IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire

DNADamage1 example

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PSE-SANTE/SDOS/LDRI

Geant4 meeting (23-27, Steptember 2019)

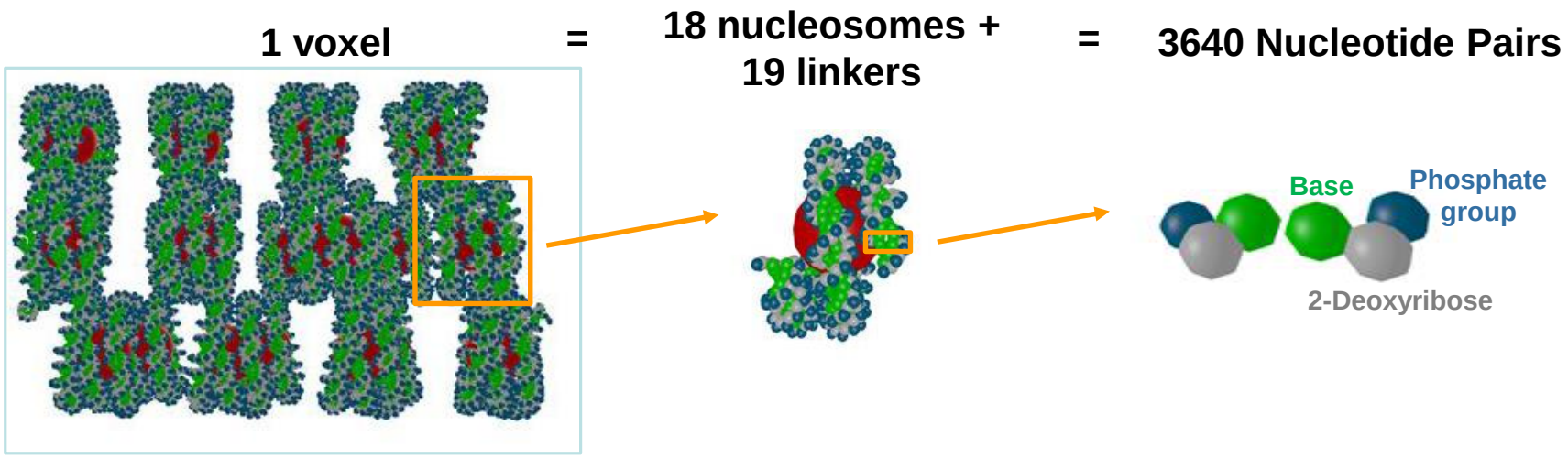
Dnadamage1 example

examples/extended/medical/dna/dnadamage1/

- Radiobiology considers DNA as the main target to understand the effect of ionizing radiations
- Geant4-DNA developments include physics, chemistry, geometric models to characterize direct and indirect damages to DNA
- Dnadamage1: first Geant4 application showing how to simulate direct and indirect DNA damages in a segment of chromatin fiber
- Adapted from the full nucleus simulation reported in Sc. Rep. 7 (2017)11923

Geometry

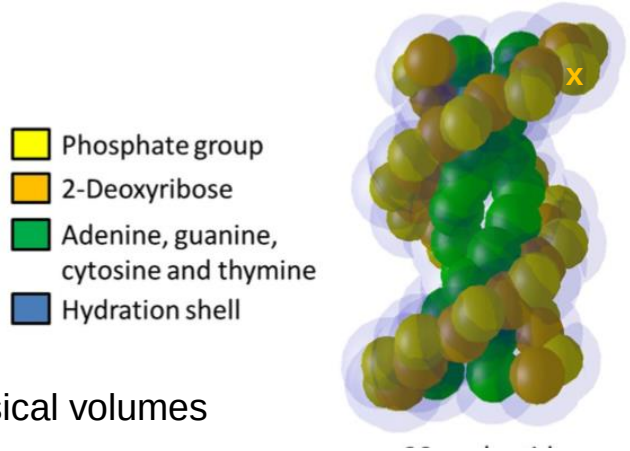
- One voxel of 40 nm fiber heterochromatin generated from DNAFabric tool
- Represents a big input file: automatically downloaded by cmake (thanks to Gunter)



