http://geant4.org

GEANT4-DNA HANDS ON

KIT Tutorial, October 25-26, 2011, Karlsruhe

3 examples

- We are going to try 3 Geant4 examples which make use of Geant4-DNA Physics processes
  - advanced examples located in $G4INSTALL/examples/advanced
    - dnaphysics
    - microdosimetry
  - extendes examples located in $G4INSTALL/examples/extended
    - TestEm12

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dnaphysics

dnaphysics advanced example

Geant4 9.5 BETA

- Located in $G4INSTALL/examples/advanced/dnaphysics

- This example teaches to Geant4 users how to use the Geant4-DNA physics processes and models in a liquid water volume
  - Produces ROOT histograms to visualize track structures
  - The PhysicsList uses the default Physics builder called G4EmDNAPhysics which contains the recommended Geant4-DNA physics, so you do not need to code the physics yourself

- It also explains how to easily change the density of the target material (liquid water) : « variable density material » new feature of Geant4
  - Possibility to investigate density change effects
    - eg. 1.06 g/cm^3 average density of cell nucleus (cf. PARTRAC)

Install dnaphysics

- For usage with Geant4 9.4, download the example from http://geant4.in2p3.fr
  - Tutorials & Teachings
  - Download « Dnaphysics Hands On »
  - Save it on your desktop

- On your Geant4 virtual machine
  - Open a terminal
  - `mv /mnt/hgfs/Desktop/dnaphysics.tar`
  - `tar -xvf dnaphysics.tar`
  - `cd dnaphysics`
  - `snavigator &`
  - `gmake`

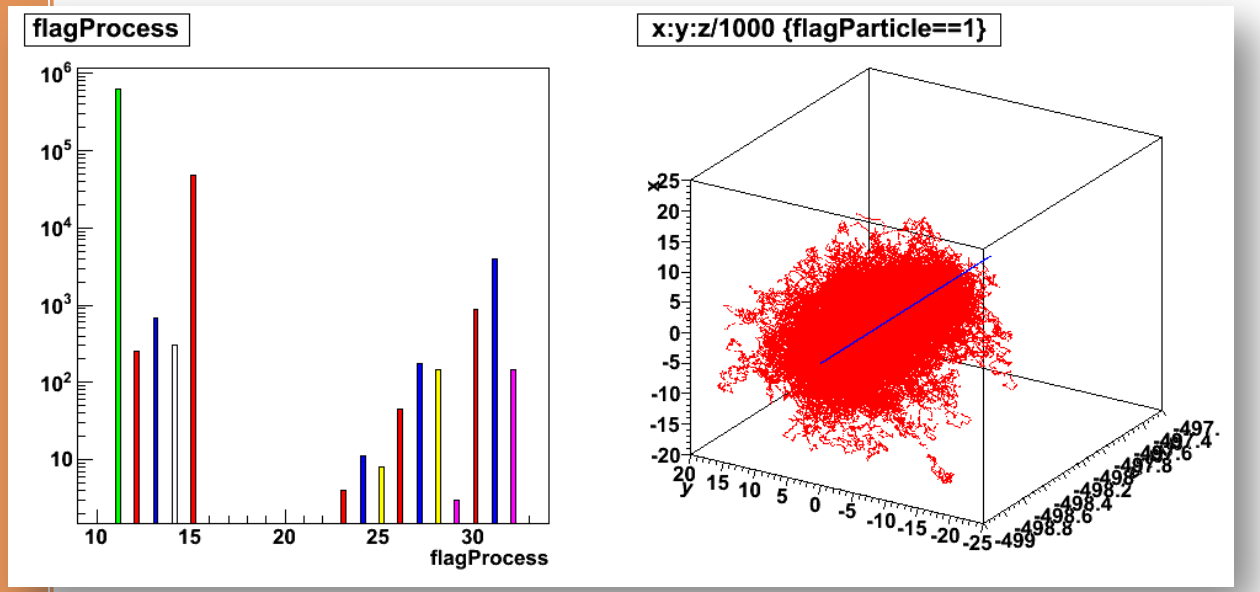
Run dnaphysics

- On your terminal
  - `$G4WORKDIR/bin/$G4SYSTEM/DNAPhysics`
    - The macro file dna.mac is read
    - 100 electrons of 1 keV are shot
    - No visualization by default
    - Results are saved in dna.root file
  - `exit`
  - `root plot.C`
    - ROOT is already installed on your system
    - ROOT macro is read to plot histograms from dna.root file

