IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

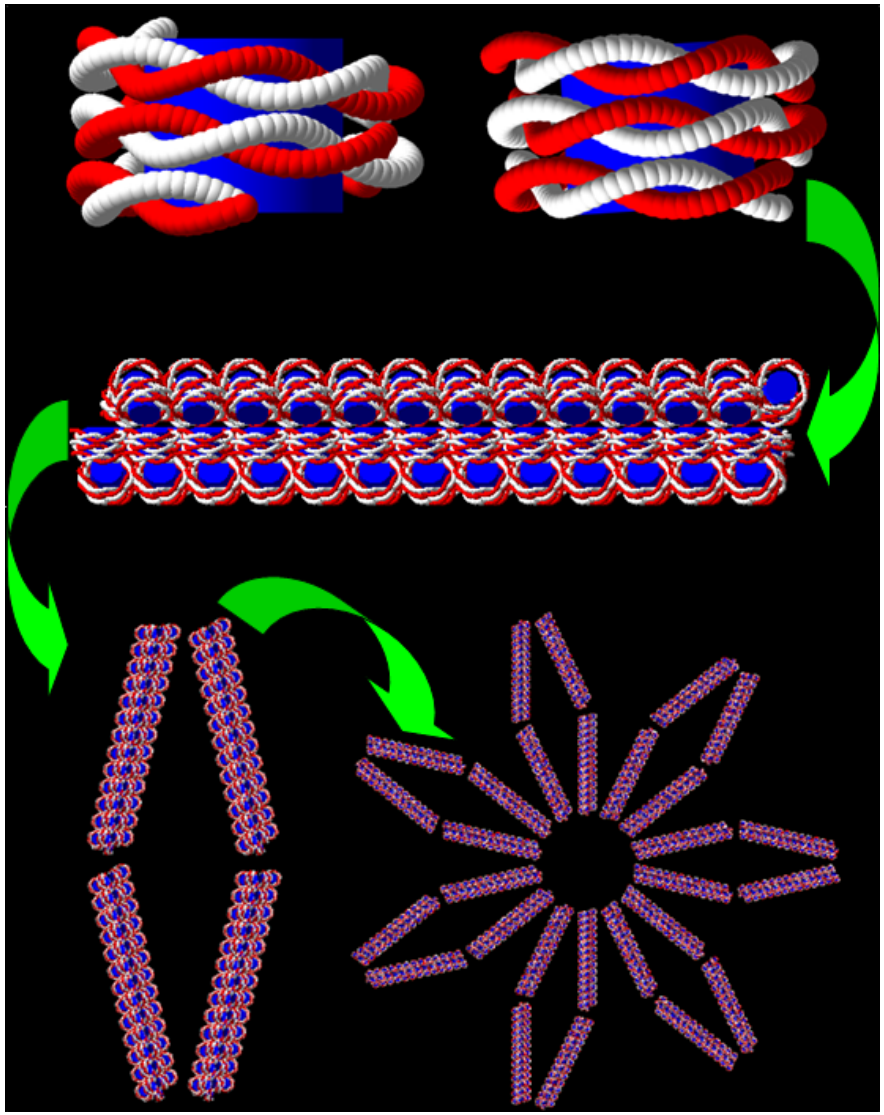
Enhancing nuclear safety

Example WholeNuclearDNA

M. Dos Santos, S. Meylan and C. Villagrasa*

Geant4-DNA Tutorial 7th November 2014.

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)



M. Dos Santos PhD. Work (IRSN/ 2013)

Nucleosome

- 200 bp / nucleosome
- DNA diameter = 2.16 nm
- Histone = cylinder of 6.5 nm in diameter and 5.7 nm in height

Chromatin fiber

- 90 nucleosomes / fiber
- 7 nucleosomes / turn
- D = 31 nm
- L = 161 nm

Chromatin fiber loop

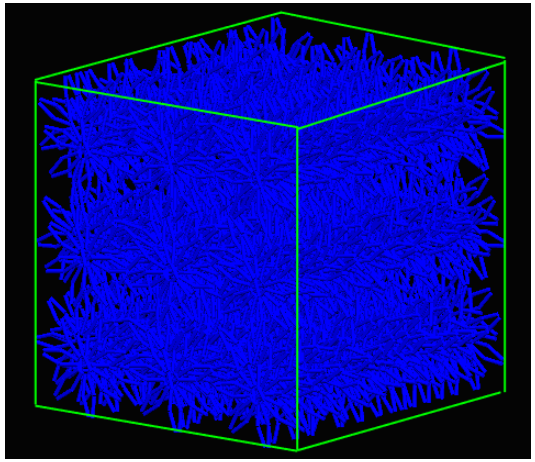
- 4 fibers / loop assembled in a diamond shape
- 7 loops to form a “flower”*

