

# Simulation Computing Workshop

## Hands-on session

**Sayak Chatterjee**  
**UMass, Amherst**

# Plans for the session

- **Setting up the environment for using REMOLL**
  - Prerequisites
  - Local machine (Linux)
  - Ifarm (Jlab computing account is needed to access)
  - Virtual box
- **Visualization of MOLLER experimental setup**
  - Using the REMOLL Graphical User Interface (GUI)
- **Run simulation with REMOLL**
  - How to submit jobs to simulate some events
- **Investigation of the simulated data**
  - Structure of the simulated data
- **Modify the simulation geometry**
  - Add or modify some materials (active or passive)
- **Analysis of the simulated data**
  - Final plots

# **Setting up the environment to use REMOLL**

# Linux (Local machine)

**Prerequisites:** git, cmake > 3.5, Geant4 >= 4.10.00 (>= 4.10.06 recommended), ROOT >= 6.0.0, python

Link of how to: [git](#), [cmake](#), [GEANT4](#), [ROOT](#), [python](#)

Once you have all the prerequisites, follow the below steps to download and compile REMOLL

Step 1: **git clone <https://github.com/JeffersonLab/remoll> directory\_name**

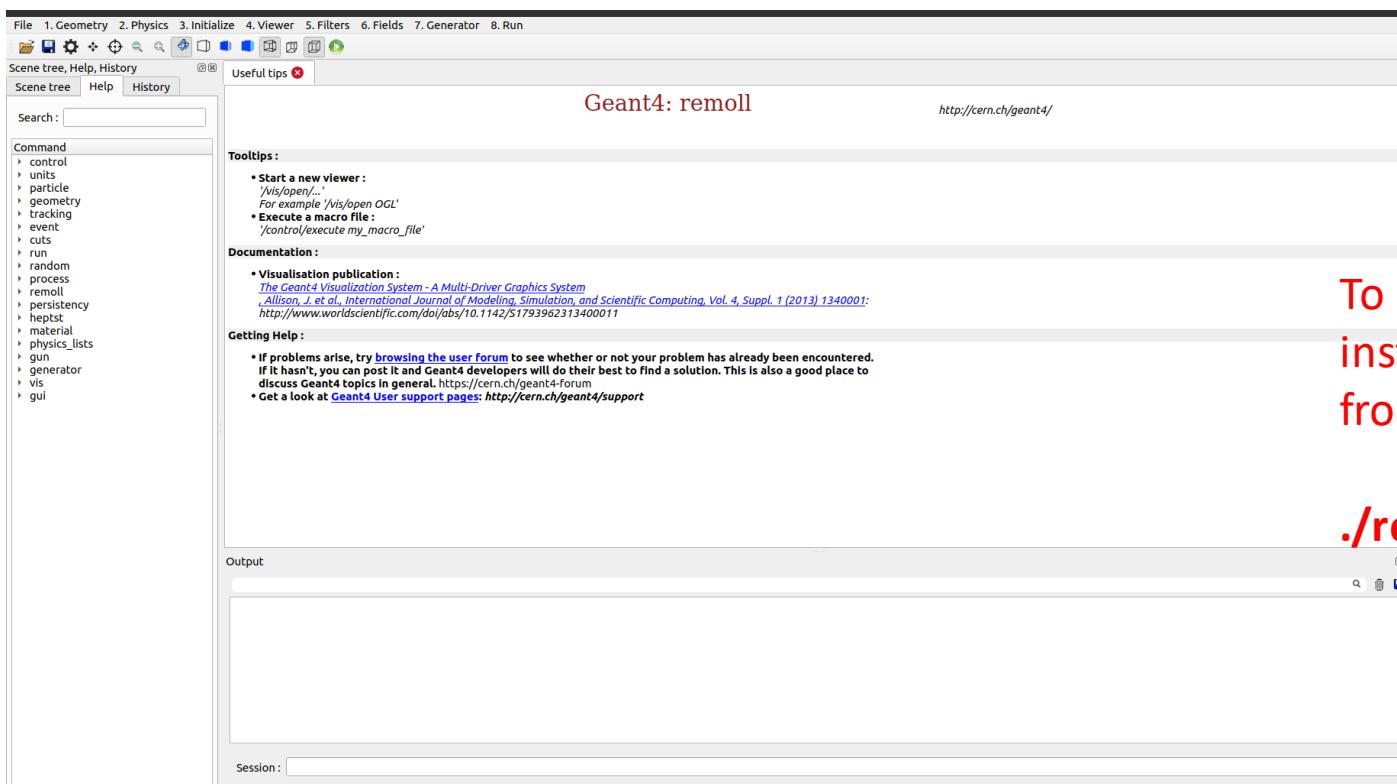
Step 2: **mkdir build**

Step 3: **cd build**

Step 4: **cmake ..**

Step 5: **make -j5**

Step 6: **make install**



To check if you have a successful installation, type the following from your **build** directory:

**./remoll**

# Ifarm (JLab computing account)

## How to get an account on ifarm:

- To get a JLab user account, each new user must fill out the Access Registration [Form](#). Be sure to fill out (and remember) the emergency contact information requested - the information will be used for identification later.
- Send an email to [helpdesk@jlab.org](mailto:helpdesk@jlab.org) and ask to create an account on ifarm. You will need to provide your name, your supervisor and institution name, and also mention that you are part of the `moller12gev` group under halla.
- Complete the [GEN034U training](#)

## Login to ifarm:

- Requires two factor authentication ([Details here](#))
- `ssh -Y username@scilogin.jlab.org` (put your set authentication password)
- `ssh -Y ifarm` (put your ifarm password)
- `cd /work/halla/moller12gev/username`
