GEANT4-DNA
A SIMULATION TOOLKIT

Hands-on on Geant4-DNA physics

geant4-dna.org

The « dnaphysics » extended example

Batmunkh MUNKHBAATAR

NUM Ulaanbaatar, Mongolia
&
JINR, Dubna, Russia
batmunkh@jinr.ru

Sébastien INCERTI

CNRS / IN2P3, Bordeaux, France
sebastien.incerti@cnrs.fr

Geant4-DNA tutorial
Princess Srisavangavadhana Faculty of Medicine,
Bangkok, Thailand
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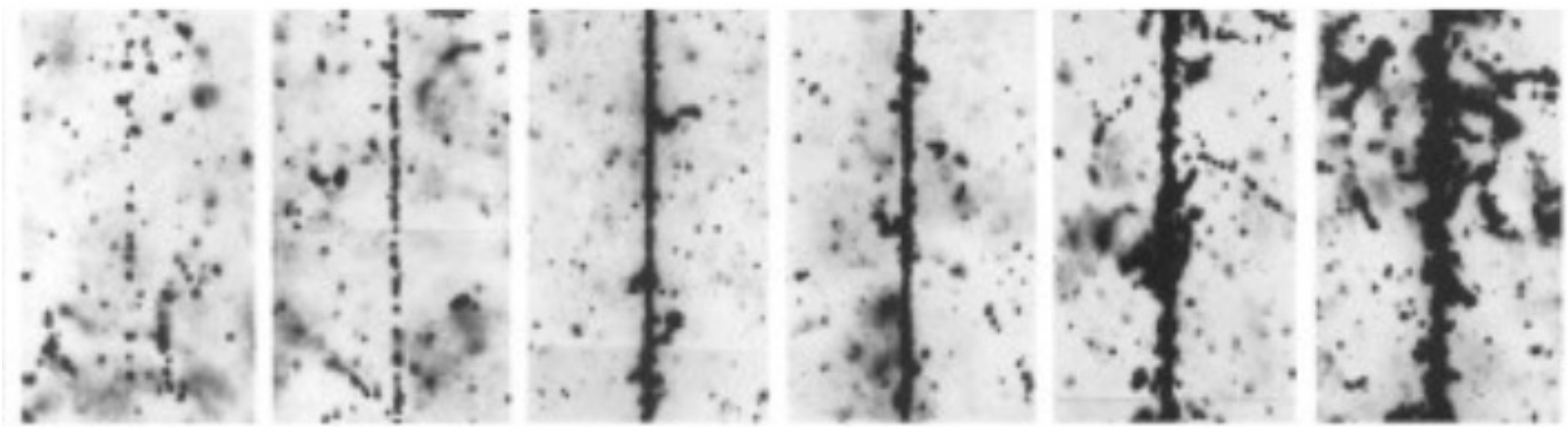
Tracks of charged particles in nuclear emulsion

- Physical information on track structure (spatial distribution of energy deposition, interaction types, etc.) is used in many domains involving ionising radiation
  - microdosimetry, radiation biology, biophysical modeling, clinical radiotherapy, space radiation, environmental science, solid state physics, accelerator design…



H^{1+} He^{2+} C^{6+} O^{8+} Si^{14+} Ca^{20+}

« Study of Elementary Particles by the Photographic Method »
C.F. Powell *et al.* (1959)

The « dnaphysics » extended example

- We are going to try the « **dnaphysics** » extended example which makes use of **Geant4-DNA Physics processes and models**
  - This is the « **simplest** » Geant4–DNA example

- This is a Geant4 « extended » example and it is located in

  `$G4INSTALL/examples/extended/medical/dna`

- Remember that all Geant4-DNA **extended & advanced** examples are listed at:

  http://geant4-dna.org

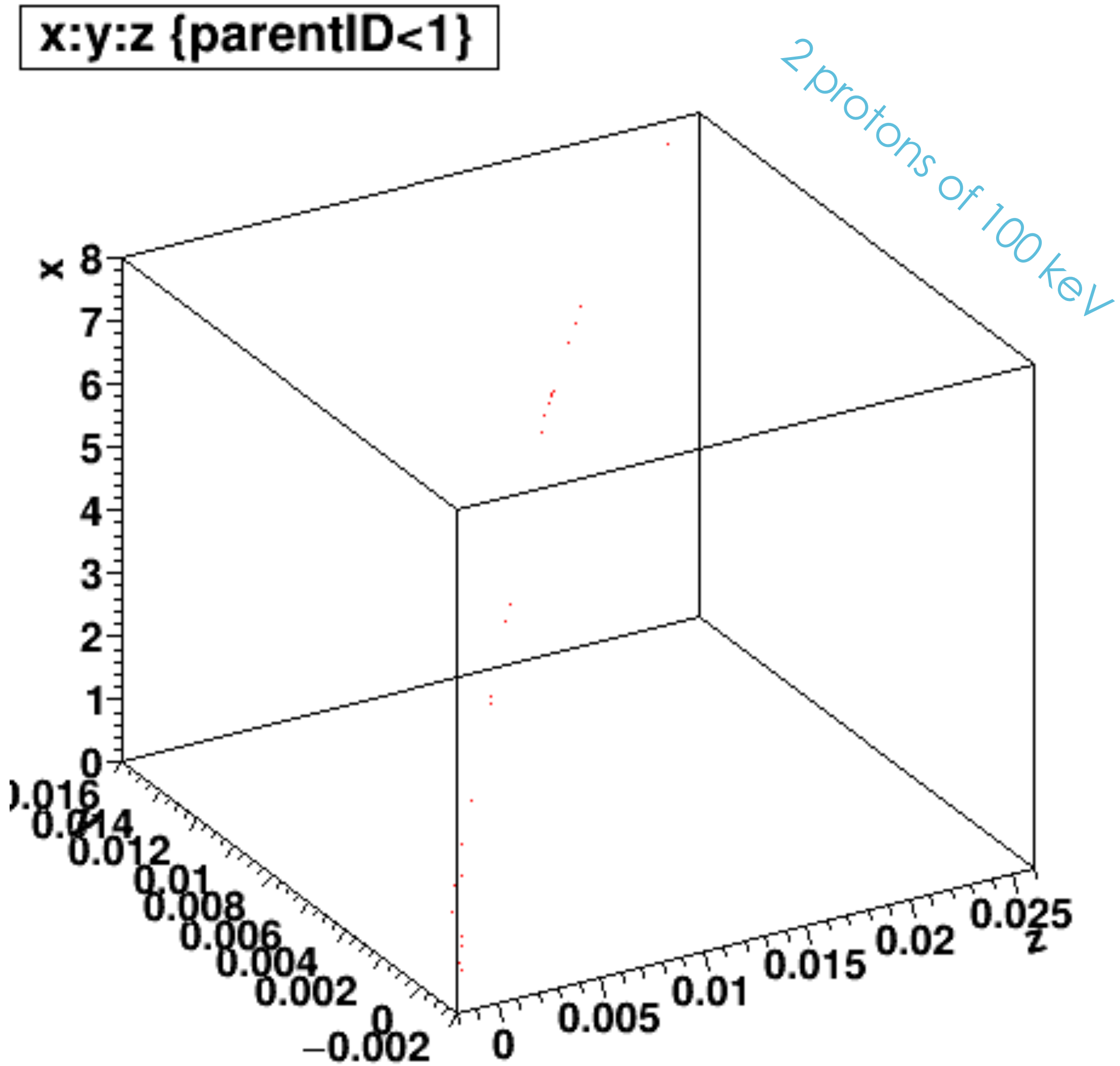
  https://geant4-userdoc.web.cern.ch/Doxygen/examples_doc/html/Examples_dna.html