Output of dnaphysics

e-_G4DNAElastic	11
e-_G4DNAExcitation	12
e-_G4DNAIonisation	13
e-_G4DNAAttachment	14
e-_G4DNAVibExcitation	15
proton_G4DNAExcitation	17
proton_G4DNAIonisation	18
proton_G4DNAChargeDec.	19
hydrogen_G4DNAExcitation	20
hydrogen_G4DNAIonisation	21
hydrogen_G4DNAChargeInc.	22
alpha_G4DNAExcitation	23
alpha_G4DNAIonisation	24
alpha_G4DNAChargeDec.	25
alpha+_G4DNAExcitation	26
alpha+_G4DNAIonisation	27
alpha+_G4DNAChargeDec.	28
alpha+_G4DNAChargeInc.	29
helium_G4DNAExcitation	30
helium_G4DNAIonisation	31
helium_G4DNAChargeInc.	32

Eg. one 100 keV He^{+}



Do more

- Try yourself to
  - Set number of incident electron to 1
  - Activate visualization
  - Zoom display by 10000
  - run again
  - Try to shhot one proton, then one hydrogen, then one helium with 10 keV incident energy
- In snavigator, look at the following classes
  - PhysicsList
    - Usage of G4EmDNAPhysics builder
  - SteppingAction
    - Recording of particles & processes
    - Positions of pre-step points
    - Energy deposit for each step
  - DetectorConstruction
    - Change of value of water density
  - HistoManager
    - Handling of histograms (creation, filling up, saving)

PhysicsList header


```
#include "G4VModularPhysicsList.hh"
#include "globals.hh »
class G4VPhysicsConstructor;
class PhysicsList: public G4VModularPhysicsList
{
  public:
    PhysicsList();
   ~PhysicsList();
    void ConstructParticle();
    void ConstructProcess();
    void SetCuts();
    void SetCutForGamma(G4double);
    void SetCutForElectron(G4double);
    void SetCutForPositron(G4double);

  private:
    G4double cutForGamma;
    G4double cutForElectron;
    G4double cutForPositron;
    G4double currentDefaultCut;
    G4VPhysicsConstructor*  emPhysicsList;
};
```

PhysicsList implementation

- In constructor
  - `emPhysicsList = new G4EmDNAPhysics();`
- In ConstructParticle()
  - `emPhysicsList->ConstructParticle();`
- In ConstructProcess()
  - `AddTransportation();`
  - `emPhysicsList->ConstructProcess();`
- Production cuts are not used by Geant4-DNA processes
  - All intercations are explicitely simulated
- Look at the Geant4-DNA Physics builder itself
  - `$G4INSTALL/source/physics_list/builders/src/G4EmDNAPhysics.cc`

What is included in the G4EmDNAPhysics builder ?


```
void G4EmDNAPhysics::ConstructParticle()
{
// bosons
  G4Gamma::Gamma();

// leptons
  G4Electron::Electron();
  G4Positron::Positron();

// baryons
  G4Proton::Proton();
  G4GenericIon::GenericIonDefinition();
  G4DNAGenericIonsManager * genericIonsManager;
  genericIonsManager=G4DNAGenericIonsManager::Instance();
  genericIonsManager->GetIon("alpha++");
  genericIonsManager->GetIon("alpha+");
  genericIonsManager->GetIon("helium");
  genericIonsManager->GetIon("hydrogen");
}
```

