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INSTITUT DE RADIOPROTECTION ET DE SÛRETÉ NUCLÉAIRE

IMPLEMENTATION OF NITROGEN CROSS-SECTIONS IN GEANT4-DNA

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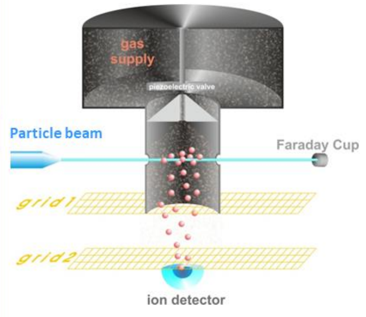
GEANT4-DNA
A SIMULATION TOOLKIT

EURADOS European Radiation Dosimetry Group

MEMBRE DE ETSON

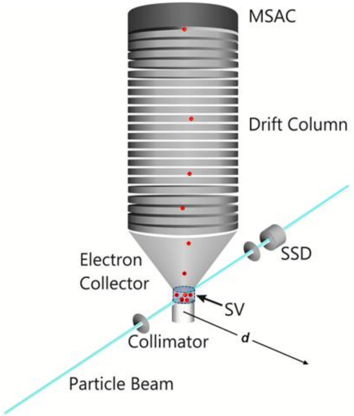
Track structure study by experimental means

Jet Counter



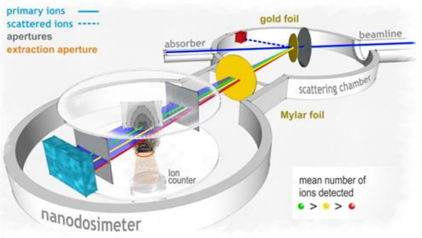
S. Pszona et al., Nucl. Instrum. and Meth. A 447, 601 (2000)

StarTrack Counter



L. De Nardo et al., Nucl. Instrum. Meth. A 484, 312 (2002)

Ion Counter



G. Garty et al., Radiat. Prot. Dosim. 99, 325 (2002)

- Objectif: study the mathematical **relations** between **nanodosimetric quantities and biological damages** (ex. DSBs, Survival curves, etc)
- Operated with **different TE gases and pressures**-> representing **different tissue volumes** in the nanometer scale
- Usual gases: N_2 and C_3H_8

Simulating nanodosimetric experiments: needs

- **PTra code (PTB)*:** Capable of track structure simulations in N2 or C3H8

**B. Grosswendt, S. Pszona, The track structure of α-particles from the point of view of ionization-cluster formation in "nanometric" volumes of nitrogen, Radiation and Environmental Biophysics 41 (2) (2002) 91–102)*

- But: simple geometry, written in Fortran, rudimentary interface => introduce gas cross-sections in Geant4-DNA

- **First cross-section data set recently implemented for electrons (13 eV-1 MeV) on N_2 in the form of look-up tables**

  PIETRZAK M., NETTELBECK H., PERROT Y., VILLAGRASA C., BANCER A., BUG M., INCERTI S.: INTERCOMPARISON OF NANODOSIMETRIC DISTRIBUTIONS IN NITROGEN SIMULATED WITH GEANT4 AND PTRA TRACK STRUCTURE CODES (2022) PHYSICA MEDICA, 102, PP. 103 – 109. DOI: 10.1016/J.EJMP.2022.09.00

N_2 cross-sections implemented in Geant4-DNA

Interaction type	Cross section type	Models
Impact ionisation	Total (including partial cross sections for 5 subshells)	Binary-Encounter-Bethe (BEB) model [1], except for K-shell onisation which uses one proposed by Casnati et al. [2].
	Impact ionisation Differential (production energy of secondaries)	Breit-Wigner formula [3].
Elastic scattering	Total	Fitted experimental data [4].
	Differential (scattering angle)	Modified Rutherford model with atomic screening corrections [4].
Electronic* excitation	Total (including 29 partial cross sections)	Formulas and cross section parameters based on Porter et al. [5]