  https://geant4.web.cern.ch/docs/advanced_examples_doc/

The « dnaphysics » extended example

- Users can simulate experimentally-observed 3D **track structure** of different particles

- They can learn how to **extract all physics information** from this track structure, for example:
  - Type of **particle**
  - Type of **physics process** at each step
  - **Coordinates** in space
  - Energy **deposit**
  - **Step length** and number
  - **Kinetic energy**
  - **Scattering angle**
  - ID of **event**, **track**, **parent track**
  - …



The « dnaphysics » extended example

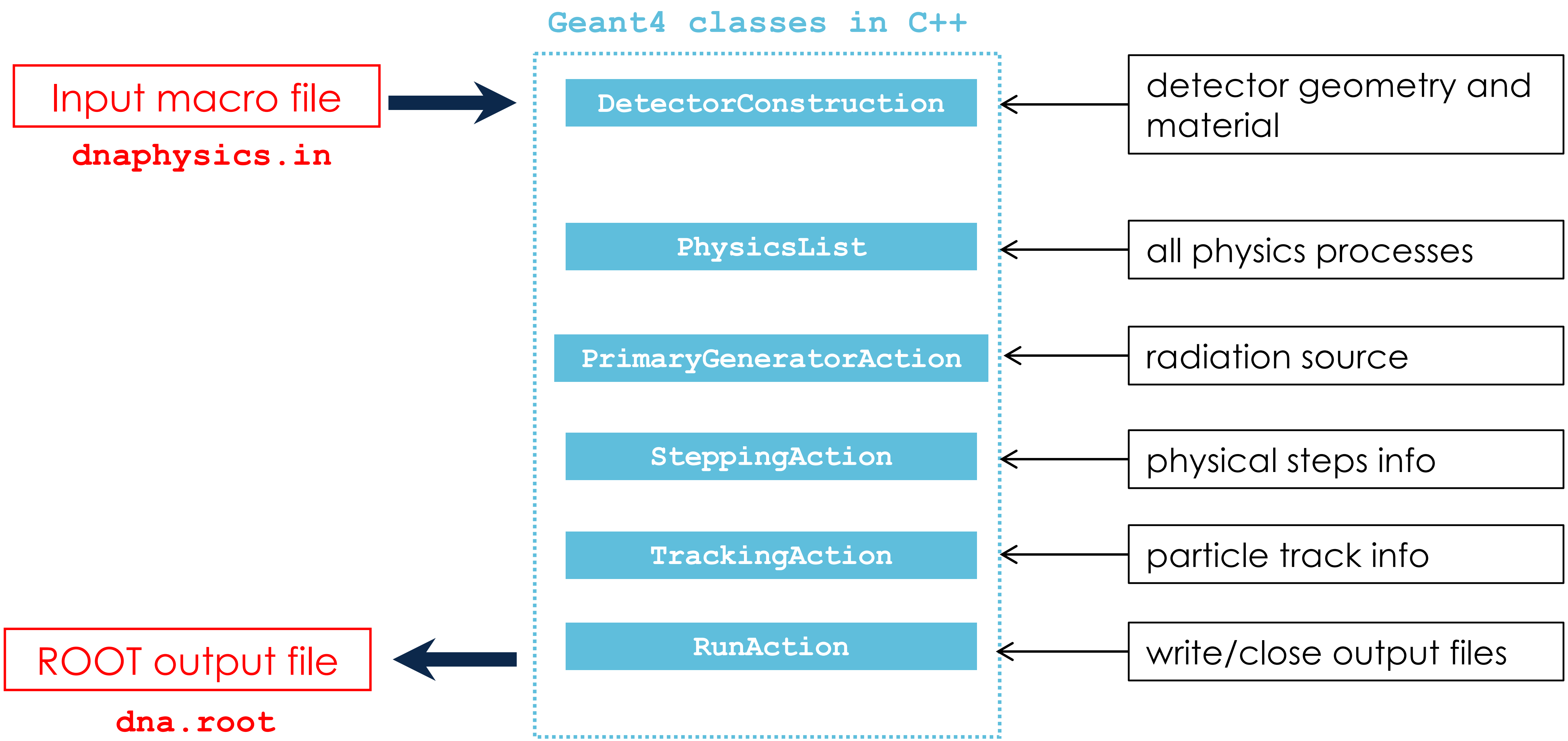
- This example aims to demonstrate how to **use the Geant4-DNA physics processes and models in a liquid water volume**
  - All particle interactions are simulated on a **step-by-step basis** (« **discrete** » processes)
    - No « condensed history » approximation
  - The PhysicsList class uses the **Geant4-DNA Physics constructor** called **`G4EmDNAPhysics_option2`**, so you do not need to code the physics yourself
    - You can easily switch from one constructor to another (e.g. **`option4`**, **`option6`**)

