JOINT INSTITUTE FOR NUCLEAR RESEARCH
Dzhelepov Laboratory of Nuclear Problems

FINAL REPORT ON THE START PROGRAMME

Simulation of X-ray spectrum using Geant4 toolkit

Supervisor:
Dr. Khushvaktov Jurabek. H.

Student:
Rasulova Dildora R.,
INP ASRU

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Abstract

A study dedicated to learn about Geant4 toolkit for the simulation of photon emission from W, Mo, and Rh material surface. The areas of application include energy from 1 keV until 10 MeV.

1. X-ray spectrum

X-rays (*X-radiation*) are a form of high-energy electromagnetic radiation. In many languages, it is referred to as ***Röntgen radiation***, after the German scientist Wilhelm Conrad Röntgen, who discovered it in 1895 and named it *X-radiation* to signify an unknown type of radiation.

X-ray wavelengths are shorter than those of ultraviolet rays and longer than those of gamma rays. There is no universally accepted, strict definition of the bounds of the X-ray band. Roughly, X-rays have a wavelength ranging from 10 nanometers to 10 picometers, corresponding to frequencies in the range of 30 petahertz to 30 exahertz (3×10^{16} Hz to 3×10^{19} Hz) and photon energies in the range of 100 eV to 100 keV, respectively.

X-rays can penetrate many solid substances such as construction materials and living tissue, so X-ray radiography is widely used in medical diagnostics (e.g., checking for broken bones) and material science (e.g., identification of some chemical elements and detecting weak points in construction materials).[3] However X-rays are ionizing radiation, and exposure to high intensities can be hazardous to health, causing damage to DNA, cancer, and at high dosages, burns and radiation sickness. Their generation and use strictly controlled by public health authorities.

Soft and hard X-rays. X-rays with high photon energies above 5–10 keV (below 0.2–0.1 nm wavelength) are called *hard X-rays*, while those with lower energy (and longer wavelength) are called *soft X-rays*.[73] The intermediate range with photon energies of several keV is often referred to as *tender X-rays*. Due to their penetrating ability, hard X-rays are widely used to image the inside of objects (e.g. in medical radiography and airport security). The term *X-ray* is metonymically used to refer to a radiographic image produced using this method, in addition to the method itself. Since the wavelengths of hard X-rays are similar to the size of atoms, they are also useful for determining crystal structures by X-ray crystallography. By contrast, soft X-rays are

easily absorbed in air; the attenuation length of 600 eV (~2 nm) X-rays in water is less than 1 micrometer.

Interaction with matter. X-rays interact with matter in three main ways, through photo-absorption, Compton scattering, and Rayleigh scattering. The strength of these interactions depends on the energy of the X-rays and the elemental composition of the material, but not much on chemical properties, since the X-ray photon energy is much higher than chemical binding energies. Photo-absorption or photoelectric absorption is the dominant interaction mechanism in the soft X-ray regime and for the lower hard X-ray energies. At higher energies, Compton scattering dominates.

*Photoelectric absorption***.** The probability of a photoelectric absorption per unit mass is approximately proportional to Z^3/E^3, where Z is the atomic number and is the energy of the incident photon. This rule is not valid close to inner shell electron binding energies where there are abrupt changes in interaction probability, so called absorption edges. However, the general trend of high absorption coefficients and thus short penetration depths for low photon energies and high atomic numbers is very strong. For soft tissue, photo-absorption dominates up to about 26 keV photon energy where Compton scattering takes over. For higher atomic number substances, this limit is higher. The high amount of calcium in bones, together with their high density, is what makes them show up so clearly on medical radiographs. A photo-absorbed photon transfers all its energy to the electron with which it interacts, thus ionizing the atom to which the electron was bound and producing a photoelectron that is likely to ionize more atoms in its path. An outer electron will fill the vacant electron position and produce either a characteristic X-ray or an Auger electron. These effects can be used for elemental detection through X-ray spectroscopy or Auger electron spectroscopy.

Compton scattering. Compton scattering is the predominant interaction between X-rays and soft tissue in medical imaging. Compton scattering is an inelastic scattering of the X-ray photon by an outer shell electron. Part of the energy of the photon is transferred to the scattering electron, thereby ionizing the atom and increasing the wavelength of the X-ray. The scattered photon can go in any direction, but a direction

similar to the original direction is more likely, especially for high-energy X-rays. The probability for different scattering angles is described by the Klein–Nishina formula. The transferred energy can be directly obtained from the scattering angle from the conservation of energy and momentum.

Rayleigh scattering. Rayleigh scattering is the dominant elastic scattering mechanism in the X-ray regime. Inelastic forward scattering gives rise to the refractive index, which for X-rays is only slightly.

Production by electrons. X-rays can be generated by an X-ray tube, a vacuum tube that uses a high voltage to accelerate the electrons released by a hot cathode to a high velocity. The high velocity electrons collide with a metal target, the anode, creating the X-rays. In medical X-ray tubes the target is usually tungsten or a more crack-resistant alloy of rhenium (5%) and tungsten (95%), but sometimes molybdenum for more specialized applications, such as when softer X-rays are needed as in mammography. In crystallography, a copper target is most common, with cobalt often being used when fluorescence from iron content in the sample might otherwise present a problem.