- `source /site/12gev_phys/softenv.csh 2.5`
- Downloading and compiling of REMOLL is the same as local machine

## Virtual Box

- Download and install the [VirtualBox Manager](#)
- [Download Virtual Machine](#) (11 GB)
- Start the VirtualBox Manager application and from the **File** menu select **Import Appliance**
- Select the Virtual Machine file MOLLER\_VM.ova from the file browser
- Click **Next**
- Click **Import** and at the end you should see the virtual machine **MOLLER\_VM** displayed on the left side of the VirtualBox application
- Click the virtual machine **MOLLER\_VM** and this will boot the Ubuntu virtual machine with all the software installed.

# **Visualization of the MOLLER experimental setup**

# Visualization

## Using GUI:

Goto following directory by: cd softwares/remoll

Run the command: ./build/remoll

Click menu 1.Geometry and select MOLLER Experiment

Click menu 3. Initialize and select Initialize

Click menu 4. Viewer and select Qt Viewer (Stored) (second item)

Now MOLLER geometry should be accessible

## Using commands:

/remoll/geometry/setfile geometry/mollerMother.gdml

/run/initialize

/vis/open OGL

/control/execute vis/vis.mac

# Visualization

File 1. Geometry 2. Physics 3. Initialize 4. Viewer 5. Filters 6. Fields 7. Generator 8. Run

Scene tree, Help, History      Useful tips      viewer-0 (OpenGLStoredQt)

Scene tree Help History

Search :

Command

- ▶ control
- ▶ units
- ▶ particle
- ▶ geometry
- ▶ tracking
- ▶ event
- ▶ cuts
- ▶ run
- ▶ random
- ▶ process
- ▶ remoll
- ▶ persistency
- ▶ heptst
- ▶ material
- ▶ physics\_lists
- ▶ gun
- ▶ generator
- ▶ vis
- ▶ gui
- ▶ hits
- ▶ physics\_engine

Output

```
Pre-step-point global time (PreT): G4BestUnit (G4double)
Pre-step Volume Path (PreVPath): G4String
Pre-step-point weight (PreW): G4double
Remaining Energy (RE): G4BestUnit (G4double)
Total Energy Deposit (TED): G4BestUnit (G4double)
WARNING: Trajectory storing has been requested. This action may be
reversed with "/tracking/storeTrajectory 0".
WARNING: The vis manager will keep up to 100 events.
This may use a lot of memory.
It may be changed with, e.g., "/vis/scene/endOfEventAction accumulate 10".
You may need to issue "/vis/viewer/update".
```