** W. Friedland & al, Simulation of DNA damage after Proton irradiation, Radiation Research 59 (2003), 401-410.*

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

Detector Construction: **Containing the description of an elliptical cell nucleus with similar dimensions of fibroblast grown in a microscopic plate at confluence.**

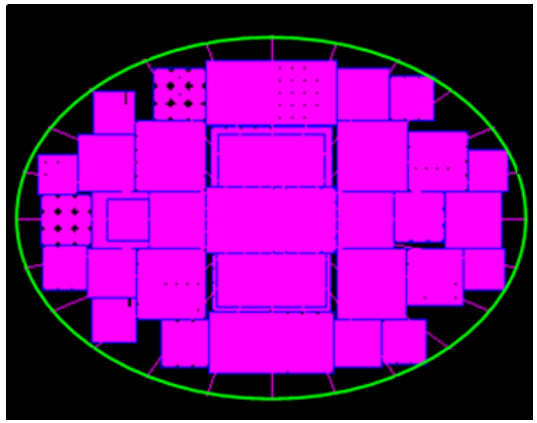
Chromosome domain example



Per nucleus:
- 23 pairs of chromosomes
- 11875 flowers or 83125 loops
- 332 500 chromatin fibers
- 29 925 000 nucleosomes
- ~ 6 Gbp

M. Dos Santos, C. Villagrasa, I. Clairand and S. Incerti. "Influence of the DNA density on the number of clustered damages created by protons of different energies". NIM B 298 (2013) 47-54.

« Fibroblast » cell nucleus



- Nucleus-> ellipsoid
- Dimensions: 23.64 * 17.04 * 6 µm
- V = 1265 µm^3
- 0.31 % of DNA / nucleus

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

Use of the G4DNAGeometry example :

Based on the existing G4DNAPhysics but including the simplified DNA geometry in the DetectorContruction

PrimaryGeneratorAction:
Default, protons of 1 keV (100 keV on wholenuclearDNA.in) traversing the nucleus in the z axis (lower axis) From z0=-2.99 nm (inside the nucleus at x=0, y=0) (x0,y0) uniform distribution in the center part of the nucleus x0 [8,-8] µm, y0 [4,-4] µm

Output: **A root file** containing an n-tuple with the following values only for those energy transfer points located on the backbone region :
-**Particle type** at the origin of the energy deposition
-**Process type (ionization, excitation)**
-Information on the **DNA strand** (flag 1 / 2)
-**Coordinates of the energy deposition** (x,y,z)
-**Energy deposition** amount

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

DetectorContruction

```
//Phosphodiester group

    G4Orb* solidSugar_48em1_nm = new G4Orb("sugar", 0.48 *
nanometer);

    G4ThreeVector posi(0.180248 * nanometer,
                       0.32422 * nanometer,
                       0.00784 * nanometer);
    G4UnionSolid* uniDNA = new G4UnionSolid("move",
                                 solidSugar_48em1_nm,
                                 solidSugar_48em1_nm,
                                 0,
                                 posi);

    G4ThreeVector posi2(-0.128248 * nanometer,
                        0.41227 * nanometer,
                        0.03584 * nanometer);
    G4UnionSolid* uniDNA2 = new G4UnionSolid("move2",
                                  solidSugar_48em1_nm,
                                  solidSugar_48em1_nm,
                                  0,
                                  posi2);

                                 .....
```

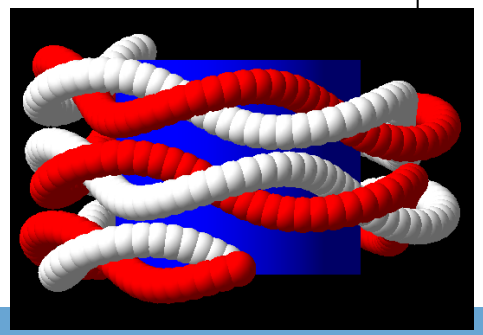
```
        /
*************************************************************************
*
      Phosphodiester group Position

*************************************************************************
*/       for (G4int n = 2; n < 200; n++)
            {
                                 .....
      uniDNA = new G4UnionSolid(name,
                                 uniDNA,
                                 solidSugar_48em1_nm,
                                 0,
                                 posSugar1);

     uniDNA2 = new G4UnionSolid(name,
                          ....uniDNA2,
                                 solidSugar_48em1_nm,
                                 0,
                                 posSugar2);
       }

 G4LogicalVolume* logicSphere3 = new G4LogicalVolume(uniDNA,
                                                     waterMaterial,
                                                     "logic sugar 2");
   G4LogicalVolume* logicSphere4 = new
G4LogicalVolume(uniDNA2,
                                                     waterMaterial,
                                                     "logic sugar 4");
```

