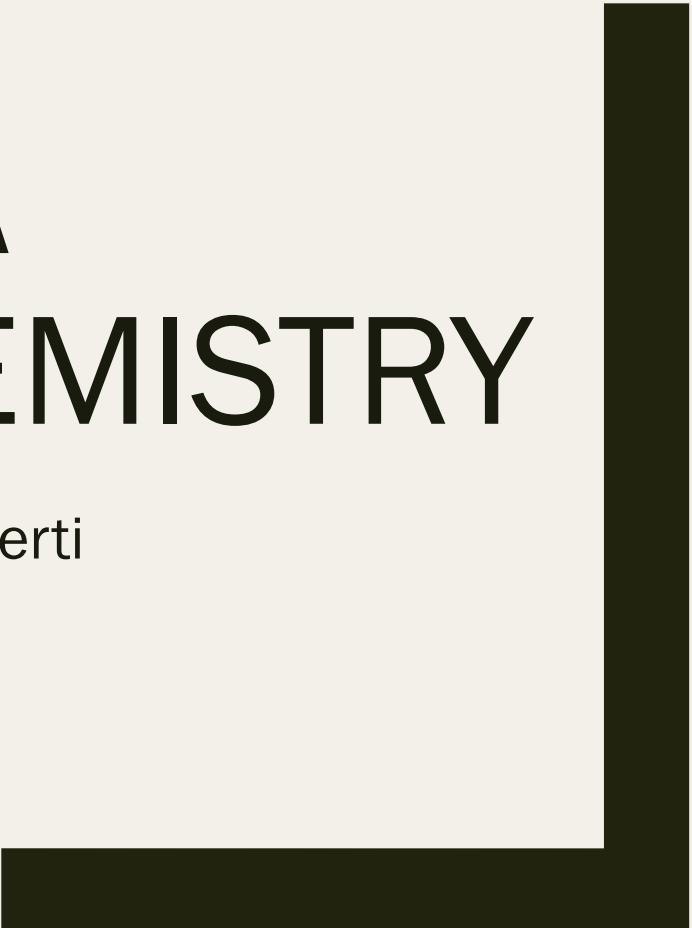




GEANT4-DNA GEOMETRY AND CHEMISTRY

Nathanael Lampe and Sebastien Incerti
Belgrade, November 2016



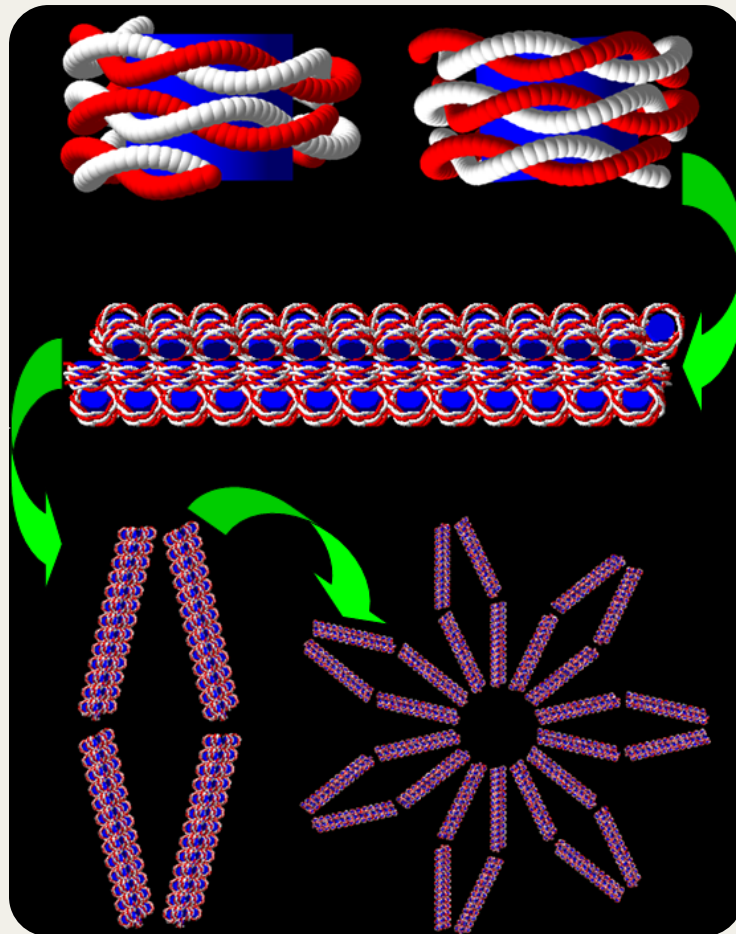
Structure

- Introduction to geometries for DNA-level simulations
 - *Hands on example: PDB4DNA*
- Introduction to the Geant4-DNA Chemistry module
 - *Hands on examples: chem1 and chem3*

Existing examples

- Whole Nuclear DNA
- PDB4DNA
- Coming Soon: MolecularDNA

« wholeNuclearDNA » extended example



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

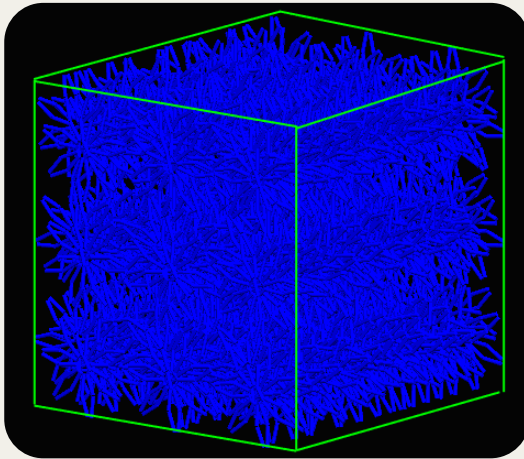
- 4 fibers / loop assembled in a diamond shape
- 7 loops to form a "flower"*

* W. Friedland et al, Rad. Res 59 (2003), 401-410

« wholeNuclearDNA » extended example

« **DetectorConstruction** » class: implementation of an **elliptical cell nucleus** with similar dimensions of **fibroblast** grown on a microscopic plate at confluence

Chromosome domain example



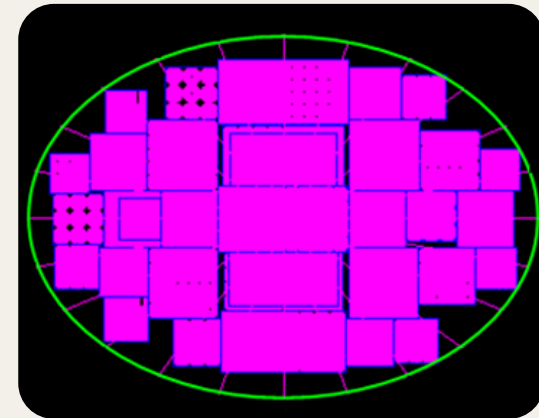
Per nucleus

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

Output: a ROOT file containing an n-tuple with the following values only for energy transfer points located in 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

« Fibroblast » cell nucleus



- Nucleus-shape: ellipsoid
- Dimensions: 19.7 * 14.2 * 5 μm^3
- V = 732 μm^3
- 0.42 % of DNA / nucleus

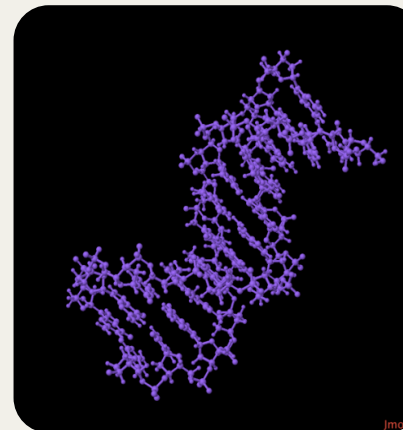
Nucl. Instrum. and Meth. B 298 (2013) 47 ([link](#))

A new interface to describe geometries in Geant4-DNA

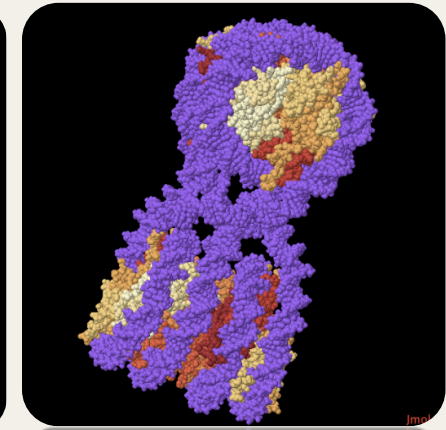
- PDB : Protein Data Bank
<http://www.rcsb.org/pdb/>
 - 3D structure of molecules
 - Proteins
 - Nucleic acids
- Description of DNA molecules
 - 1FZX.pdb
- Dodecamer
- 12 DNA base pairs
- (2,8 x 2,3 x 4,01 nm³)
- 1ZBB.pdb
- Tetranucleosome
 - 2 nucleosomes : 347 pairs of bases
 - (9,5 x 15,0 x 25,1 nm³)

```

HEADER  STRUCTURAL PROTEIN/DNA          08-APR-05  1ZBB
TITLE   STRUCTURE OF THE 4_601_167 TETRANUCLEOSOME
...
ATOM    1  O5'  DA I  1    70.094 16.969 123.433 0.50238.00  O
ATOM    2  C5'  DA I  1    70.682 18.216 123.054 0.50238.00  C
ATOM    3  C4'  DA I  1    69.655 19.289 122.776 0.50238.00  C
...
TER     14223      DT J 347
...
HELIX   1  1 GLY A  44 SER A  57  1          14
HELIX   2  2 ARG A  63 ASP A  77  1          15
...
SHEET   1  A 2 ARG A  83 PHE A  84  0
SHEET   2  A 2 THR B  80 VAL B  81  1 O VAL B  81  N ARG A  83
  