[1] W. Hwang, Y. Kim, andM. E. Rudd, New model for electron-impact ioniza505 tion cross sections of molecules, J. Chem. Phys. 104 (8) (1996) 2956–2966
[2] E. Casnati, A. Tartari, and C. Baraldi, An empirical approach to K-shell 508 ionisation cross section by electrons, J. Phys. B 16 (3) (1983) 505–505
[3] A. Green and T. Sawada, Ionization cross sections and secondary electron 54 distributions, J. Atmos. Terr. Phys. 34 (10) (1972) 1719–1728
[4] B. Grosswendt and E.Waibel, Transport of low energy electrons in nitrogen 446 and air, Nucl. Instrum. Methods 155 (1-2) (1978) 145–156
[5] H. Porter, C. Jackman, and A. Green, Efficiencies for production of atomic 514 nitrogen and oxygen by relativistic proton impact in air, J. Chem. Phys. 515 65 (1) (1976) 154–167

***Auto-ionsation process included in the excitation model**

N_2 cross-sections implemented in Geant4-DNA

[MODELS ARE DESCRIBED IN THE G4DNAPTBXXXMODEL.CC .hh CLASSES

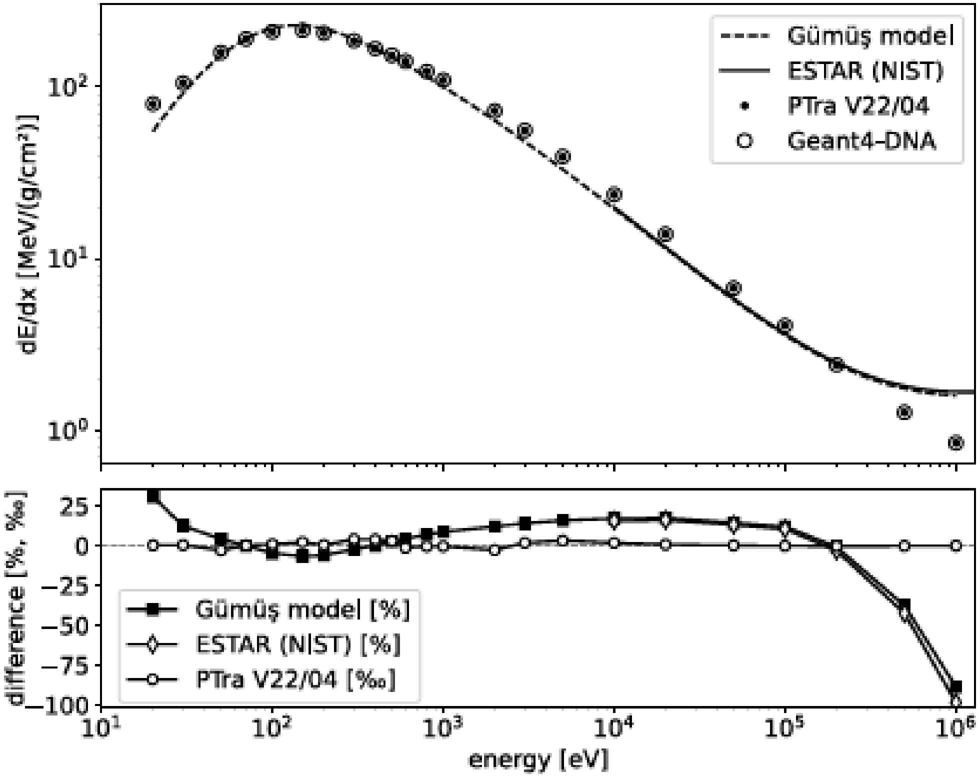
- **Used to handled materials different from liquid water**

- **Introduced for the first time in Geant4 10.4 for the use of DNA precusors material‘s cross-sections: THF, TMP, PU and PY (** *M. Bug et al, Rad. Phys and Chem. 130, 459-479 (2017))*