DNA Geometry from DNAFabric software (IRSN) : www.symalgo-tech.com

Physical stage

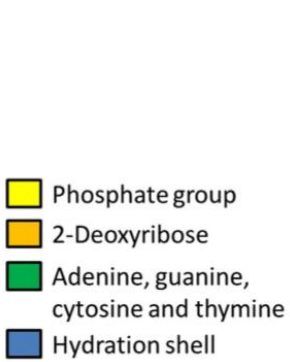
- G4EmDNAPhysics by default is used
- Direct SB defined when energy deposit in “2-Deoxryibose” or “Phosphate” volume (including hydration shell) above a given threshold
- The position and volume of each DNA element are used from input file
- Energy deposits and “damaged” DNA volumes are saved from SteppingAction

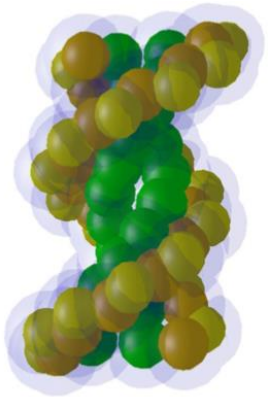


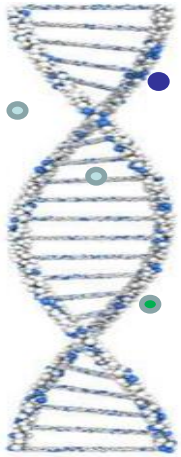
Physical volumes

Chemistry and DNA reaction

- The idea is to consider the DNA model not as a group of Geant4 physical volumes but as a set of spatially ordered molecules that should not diffuse over time
- A chemical stage duration is limited by 2.5 ns.
- The chemical reactions between OH• and a sugar (2-deoxyribose and phosphate) give rise to indirect SSB.
- After a reaction, the radical is killed and the affected DNA molecule is assumed to no longer participate in other reactions
- G4EmDNAChemistry_option2 is used for this example.



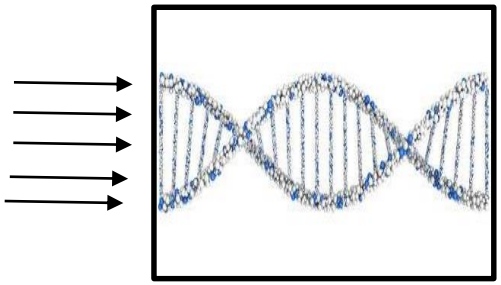




Reaction	Reaction rate ($10^9 M^{-1} \cdot s^{-1}$)
2-deoxyribose + $OH^•$	2.5
Adenine + $OH^•$	6.10
Guanine + $OH^•$	9.20
Thymine + $OH^•$	6.40
Cytosine + $OH^•$	6.10
Histone + molecule → $\text{histone}_{\text{modified}}$	—

“Parallel world” for chemistry

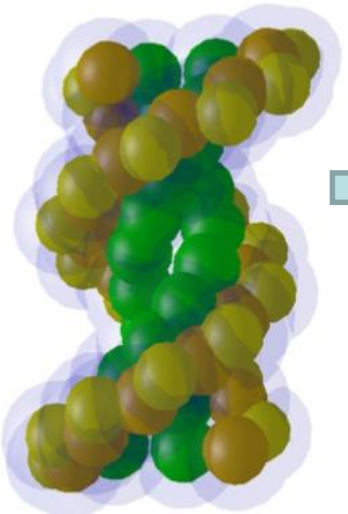
Navigators: physics and chemistry



Voxel «Straight»

- Reduce time consuming for navigator of chemical molecule in the physical DNA molecule
- Shift to “Parallel world” at the beginning of chemical stage

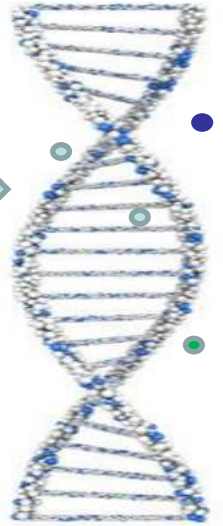
Physical volumes



navigator

Stop navigating
DNA Geometry

Molecule



Analyse SSB damage in ROOT

- Analyse DNA hits using ROOT
  - A 17.5 eV threshold for the energy deposit in the backbone of a nucleotide to determine a direct SSB.
  - 40% of the chemical reactions between OH• and a sugar (2-deoxyribose) give rise to an indirect SSB.
  - Merging direct and indirect SSB
- Output file gives the distribution of DNA damage using the Standard DNA Damage data format (Shuemann et al. 2019 Rad. Res. (191) 76-92)

To improve for the next release

- Optimization by not treating DNA molecules in the same way as other chemical molecules
- Can be used with other chemical molecular reaction list as **G4EmDNAChemistry_option1**
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