```



1FZX.pdb

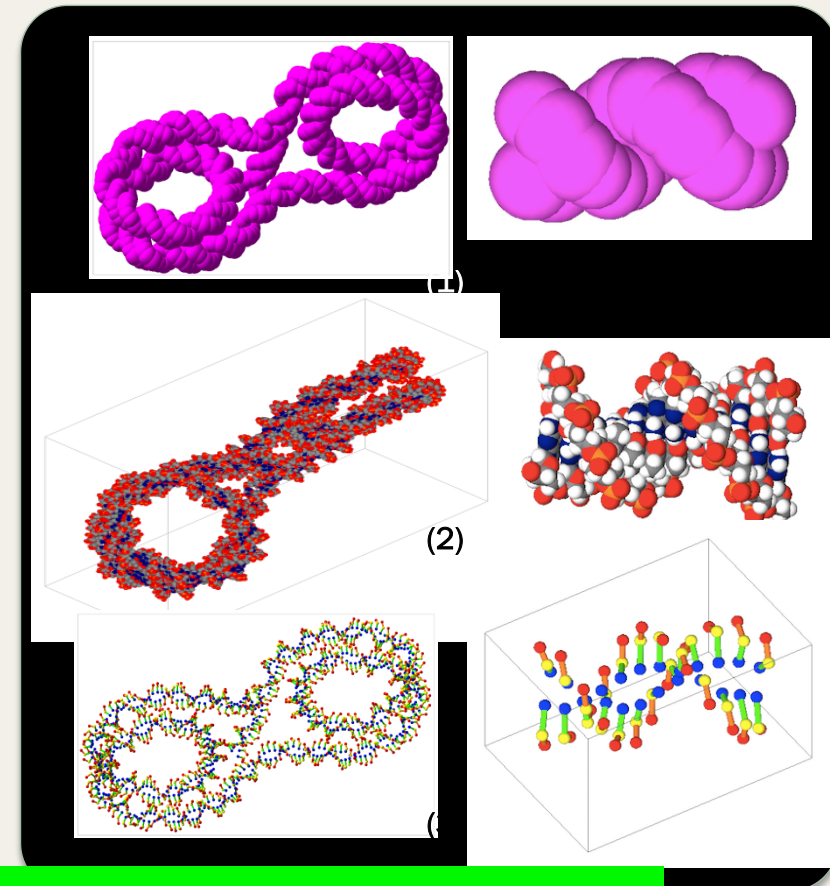


1ZBB.pdb

« PDB4DNA » suite

Click

- 1) A C++ library
 - Reading of *PDB files*
 - Build *bounding boxes* from atom coordinates
 - Search for *closest atom* from a given point
 - Geometry and visualization : *3 granularities*
- (1) Barycenter of nucleotides
- (2) Atomistic
- (3) Barycenter of nucleotide components
- 2) A Geant4-DNA example
 - Water box surrounding the molecule
 - The output results consists in a *ROOT* file, containing for each event:
 - energy deposit in bounding boxes
 - number of single strand breaks (SSB)
 - number of double strand breaks (DSB)
- Available on-line under Geant4 license



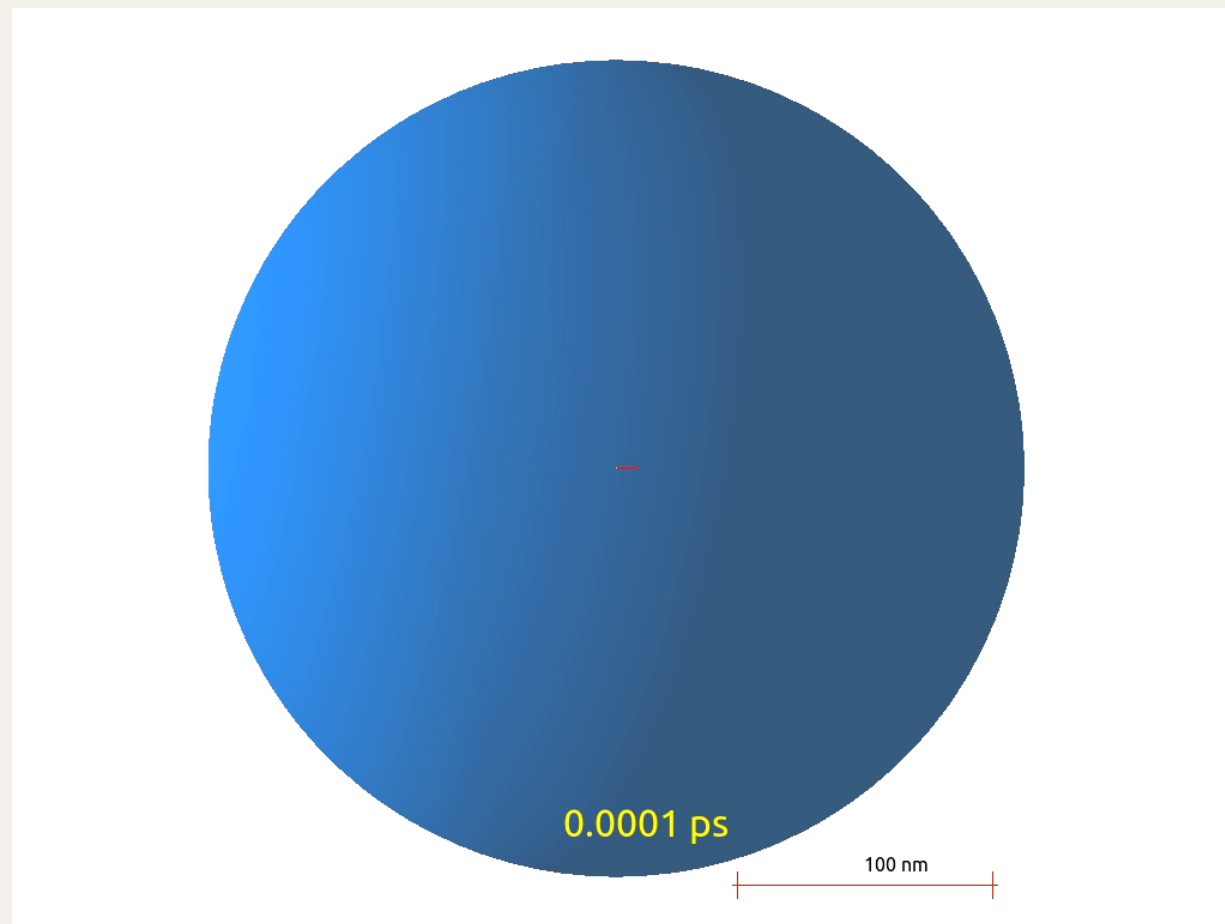
Comput. Phys. Comm. 192 (2015) 282 ([link](#))

CHEM3

Geant4-DNA generated track of **1 keV electron**, followed up to **100 ns** during chemical stage. Using pre-release Geant4 10.1 code.

First, the **physical stage** is modeled, using Geant4-DNA physics: the 1 keV electron track is fully slowed down and thermalized in a **150 nm sphere** of liquid water. **Yellow points** correspond to interaction events in liquid water.

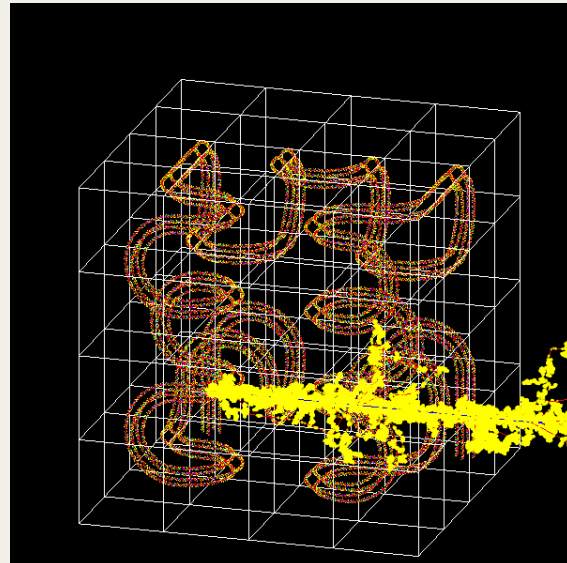
Next, the **physico-chemical / chemical stage** is simulated for the first 100 ns. **Individual radical species** diffusing in space and reacting with each other are shown as colour trails, the color coding chemical species type.