- It also explains how to **easily change the density of the target material** (liquid water): this is the « **variable density material** » feature of Geant4
  - Users can investigate density change effects
    - E.g. 1.06 g/cm3 average density of cell nucleus (cf. PARTRAC code)

- Produces a **ROOT ntuple** to analyze & visualize track structures

https://root.cern

Structure of the « dnaphysics » extended example



« dnaphysics » extended example: input macro commands (UI)

dnaphysics.in

```
# Verbosity
/tracking/verbose 0
/run/verbose 2
/control/verbose 2
#
# MT
/run/numberOfThreads 2
#
# Material
/dna/test/setMat G4_WATER
# or alternatively
#/dna/test/setMatDens G4_WATER_MODIFIED 1.200 g/cm3
#
# Size of World volume
/dna/test/setSize 100 um
#
# Atomic deexcitation
/process/em/fluo true
/process/em/auger true
/process/em/augerCascade true
/process/em/deexcitationIgnoreCut true
#
# Physics
# - To use Geant4-DNA constructor X, X=0, 2, 4, or 6 (recommended)
#/dna/test/addPhysics DNA_Opt0
/dna/test/addPhysics DNA_Opt2
#/dna/test/addPhysics DNA_Opt4
#/dna/test/addPhysics DNA_Opt6
#
# - To add radioactive radioactive decay
/dna/test/addPhysics raddecay
#
# Heavy ions tracking cut
#/dna/test/addIonsTrackingCut false
#
# Run initialization
/run/initialize
#
# Visualization
#/control/execute vis.mac
#
# Incident particle type
#/gun/particle e-
/gun/particle proton
#/gun/particle hydrogen
#/gun/particle alpha
#/gun/particle alpha+
#/gun/particle helium
#/gun/particle ion
#/gun/ion 14 28
#
# Incident particle energy
/gun/energy 100 keV
#
# Beam on
/run/beamOn 2
```

- Verbosity commands → Control of verbosity
- MT commands → Select number of threads
- Material commands → Select the target material
- Size of World volume commands → Set World size
- Atomic deexcitation commands → Activate fluorescence, Auger electron production and Auger cascade, without production cuts
- Physics commands → Select Geant4-DNA Physics constructor
- Radioactive decay commands → Add radioactive decay physics
- Heavy ions tracking cut commands → Tracking cut for heavy ions
- Visualization commands → Activate visualization
- Incident particle type commands → Choose incident particle
- Incident particle energy commands → Set incident particle energy
- Beam on commands → Shoot particles

« dnaphysics » extended example: DetectorConstruction class

- Detector material:
  - The « World » volume contains liquid water, defined as « **G4_WATER** » (= Geant4 NIST material* for liquid water). Density is 1 g/cm3

```
// Water is defined from NIST material database
G4NistManager * man = G4NistManager::Instance();

G4Material * H2O = man->FindOrBuildMaterial("G4_WATER");

/*
 If one wishes to test other density value for water material,
 one should use instead:
 G4Material * H2O = man->BuildMaterialWithNewDensity("G4_WATER_MODIFIED",
 "G4_WATER",1.100*g/cm3);
```

See source file
dnaphysics/src/DetectorConstruction.cc

Users can **change density** value here (**C++**) or in **dnaphysics.in** (**UI**)

* See https://geant4-userdoc.web.cern.ch/UsersGuides/ForApplicationDeveloper/html/Appendix/materialNames.html

« dnaphysics » extended example: DetectorConstruction class

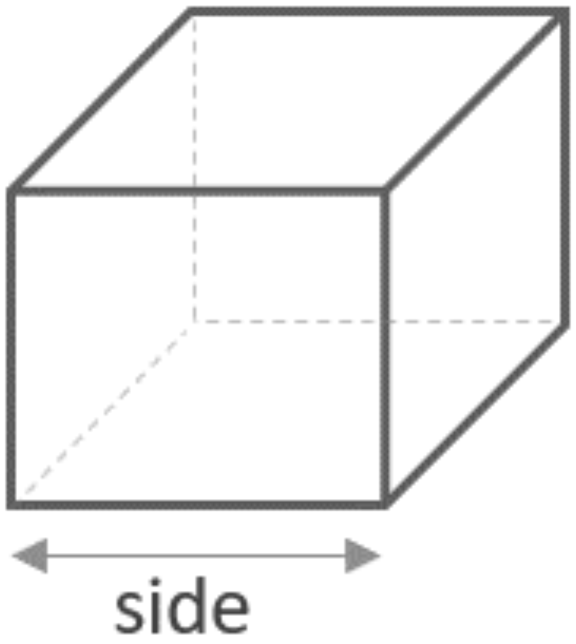
- Detector geometry:
  - The « World » volume is a cube (side size is 100 micrometer, see constructor)

```
// World volume
G4double worldSizeX = fWorldSize;
G4double worldSizeY = worldSizeX;
G4double worldSizeZ = worldSizeX;

G4Box* solidWorld = new G4Box("World",  // its name
                              worldSizeX / 2, worldSizeY / 2, worldSizeZ / 2);
                              // its size

fLogicWorld = new G4LogicalVolume(solidWorld,  // its solid
                                  fpWaterMaterial,  // its material
                                  "World");  // its name

fPhysiWorld = new G4PVPlacement(0,  // no rotation
                                G4ThreeVector(),  // at (0,0,0)
                                "World",  // its name
                                fLogicWorld,  // its logical volume
                                0,  // its mother volume
                                false,  // no boolean operation
                                0);  // copy number
```



See source file
`dnaphysics/src/DetectorConstruction.cc`

« dnaphysics » extended example: PhysicsList class

- Physics constructor and cut-off parameters:
  - The PhysicsList class uses the default `G4EmDNAPhysics_option2` Physics constructor

G4EmDNAPhysics_option2 constructor

```
PhysicsList::PhysicsList() : G4VModularPhysicsList()
{
  SetDefaultCutValue(1.0 * micrometer);
  SetVerboseLevel(1);

  fEmPhysics = "DNA_Opt2";
  fEmPhysicsList = new G4EmDNAPhysics_option2();
  fDecayPhysicsList = new G4DecayPhysics();

  G4ProductionCutsTable::GetProductionCutsTable()->SetEnergyRange(100 * eV, 1 * GeV);
  G4EmParameters* param = G4EmParameters::Instance();
  param->SetMinEnergy(100 * eV);
  param->SetMaxEnergy(1 * GeV);
}
```