Session :

# **Running simulation**

# Where to find what?

```
sayak@Sayak: ~/Desktop/Moll... × sayak@Sayak: ~/Desktop/Moll... × sayak@Sayak: ~/Desktop/Moll... ×
ifarm1802.jlab.org> ls
analysis           Dockerfile      lib64          README.FAQ.md    remoll.cc
bin                Doxyfile       logfiles        README.hitdet.md  reroot.cc
build              Gemfile        macros         README.md       rootfiles
cmake              generators     manual.txt     README.optical.md scripts
CMakeLists.txt     geometry      map_directory README.pion      share
_config.yml        geometry_sandbox pullgitinfo.py README.replay.md src
CONTRIBUTORS.md   include        README.Compiling.md README.Running.md vis
doc                initialize.sh README.Contributing.md README.Singularity.md
docker             jobs          README.Docker.md  README.variables.md
```

**geometry** -> Contains all the GDML files for the individual sub-systems

Position of the different sub-systems: `geometry/positions.xml`

Geometry for the sensitive volumes: `geometry/mollerParallel.gdml`

**map\_directory** -> Contains the magnetic field files

**macros** -> Different macros to run simulations

**analysis** -> Contains various example analysis scripts

**vis** -> Different macros for visualization

## Simulation in batch mode

- Simulate multiple events according to input macro file to generate the root output
- Input macro file provide what physics models, event types to generate, geometry, magnetic field, output destination, and number of events to simulate
- Standard input files are available in macros directory remoll/macros
- Hands-On-Remoll directory has three such files that we will use HandsOn\_run\_moller.mac, HandsOn\_run\_ep.mac HandsOn\_kryptonite.mac
- Copy these files to you VM or to ifarm remoll/macros
  - For VM, just open a browser in your VM and download the files
  - For ifarm (from local machine to ifarm):  
`scp -r file_name username@login1.jlab.org:/u/home/username/`
  - For ifarm (from ifarm to local machine):  
`scp -r username@login1.jlab.org:/u/home/username directory_at_the_local_machine`

# Standard input macro file (.mac)

```
HandsOn_run_moller.mac
```

1 # Hands-On tutorial moller generator macro file  
2  
3  
4 # This must be called before initialize  
5 /remoll/geometry/setfile geometry/mollerMother.gdml ← Geometry files  
6 # Parallel world geometry is optional - detector 28 (the primary detector array's idealize vacuum detector) is included in this parallel world now.  
7 /remoll/parallel/setfile geometry/mollerParallel.gdml ←  
8  
9 /remoll/physlist/parallel/enable ← Enable physics list  
10  
11 # This must be explicitly called  
12 /run/initialize ← Initialization  
13  
14 /remoll/printgeometry true  
15  
16 /control/execute macros/load\_magnetic\_fieldmaps.mac ← Magnetic field  
17  
18 # Raster and initial angle stuff  
19 {  
20 /remoll/oldras true ← Raster settings  
21 /remoll/rasx 5 mm  
22 /remoll/rasy 5 mm  
23 }  
24  
25 /remoll/evgen/set moller ← Event generators  
26 /remoll/evgen/thcommmin 80.0 deg  
27 /remoll/evgen/thcommmax 100.0 deg  
28  
29 /remoll/beamene 11 GeV ← Beam parameters  
30  
31 /remoll/beamcurr 85 microampere  
32  
33 # Make interactions with W, Cu, and Pb  
34 # realistic rather than pure absorbers  
35 /control/execute macros/HandsOn\_kryptonite.mac ← Setting Kryptonite material  
36  
37 ##disable all detectors,  
38 /remoll/SD/disable\_all ← Detector list  
39 /remoll/SD/enable 28  
40 /remoll/SD/enable 47  
41 /remoll/SD/print\_all  
42  
43 /process/list  
44  
45 # Specify random number seed  
46 /remoll/seed 123456  
47  
48 /remoll/filename remollout\_Moller\_gen\_2k.root ← Output file  
49 /remoll/target/print  
50 /run/beamOn 2000 ← # events to be simulated