<http://dx.doi.org/10.6084/m9.figshare.978887>

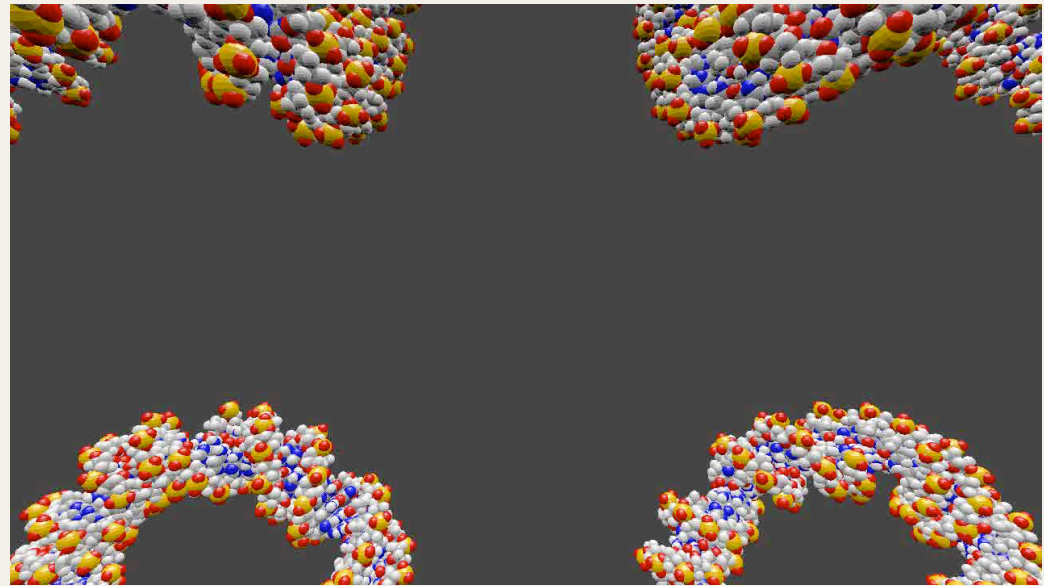
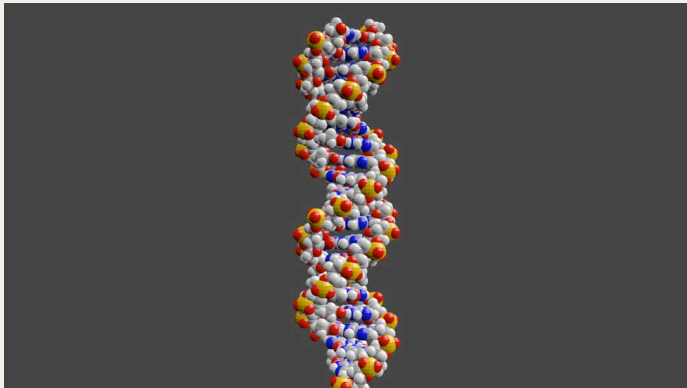
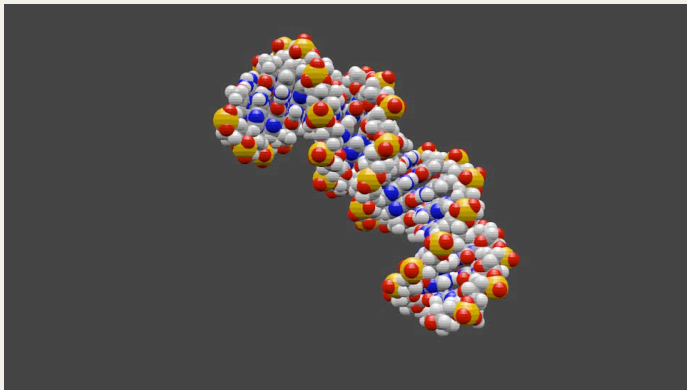
Coming Soon: MolecularDNA

- A complete approach to model physics and chemistry with a simple specification of DNA geometries
- The idea is to quantify direct DNA damage (from physics) and indirect damage (from radicals)



Geometry Definition

- Repeating geometries are used to describe the DNA macro-molecule.



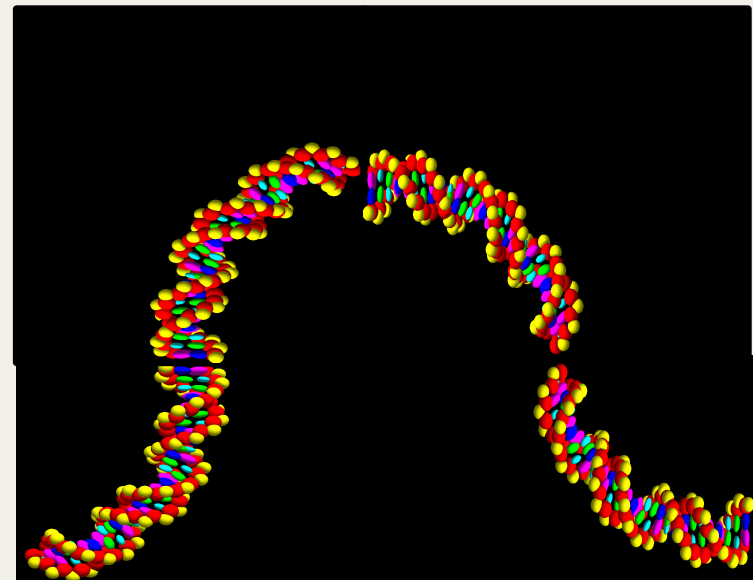
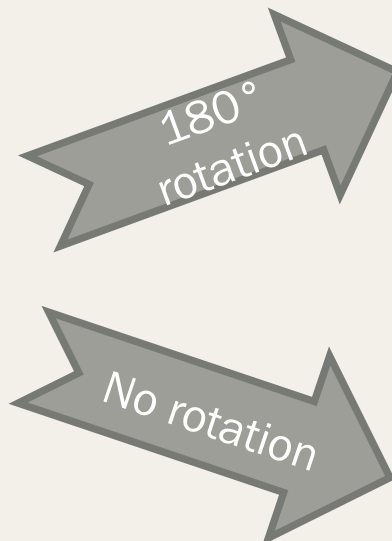
One continuous chain can be made from these two repeating units. Here the DNA is represented atomistically (and turns are exaggerated for clarity)

Geometry Definition

- Two types of files permit the definition of arbitrary geometries.
 - *One file to specify the position of molecules within each placement volume*
 - *One file to specify the position and rotation of each placement volume*
 - *DNA is built based on a molecular representation of the chain*
- One base pair = 2 sugars, 2 phosphates, 2 bases



One file specifies this curved geometry



One file places the curved geometries in the simulation

Implementation

```
34 MolecularDetectorConstruction::MolecularDetectorConstruction():  
35     G4VUserDetectorConstruction()  
36 {  
37     fpDNAGeometry = new MolecularDNAGeometry();  
38 }  
39
```

All DNA geometry classes are contained in and initialised in MolecularDNAGeometry.
Importantly, this activates a number of G4Messengers

```
17 /dnageom/placementSize 50 nm  
18 /dnageom/definitionFile geometries/bacteria-XFXFX-4.txt  
19 /dnageom/placementVolume turn geometries/fourstrands_50nm_turn.txt  
20 /dnageom/placementVolume turntwist geometries/fourstrands_50nm_turn.txt true  
21 /dnageom/placementVolume straight geometries/fourstrands_50nm_straight.txt
```

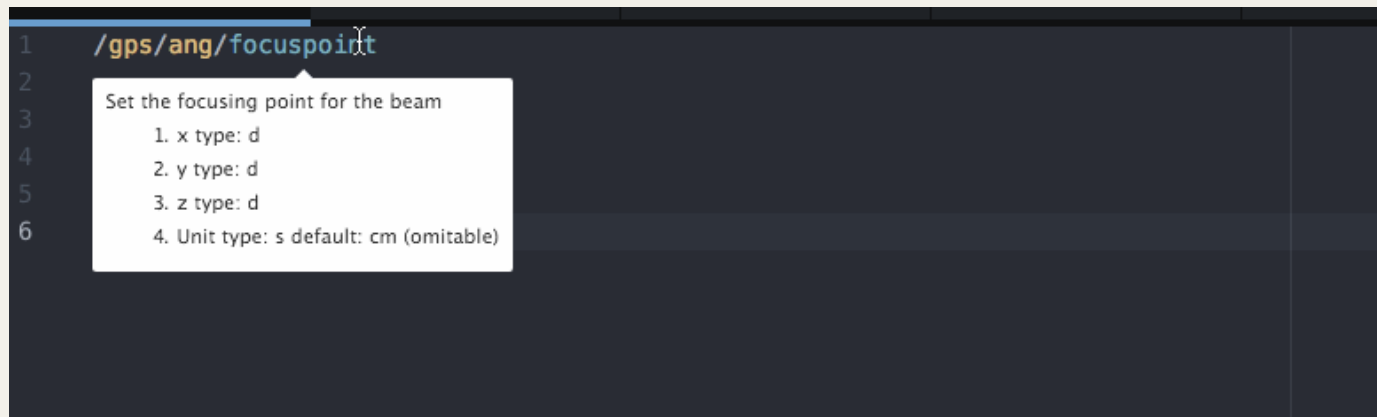
These messengers set the data files for when the DNA is constructed

```
62 G4VPhysicalVolume* MolecularDetectorConstruction::ConstructDetector()  
63 {  
64     // Define world logical and physical volume  
65  
66     this->GetDNAGeometry()->BuildDNA(worldLogical);  
67     return world;  
68 }
```

The DNA is constructed in a logical volume which contains it entirely.