Proton and He^{2+} nuclei can gain electrons and become H, He^{+}, He^{0}

G4EmDNAPhysics: Physics processes & models for electrons


```
void G4EmDNAPhysics::ConstructProcess()
{
  G4PhysicsListHelper* ph = G4PhysicsListHelper::GetPhysicsListHelper();
  theParticleIterator->reset();
  while( (*theParticleIterator)() )
  {
    G4ParticleDefinition* particle = theParticleIterator->value();
    G4String particleName = particle->GetParticleName();

    if (particleName == "e-") {
      // *** Elastic scattering (two alternative models available) ***
      G4DNAElastic* theDNAElasticProcess = new G4DNAElastic("e-_G4DNAElastic");
      theDNAElasticProcess->SetModel(new G4DNAChampionElasticModel());

      // or alternative model
      //theDNAElasticProcess->SetModel(new G4DNAScreenedRutherfordElasticModel());
      ph->RegisterProcess(theDNAElasticProcess, particle);

      // *** Excitation ***
      ph->RegisterProcess(new G4DNAExcitation("e-_G4DNAExcitation"), particle);
      // *** Ionisation ***
      ph->RegisterProcess(new G4DNAIonisation("e-_G4DNAIonisation"), particle);
      // *** Vibrational excitation ***
      ph->RegisterProcess(new G4DNAVibExcitation("e-_G4DNAVibExcitation"), particle);
      // *** Attachment ***
      ph->RegisterProcess(new G4DNAAttachment("e-_G4DNAAttachment"), particle);
```

We have two models for electron elastic scattering in liquid water

PROCESS

MODEL

G4EmDNAPhysics: Physics processes & models for other Geant4-DNA particles

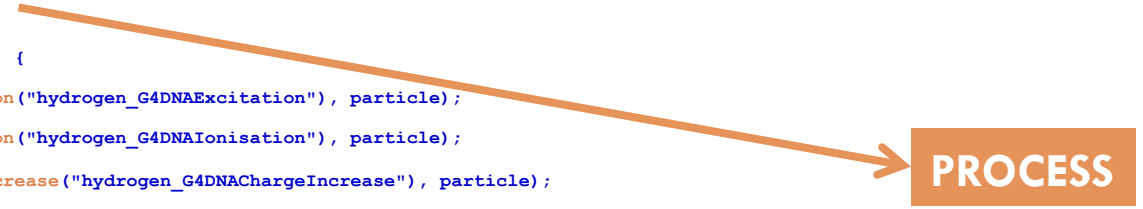

```
} else if ( particleName == "proton" ) {
    ph->RegisterProcess(new G4DNAExcitation("proton_G4DNAExcitation"), particle);
    ph->RegisterProcess(new G4DNAIonisation("proton_G4DNAIonisation"), particle);
    ph->RegisterProcess(new G4DNAChargeDecrease("proton_G4DNAChargeDecrease"), particle);

  } else if ( particleName == "hydrogen" ) {
    ph->RegisterProcess(new G4DNAExcitation("hydrogen_G4DNAExcitation"), particle);
    ph->RegisterProcess(new G4DNAIonisation("hydrogen_G4DNAIonisation"), particle);
    ph->RegisterProcess(new G4DNAChargeIncrease("hydrogen_G4DNAChargeIncrease"), particle);

  } else if ( particleName == "alpha" ) {
    ph->RegisterProcess(new G4DNAExcitation("alpha_G4DNAExcitation"), particle);
    ph->RegisterProcess(new G4DNAIonisation("alpha_G4DNAIonisation"), particle);
    ph->RegisterProcess(new G4DNAChargeDecrease("alpha_G4DNAChargeDecrease"), particle);

  } else if ( particleName == "alpha+" ) {
    ph->RegisterProcess(new G4DNAExcitation("alpha+_G4DNAExcitation"), particle);
    ph->RegisterProcess(new G4DNAIonisation("alpha+_G4DNAIonisation"), particle);
    ph->RegisterProcess(new G4DNAChargeDecrease("alpha+_G4DNAChargeDecrease"), particle);
    ph->RegisterProcess(new G4DNAChargeIncrease("alpha+_G4DNAChargeIncrease"), particle);

  } else if ( particleName == "helium" ) {
    ph->RegisterProcess(new G4DNAExcitation("helium_G4DNAExcitation"), particle);
    ph->RegisterProcess(new G4DNAIonisation("helium_G4DNAIonisation"), particle);
    ph->RegisterProcess(new G4DNAChargeIncrease("helium_G4DNAChargeIncrease"), particle);
  }
```



More on Geant4-DNA Physics

- Some DNA models « kill » the particle below a certain energy threshold because the models are not validated or defined below this threshold
  - In this case, tracking is stopped and kinetic energy is locally deposited
  - Electrons below 4 eV (by G4DNAChampionElasticModel) or below 9 eV (by G4DNAScreenedRutherfordElasticModel)
  - Protons & H below 100 eV by G4DNAIonisation
  - He^{2+}, He^{+} and He^{0} below 1 keV by G4DNAIonisation