## Modifying the Input macro file

- Simulation output file size can be reduced, if you know what sensitive detectors you want to record data
- We can first disable all the detector
- disable all detectors, /remoll/SD/disable\_all
- Then enable ones you want

/remoll/SD/enable 28

/remoll/SD/enable 470

- You can control what data you want to record for each detector

/remoll/SD/detect lowenergyneutral 28

/remoll/SD/detect secondaries 28

/remoll/SD/detect boundaryhits 28

- Enable kryptonite feature

/remoll/kryptonite/enable

- Then you can either turn certain materials into kryptonite

/remoll/kryptonite/add Tungsten

/remoll/kryptonite/add Copper

- You can also turn certain volumes into kryptonite by giving the name of the GDML solid shape

/remoll/kryptonite/volume name\_of\_the\_GDML\_solid\_shape

## How to run the simulation

- Goto remoll directory
- `./build/remoll destination+macro file name`
- This will start the simulation in batch mode
- We will do following simulations
  - a.Run 2000 moller electrons events
  - b.Run 2000 ep elastic electron events
- The output root files from these two jobs are also available at [Hands-On Materials](#) (Rootfilesremollout\_Moller\_gen\_2k.root and remollout\_Ep\_gen\_2k.root)
- Let us now try to see how the simulated data look like!

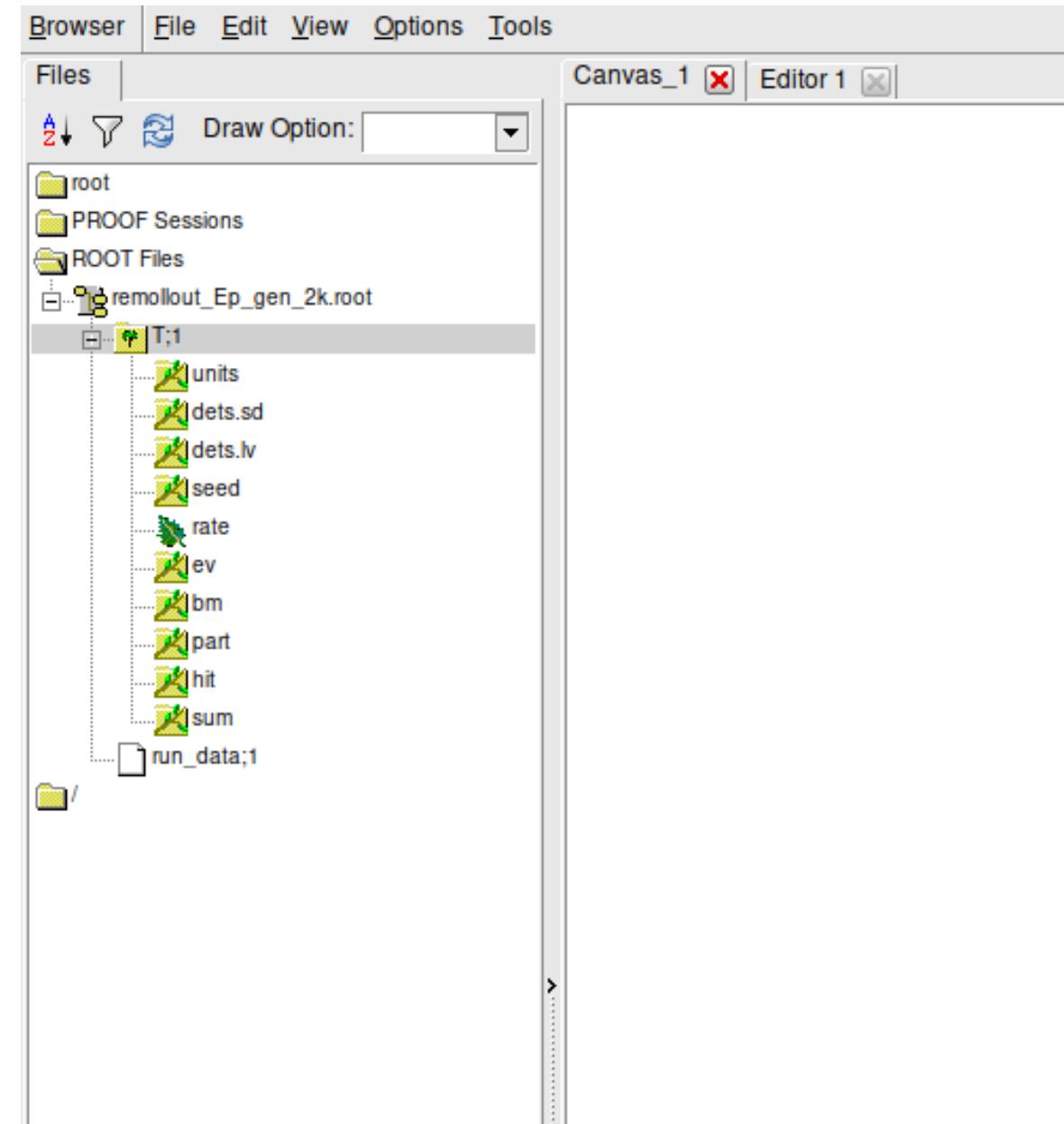
# Opening the root file generated after simulation & understanding the data structure

