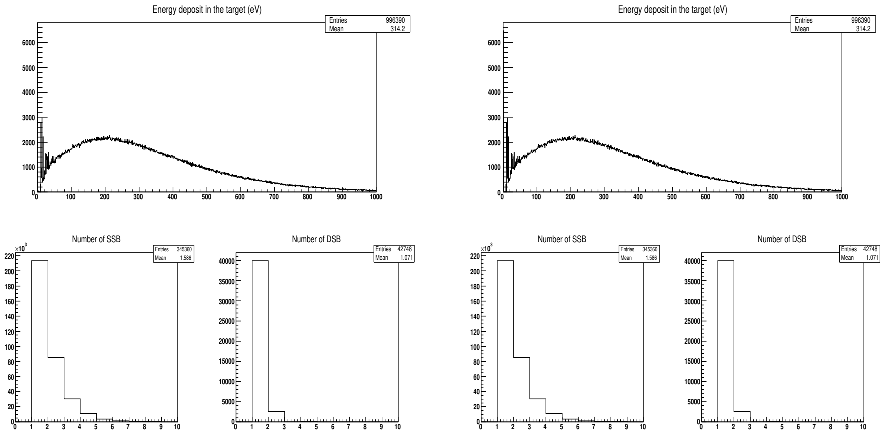


Figure: 1ZBB,PDB4DNA(left), PDB4DNA-C.M(righ), beam partícle (*proton*),1000000 events @ 600 keV, bond breaking at 8.22eV

Counting for baricenters and centers of mass

Energy deposition and Double and single breaking bonds

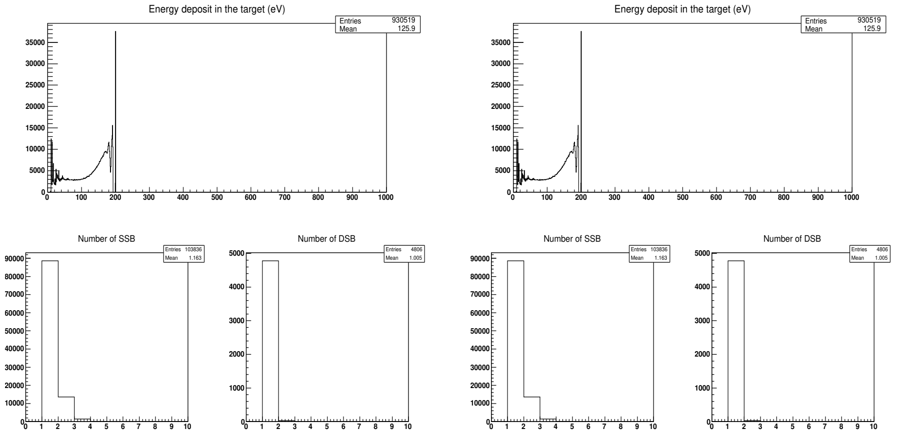
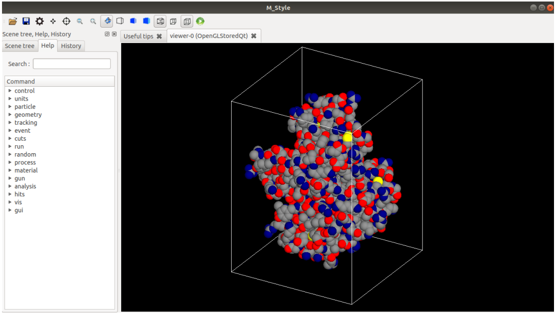
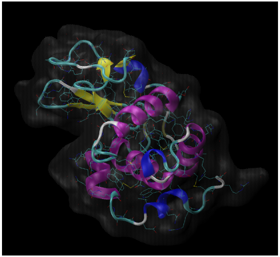


Figure: 1ZBB,PDB4DNA(left), PDB4DNA-C.M(righ), beam partícle (*proton*),1000000 events @ 200 keV, bond breaking at 8.22eV

We have *M_style*, an algorithm that preserves the general structure of a Geant4 format and some of the main functions of *PDB4DNA*. This code allows DNA, proteins and lipids to be irradiated, bringing us closer to the approximations of adverse effects generated in biological molecules due to the action of ionizing radiation.





Energy deposition PDB4DNA-modified vs M_style

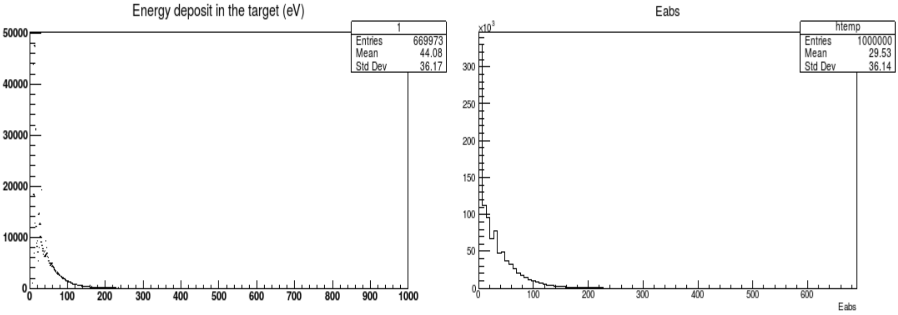


Figure: Energy deposition for electrons of $1keV$ PDB4DNA y M_Style, 1′000.000 events

Energy deposition PDB4DNA-modified vs M_style

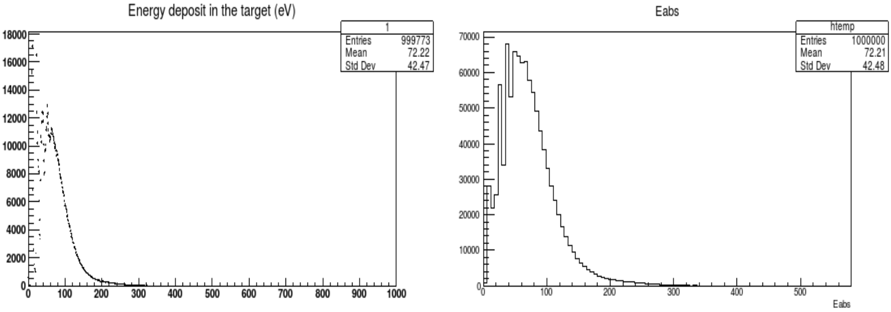


Figure: Energy deposition for protons of $1keV$ PDB4DNA y M_Style, $1'000.000$ events

Conclusions

- The characterization of the neutron capture reaction by Gadolinium via Geant4 is suitable
- We obtain the energy and angular distribution of the Gd-NCR
- It can be seen that the angular distribution for the final state of GdNCR is generated isotropically in Geant4

THANKS FOR YOUR ATTENTION
ANY QUESTIONS?