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

DetectorContruction

```
//base pairs


 G4Orb* solidBp1 = new G4Orb("blue sphere", 0.17 *
nanometer);
     G4LogicalVolume* logicBp1 = new
G4LogicalVolume(solidBp1,
                                        waterMaterial,
                                        "logic blue sphere");
     G4Orb* solidBp2 = new G4Orb("pink sphere", 0.17 *
nanometer);
     G4LogicalVolume* logicBp2 = new
G4LogicalVolume(solidBp2,
                                        waterMaterial,
                                        "logic pink sphere");
```

.....



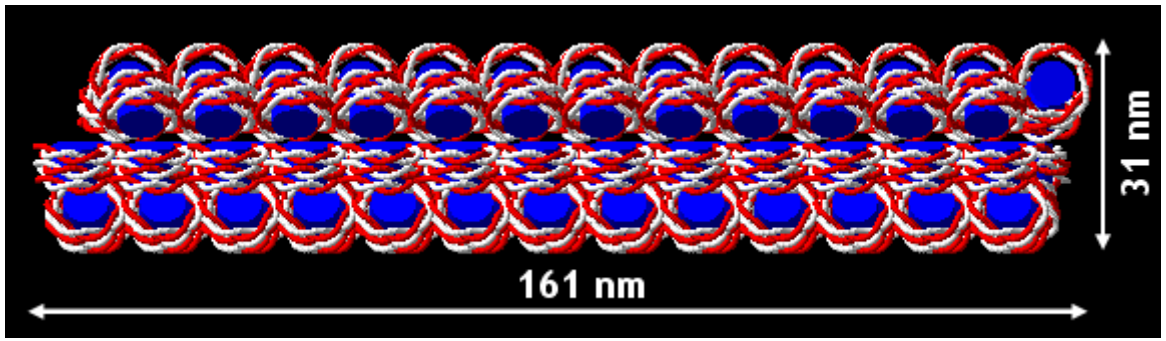
```
/
*****************************************************************************
    Base pair Position
*****************************************************************************
/                          .....
     for (G4int n = 0; n < 200; n++)
     {
                           .....

 new G4PVPlacement(0,
                        position1,
                        logicBp1,
                        "physi blue sphere",
                        logicSphere3,
                        false,
                        0);
       new G4PVPlacement(0,
                        position2,
                        logicBp2,
                        "physi pink sphere",
                        logicSphere4,
                        false,
                        0);
     }
```

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

DetectorContruction

```
 /
**************************************************************************
**/
  //              Initial position of different elements
  /
**************************************************************************
**/
      // DNA and histone positions
      for (int j = 0; j < 90; j++)
      {
                        .....

  new G4PVPlacement(rotStrand1,
                    posStrand1,
                    logicSphere3,
                    "physi sugar 2",
                    logicEnv,
                    false,
                    0);

new G4PVPlacement(rotStrand2,
                  posStrand2,
                  logicSphere4,
                  "physi sugar 4",
                  logicEnv,
                  false,
                  0);
```

```
new G4PVPlacement(rotHistone,
                  posHistone,
                  logicHistone,
                  "PV histone",
                  logicEnv,
                  false,
                  0);
```