- ***/examples/extended/medical/dna/icsd shows how to build a PhysicsList using these models and mixed with liquid water Geant4DNA classical models:***

```
G4DNAEmfietzoglouIonisationModel *e_modelDNAEmfietzoglouIonisation = new G4DNAEmfietzoglouIonisationModel();
G4DNAPTBIonisationModel *modelDNAPTBIonisation =  new G4DNAPTBIonisationModel("THF/TMP/PY/PU/N2", particle);
G4DNAModelInterface *e_ionisationInteraction =  new G4DNAModelInterface("e-_ionisation_interaction");
e_ionisationInteraction-> RegisterModel(e_modelDNAEmfietzoglouIonisation, particle);
e_ionisationInteraction->RegisterModel(modelDNAPTBIonisation);
G4DNAIonisation *e_DNAIonisationProcess = new G4DNAIonisation("e-_G4DNAIonisation");
e_DNAIonisationProcess->SetEmModel(e_ionisationInteraction);
ph->RegisterProcess(e_DNAIonisationProcess, particle);
```

Validation of the implemented cross-sections



- Electronic stopping power in N2 compared to NIST ESRAR data base and Gümus model (H. Gümüş, Simple stopping power formula for low and intermediate energy electrons, Radiation Physics and Chemistry 72 (1) (2005) 7–12.)

- Results have also been compared to electron ranges in N2 with relative differences <10% in general

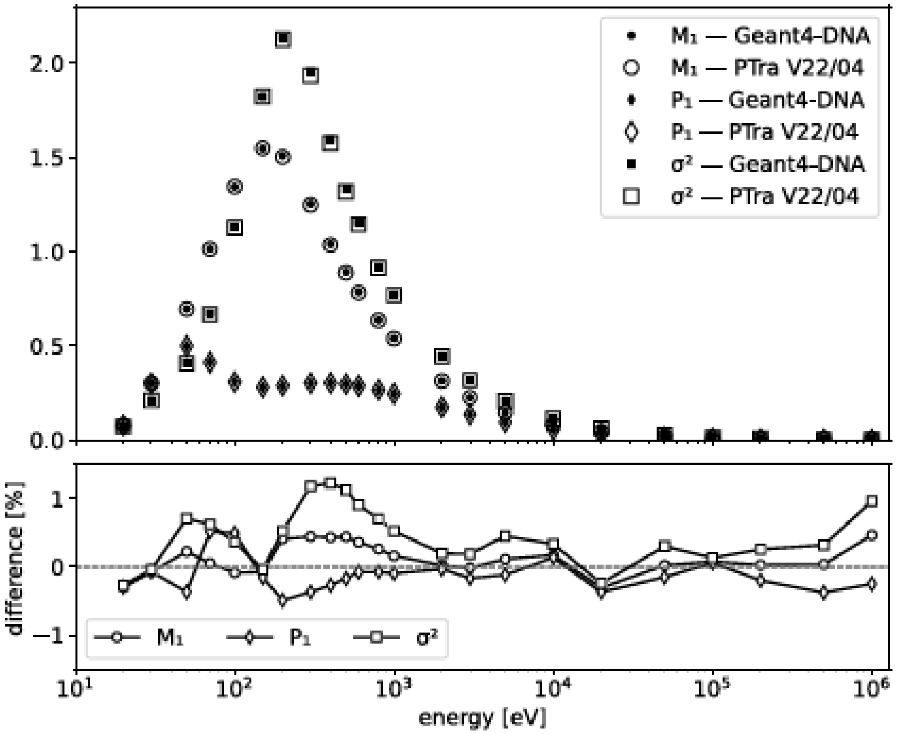
Geant4-DNA/ PTra benchmark and experimental validation