The maximum energy of the produced X-ray photon is limited by the energy of the incident electron, which is equal to the voltage on the tube times the electron charge, so an 80 kV tube cannot create X-rays with an energy greater than 80 keV. When the electrons hit the target, X-rays are created by two different atomic processes:

1. *Characteristic X-ray emission* (X-ray electroluminescence): If the electron has enough energy, it can knock an orbital electron out of the inner electron shell of the target atom. After that, electrons from higher energy levels fill the vacancies, and X-ray photons are emitted. This process produces an emission spectrum of X-rays at a few discrete frequencies, sometimes referred to as spectral lines. Usually, these are transitions from the upper shells to the K shell (called K lines), to the L shell (called L lines) and so on. If the transition is from 2p to 1s, it is called Kα, while if it is from 3p to 1s it is Kβ. The frequencies of these lines

depend on the material of the target and are therefore called characteristic lines. The Kα line usually has greater intensity than the Kβ one and is more desirable in diffraction experiments. Thus, the Kβ line is filtered out by a filter. The filter is usually made of a metal having one proton less than the anode material (e.g., Ni filter for Cu anode or Nb filter for Mo anode).

2. *Bremsstrahlung*: This is radiation given off by the electrons as they are scattered by the strong electric field near the nuclei. These X-rays have a continuous spectrum. The frequency of *Bremsstrahlung* is limited by the energy of incident electrons.

So, the resulting output of a tube consists of a continuous *Bremsstrahlung* spectrum falling off to zero at the tube voltage, plus several spikes at the characteristic lines. The voltages used in diagnostic X-ray tubes range from roughly 20 kV to 150 kV and thus the highest energies of the X-ray photons range from roughly 20 keV to 150 keV.

Both of these X-ray production processes are inefficient, with only about one percent of the electrical energy used by the tube converted into X-rays, and thus most of the electric power consumed by the tube is released as waste heat. When producing a usable flux of X-rays, the X-ray tube must be designed to dissipate the excess heat. A specialized source of X-rays which is becoming widely used in research is synchrotron radiation, which is generated by particle accelerators. Its unique features are X-ray outputs many orders of magnitude greater than those of X-ray tubes, wide X-ray spectra, excellent collimation, and linear polarization.[89] Short nanosecond bursts of X-rays peaking at 15 keV in energy may be reliably produced by peeling pressure-sensitive adhesive tape from its backing in a moderate vacuum. This is likely to be the result of recombination of electrical charges produced by triboelectric charging. The intensity of X-ray triboluminescence is sufficient for it to be used as a source for X-ray imaging.