See source file `dnaphysics/src/PhysicsList.cc`

Note

- For energies above than the maximum energy covered by Geant4-DNA models, Geant4 standard electromagnetic models are used

« dnaphysics » extended example: PrimaryGeneratorAction class

- Radiation source:
  - This class describes the source of incident particles:
    - type, kinetic energy, position, angular distribution…

```
#include "PrimaryGeneratorAction.hh"

//....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo...

PrimaryGeneratorAction::PrimaryGeneratorAction()
 : G4VUserPrimaryGeneratorAction(),
   fpParticleGun(0)
{
  G4int n_particle = 1;
  fpParticleGun  = new G4ParticleGun(n_particle);
}
```

See source file
`dnaphysics/src/PrimaryGeneratorAction.cc`

The macro file (`dnaphysics.in`) contains UI* commands:

```
/gun/particle proton
/gun/energy 100 keV
/gun/position 0 0 0 um
/gun/direction 0 0 1
/run/beamOn 1
```

* See e.g. http://www.hep.ph.ic.ac.uk/~yoshiu/COMET/comet_g4HTMLdoc/_gun_.html

« dnaphysics » extended example: SteppingAction class

- Physical steps of particle track:
  - This class records useful information about each physical interaction: particle type, kinetic energy, position, energy deposition, etc.

```
if (partDef == G4Electron::ElectronDefinition())
   flagParticle = 1;
```

Users can flag a particle

```
G4int procID = postStep->GetProcessDefinedStep()->GetProcessSubType();
```

```
else if (flagParticle == 1) {
  if (procID == 58)
    flagProcess = 10;
```

Users can flag a process (see **README** for numbering)

(Note: string comparison of process name is possible but is not recommended)

G4AnalysisManager

```
G4AnalysisManager* analysisManager = G4AnalysisManager::Instance();

// fill ntuple
analysisManager->FillNtupleDColumn(0, flagParticle);
analysisManager->FillNtupleDColumn(1, flagProcess);
analysisManager->FillNtupleDColumn(2, xp);
analysisManager->FillNtupleDColumn(3, yp);
analysisManager->FillNtupleDColumn(4, zp);
analysisManager->FillNtupleDColumn(5, step->GetTotalEnergyDeposit() / eV);
```

Users can extract step information about primary/secondary particles, process, position of energy depositions… and fill ROOT ntuple(s) or histograms with such information

« dnaphysics » extended example: TrackingAction class

- Physical properties of particle track:
  - This class records useful information about each physical track

G4AnalysisManager

```
// Call analysis manager
G4AnalysisManager* analysisManager = G4AnalysisManager::Instance();

// Fill track information ntuple
analysisManager->FillNtupleDColumn(1, 0, flagParticle);
analysisManager->FillNtupleDColumn(1, 1, x);
analysisManager->FillNtupleDColumn(1, 2, y);
analysisManager->FillNtupleDColumn(1, 3, z);
analysisManager->FillNtupleDColumn(1, 4, dirx);
analysisManager->FillNtupleDColumn(1, 5, diry);
analysisManager->FillNtupleDColumn(1, 6, dirz);
analysisManager->FillNtupleDColumn(1, 7, aTrack->GetKineticEnergy() / eV);
analysisManager->FillNtupleIColumn(1, 8, aTrack->GetTrackID());
analysisManager->FillNtupleIColumn(1, 9, aTrack->GetParentID());
analysisManager->AddNtupleRow(1);
```

Users can extract track information such as: type of particle for the current track, track position, momentum direction, kinetic energy, ID and parent track ID

« dnaphysics » extended example: RunAction class

- Write and close simulation results:
  - This class is used to create ROOT ntuple(s) and histograms, and to save them in a ROOT file (`dna.root`) at the end of the run
  - The singleton `G4AnalysisManager` is the entity in charge of collecting and accumulating and saving all information

G4AnalysisManager

```
void RunAction::EndOfRunAction(const G4Run* aRun)
{
  G4int nofEvents = aRun->GetNumberOfEvent();
  if (nofEvents == 0) return;

  // Print histogram statistics
  auto analysisManager = G4AnalysisManager::Instance();

  // Save histograms
  analysisManager->Write();
  analysisManager->CloseFile();
}
```

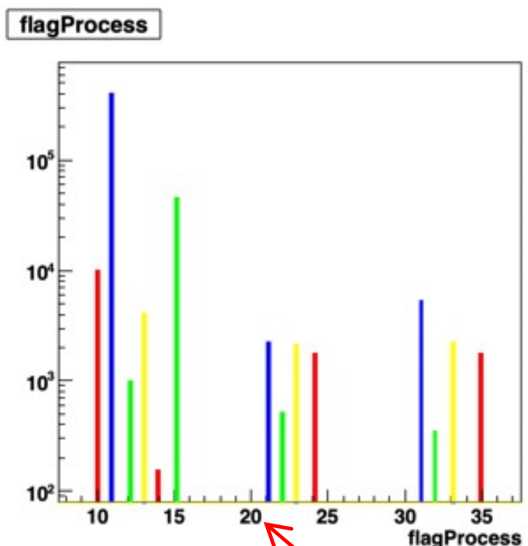
Note
- Save histograms in method `EndOfRunAction()`
- In MT mode, each thread creates and fills a local ROOT file; all files are then merged automatically at the end of the simulation