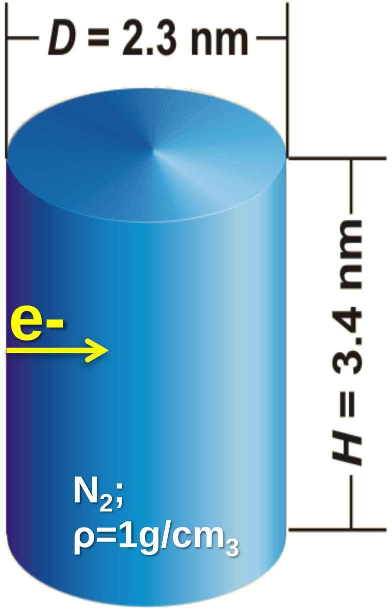
ICSD IN A VOLUME REPRESNETING 10 BASE PAIRS

Cylindical target 2.3 nm in diameter and 3.4 nm in height

Density= 1 g/cm^3

Benchmark 1: 10 DNA-base pairs volume





Geant4-DNA/ PTra benchmark and experimental validation

ICSD IN A VOLUME REPRESNETING 10 BASE PAIRS

Cylindical target 2.3 nm in diameter and 3.4 nm in height

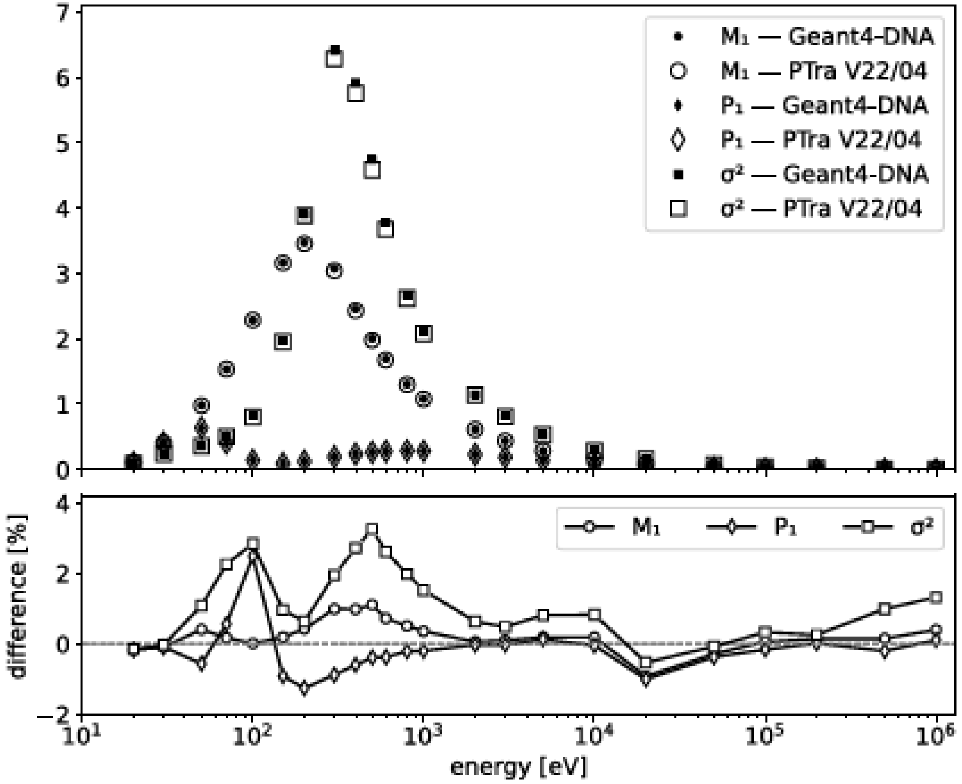
Density= 1 g/cm^3

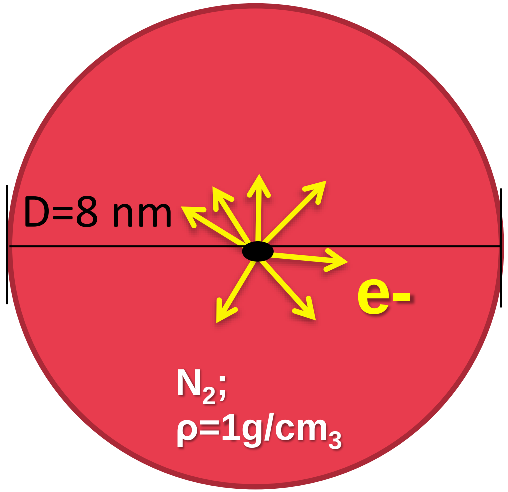
ICSD IN A VOLUME REPRESNETING 1 NUCLEOSOME