- Open a terminal using Alt+Crtl+T
- Goto ~/softwares/remoll
- Now we will open the root file using
- ./build/reroot HandsOn\_remollout\_10k.root  
reroot is root compiled with remoll libraries
- Type new TBrowser()

This will open the browser to see the data inside the root file

- Click on the tree elements (branches) to see the data in the form of histograms
- We can also access the data using the root command line:

- T->Print()
- T->Draw ("hit.p","hit.pid==11 && hit.det==28")
- T->Draw("hit.r","(hit.pid==11 && hit.det==28)\*rate","hist")
- Etc...



## Some examples on how to visualize the data using the ROOT command line!

Plot hit.vz (startZ vertex) of electrons hitting detector 28:

```
T->Draw("hit.vz","hit.pid==11 && hit.det==28")
```

Plot hit.p (momentum) of electrons hitting detector 28:

```
T->Draw("hit.p","hit.pid==11 && hit.det==28")
```

```
T->Draw("hit.p/GeV","hit.pid==11 && hit.det==28")
```

Plot hit.p (momentum) of electrons hitting detector 28 weighted by the rate so higher rate events gets higher weights and lower rate events gets a lower weight:

```
T->Draw("hit.p","(hit.pid==11 && hit.det==28)*rate","hist")
```

Plot hit.r (radius of hit) of electrons hitting detector 28 weighted by the rate so higher rate events gets higher weights and lower rate events gets a lower weight:

```
T->Draw("hit.r","(hit.pid==11 && hit.det==28)*rate","hist")
```

Plot 2D histogram to see correlation between momentum and radius at the detector 28:

```
T->Draw("hit.r:hit.p","(hit.pid==11 && hit.det==28)*rate","","")
```

```
T->Draw("hit.r:hit.p","(hit.pid==11 && hit.det==28)*rate","","")
```

How do we automate these steps? Use a root script (basicRootScript.C -> basic root script that we'll be using)

# ROOT scripting: Defining histograms

[basicRootScript.C](#) is our template script, we will create histograms of hit radius, xy 2D distribution and source vertex of these hits

Declare 1D histograms for radius and source vertex:

```
TH1D *r;  
TH1D *sourceZ;  
TH1D *rRate; //for rate weighted radial distribution
```