- See other hints from the Geant4-DNA web page
  - https://twiki.cern.ch/twiki/bin/view/Geant4/LoweMigratedDNAProcesses
  - How to access total cross sections
  - How to « kill » particles below a certain energy threshold
  - …

SteppingAction

- Flag of particle
  - ```
    if (s->GetTrack()->GetDynamicParticle()->GetDefinition() ->GetParticleName() == "e-")
    flagParticle = 1;
    ```
- Flag of process
  - ```
    if (s->GetPostStepPoint()->GetProcessDefinedStep()->GetProcessName()=="hydrogen_G4DNAExcitation")
      flagProcess =20;
    ```
- Step information
  - `x=s->GetPreStepPoint()->GetPosition().x()/nanometer;`
  - `y=s->GetPreStepPoint()->GetPosition().y()/nanometer;`
  - `z=s->GetPreStepPoint()->GetPosition().z()/nanometer;`
  - `s->GetTotalEnergyDeposit()/eV`

DetectorConstruction

- Definition of water material
  - `// Water is defined from NIST material database`
  - `G4NistManager * man = G4NistManager::Instance();`
  - `G4Material * H2O = man->FindOrBuildMaterial("G4_WATER");`

- Change of density value (from Geant4 9.5 BETA)
  - `// If one wishes to test other density value for water material, one should use instead:`
  - `// G4Material * H2O = man->BuildMaterialWithNewDensity("G4_WATER_MODIFIED","G4_WATER", 1000*g/cm/cm/cm);`
  - `// Note: any string for "G4_WATER_MODIFIED" parameter is accepted`
  - `// and "G4_WATER" parameter should not be changed`

- Display density
  - `G4cout << "-> Density of water material (g/cm3)=" << waterMaterial->GetDensity()/(g/cm/cm/cm) << G4endl;`

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microdosimetry

microdosimetry advanced example

- Shows the multi-scale combination of
  - Geant4 Standard EM Physics (condensed/discrete)
    - Geant4 Standard EM
  - Purely discrete processes
    - Geant4-DNA
  - For protons/hydrogen
  - In two regions (the « World » and « Target »)

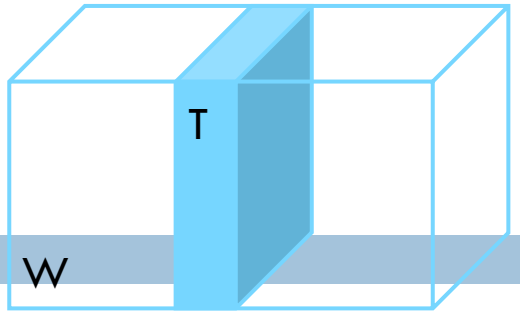
- Useful when the user in interested in simulating efficiently high energy incident particles with Geant4 EM Standard Physics, providing a space phase input for Geant4-DNA simulations applied to much small volumes

- Also shows how to create a process to kill particles below a certain energy threshold
  - G4ElectronCapture

Install microdosimetry

- Open a terminal on your virtual machine
- Type the following commands:
- `cp -R $G4INSTALL/examples/advanced/microdosimetry .`
- `cd microdosimetry`
- `gmake`
- `$G4WORKDIR/bin/$G4SYSTEM/Microdosimetry`
  - A 5 MeV proton is shot (see microdosimetry.mac)
- `exit`
- `root plot.C`

Geometry



- A 50 µm thick « Target » volume placed in a 1 mm thick « World » mother volume
- Both contain liquid water only
- We would like to use
  - EM Standard models in the « World »
  - Geant4-DNA models in the « Target » below 1 MeV for e-

1) Create a Region for the target volume in DetectorConstruction


```
fRegion = new G4Region("Target");

G4ProductionCuts* cuts = new G4ProductionCuts();

G4double defCut = 1*nanometer;
cuts->SetProductionCut(defCut,"gamma");
cuts->SetProductionCut(defCut,"e-");
cuts->SetProductionCut(defCut,"e+");
cuts->SetProductionCut(defCut,"proton");

fRegion->SetProductionCuts(cuts);
fRegion->AddRootLogicalVolume(logicTarget);
```