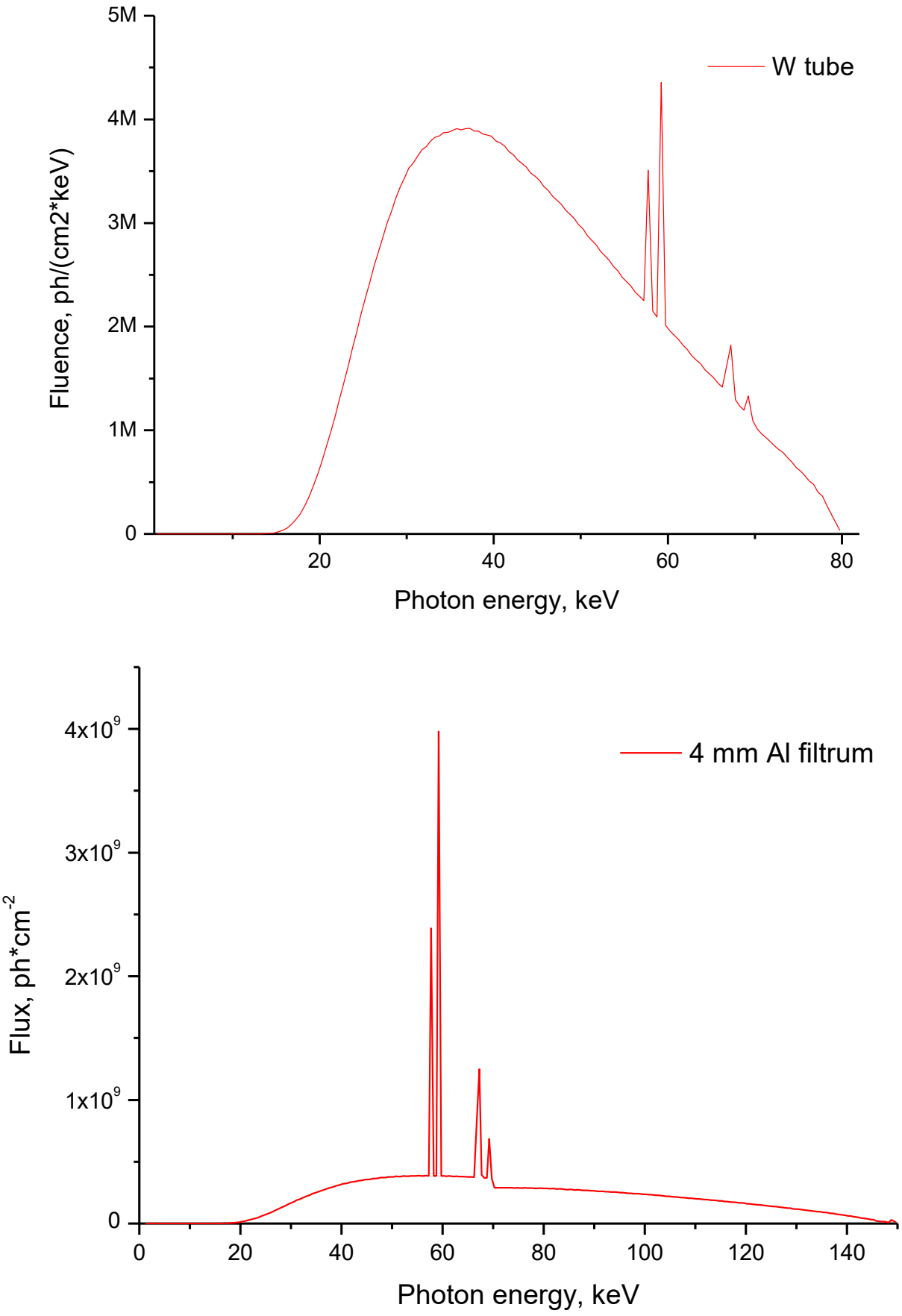


Figure 1. Spectrum of X-tubes simulated using Geant program toolkit.

2. Geant4 toolkit

2.1. Electromagnetic Physics

The GEANT4 set of electromagnetic (EM) physics processes and models are used in practically all types of simulation applications including high energy and nuclear physics experiments, beam transport, medical physics, cosmic ray interactions and radiation effects in space. In addition to models for low and high energy EM physics for simulation of radiation effects in media, a sub-library of very low energy models was developed within the framework of the GEANT4-DNA project, with the goal of simulating radiation effects involving physics and chemistry at the sub-cellular level. In the early stages of GEANT4, low and high energy EM processes were developed independently, with the result that these processes could not be used in the same run. To resolve this problem, the interfaces were unified so that the standard, muons, highenergy, lowenergy, and dna EM physics sub-packages now follow the same design. Migration to this common design resulted in an improvement of overall CPU performance, and made it possible to provide several helper classes which are useful for a variety of user applications (for example G4EmCalculator).

General design. The electromagnetic processes of GEANT4 follow the basic interfaces:

- G4VEnergyLossProcess;
- G4VEmProcess;
- G4VMultipleScattering.

The class diagram is shown in Fig.1. These common interfaces for all EM sub-packages enabled the full migration of EM classes to multi-threading without significant modification of existing physics model codes. Initialization of the energy loss, stopping power and cross section tables is carried out only once in the master thread at the beginning of simulation.

These tables are shared between threads in run time.