* See e.g. https://root.cern.ch

« dnaphysics » extended example: output

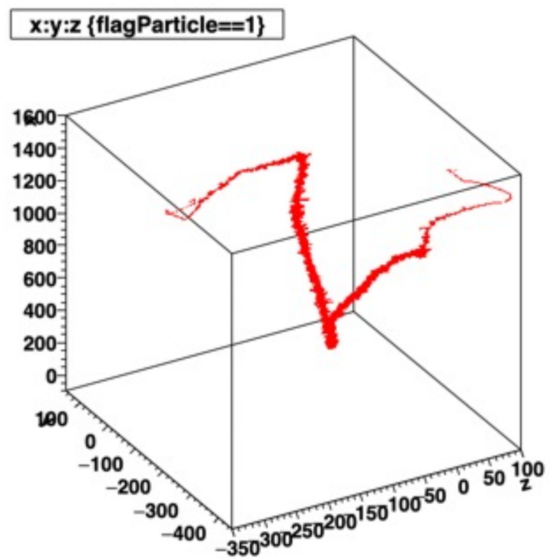
- Results are saved in the `dna.root` file and can be analyzed using ROOT*
  - Type `root plot.C`

Number of occurences of physical processes	3D visualization of 2 proton tracks	Occurring processes along x-axis	Energy distribution of electrons

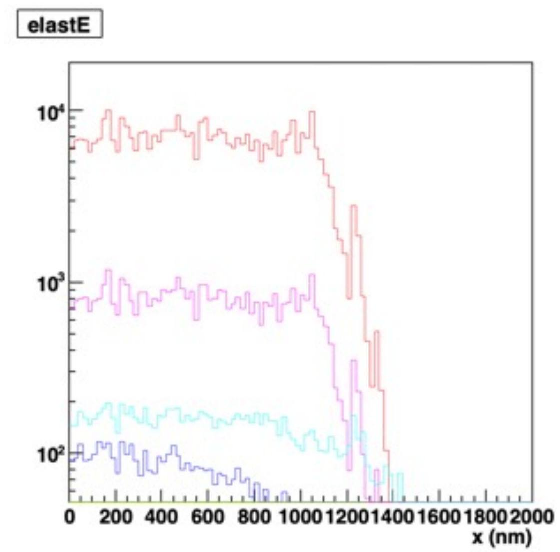


(See `README` for process numbers)

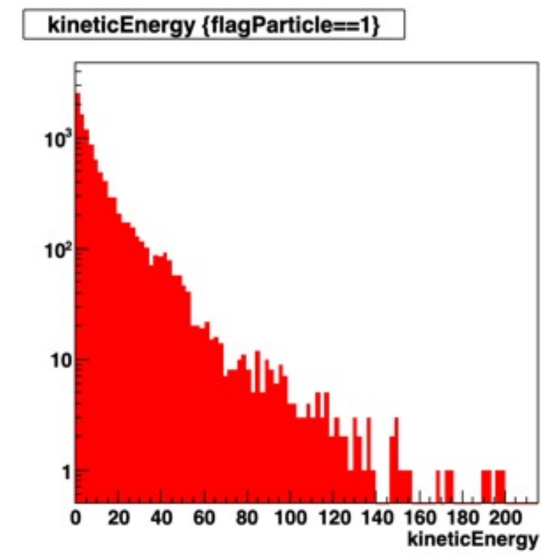
```
proton_G4DNAElastic: 21
proton_G4DNAExcitation: 22
proton_G4DNAIonisation: 23
proton_G4DNAChargeDecrease: 24
```



2 protons
(100 keV)



Elastic
Vib. excitation
Solvation
Ionisation
...



Note: We also provide the `deexcitation.in` and `plotDeexcitation.C` macros to illustrate atomic deexcitation (fluorescence photons and Auger electrons)

Hands-on practice with the « dnaphysics » extended example

GEANT4-DNA

Hands-on practice with the « dnaphysics » extended example

- **Copy** the dnaphysics extended example to your local directory, **create** your build directory and **compile** dnaphysics

```
cd
cp -r $G4EXAMPLES/extended/medical/dna/dnaphysics .
cd dnaphysics
mkdir build-dnaphysics
cd build-dnaphysics
cmake ../
make
```

or `make -jN` if you have N cores

```
localhost.localdomain:/build-dnaphysics < 80 >make -j2
[ 22%] Building CXX object CMakeFiles/dnaphysics.dir/src/ActionInitialization.cc.o
[ 22%] Building CXX object CMakeFiles/dnaphysics.dir/dnaphysics.cc.o
[ 33%] Building CXX object CMakeFiles/dnaphysics.dir/src/DetectorConstruction.cc.o
[ 44%] Building CXX object CMakeFiles/dnaphysics.dir/src/DetectorMessenger.cc.o
[ 55%] Building CXX object CMakeFiles/dnaphysics.dir/src/PhysicsList.cc.o
[ 66%] Building CXX object CMakeFiles/dnaphysics.dir/src/PrimaryGeneratorAction.cc.o
[ 77%] Building CXX object CMakeFiles/dnaphysics.dir/src/RunAction.cc.o
[ 88%] Building CXX object CMakeFiles/dnaphysics.dir/src/SteppingAction.cc.o
[100%] Linking CXX executable dnaphysics
[100%] Built target dnaphysics
```

Hands-on practice with the « dnaphysics » extended example

- **Run** dnaphysics using the provided macro file:

  `./dnaphysics dnaphysics.in`

```
# Verbosity
/tracking/verbose 0
/run/verbose 2
/control/verbose 2
#
# MT
/run/numberOfThreads 2
#
# Material
/dna/test/setMat G4_WATER
# or alternatively
#/dna/test/setMatDens G4_WATER_MODIFIED 1.200 g/cm3
#
# Size of World volume
/dna/test/setSize 100 um
#
# Atomic deexcitation
/process/em/fluo true
/process/em/auger true
/process/em/augerCascade true
/process/em/deexcitationIgnoreCut true
#
# Physics
# - To use Geant4-DNA constructor X, X=0, 2, 4, or 6 (recommended)
#/dna/test/addPhysics DNA_Opt0
/dna/test/addPhysics DNA_Opt2
#/dna/test/addPhysics DNA_Opt4
#/dna/test/addPhysics DNA_Opt6
#
# - To add radioactive radioactive decay
/dna/test/addPhysics raddecay
#
# Heavy ions tracking cut
#/dna/test/addIonsTrackingCut false
#
# Run initialization
/run/initialize
#
# Visualization
#/control/execute vis.mac
#
# Incident particle type
#/gun/particle e-
/gun/particle proton
#/gun/particle hydrogen
#/gun/particle alpha
#/gun/particle alpha+
#/gun/particle helium
#/gun/particle ion
#/gun/ion 14 28
#
# Incident particle energy
/gun/energy 100 keV
#
# Beam on
/run/beamOn 2
```