Declare 2D histograms for XY distribution:

```
TH2D *hXY;  
TH2D *hXYrate; //for rate weighted XY distribution
```

Let's define their parameters and create them initHisto() routine:

```
r = new TH1D("r","radial distribution;r[mm]",200,500,1500);  
sourceZ = new TH1D("sourceZ","initial vertex for hit ;z position [mm]",5000,-5500,-3500);  
hXY = new TH2D("hXY","2D hit distribution;x[mm];y [mm]",200,-2100,2100,200,-2100,2100);
```

Define rate weighted histograms:

```
rRate = new TH1D("rRate","rate weighted distribution;r[mm]",200,500,1500);  
hXYrate = new TH2D("hXYrate","rate weighted 2D hit distribution;x [mm];y [mm]",200,-2100,2100,200,-2100,2100);
```

## **ROOT scripting: Filling the histograms, scaling & plotting**

**Let's fill these histograms with data from the Tree in at the processOne(...) routine**

```
r->Fill(hit->at(j).r);
sourceZ->Fill(hit->at(j).vz);
hXY->Fill(hit->at(j).x,hit->at(j).y);
rRate->Fill(hit->at(j).r,rate);
hXYrate->Fill(hit->at(j).x,hit->at(j).y,rate);
```

**Scale rate weighted histograms if we have used chain of root files (more than one root file linked) in the void scale() routine:**

```
r->Scale(1./nFiles);
sourceZ->Scale(1./nFiles);
hXY->Scale(1./nFiles);
rRate->Scale(1./nFiles);
hXYrate->Scale(1./nFiles);
```

**Let's create few canvases to visualize the data:**

```
TCanvas *c1 = new TCanvas(); c1->Divide(1,2);
c1->cd(1); r->DrawCopy();
c1->cd(2); rRate->DrawCopy();
```

## **ROOT scripting: Saving plots as a root file**

**Output written in this step can be accessed later in a root file “basicRootScript.root”:**

```
r->Write();  
sourceZ->Write();  
hXY->Write();  
rRate->Write();  
hXYrate->Write();
```

**Output written in this step can be accessed later in a root file “basicRootScript.root”**

**This file name is set in the routine:**

```
void initHisto()  
string foutNm = Form("basicRootScript.root");
```

**You can access the saved histograms using the command:**

```
root basicRootScript.root  
or  
.build/reroot basicRootScript.root
```

## **Executing the analysis script**

**Load the script BasicRootScript.C:**

```
.L Analysis/basicRootScript.C
```

**Execute the script:**

```
basicRootScript("HandsOn_remollout_10k.root")
```

# **Modification of REMOLL geometry**

## Handling the GDML files

- Main geometry is kept in geometry/mollerMother.gdml parent file
- The parent or mother GDML file has set of daughter volumes containing different regions of the experiment
- A parallel GDML geometry is kept for intercept type sensitive detectors to observe particles crossing certain z-location
- Let us try to create a new sensitive detector of radius 600 mm with detector id of 470 located at 4600 mm in hall coordinates.
  - We use the parallel world to implement it

# **Steps to implement new sensitive detector in the geometry using GDML**

**Positioning : In the positions.xml file:**

```
<position name="TestSensDetVirtualPlane_pos" z="4600.0" unit="mm"/>
```

**Create the solid in the mollerParallel.gdml:**

```
<tube name="TestSensDetVirtualPlane_solid" startphi="0" deltaphi="360" aunit="deg" rmax="600" rmin="0" z="1" lunit="mm"/>
```

**Create the logical volume:**

```
<volume name="TestSensDetVirtualPlane_log">
  <materialref ref="G4_Galactic"/>
  <solidref ref="TestSensDetVirtualPlane_solid"/>
  <auxiliary auxtype="SensDet" auxvalue="planeDet"/>
  <auxiliary auxtype="DetNo" auxvalue="470"/>
</volume>
```