Specialised Run/Event/Stepping Actions handle analysis

- Users of the Atom text editor can access syntax highlighting and auto-completion for G4 macros.
- Want to find out more:
<http://goodfoodgoodcode.com> contains some more explanations of what I do.
- Interested in modelling plasmids/human DNA/other DNA using this approach?
Come speak to me.



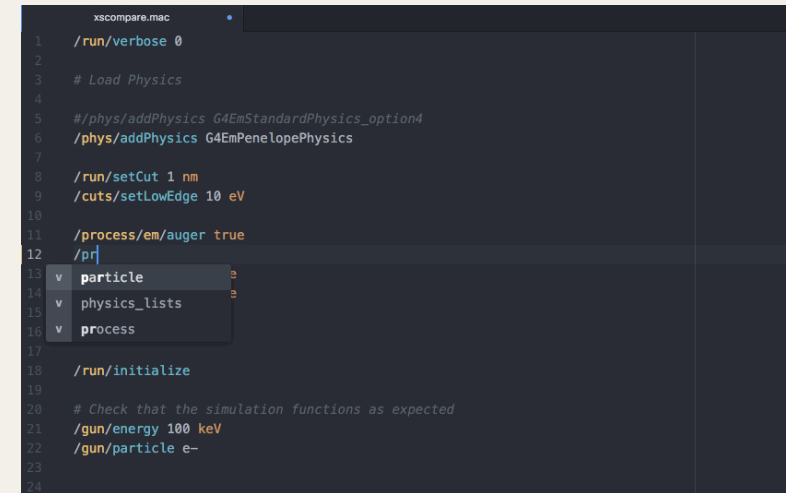
```

1 /gps/ang/focuspoint
2
3
4
5
6

```

Set the focusing point for the beam

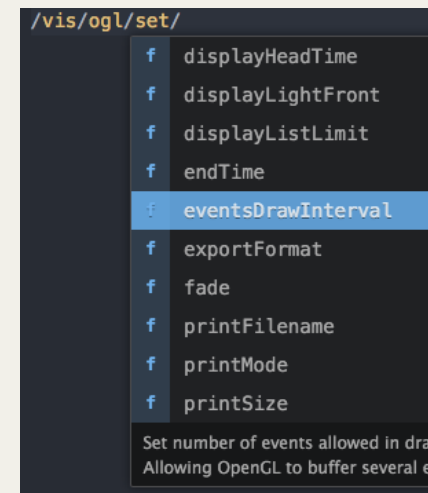
1. x type: d
2. y type: d
3. z type: d
4. Unit type: s default: cm (omitable)



```

xscompare.mac
1 /run/verbose 0
2
3 # Load Physics
4
5 #/phys/addPhysics G4EmStandardPhysics_option4
6 /phys/addPhysics G4EmPenelopePhysics
7
8 /run/setCut 1 nm
9 /cuts/setLowEdge 10 eV
10
11 /process/em/augetrue
12 /pr
13 v particle
14 v physics_lists
15 v process
16
17
18 /run/initialize
19
20 # Check that the simulation functions as expected
21 /gun/energy 100 keV
22 /gun/particle e-
23
24

```



```

/vis/ogl/set/
f displayHeadTime
f displayLightFront
f displayListLimit
f endTime
f eventsDrawInterval
f exportFormat
f fade
f printFilename
f printMode
f printSize

```

Set number of events allowed in draw
Allowing OpenGL to buffer several e

<http://atom.io/packages/language-geant4-macros>



Follow me on Twitter:
@natlampe

PDB4DNA

Sebastien Incerti (CNRS) and Nathanael Lampe (LPC Clermont/CENBG)
based on material provided by
E. Delage and Y. Perrot (LPC Clermont)

National Cancer Center – Oct. 30 – Nov 1st, 2015


Protein Data Bank

<http://www.rcsb.org/>

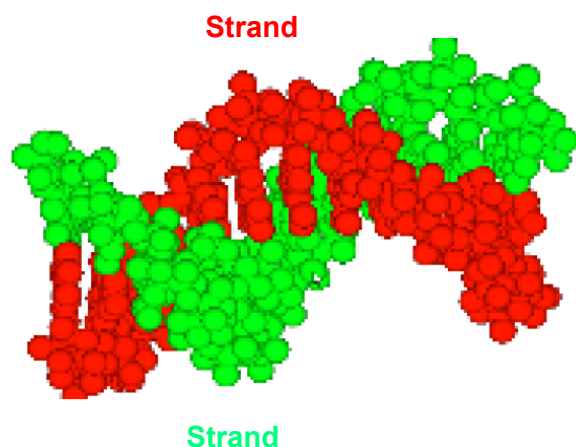
- Protein Data Bank **files**
 - A way to **store and exchange** polyatomic structures (proteins, **DNA**)
 - File describing the **3D structural information** of molecules
 - A **worldwide free access** to files obtained experimentally by crystallography techniques or computed with geometry optimization codes:

- File format
 - ASCII file **‘.pdb’**
 - We mainly extract information from **ATOM** keyword

```
HEADER TRANSFERASE 19-APR-13 4BJP
TITLE CRYSTAL STRUCTURE OF E. COLI PENICILLIN BINDING PROTEIN 3
...
JRNL DOI 10.1371/JOURNAL.PONE.0098042
...
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
...
ATOM 265 C ASP A 149 -38.902 78.078 31.778 C
ATOM 266 O ASP A 149 -39.587 78.804 32.500 O
ATOM 267 CB ASP A 149 -36.407 78.326 31.747 C
...
TER 3106 ALA A 567
...
END
```



10 base pairs: two whole DNA strands



HEADER DNA

...

10BP EXAMPLE

MODEL 1

ATOM 1 O5' A 1 9.256 -9.769 4.573 O

ATOM 2 C5' A 1 10.679 -9.579 4.526 C

...

ATOM 33 OP1 A 2 12.795 -8.381 9.736 O

...

ATOM 65 P A 3 11.850 -2.418 12.300 P

...

ATOM 445 O5' A 10 1.100 5.570 32.583 O

TER 445 A 10

ATOM 446 O5' B 14 -9.356 10.980 33.794 O

...

ATOM 688 C4 B 20 2.805 3.343 8.223 C

TER 688 B 20

ENDMDL

} This file encodes
DNA molecule

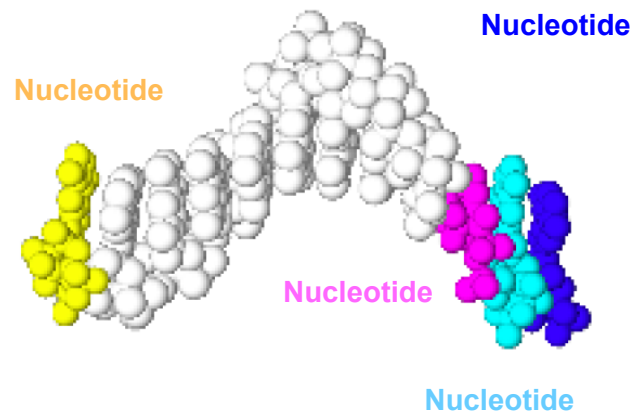
} Start molecule

} Atom coordinates –
first strand (A)

} Atom coordinates –
second strand (B)

} End molecule

10 base pairs: individual **nucleotides**



```
HEADER  DNA                                10BP EXAMPLE
...

MODEL  1

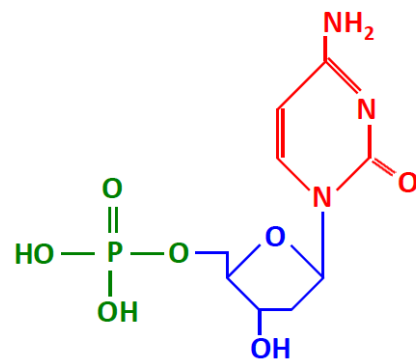
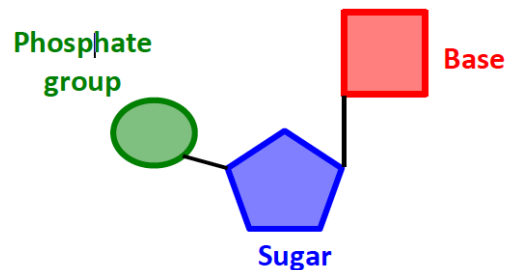
ATOM    1  O5'  A  1  9.256 -9.769  4.573  O
ATOM    2  C5'  A  1 10.679 -9.579  4.526  C
...
ATOM   33  OP1  A  2 12.795 -8.381  9.736  O
...
ATOM   65  P    A  3 11.850 -2.418 12.300  P
...
ATOM  445  O5'  A 10  1.100  5.570 32.583  O
TER      445    A 10

ATOM  446  O5'  B 14 -9.356 10.980 33.794  O
...
ATOM  688  C4   B 20  2.805  3.343  8.223  C
TER      688    B 20

ENDMDL
```