Geant4-DNA physics option 2

Incident particle is proton

2 protons of 100 keV are shot

Hands-on practice with the « dnaphysics » extended example

- Results are saved in `dna.root` and can be analyzed using ROOT (`plot.C`)

`root plot.C`

```
// All
ntuple->SetFillStyle(1001);
ntuple->SetFillColor(2);
ntuple->Draw("flagProcess","","B");

// Excitation
ntuple->SetFillStyle(1001);
ntuple->SetFillColor(3);
ntuple->Draw("flagProcess","flagProcess==12||flagProcess==15||flagProcess==22|

// Elastic
ntuple->SetFillStyle(1001);
ntuple->SetFillColor(4);
ntuple->Draw("flagProcess","flagProcess==11||flagProcess==21||flagProcess==31|

// Ionisation
ntuple->SetFillStyle(1001);
ntuple->SetFillColor(5);
ntuple->Draw("flagProcess","flagProcess==13||flagProcess==23||flagProcess==33|
```

← Plot occurring physical processes

e-_G4DNAElectronSolvation	10
e-_G4DNAElastic	11
e-_G4DNAExcitation	12
e-_G4DNAIonisation	13
e-_G4DNAAttachment	14
e-_G4DNAVibExcitation	15
proton_G4DNAElastic	21
proton_G4DNAExcitation	22
proton_G4DNAIonisation	23
proton_G4DNAChargeDecrease	24

(See `README` for process numbers)

```
c1->cd(2);

ntuple->SetMarkerColor(2);

ntuple->Draw("x:y:z","flagParticle==1");

//ntuple->SetMarkerColor(4);
//ntuple->SetMarkerSize(4);
//ntuple->Draw("x:y:z/1000","flagParticle==4 || flagParticle==5 || flagParticle==6","same");
```

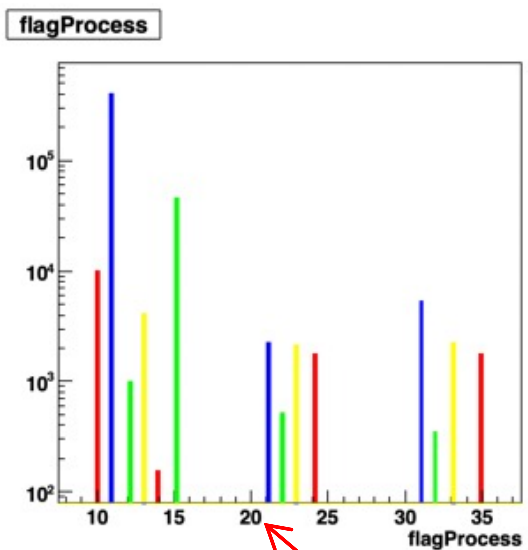
← Draw processes in track

* See e.g. https://root.cern.ch

« dnaphysics » extended example: output

- Results are saved in the `dna.root` file and can be analyzed using ROOT*
  - Type `root plot.C`

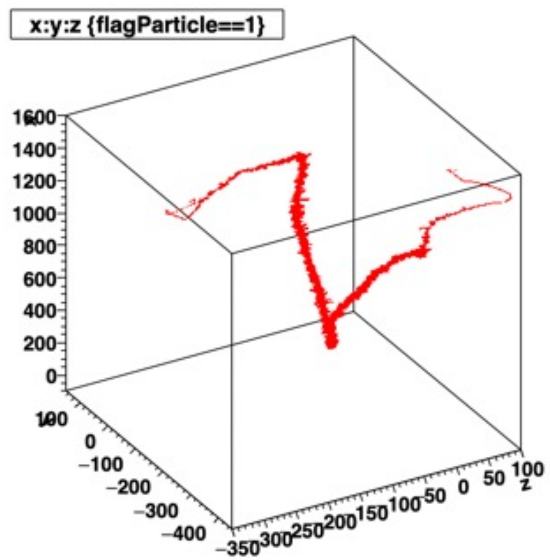
Number of occurences of physical processes



(See `README` for process numbers)

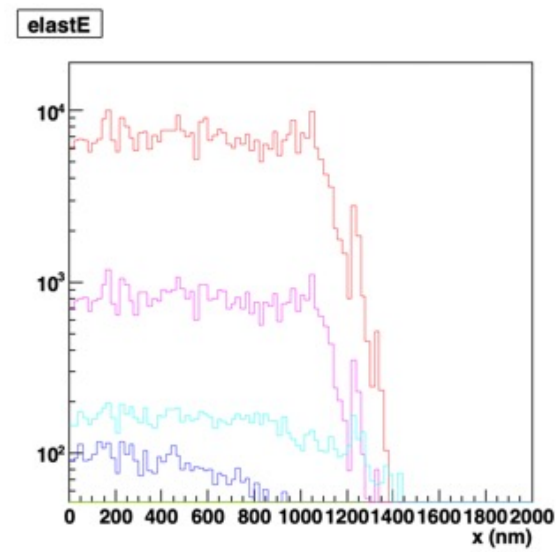
```
proton_G4DNAElastic: 21
proton_G4DNAExcitation: 22
proton_G4DNAIonisation: 23
proton_G4DNAChargeDecrease: 24
```

3D visualization of 2 proton tracks



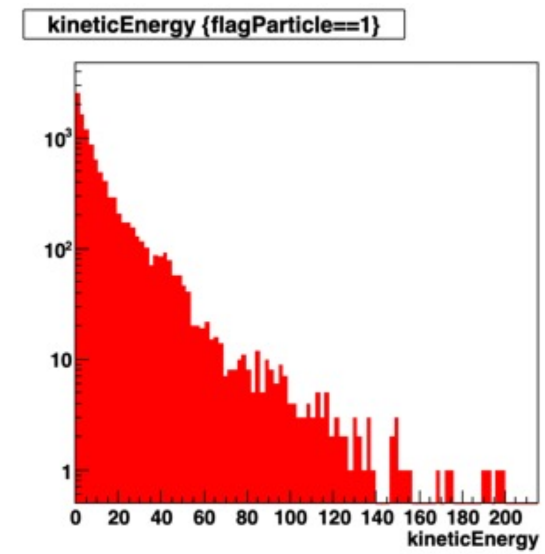
2 protons
(100 keV)

Occurring processes along x-axis



Elastic
Vib. excitation
Solvation
Ionisation
...