**Create the physical volume that will be placed within the simulation:**

```
<physvol name="TestSensDetVirtualPlane_phys">
  <volumeref ref="TestSensDetVirtualPlane_log"/>
  <positionref ref="TestSensDetVirtualPlane_pos"/>
</physvol>
```

# **Simulation & Analysis**

## A small simulation to get started with REMOLL

- Run simulation in batch mode to produce 2000 moller events with realistic materials
- Modify input macro file to change some realistic materials into Kryptonite
- Run simulation in batch mode to produce 2000 moller events with some materials converted to Kryptonite
- Run remoll in batch mode:  
`./build/remoll macros/HandsOn_run_moller.mac`
- Open macros/HandsOn\_run\_moller.mac in a text editor
- Remove # to uncomment the line /control/execute macros/HandsOn\_kryptonite.mac
- Change the output root file name to remollout\_Moller\_gen\_2k\_kryptonite.root
- Run remoll in batch mode:  
`./build/remoll macros/HandsOn_run_moller.mac`

[The output root files are available to download from here](#)

## Analysis of the simulated data

- We will look at Photons (pid=22) hitting the sensitive detector (det id 470) we created previously using GDML
- Use [RootScript.C](#) as a template script and create a root script relevant for above study
- Declare 1D & 2D histograms for radius, source vertex and XY distributions

```
TH1D *r;  
TH1D *sourceZ;  
TH1D *rRate; //for rate weighted radial distribution  
TH2D *hXY;  
TH2D *hXYrate; //for rate weighted XY distribution
```

- Defining the histograms

```
r = new TH1D("r","Det470 radial distribution;r[mm]",200,0,600);  
rRate = new TH1D("rRate","Det 470 rate weighted distribution;r[mm]",200,0,600);  
hXY = new TH2D("hXY","2D hit distribution;x [mm];y [mm]",200,-600,600,200,-600,600);  
hXYrate = new TH2D("hXYrate","rate weighted 2D hit ditribution;x [mm];y [mm]",200,-600,600,200,-600,600);  
sourceZ = new TH1D("sourceZ","initial vertex for hit ;z position [mm]",10000,-5300,8000);
```

- Cuts

```
if(hit->at(j).pid!=22) continue;  
if(hit->at(j).det != 470) continue;
```

## Analysis of the simulated data

- Fill the histograms

```
r->Fill(hit->at(j).r);
sourceZ->Fill(hit->at(j).vz);
hXY->Fill(hit->at(j).x,hit->at(j).y);
rRate->Fill(hit->at(j).r,rate);
hXYrate->Fill(hit->at(j).x,hit->at(j).y,rate);
```

- Create a canvas

```
Double_t w = 600;//width
Double_t h = 600;//height
TCanvas *p1 = new TCanvas("TCan_sourceZ","Source Z Canvas",w,h);
```

## Analysis of the simulated data

- Use the function: `gStyle->SetOptStat("nemr");` to format histogram stat box information: n-name, e-events, m-mean, r-rms
- Draw the vertex histogram on the p1 Canvas :

```
sourceZ->DrawCopy();
```

- You can save the canvas as an image to formats including pdf or png:

```
p1->SaveAs("TCan_sourceZ.png");
```

- Canvas with multiple pads:

```
TCanvas *p2 = new TCanvas("TCan_rate_xy","Radial and XY hits",w,h);
p2->Divide(2,2);
p2->cd(1);
r->DrawCopy();
p2->cd(2);
rRate->DrawCopy();
p2->cd(3);
hXY->DrawCopy();
p2->cd(4);
hXYrate->DrawCopy();
```

## Analysis of the simulated data

- How to run the analysis script
  - We will first run the script RootScript.C with root file remollout\_Moller\_gen\_2k.root
  - Give a unique name at string

```
foutNm = Form("RootScript_real.root");
```
  - Load the script RootScript.C

```
.L analysis/RootScript.C
```
  - Execute the script

```
RootScript("remollout_Moller_gen_2k.root")
```

**So now you have all the plots or at least you know how to make your required plots, so the next task is to explain them!!!**