Spherical target of 8 nm diameter in the center of a 20x 20x 20 nm cubic world

Density= 1 g/cm^3

Benchmark 2: nucleosome volume





Geant4-DNA/ PTra benchmark and experimental validation

ICSD IN A VOLUME REPRESNETING 10 BASE PAIRS

Cylindical target 2.3 nm in diameter and 3.4 nm in height

Density= 1 g/cm^3

ICSD IN A VOLUME REPRESNETING 1 NUCLEOSOME

Spherical target of 8 nm diameter in the center of a 20x 20x 20 nm cubic world

Density= 1 g/cm^3

EXPERIMENTAL VALIDATION

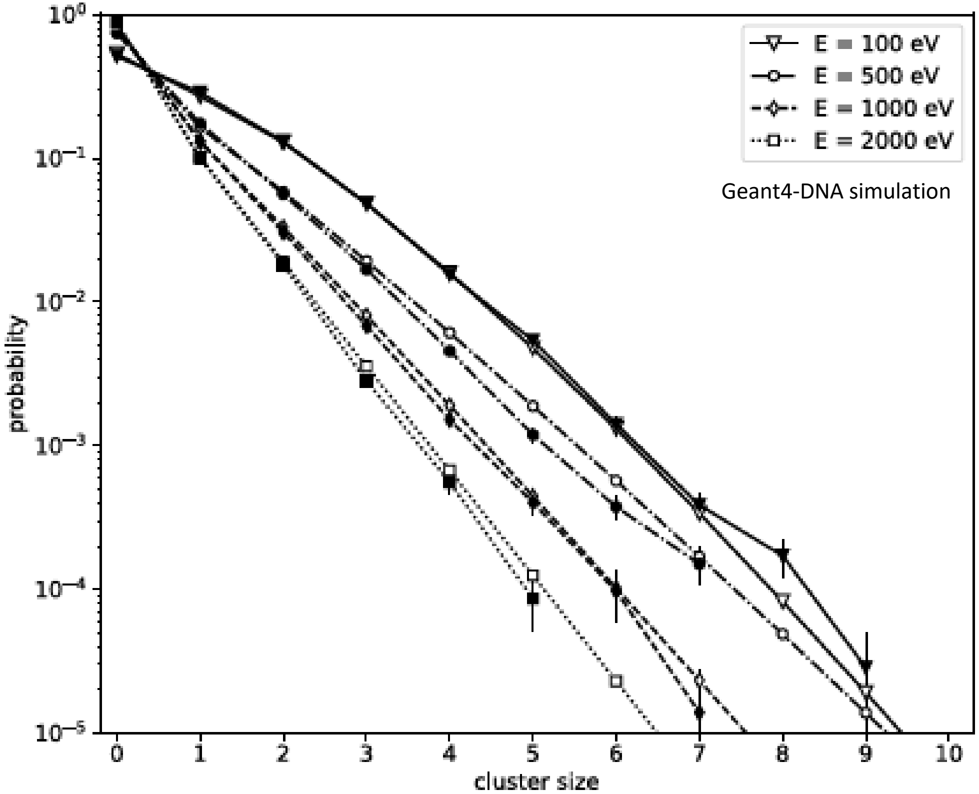
Comparison to ICSD experimentally obtained with the Jet Counter.