10 base pairs: atomistic content of nucleotides

Nucleotide structure



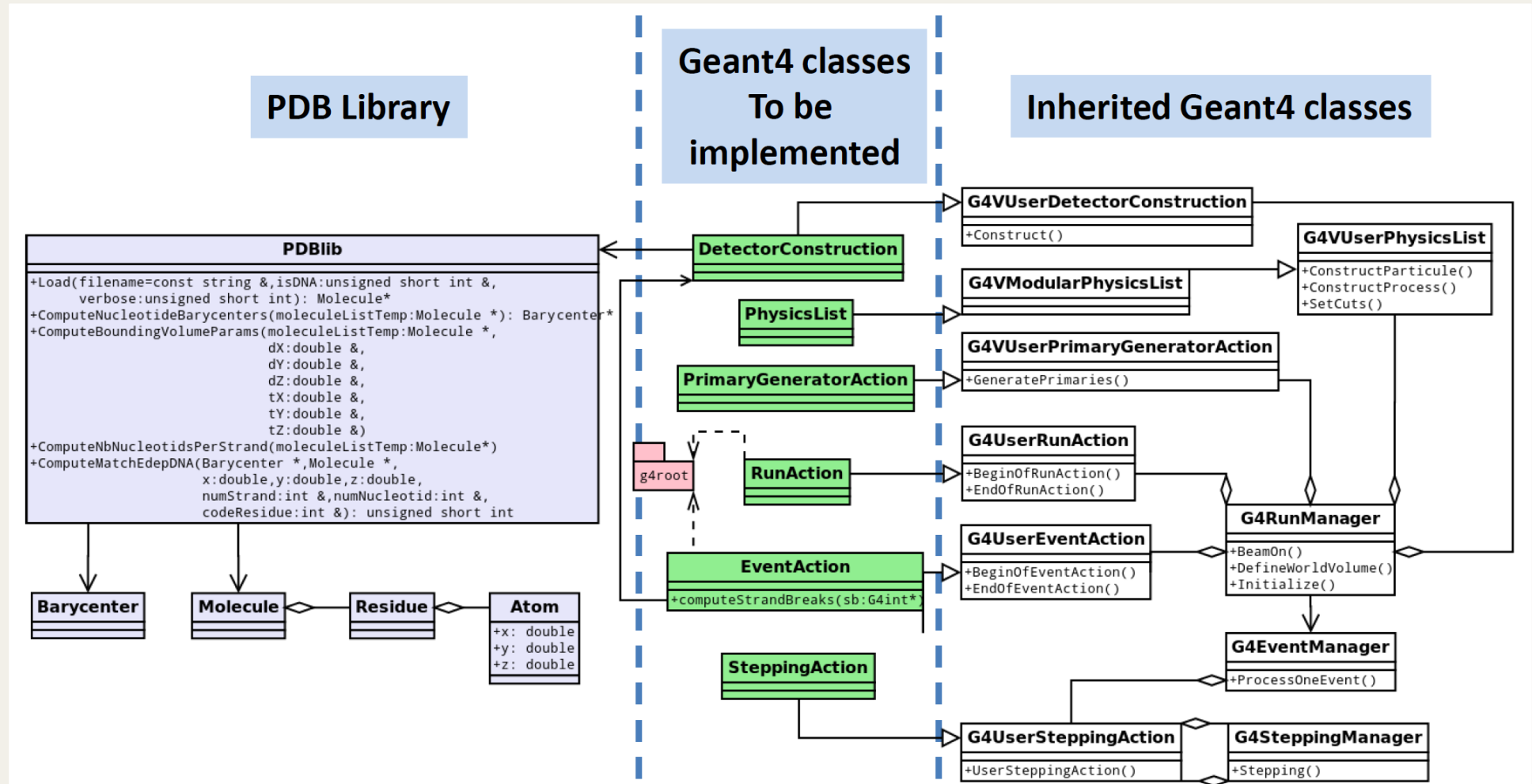
HEADER DNA

10BP EXAMPLE

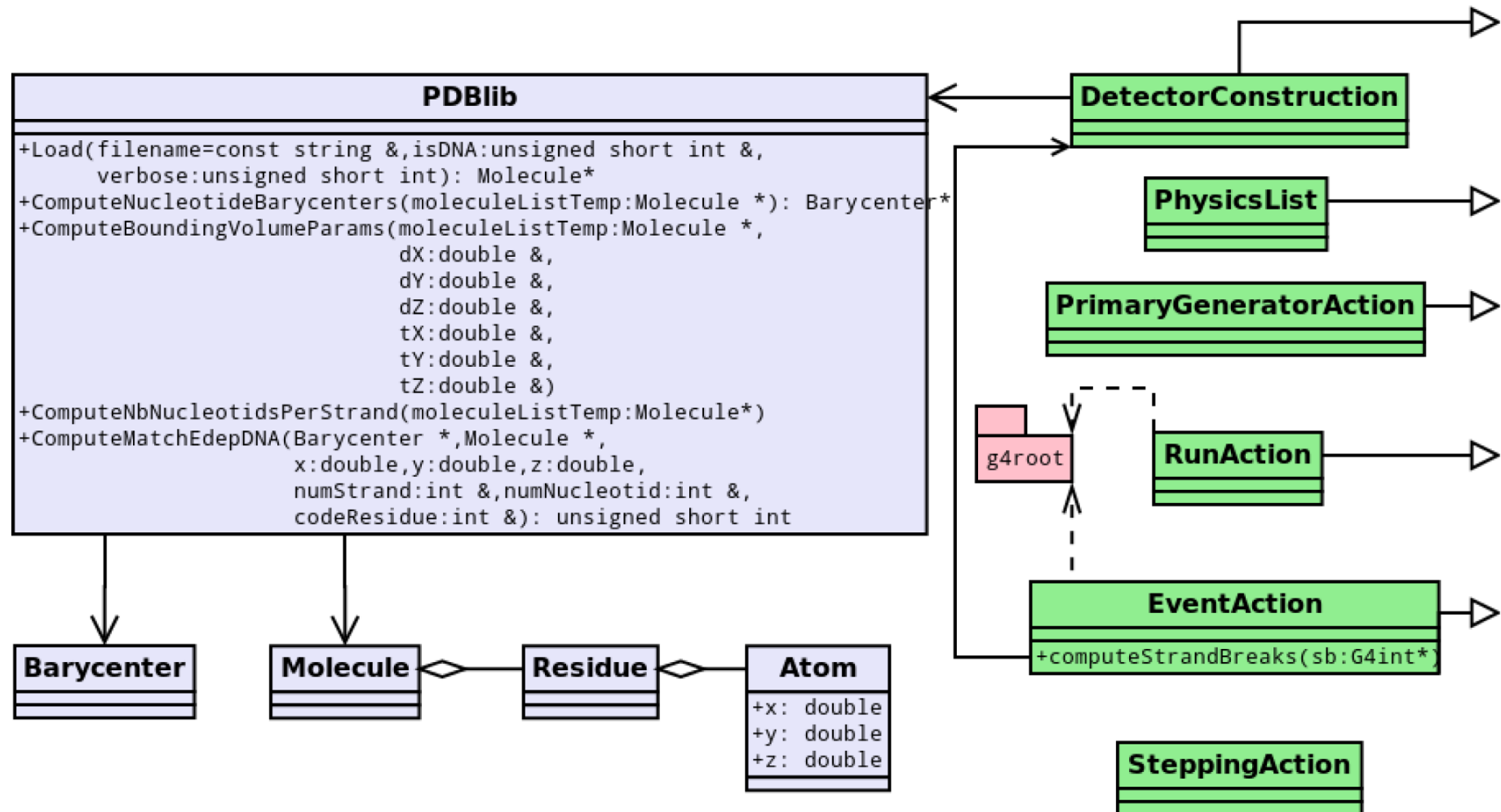
...

ATOM	65	P	DC A	3	11.850	-2.418	12.300	P	} Phosphate group
ATOM	66	OP1	DC A	3	15.242	-2.080	12.670	O	
ATOM	67	OP2	DC A	3	11.107	-3.437	11.073	O	
ATOM	68	O5'	DC A	3	12.981	-1.059	12.299	O	
ATOM	69	C5'	DC A	3	11.563	0.189	11.896	C	} Sugar
ATOM	70	C4'	DC A	3	12.527	1.314	11.875	C	
ATOM	71	O4'	DC A	3	11.455	0.915	11.029	O	
ATOM	72	C3'	DC A	3	11.954	1.427	11.278	C	
ATOM	73	O3'	DC A	3	12.405	2.645	11.894	O	
ATOM	74	C2'	DC A	3	10.453	1.552	11.042	C	
ATOM	75	C1'	DC A	3	10.249	1.499	11.527	C	
ATOM	76	N1	DC A	3	9.058	0.693	11.174	N	} Base
ATOM	77	C2	DC A	3	7.998	1.341	10.557	C	
ATOM	78	O2	DC A	3	8.060	2.547	10.316	O	
ATOM	79	N3	DC A	3	6.897	0.610	10.230	N	
ATOM	80	C4	DC A	3	6.836	-0.699	10.496	C	
ATOM	81	N4	DC A	3	5.745	-1.381	10.158	N	
ATOM	82	C5	DC A	3	7.924	-1.372	11.112	C	
ATOM	83	C6	DC A	3	9.008	-0.643	11.454	C	

Integration into Geant4 (1/2)



Integration into Geant4 (2/2)