2) Define Physics for the World

- In the loop over particles, activate EM standard processes
  - they will be ACTIVE IN THE WORLD

```
if (particleName == "e-") {

// msc is active in the world
G4eMultipleScattering* msc = new G4eMultipleScattering();
pmanager->AddProcess(msc, -1, 1, 1);

// standard ionisation is active in the world
G4eIonisation* eion = new G4eIonisation();
eion->SetEmModel(new G4MollerBhabhaModel(), 1);
pmanager->AddProcess(eion, -1, 2, 2);
```

Define Physics for the World

- then INACTIVATE Geant4-DNA processes using a G4DummyModel and the SetModel method. They will be INACTIVE IN THE WORLD.

```
// DNA elastic is not active in the world
G4DNAElastic* theDNAElasticProcess = new G4DNAElastic("e-_G4DNAElastic");
theDNAElasticProcess->SetModel (new G4DummyModel(),1);
pmanager->AddDiscreteProcess(theDNAElasticProcess);
// DNA excitation is not active in the world
G4DNAExcitation* dnaex = new G4DNAExcitation("e-_G4DNAExcitation");
dnaex->SetModel (new G4DummyModel(),1);
pmanager->AddDiscreteProcess(dnaex);
// DNA ionisation is not active in the world
G4DNAIonisation* dnaioni = new G4DNAIonisation("e-_G4DNAIonisation");
dnaioni->SetModel (new G4DummyModel(),1);
pmanager->AddDiscreteProcess(dnaioni);
// DNA attachment is not active in the world
G4DNAAttachment* dnaatt = new G4DNAAttachment("e-_G4DNAAttachment");
dnaatt->SetModel (new G4DummyModel(),1);
pmanager->AddDiscreteProcess(dnaatt);
// DNA vib. excitation is not active in the world
G4DNAVibExcitation* dnavib = new G4DNAVibExcitation("e-_G4DNAVibExcitation");
dnavib->SetModel (new G4DummyModel(),1);
pmanager->AddDiscreteProcess(dnavib);
```

3) Define Physics for the Target

- Inactivate EM Standard processes in the TARGET Region below 1 MeV by registering corresponding EM Standard models to the G4EmConfigurator

```
G4EmConfigurator* em_config = G4LossTableManager::Instance()->EmConfigurator();
G4VEmModel* mod;

mod =  new G4UrbanMscModel93();
mod->SetActivationLowEnergyLimit(1*MeV);
em_config->SetExtraEmModel("e-","msc",mod,"Target");

mod = new G4MollerBhabhaModel();
mod->SetActivationLowEnergyLimit(1*MeV);
em_config->SetExtraEmModel("e-","eloni",mod,"Target",0.0,100*TeV, new G4UniversalFluctuation());
```

Specify low enery limit of activation

Specify particle name, process name, model and region name and energy interval (option if more than one models are used)

Define Physics for the Target

- Activate Geant4-DNA processes in the TARGET Region by registering the corresponding Geant4-DNA models to the G4EmConfigurator

```
mod = new G4DNAChampionElasticModel();
em_config->SetExtraEmModel("e-","e-_G4DNAElastic",mod,"Target",0.0,1*MeV);

mod = new G4DNABornIonisationModel();
em_config->SetExtraEmModel("e-","e-_G4DNAIonisation",mod,"Target",11*eV,1*MeV);

mod = new G4DNABornExcitationModel();
em_config->SetExtraEmModel("e-","e-_G4DNAExcitation",mod,"Target",9*eV,1*MeV);

mod = new G4DNAMeltonAttachmentModel();
em_config->SetExtraEmModel("e-","e-_G4DNAAttachment",mod,"Target",4*eV,13*eV);

mod = new G4DNASancheExcitationModel();
em_config->SetExtraEmModel("e-","e-_G4DNAVibExcitation",mod,"Target",2*eV,100*eV);
```