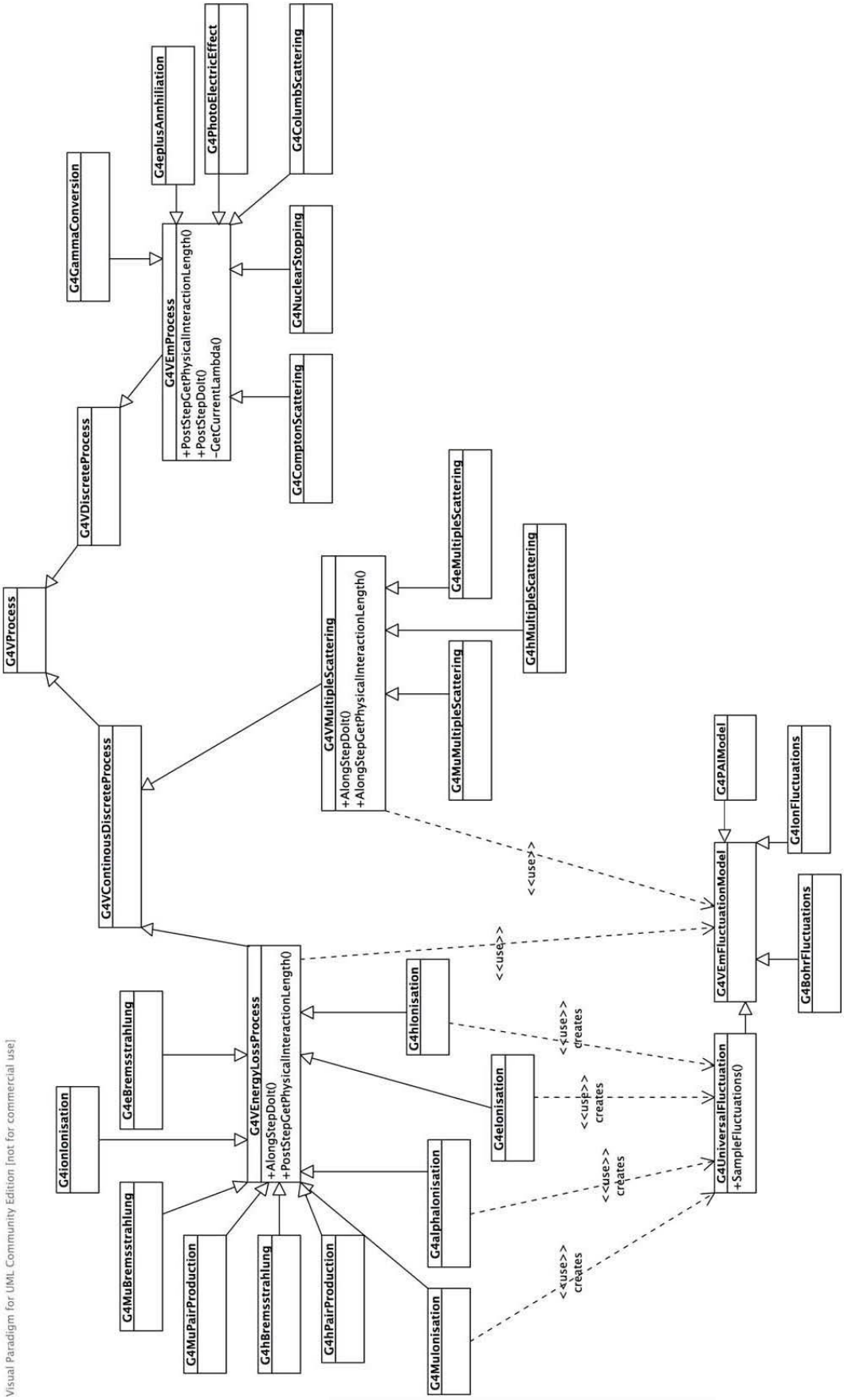


Figure 1. Design of EM physics processes

Electromagnetic processes. These base classes provide all management work of initialisation of processes, creation and filling of physics tables, and generic run-time actions. Concrete process classes are responsible for the initialisation of parameters and defining the set of models for the process. It is strongly recommended to use existing processes and not create a new one for each new model. Here is a list of main EM processes:

• G4PhotoelectricEffect;
• G4ComptonScattering;
• G4GammaConversion;
• G4GammaConversion;
• G4RayleighScattering;
• G4eIonisation;
• G4eBremsstrahlung;
• G4hIonisation;
• G4MuIonisation;
• G4hIonisation;
• G4MuBremsstrahlung;
• G4eMultipleScattering;
• G4MuMultipleScattering.

More processes are provided in lowenergy, polarisation, and adjoint sub-libraries. In some specific cases, interfaces described above are not applicable and the high-level interface G4VProcess is used. Any concrete physics process class may need custom parameters. It is recommended to define following parameters specific to the class in the class constructor:

- process sub-type;
- buildTables flag;
- secondary particle type;
- min/max energy of cross section tables;
- number of bins in tables;

• flag to force zero cross section in the low edge ofa table.

Any EM process should implement following methods:

• IsApplicable(const G4ParticleDefinition& p)

• ProcessDescription()

Main initialisation of a process is performed by initialisation methods:

• InitialiseEnergyLossProcess

• InitialiseProcess

In these methods a default set of EM models and their energy intervals of applicability may be defined. It is strongly recommended that a process class cannot change EM parameters in G4EmParameters class or status of the deexcitation module. EM parameters can be modified in physics lists or via UI commands.

3. Simulation algorithm

Implementation of the Sensitive Detector in Geant4

In the MySensitiveDetector() class, the primary goal is to capture and record the kinetic energy of the particles passing through a specified detector volume. The following steps outline the process implemented in the code.

*Tracking Particle Information***.** The class first retrieves the current particle track using the G4Track object. Specifically, the kinetic energy of the particle is extracted using the GetKineticEnergy() method. This energy is then converted to units of keV by dividing by the constant CLHEP::keV.

Storing Data. To record the kinetic energy, the Geant4 G4AnalysisManager is used. This class handles the output of data to an ntuple for further analysis. The energy value is stored in the first column (indexed as 0) of the ntuple with the FillNtupleDColumn() function, followed by the addition of a new row in the ntuple via the AddNtupleRow() method.

Returning the Result. The function then returns true, signaling that the sensitive detector has successfully processed the current step.

This implementation allows for efficient data collection of kinetic energy during the simulation, ensuring that relevant information about particle interactions is stored for subsequent analysis.

```
14
15  G4bool MySensitiveDetector::ProcessHits(G4Step* step, G
16  {
17    G4Track* track = step->GetTrack();
18    auto kine = track->GetKineticEnergy()/CLHEP::keV;
19
20      G4AnalysisManager* analysisManager = G4AnalysisMana
21      analysisManager->FillNtupleDColumn(0, 0, kine);
22      analysisManager->AddNtupleRow(0);
23      return true;
24  }
```

Figure 2. Code written in MySensitiveDetector.hh

Physical Model Description. In the following section, we describe the construction of the simulation geometry and the materials used for defining the experimental setup in Geant4.