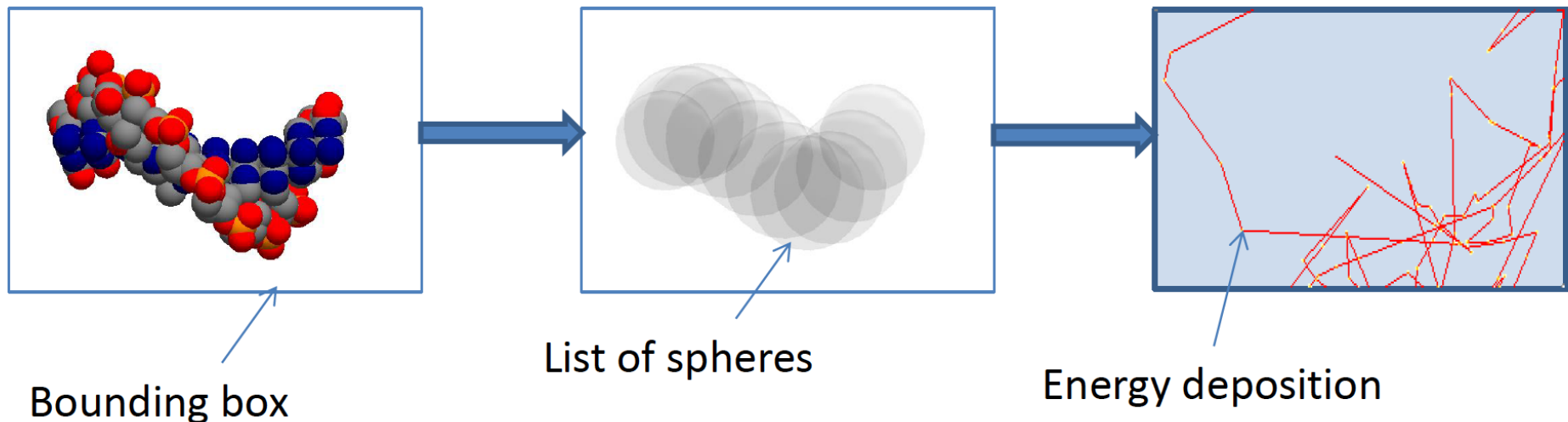


- **DetectorConstruction** call PDBlib to construct molecule geometry
- **EventAction** compute match between Edep and DNA via Detector construction

Algorithm to find the closest atom (1/2)

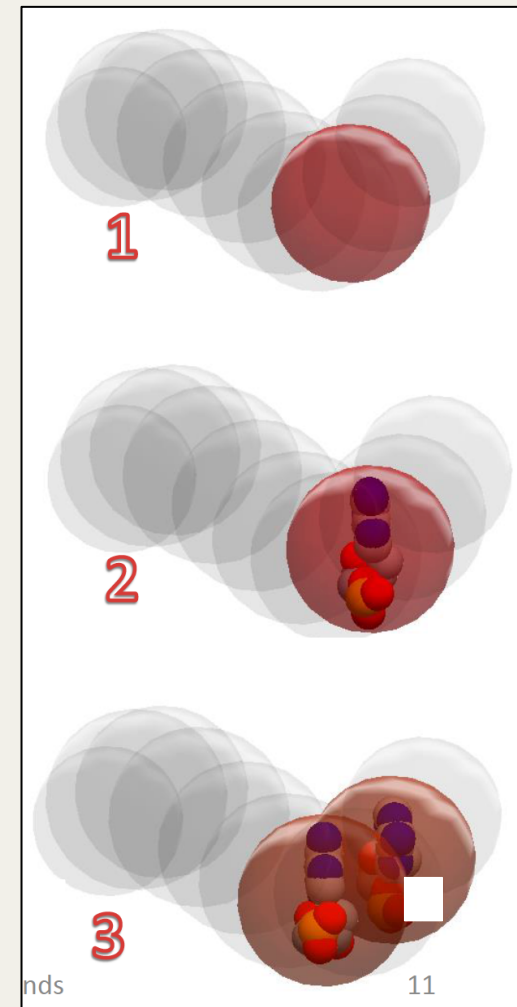
GOAL : allocate energy depositions to a geometrical element [sugar, phosphate, base] of nucleotides and then deduce SSB and DSB

- A bounding box is calculated with atoms coordinates
- No other Geant4 solid is needed for simulation
- We consider that a sphere is a good approximation to englobe a nucleotide. A list of spheres representing nucleotides is calculated
- DNA specific



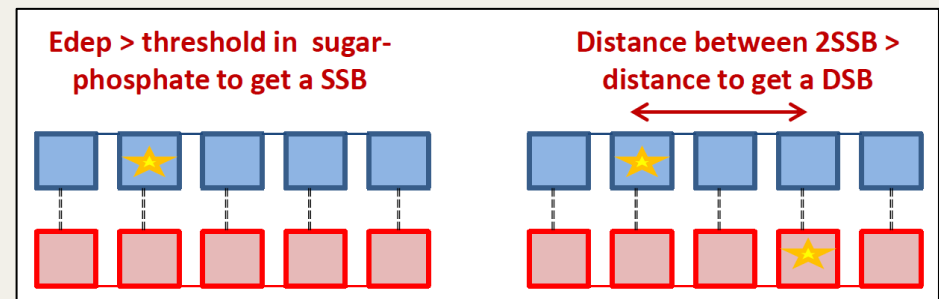
Algorithm to find the closest atom (2/2)

1. Find the **closest nucleotide** from the energy deposition inside the two strands
2. Find the **closest atom** from the energy deposition
 - atom by atom inside the selected nucleotide
 - considering Van der Waals radii
3. Due to sphere overlapping, **find a better match** in the next two nucleotides in the list
4. Return algorithm response:
 - *No DNA hit*
 - *or DNA hit, return **nucleotide ID, DNA strand, group type** (sugar, phosphate or base)*



Strand **breaks**

- Begin of **event**
 - A map for each strand is created to store *nucleotide ID* and *associated energy deposition*
- For each **step**
 - If the step is in the bounding volume, increment energy deposition per event
 - Ask to PDBlib to *check the step position*
- If the step is in a sugar or a phosphate: get nucleotide ID, strand number, energy deposit, *update the map* (ID, Edep+=StepEdep)
- End of **event**
 - Compute and store strand breaks
 - Store energy deposit in the bounding volume



« PDB4DNA » HANDS-ON

Directory content

11 \$G4EXAMPLES/extended/medical/dna/pdb4dna/

```
2266137 Jun 26 12:11 1ZBB.pdb
1380 Jun 26 12:11 analysis.C
2222 Jun 26 12:11 CMakeLists.txt
420 Jun 26 12:11 GNUmakefile
1819 Jun 26 12:11 gui.mac
2197 Jun 26 12:11 History
4096 Jun 29 09:16 include/
201 Jun 26 12:11 init.mac
197 Jun 26 12:11 init_vis.mac
8202 Jun 26 12:11 pdb4dna.cc
341 Jun 26 12:11 pdb4dna.in
11786 Jun 26 12:11 pdb4dna.out
4744 Jun 26 12:11 README
274 Jun 26 12:11 runInGUI.mac
4096 Jun 29 09:16 src/
2722 Jun 26 12:11 vis.mac
```

→ PDB file
→ ROOT macro file
→ Macro to run in batch mode

```
Jun 26 12:11 ActionInitialization.hh
Jun 26 12:11 Analysis.hh
Jun 26 12:11 CommandLineParser.hh
Jun 26 12:11 DetectorConstruction.hh
Jun 26 12:11 DetectorMessenger.hh
Jun 26 12:11 EventAction.hh
Jun 26 12:11 EventActionMessenger.hh
Jun 26 12:11 PDBatom.hh
Jun 26 12:11 PDBbarycenter.hh
Jun 26 12:11 PDBlib.hh
Jun 26 12:11 PDBmolecule.hh
Jun 26 12:11 PDBresidue.hh
Jun 26 12:11 PhysicsList.hh
Jun 26 12:11 PrimaryGeneratorAction.hh
Jun 26 12:11 RunAction.hh
Jun 26 12:11 RunInitObserver.hh
Jun 26 12:11 SteppingAction.hh
```

Compile and link the application

```
cd
```

```
cp -R $G4EXAMPLES/extended/medical/dna/pdb4dna/ .
```

```
mkdir build-pdb4dna
```

```
cd build-pdb4dna
```

```
cmake ../pdb4dna
```

```
make -j2
```

```
localhost.localdomain:/build-pdb4dna < 482 >make -j2
Scanning dependencies of target pdb4dna
[ 5%] [ 11%] Building CXX object CMakeFiles/pdb4dna.dir/pdb4dna.cc.o
Building CXX object CMakeFiles/pdb4dna.dir/src/RunInitObserver.cc.o
[ 17%] Building CXX object CMakeFiles/pdb4dna.dir/src/ActionInitialization.cc.o
[ 23%] Building CXX object CMakeFiles/pdb4dna.dir/src/PDBmolecule.cc.o
[ 29%] Building CXX object CMakeFiles/pdb4dna.dir/src/PDBatom.cc.o
[ 35%] Building CXX object CMakeFiles/pdb4dna.dir/src/CommandLineParser.cc.o
[ 41%] Building CXX object CMakeFiles/pdb4dna.dir/src/PrimaryGeneratorAction.cc.o
[ 47%] Building CXX object CMakeFiles/pdb4dna.dir/src/DetectorMessenger.cc.o
[ 52%] Building CXX object CMakeFiles/pdb4dna.dir/src/SteppingAction.cc.o
[ 58%] Building CXX object CMakeFiles/pdb4dna.dir/src/PhysicsList.cc.o
[ 64%] Building CXX object CMakeFiles/pdb4dna.dir/src/PDBresidue.cc.o
[ 70%] Building CXX object CMakeFiles/pdb4dna.dir/src/RunAction.cc.o
[ 76%] Building CXX object CMakeFiles/pdb4dna.dir/src/PDBbarycenter.cc.o
[ 82%] Building CXX object CMakeFiles/pdb4dna.dir/src/DetectorConstruction.cc.o
[ 88%] Building CXX object CMakeFiles/pdb4dna.dir/src/EventActionMessenger.cc.o
[ 94%] Building CXX object CMakeFiles/pdb4dna.dir/src/EventAction.cc.o
[100%] Building CXX object CMakeFiles/pdb4dna.dir/src/PDBlib.cc.o
Linking CXX executable pdb4dna
[100%] Built target pdb4dna
localhost.localdomain:/build-pdb4dna < 483 >
```