Bottomless cylinder, 10 mm in diameter and 10 mm in heigh. 100% sensitive volume

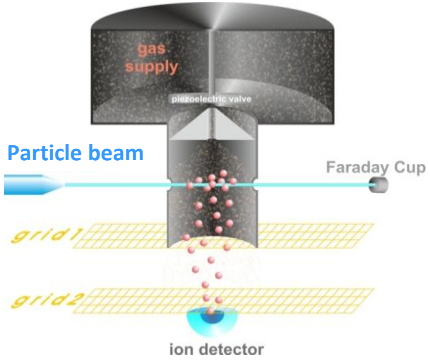
Density: 0.34 µg/cm^3

(equivalent water target of 2.3 nm in diameter and heigh)

Validation 3: experimental (Geant4-DNA)



Jet Counter



S. Pszona et al., Nucl. Instrum. and Meth. A 447, 601 (2000)

Conclusion

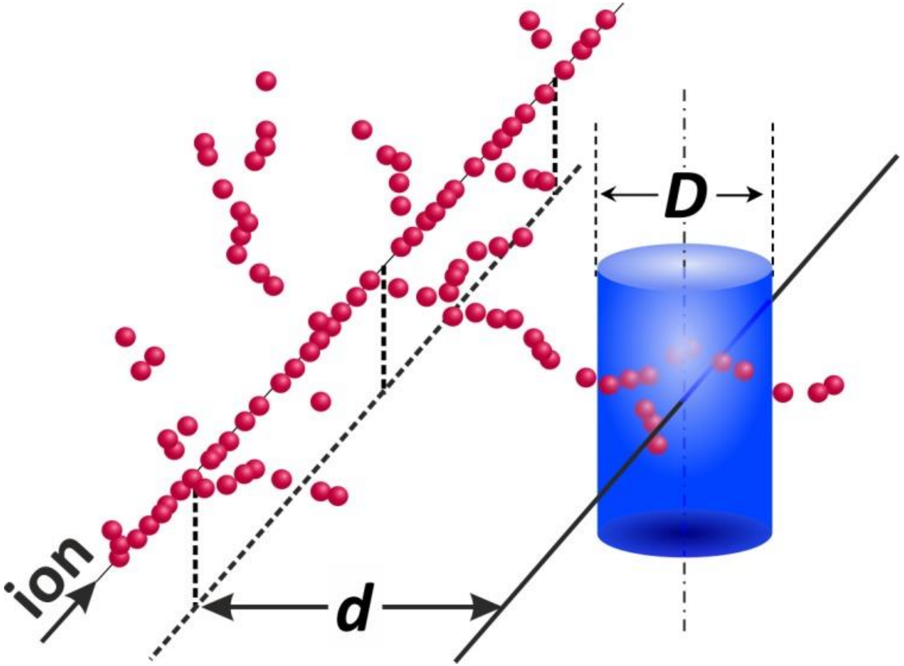
- **N_2 gas cross-section** have successfully been implemented in Geant4-DNA. This will allow the use of the code for simulating micro- and nanodosimetry experiments.

- They will be available in next Geant4.11.1 release through an updated version of the ICSD example ***/examples/extended/medical/dna/icsd***

- Further work is ongoing to extend the available cross-sections for electron transport **on propane**

Thank you for your attention

Track structure study by experimental means



The number ν of ionisations inside the target volume is counted event by event.

Nanodosimetric Quantities

distribution:

$$P(\nu|Q)$$

i-th moment:

$$M_i(Q) = \sum_{\nu=0}^{\infty} \nu^i \cdot P(\nu|Q)$$

i-th cumulative probability:

$$F_i(Q) = \sum_{\nu=i}^{\infty} P(\nu|Q)$$

N_2 cross-sections implemented in Geant4-DNA

[AUTOIONISATION PROCESS INCLUDED IN THE EXCITATION MODEL:

The auto-ionisation process is part of the excitation model in both MC codes, where a probability of 50% auto-ionisation is assumed if the excitation energy of a Rydberg state is greater than the 15.58 eV ionisation threshold for nitrogen. The secondary electrons produced by auto-ionisation are emitted isotropically and their kinetic energy is calculated from the given excitation energy minus the ionisation threshold.