Materials. The materials are initialized using the G4NistManager, which provides predefined materials based on the NIST database. In this simulation, the following materials are used:

- **Vacuum**: Represented by "G4_Galactic", used for the world volume and sensitive detector.
- **Tungsten (W)**: Used in other parts of the setup, although not specifically placed in this version of the code.
- **Molybdenum (Mo)**: Another material available but not directly used in the code snippet.
- **Rhodium (Rh)**: This material is used for the target

Geometry Construction. The geometry consists of three primary components: the world volume, the target, and the sensitive detector.

- **World Volume**:

  The world volume is a simple cubic box with dimensions of 1 cm×1 cm×2 cm1. It is filled with vacuum ("G4_Galactic") and serves as the container for all other physical volumes.
- **Target**:

  The target is a small rhodium layer with dimensions of 1 cm×1 cm×100 μm. The target volume is placed at the origin inside the world volume.
- **Sensitive Detector**:

  The sensitive detector is represented by a vacuum volume of dimensions, placed at a distance of 200 μm from the target. This detector will capture interactions of interest during the simulation.
- **Sensitive Detector Setup**:

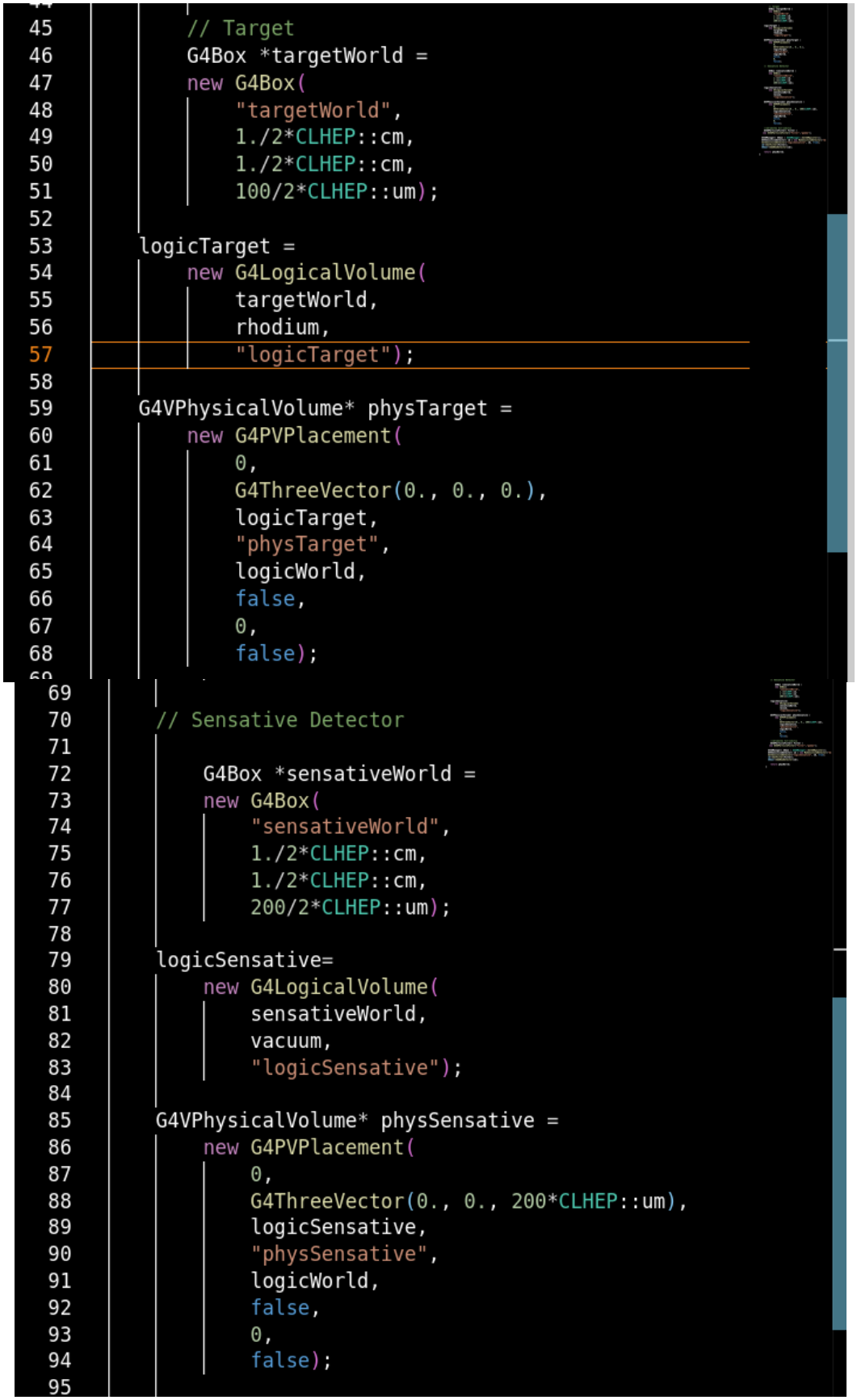
  To monitor particle interactions within the sensitive detector, a custom sensitive detector class (MySensitiveDetector) is implemented. A particle filter is applied

to restrict detection to gamma particles, ensuring that only relevant interactions are recorded.