Energy distribution of electrons

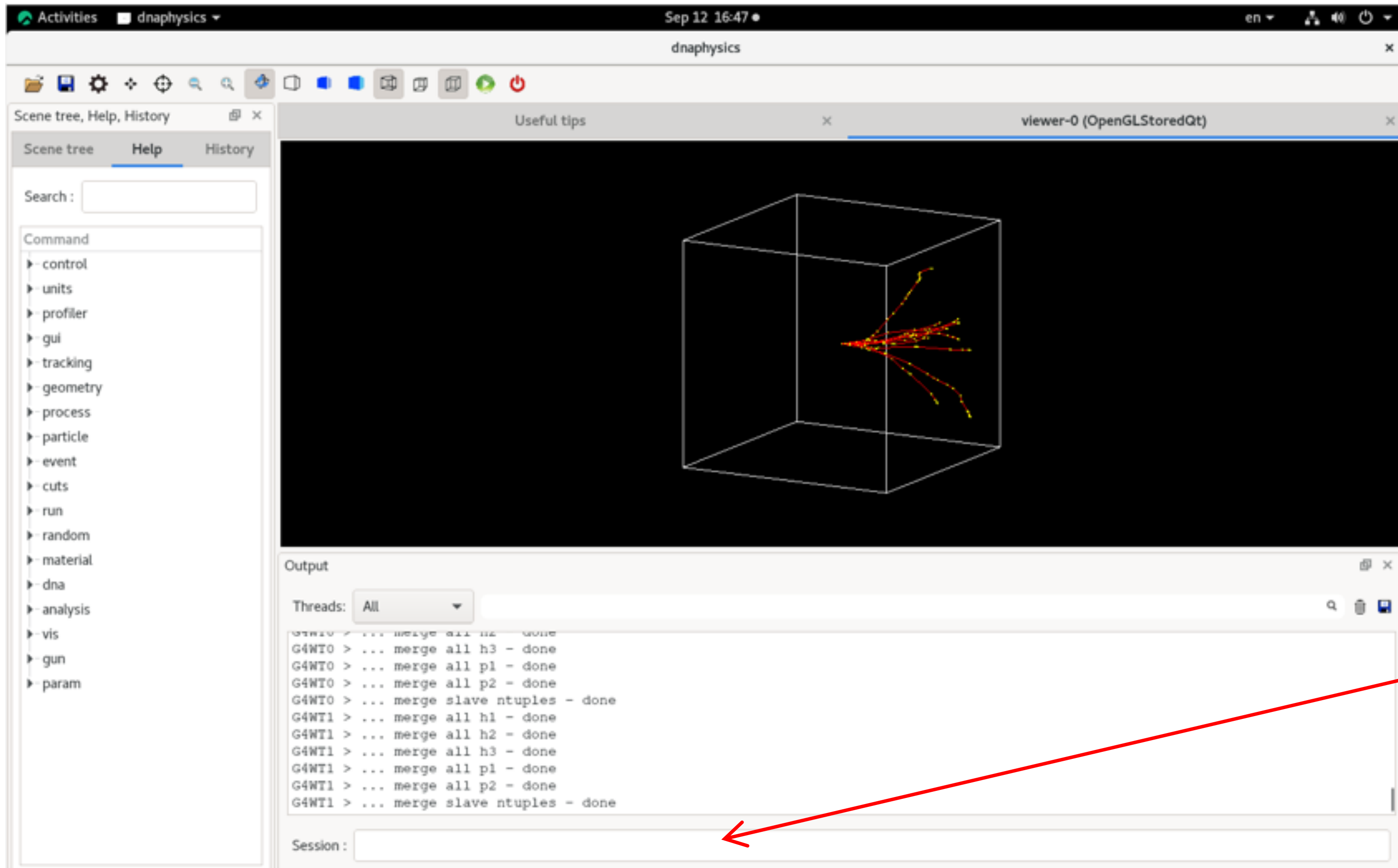


Note: We also provide the `deexcitation.in` and `plotDeexcitation.C` macros to illustrate atomic deexcitation (fluorescence photons and Auger electrons)

Hands-on practice with the « dnaphysics » extended example

- Run dnaphysics in **interactive mode** (allows GUI commands)

```
./dnaphysics
```



You can enter your commands in the **GUI session**:

```
/gun/particle e-
/gun/energy 100 keV
/run/beamOn 10
```

Type of particles and physical processes (see README)

Particles

```
- particles:
gamma: 0
e-: 1
proton: 2
hydrogen: 3
alpha: 4
alpha+: 5
helium: 6
GenericIon (above helium): 7
```

Processes

```
- processes:

Capture: 1

RadioactiveDecay: 2

e-_G4DNAElectronSolvation: 10
e-_G4DNAElastic: 11
e-_G4DNAExcitation: 12
e-_G4DNAIonisation: 13
e-_G4DNAAttachment: 14
e-_G4DNAVibExcitation: 15
msc: 110
CoulombScat: 120
eIoni: 130

proton_G4DNAElastic: 21
proton_G4DNAExcitation: 22
proton_G4DNAIonisation: 23
proton_G4DNAChargeDecrease: 24
msc: 210
CoulombScat: 220
hIoni: 230
nuclearStopping: 240

hydrogen_G4DNAElastic: 31
hydrogen_G4DNAExcitation: 32
hydrogen_G4DNAIonisation: 33
hydrogen_G4DNAChargeIncrease: 35
```

```
alpha_G4DNAElastic: 41
alpha_G4DNAExcitation: 42
alpha_G4DNAIonisation: 43
alpha_G4DNAChargeDecrease:  44
msc: 410
CoulombScat: 420
ionIoni: 430
nuclearStopping: 440

alpha+_G4DNAElastic: 51
alpha+_G4DNAExcitation: 52
alpha+_G4DNAIonisation: 53
alpha+_G4DNAChargeDecrease: 54
alpha+_G4DNAChargeIncrease: 55
msc: 510
CoulombScat: 520
hIoni: 530
nuclearStopping: 540

helium_G4DNAElastic: 61
helium_G4DNAExcitation: 62
helium_G4DNAIonisation: 63
helium_G4DNAChargeIncrease: 65

GenericIon_G4DNAIonisation: 73
msc: 710
CoulombScat: 720
ionIoni: 730
nuclearStopping: 740

phot: 81
compt: 82
conv: 83
Rayl: 84
```