Preparation before run (1/2)

Visit PDB web site

<http://www.rcsb.org>

The screenshot shows the RCSB PDB website homepage. At the top is a dark blue navigation bar with links: Deposit, Search, Visualize, Analyze, Download, Learn, and More. On the right of this bar is a 'MyPDB Login' button. Below the navigation bar is a large banner area. On the left of the banner is the RCSB PDB logo and the text 'An Information Portal to 111241 Biological Macromolecular Structures'. To the right of the logo is a search bar with the placeholder text 'Search by PDB ID, author, macromolecule, sequence, or ligand' and a 'Go' button. Below the search bar are links for 'Advanced Search' and 'Browse by Annotations'. Further down the banner are logos for PDB-101, Worldwide PDB, EMDatabank, and Structural Biology Knowledgebase. On the far right of the banner are social media icons for Facebook, Twitter, YouTube, Apple, and Android. Below the banner is a main content area. On the left is a dark blue sidebar with a 'Welcome' message and icons for Deposit, Search, Visualize, Analyze, Download, and Learn. The main content area has three columns. The first column is titled 'A Structural View of Biology' and contains text about the PDB archive and its use in education and research. The second column is titled '2015 High School Video Challenge Awards' and shows two video thumbnails: 'Battling the Virus' (Judge's Award, First Place) and 'Virus' (Judge's Award, Second Place). The third column is titled 'August Molecule of the Month' and features a 3D molecular model of Tetrahydrobiopterin Biosynthesis, showing three subunits labeled GTPCH, PTPS, and SR. At the bottom right of the main content area is a 'Feedback' link.

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB Login

RCSB PDB An Information Portal to 111241 Biological Macromolecular Structures

Search by PDB ID, author, macromolecule, sequence, or ligand Go

Advanced Search | Browse by Annotations

PDB-101 Worldwide PDB EMDatabank Structural Biology Knowledgebase

Facebook Twitter YouTube Apple Android

Welcome

Deposit Search Visualize Analyze Download Learn

A Structural View of Biology

This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

2015 High School Video Challenge Awards

Battling the Virus
Judge's Award, First Place

Virus
Judge's Award, Second Place

August Molecule of the Month

GTPCH
PTPS
SR

Tetrahydrobiopterin Biosynthesis

Feedback

Preparation before run (2/2)

RCSB PDB Deposit Search Visualize Analyze Download Learn More

PDB An Information Portal to 111241 Biological Macromolecular Structures

Search by PDB ID, author, macromolecule, sequence, etc.

Advanced Search | Browse by Annotations

Search for 1ZBB = dinucleosome

Search for 1ZFX = 12bp of DNA

Summary PDB-101 3D View Sequence Annotations Seq. Similarity 3D Similarity Literature Biol. & Chem. Methods Links

Structure of the 4_601_167 Tetranucleosome

DOI:10.2210/pdb1zbb/pdb NDB ID: PD0639

1ZBB

Display Files Download Files Download Citation

Primary Citation

X-ray structure of a tetranucleosome and its implications for the chromatin fibre.

Schalch, T., Duda, S., Sargent, D.F., Richmond, T.J.

Journal: (2005) Nature **436**: 138-141

PubMed: 16001076

DOI: 10.1038/nature03686

Search Related Articles in PubMed

PubMed Abstract:

DNA in eukaryotic chromosomes is organized in arrays of nucleosomes compacted into chromatin fibres. This higher-order structure of nucleosomes is the substrate for DNA replication, recombination, transcription and repair. Although the structure of the nucleosome core is known at near-atomic... [Read More & Search PubMed Abstracts]

Reference

Molecular Description

Hide

Classification: Structural Protein/dna

Biological Assembly

Download file

- FASTA Sequence
- PDB File (Text)
- PDB File (gz)
- PDBx/mmCIF File
- PDBx/mmCIF File (gz)
- PDBML/XML File
- PDBML/XML File (gz)
- Structure Factor (Text)
- Structure Factor (gz)
- Biological Assembly (gz) (A)

3D View: J More Info

Symmetry: D2

Stoichiometry: Hetero 32-mer - A8B8C8D8

View

Running with GUI

29

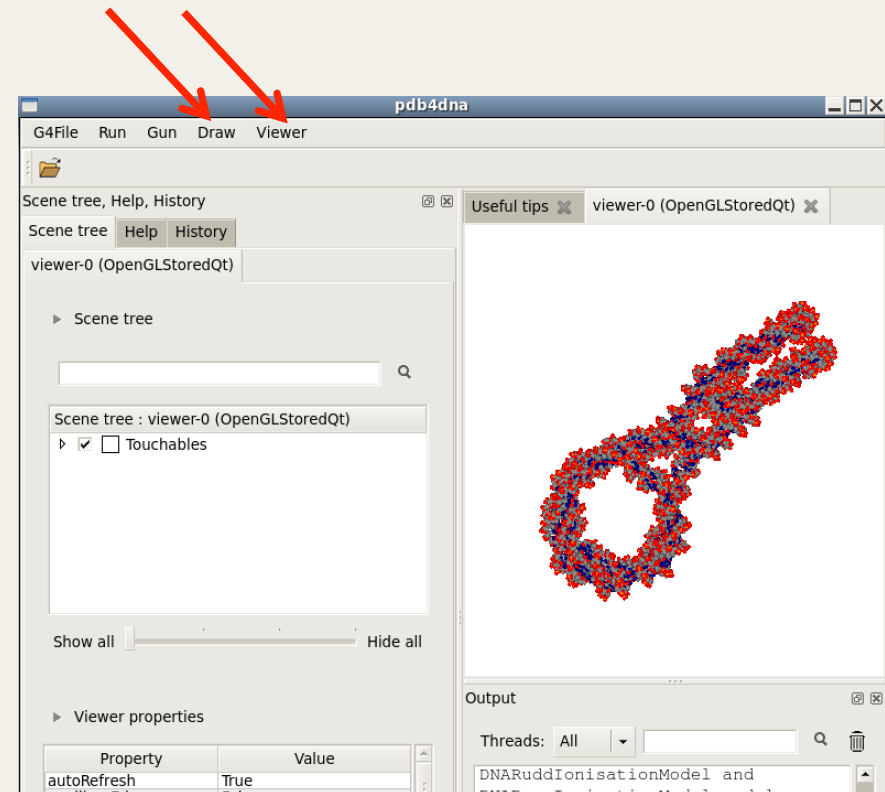
- Rename your PDB file (extension « pdb ») as a macro file (« mac » extension)

```
cp 1ZBB.pdb 1ZBB.mac
```

- Open GUI

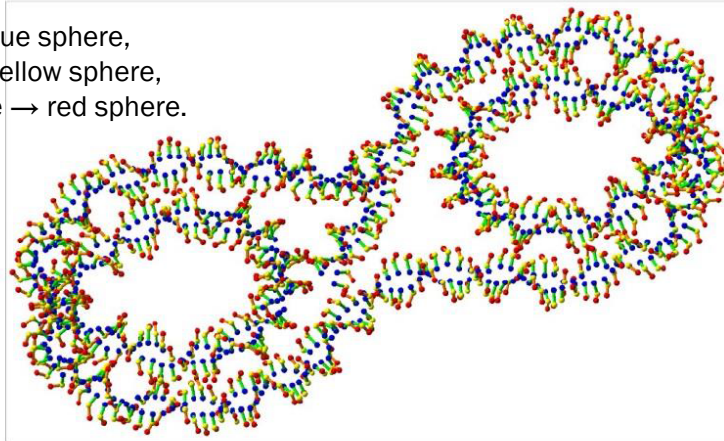
```
./pdb4dna -gui
```

- Open the 1ZBB.mac file
- Click on **Viewer** → **Set style surface**
- Click on **Draw** and try different options...