The sensitive detector is created and assigned to the logical volume of the sensitive detector.A filter for gamma particles ("gamma") is applied using the G4SDParticleFilter class.

This setup ensures that the necessary materials and detector geometry are properly defined and ready for further simulations involving particle interactions.

```
10  void PhysicalConstruction::DefineMaterials() {
11      G4NistManager* nist = G4NistManager::Instance();
12
13      vacuum = nist->FindOrBuildMaterial("G4_Galactic");
14      wolfram = nist->FindOrBuildMaterial("G4_W");
15      molibden = nist->FindOrBuildMaterial("G4_Mo");
16      rhodium = nist->FindOrBuildMaterial("G4_Rh");
17
18  }
19
20  G4VPhysicalVolume* PhysicalConstruction::Construct() {
21      G4Box *solidWorld =
22          new G4Box(
23              "solidWorld",
24              1./2*CLHEP::cm,
25              1./2*CLHEP::cm,
26              2/2*CLHEP::cm);
27
28      logicWorld =
29          new G4LogicalVolume(
30              solidWorld,
31              vacuum,
32              "logicWorld");
33
34      G4VPhysicalVolume* physWorld =
35          new G4PVPlacement(
36              0,
37              G4ThreeVector(0., 0., 0.),
38              logicWorld,
39              "physWorld",
40              0,
41              false,
42              0,
43              false);
```



```
45          // Target
46          G4Box *targetWorld =
47          new G4Box(
48              "targetWorld",
49              1./2*CLHEP::cm,
50              1./2*CLHEP::cm,
51              100/2*CLHEP::um);
52
53      logicTarget =
54          new G4LogicalVolume(
55              targetWorld,
56              rhodium,
57              "logicTarget");
58
59      G4VPhysicalVolume* physTarget =
60          new G4PVPlacement(
61              0,
62              G4ThreeVector(0., 0., 0.),
63              logicTarget,
64              "physTarget",
65              logicWorld,
66              false,
67              0,
68              false);
69
70      // Sensative Detector
71
72          G4Box *sensativeWorld =
73          new G4Box(
74              "sensativeWorld",
75              1./2*CLHEP::cm,
76              1./2*CLHEP::cm,
77              200/2*CLHEP::um);
78
79      logicSensative=
80          new G4LogicalVolume(
81              sensativeWorld,
82              vacuum,
83              "logicSensative");
84
85      G4VPhysicalVolume* physSensative =
86          new G4PVPlacement(
87              0,
88              G4ThreeVector(0., 0., 200*CLHEP::um),
89              logicSensative,
90              "physSensative",
91              logicWorld,
92              false,
93              0,
94              false);
95
```

Figure 3. Code written in PhysicalConstruction.hh

Run Action Implementation. The RunAction class in Geant4 manages the initialization and finalization of data processing during the simulation. In this case, the class handles the opening and closing of the output file, as well as writing the collected data to the file at the appropriate times. The following outlines the functionality implemented in the RunAction class:

1. **Beginning of Run**:

   At the start of each run, the BeginOfRunAction() method is called. In this method, the G4AnalysisManager instance is used to open a ROOT file (output.root), where all the analysis results will be stored. The file remains open throughout the run, allowing the collection of data from the simulation.
2. **End of Run**:

   Once the simulation run is complete, the EndOfRunAction() method is invoked. This method instructs the G4AnalysisManager to write all the recorded data (such as histograms and ntuples) to the ROOT file and then closes the file to ensure data integrity and proper storage.

RunAction class is essential for managing the output of simulation data. By opening the file at the beginning and closing it at the end of the run, it ensures that all the data is properly collected and stored for later analysis.

```
14  void RunAction::BeginOfRunAction(const G4Run* aRun) {
15      G4AnalysisManager* analysisManager = G4AnalysisMana
16      analysisManager->OpenFile("output.root");
17      //fHistoManager->Book();
18  }
19
20  void RunAction::EndOfRunAction(const G4Run* aRun) {
21      G4AnalysisManager* analysisManager = G4AnalysisMana
22      analysisManager->Write();
23      analysisManager->CloseFile();
24      //fHistoManager->Save();
25  }
```

Figure 4. Code written in RunAction.hh

Particle Source Setup. The particle source in this simulation is configured using the Geant4 General Particle Source (GPS) commands. The following configuration defines an electron beam with specific energy, position, and direction for the simulation. The key components of the setup are as follows:

1. **Particle Type**:
   The particle type is set to electrons (e-) using the /gps/particle command.
2. **Energy**:
   A monoenergetic source is used, meaning that all particles are generated with the same kinetic energy of 10 MeV. This is defined by the following commands:
3. **Position**:
   The source of the electrons is placed at a specific point in space, located at coordinates (0, 0, -1 cm). This is specified using the /gps/pos/type Point and /gps/pos/centre commands.
4. **Angular Distribution**:
   The angular distribution is set to be planar, meaning that the particles are emitted along a specific direction. In this case, all particles travel along the positive z-axis, defined by the vector (0, 0, 1).
5. **Simulation Run**:
   The /run/beamOn command is used to initiate the simulation with a total of 1,000,000 electron events. This ensures that a sufficient number of particles are simulated to gather statistically significant results.