Try to change the Physics constructor…

- Can be selected in `dnaphysics.in` …

```
#
# Physics
# - To use Geant4-DNA constructor X, X=0, 2, 4, or 6 (recommended)
#/dna/test/addPhysics DNA_Opt0
/dna/test/addPhysics DNA_Opt2
#/dna/test/addPhysics DNA_Opt4
#/dna/test/addPhysics DNA_Opt6
#
```

- Run the simulation and display ROOT results

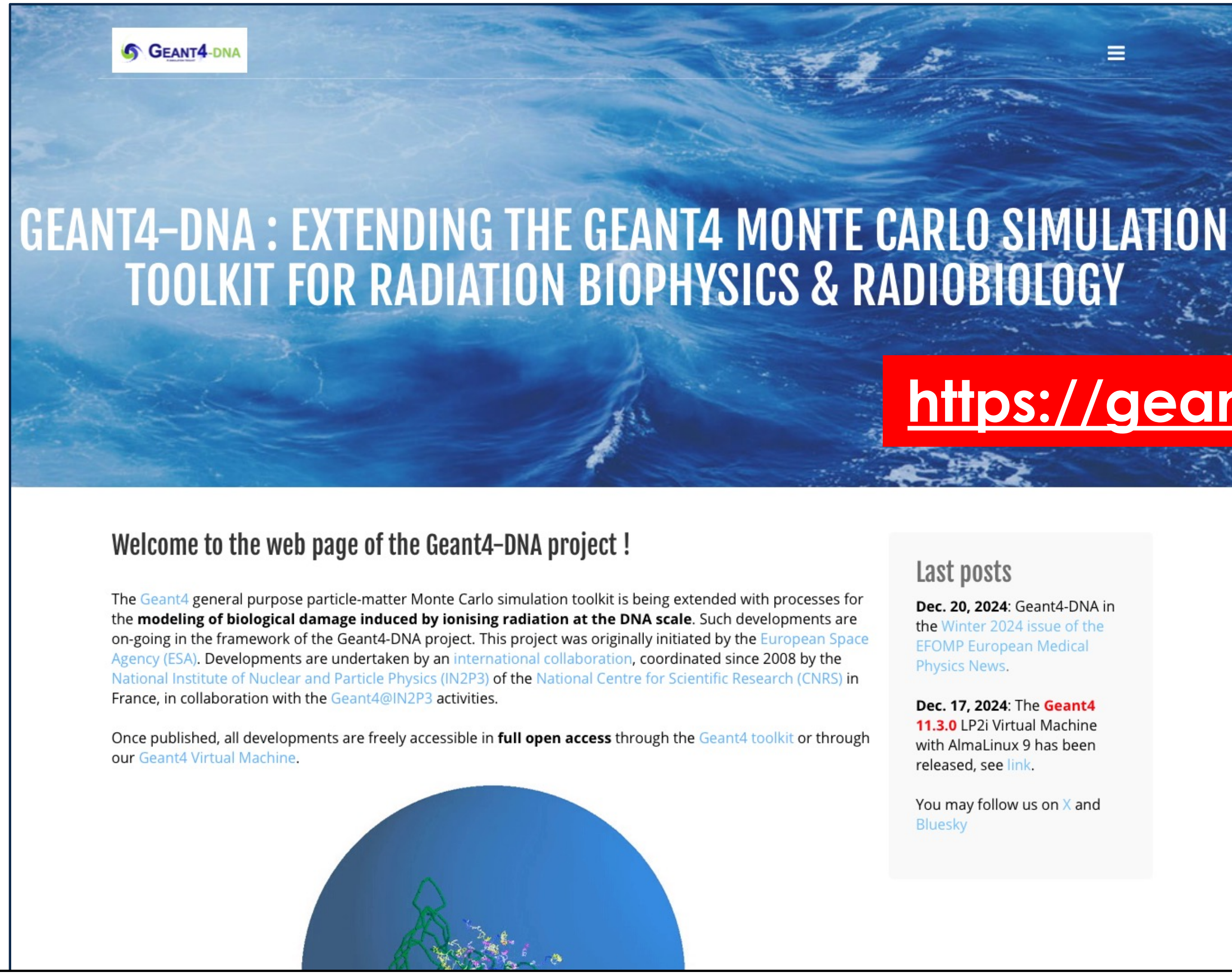
Try to change the density value of the target material

- Can be selected in `dnaphysics.in` …

```
#
# Material
/dna/test/setMat G4_WATER
# or alternatively
#/dna/test/setMatDens G4_WATER_MODIFIED 1.200 g/cm3
#
```

- Run the simulation and display ROOT results

Thank you for your attention


GEANT4-DNA

GEANT4-DNA : EXTENDING THE GEANT4 MONTE CARLO SIMULATION TOOLKIT FOR RADIATION BIOPHYSICS & RADIOBIOLOGY

Welcome to the web page of the Geant4-DNA project !

The Geant4 general purpose particle-matter Monte Carlo simulation toolkit is being extended with processes for the **modeling of biological damage induced by ionising radiation at the DNA scale**. Such developments are on-going in the framework of the Geant4-DNA project. This project was originally initiated by the European Space Agency (ESA). Developments are undertaken by an international collaboration, coordinated since 2008 by the National Institute of Nuclear and Particle Physics (IN2P3) of the National Centre for Scientific Research (CNRS) in France, in collaboration with the Geant4@IN2P3 activities.

Once published, all developments are freely accessible in **full open access** through the Geant4 toolkit or through our Geant4 Virtual Machine.

Last posts

Dec. 20, 2024: Geant4-DNA in the Winter 2024 issue of the EFOMP European Medical Physics News.

Dec. 17, 2024: The Geant4 11.3.0 LP2i Virtual Machine with AlmaLinux 9 has been released, see link.

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https://geant4-dna.org/