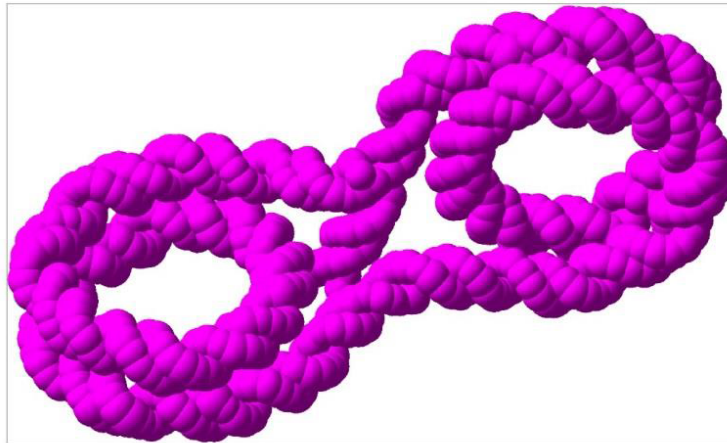


3 visualizations

- Base → blue sphere,
- Sugar → yellow sphere,
- Phosphate → red sphere.



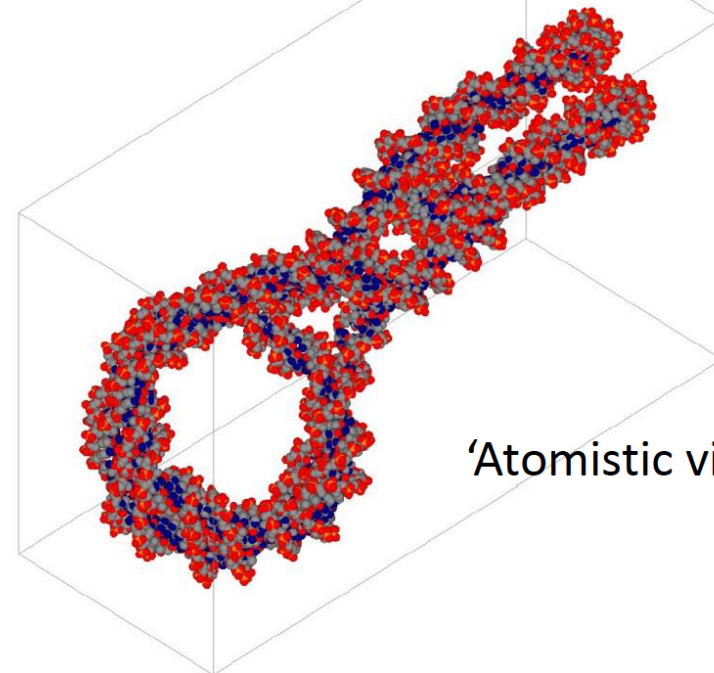
'Residue view'



'Barycenter view'

CPK coloring

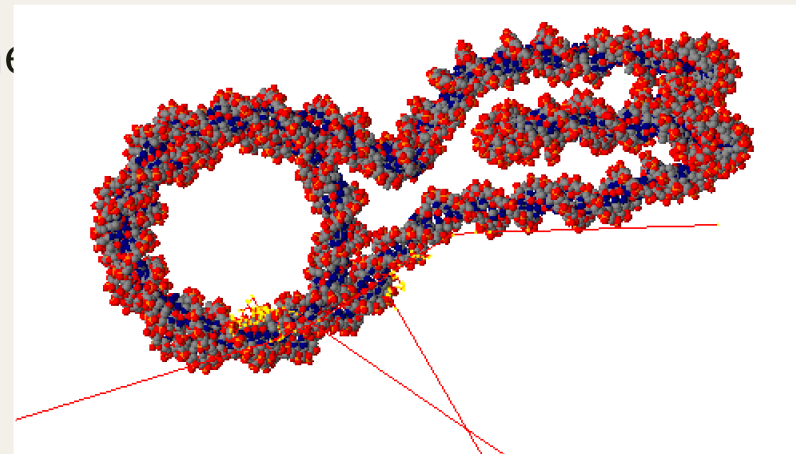
- Hydrogen(H) → white sphere,
- Carbon(C) → gray sphere,
- Oxygen(O) → red sphere,
- Nitrogen(N) → dark blue sphere,
- Sulfur(S) → yellow sphere,
- Phosphorus(P) → orange sphere,
- others/undefined → pink sphere



'Atomistic view'

Running with GUI

- Once you have loaded your PDB file, go to the
/gun/particle e-
/gun/energy 1 keV
/run/initialize
/run/beamOn 1
- Might be a bit slow with visualization
- Nice for visualization, but switch to **batch mode** for energy deposition scoring...



Running in **batch mode** (1/2)

1. Prepare your macro file using an editor (nedit, geany)
 - You can alternatively use pdb4dna.in

```
localhost.localdomain:/build-pdb4dna < 540 >more pdb4dna.in
#/control/execute vis.mac

/run/initialize

/tracking/verbose 0

/PDB4DNA/det/loadPDB 1ZBB.pdb
/PDB4DNA/det/buildBoundingV

/PDB4DNA/event/setEnergyThres 8.22 eV #default value: 8.22 eV
/PDB4DNA/event/setDistanceThres 10    #default value: 10

/gun/particle e-
/gun/energy 100 keV

/run/initialize
/run/printProgress 100
/run/beamOn 10000
localhost.localdomain:/build-pdb4dna < 541 >
```

→ Select your PDB file

→ Construct bounding volume

} Set thresholds for strand breaks: energy, distance

} Primaries

} Run control

Running in batch mode (2/2)

2. Run the simulation

```
./pdb4dna -mac pdb4dna.in -mt 2
```



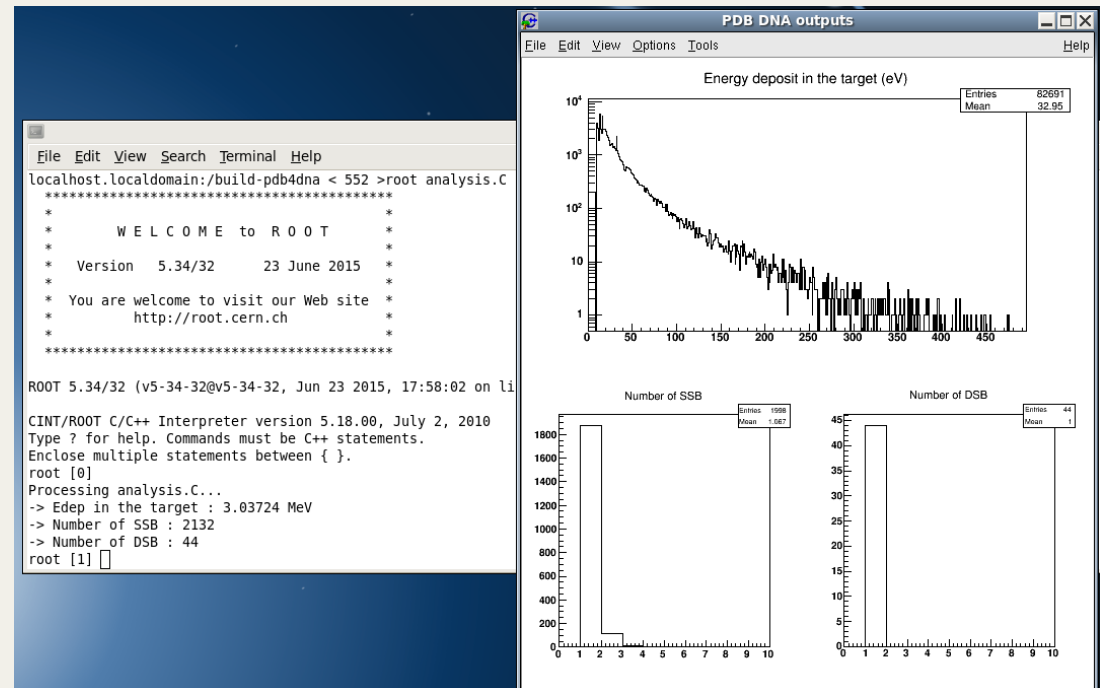
Macro file



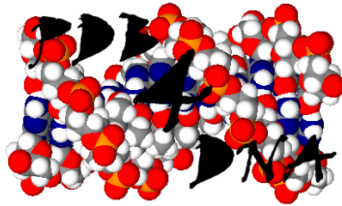

Number of
threads

Analysis of results

- All results are stores in the file `pdb4dna_output.root`
- A ROOT macro file is provided for easy analysis: `3 histograms`
 - For *each event*
- energy deposits in the bounding volume
- # SSB
- # DSB
- Quit Geant4
`Idle> exit`
- Do
`root analysis.C`



Dedicated **web site**



Geant 4

Last update : December 8, 2014
[Examples & tutorials](#) from Geant4-DNA

The **pdb4dna** example can be found in 'extended/medical/dna' Geant4 10.1 example directory.
It simulates energy deposits in a target volume generated from a PDB file representing DNA geometry.
Position of energy deposits are used to compute strand breaks in the DNA geometry.
Geant4-DNA physical processes and models are used.

Authors: Emmanuel Delage, Yann Perrot, Quang Trung Pham.

- **Download** the package [here](#) or preferably with whole Geant4 package,
- [PDB4DNA: Implementation of DNA geometry from the Protein Data Bank \(PDB\) description for Geant4-DNA Monte-Carlo simulations](#) Computer Physics Communications,
- Limitations: this example works only with Geant4.10.0 and later,
- Download whole [Geant4](#) package including pdb4dna.
- License: [Geant4](#).

~~PDBlib~~

HOT SPOT
Geant4 DNA
[tutorial](#)
ESA/ESTEC
November 2014

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LINKS
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