In summary, this configuration creates a monoenergetic electron beam with a well-defined position and direction, simulating a beam directed along the z-axis towards the target. The high number of simulated events ensures the collection of a robust dataset for subsequent analysis.

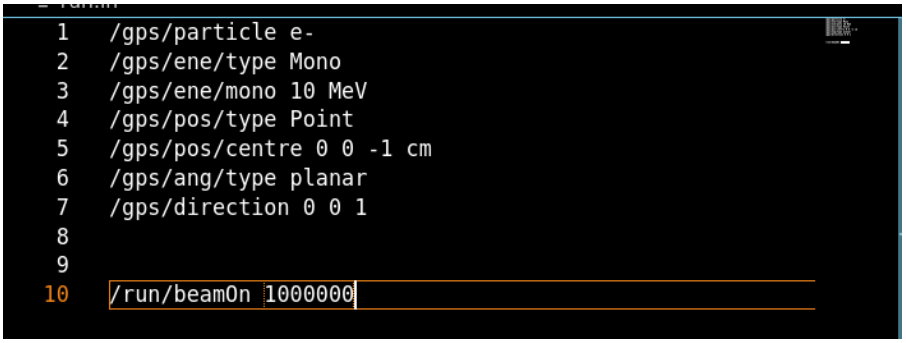


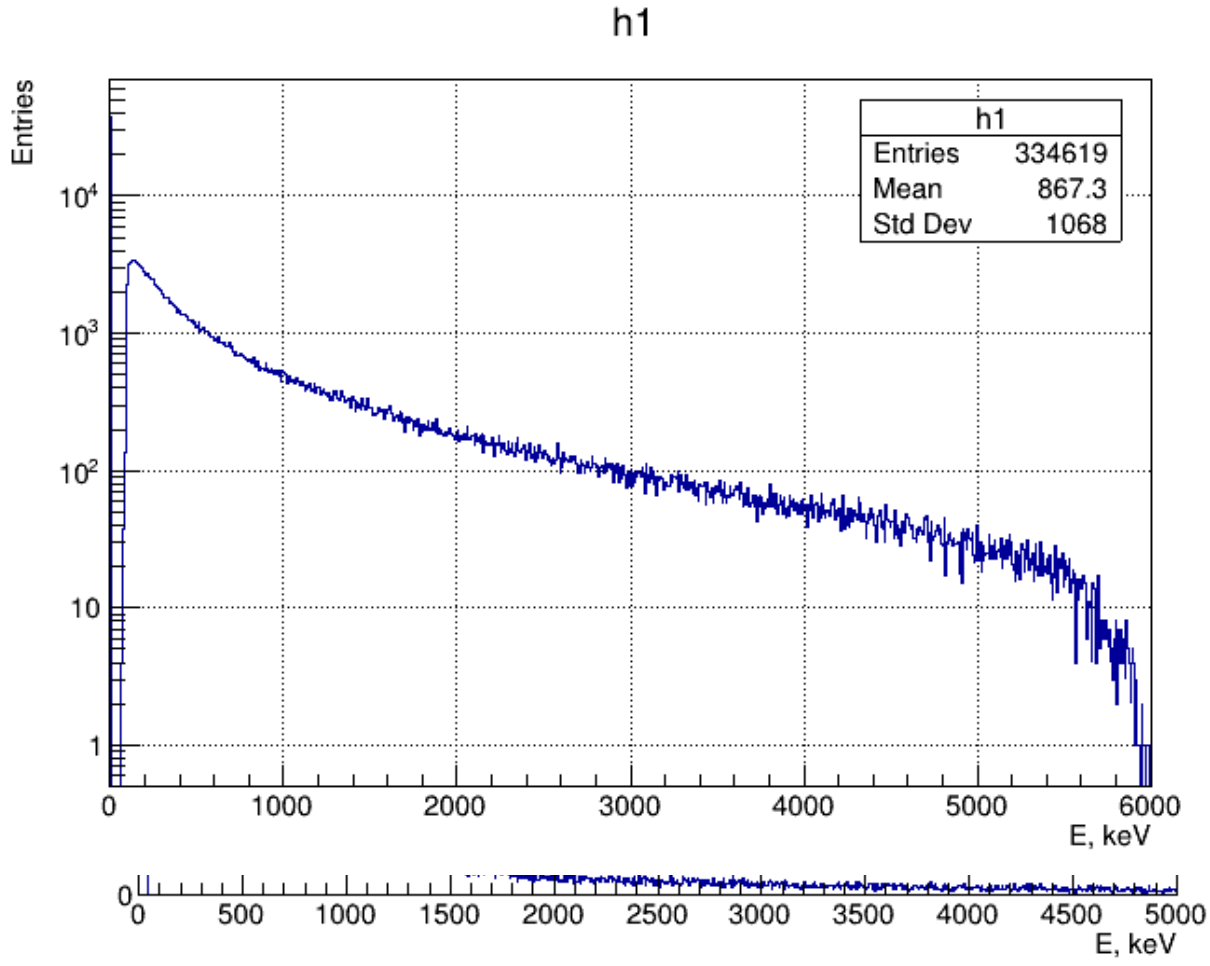
Figure 5. Code written in run,in

4. Results

The simulations were conducted for various X-ray tube target materials, including **tungsten (W)**, **rhodium (Rh)**, and **molybdenum (Mo)**. These materials were chosen due to their widespread use in medical imaging and radiation therapy applications. The incident electron beam energies used in the simulations were **6 MeV**, **5 MeV**, **8 MeV**, and **10 MeV**.