Specify energy range of applicability

TestEm12

TestEm12 purpose

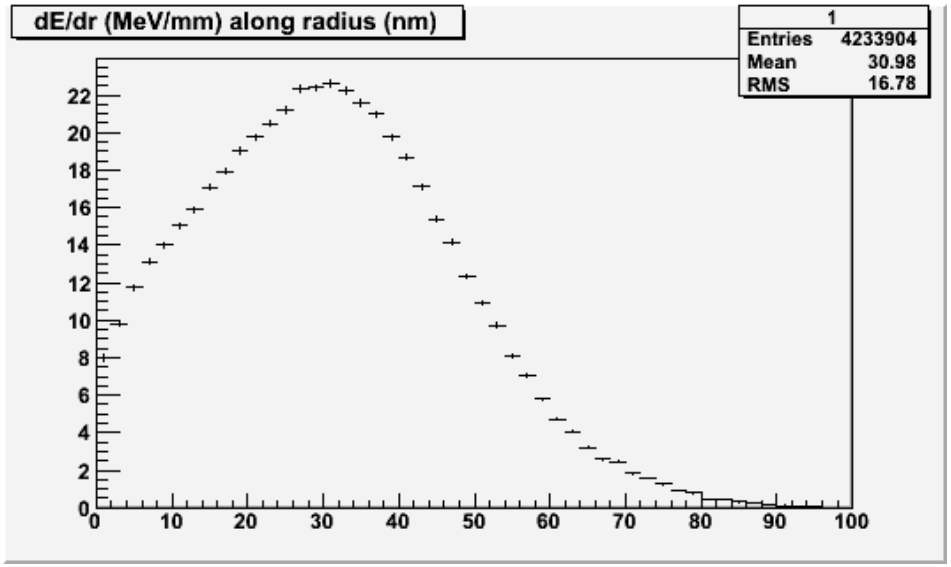
- Shows how to get energy deposit distribution for electrons shot within the center of a liquid water sphere
- Uses Physics builders
  - Standard EM
  - Low Energy EM
  - Geant4-DNA
    - To be run with macro dna.mac
- Produces histograms
- Can be fully run & configurated through UI commands

Install and run TestEm12

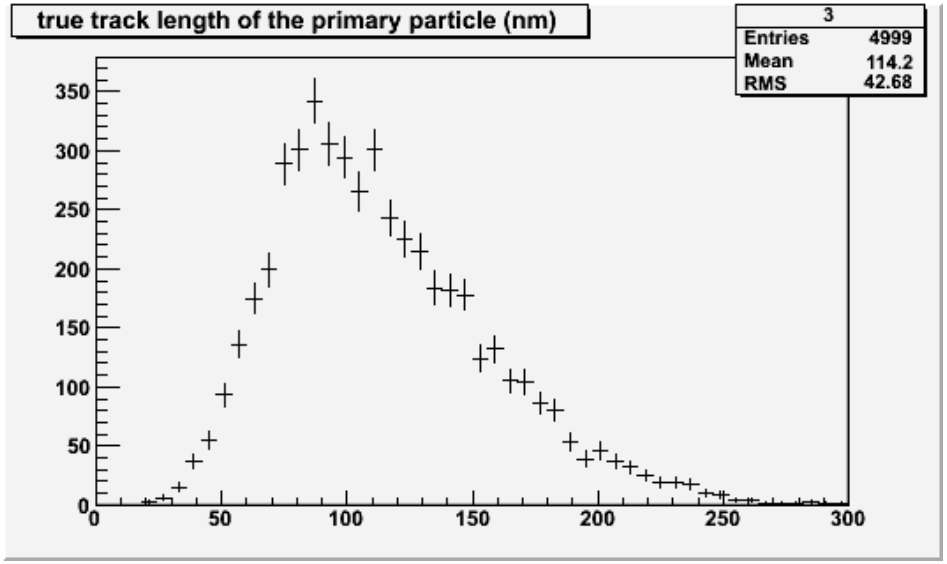
- Open a terminal on your virtual machine
- Type the following commands:
- `cp -R $G4INSTALL/examples/extended/electromagnetic/TestEm12 .`
- `cd TestEm12`
- `gmake`
- `$G4WORKDIR/bin/$G4SYSTEM/TestEm12 dna.mac`
  - 5000 electrons of 1 keV are shot from the center of a liquid water sphere of radius 100 nm (see dna.mac)
- `exit`
- `root`
- `Tbrowser g`
- Open the dna.root file in the browser

Example of results

dE/dr along radius



Track length of primary



Thank you for your attention