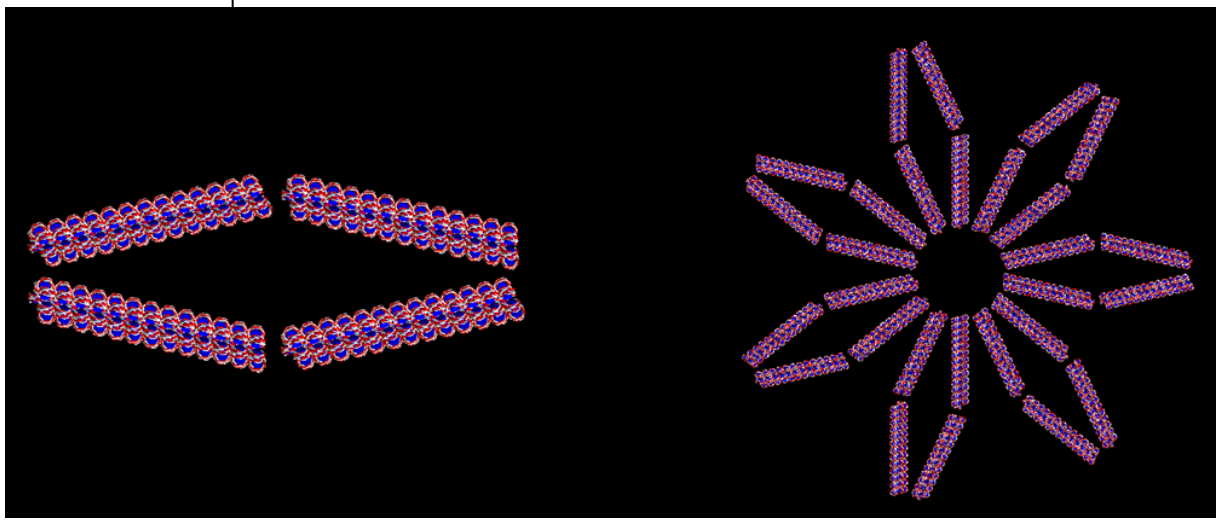


G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

DetectorContruction

```
// Chromatin fiber position
  for (G4int i = 0; i < 7; i++)
  {

 G4ThreeVector posFiber = G4ThreeVector(0, 152 *
nanometer, 0);
    posFiber.rotateZ(i * 25.72 * degree);

 new G4PVPlacement(rotFiber,
                   posFiber,
                   logicEnv,
                   "physi env",
                   logicBoxros,
                   false,
                   0);

            .....
 posFiber = G4ThreeVector(0, 152 *
nanometer, 0);
    posFiber.rotateZ((7 + i) * 25.72 *
degree);


            .....
```

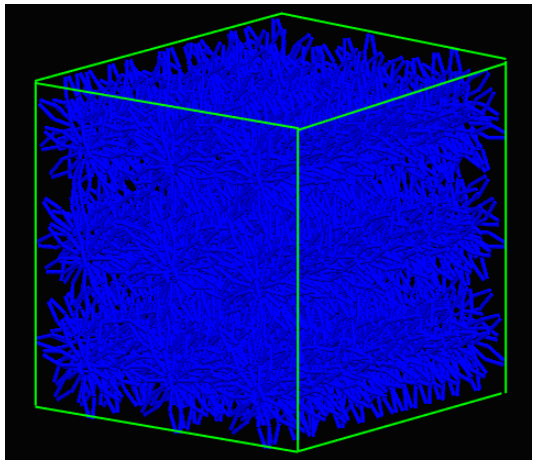
```
 rotFiber->rotateY((25.72 + (i - 14) * 51.43) * degree);
    posFiber = G4ThreeVector(-36.5 * nanometer, 312 *
nanometer, 0);

                    .....


 posFiber = G4ThreeVector(-103 * nanometer, 297 * nanometer,
0);
    posFiber.rotateZ((i - 21) * 51.43 * degree);

  }
```



G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

DetectorContruction

```
 /
**************************************************************************
/
  //              Box containing the chromatin flowers
  /
**************************************************************************
/

  for (int k = 0; k < 22; k++)
  {


     ostringstream oss;
       oss << "chromo" << k + 1 << ".dat";
       name = oss.str();
       oss.str("");
       oss.clear();


    LoadChromosome(name.c_str(), physiBox[k * 2], logicBoxros);
   LoadChromosome(name.c_str(), physiBox[k * 2 + 1], logicBoxros);
  }

LoadChromosome("chromoY.dat", physiBox[44], logicBoxros);
LoadChromosome("chromoX.dat", physiBox[45], logicBoxros);
```



Parameterization of the position of the flowers for each chromosome domain

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

DetectorContruction

```
DetectorConstruction::DetectorConstruction() :
    fBuildChromatineFiber(true),
    fBuildBases(false)
{
}
```

vis.mac-> Visualization is very time consuming: therefore, we recommend to only « place » (G4PVplacement) those volumes that you want to visualize

plot.C ->Draws the positions(x,y,z) of ionizations happening in the backbone region (strands 1 and 2 with different colors) from the ntuple information

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

Hands-on

Copy the example in your work directory

As it is,

- mkdir build
- cd build
- Module load geant4/10.01-mt
- cmake ../
- Make
- ./wholeNuclearDNA

(vis.mac is used) you can only see the nucleus and the chromosome territories.

G4DNAGeometry (advanced examples)
WholeNuclearDNA (extended examples)

Hands-on

To make a calculation:

```
DetectorConstruction::DetectorConstruction() :
   fBuildChromatineFiber(true),
   fBuildBases(true)
{
}
```

- cmake ../wholeNuclearDNA
- make
- ./wholeNuclearDNA wholeNuclearDNA.in

And WAIT …….

a root file with the ntuple is created

To see the results

- root
- .X plot.C