

# « molecularDNA » example

Hoang Tran

Univ. Bordeaux, CNRS, LP2I Bordeaux, UMR 5797, F-33170 Gradignan, France

# **Geant4-DNA for radiobiology**





Extension of the Geant4 Monte Carlo simulation toolkit for radiobiology

- Track structure code: simulate each particle-matter interaction
  - ➤ physical stage
- Simulate the production and tracking of radiolytic species, together with their mutual interactions
  - > physico-chemical and chemical stages
- ➤DNA-scale geometries

# MolecularDNA: can simulate early DNA damage using only Geant4 macro commands - No C++ skills needed



Simulation of physics, physico-chemistry and chemistry processes in DNA geometries.



### Physical stage

G4EmDNAPhysics\_option2, G4EmDNAPhysics\_option4 or G4EmDNAPhysics\_option6 constructors are recommended to use in the molecularDNA example.

### Chemistry stage

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.
- No longer necessary to diffuse the molecular species and to calculate the possible reactions between the species at each time step.
- A « synchronous » alternative hybrid version (« IRT-sync ») which gives all spatio-temporal info. on radicals required for combination with geometries



# Geometry model

### **Design principle**

The molecularDNA application was made to make it easy to define a DNA geometry, and then place it repeatedly to model a complex geometry at large scales, as below.





It will join chains together correctly even when placement volumes are rotated along the lines of the image

## Damage model



**Direct Damage** occurs when energy from physical processes is deposited near a DNA molecule. In moleculardna, we associate damage either with a 'strand' molecule (sugar or phosphate placement) or a base molecule.

**Indirect damage** is scored when a chemical reaction leads to a strand break.





Strand breakage scheme (Nikjoo et al.1997) DNA segment complexity can be considered



# Geometry library



### Benchmarking and will need more...



1.00E-15

10

100

1000

10000

Fragment Length (kbp)

#### **Documentations**



Built using Just The Docs.

This site uses Just the Docs, a documentation theme for Jekyli

#### 希 FractalDN

Structure Models

DNA Models

API Reference

Examples

#### 希 » FractalDNA

View page source

#### FractalDNA

FractalDNA is a Python package to make DNA geometries that can be joined together like jigsaw puzzles. Both simple, sections of DNA and Solenoidal DNA can be built. This module was built to enable DNA-level simulations to be run in Geant4-DNA, part of the Geant4 project.

Structure models define the large scale structure of DNA, seeded from fractals. An example seeding fractal is below:



DNA Models provide straight and curved segments that can come together to make DNA for use in simulations.



Documentation is divided into three main sections, focused on building DNA models, high level structure models, and then some notebook examples. showing how the code works.

Structure Models

DNA Models

# Thank you to contributors

- J.M.C. Brown
- K. Chatzipapas
- M. Dordevic
- S. Incerti
- M. Karamitros
- N. Lampe
- D. Sakata
- W.G. Shin