Each simulation evaluated the interaction of high-energy electrons with the respective material targets, focusing on the resulting X-ray spectra and energy deposition profiles. The electron beam was configured to be monoenergetic and directed towards the target. These simulations provide insight into the efficiency and behavior of these materials under varying energy conditions.

In the Fig.6 , the graphical results will be presented, showing the X-ray spectra and energy distributions for each material at the specified electron energies.



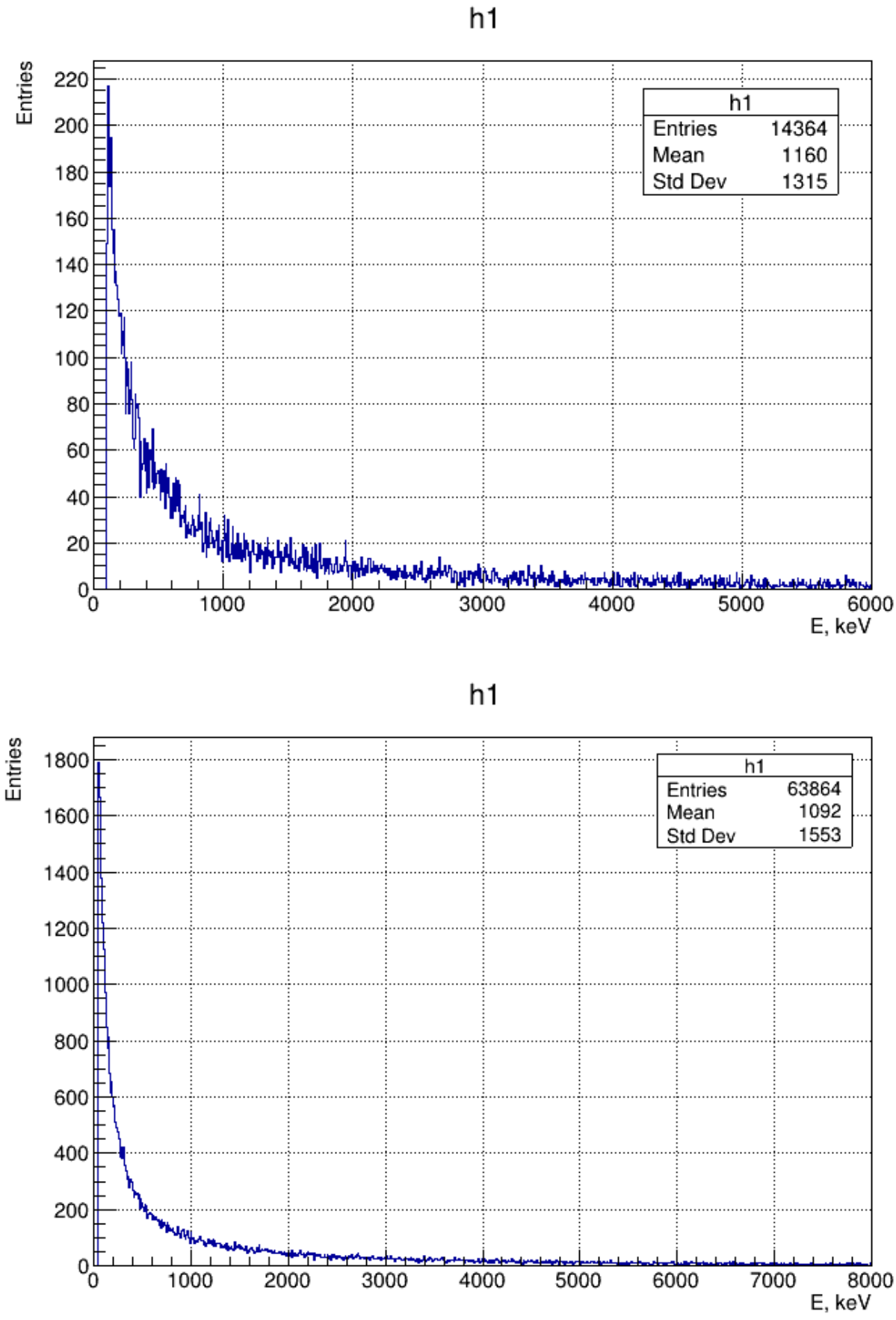


Figure 6. Energy of emitted photon fron W, Mo, and Rh material surface

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