- $_typical_2012 _neutron_2010 _neutron_1999 _comparative_1982 _geant4simulation_2003 _collaboration_1982 _geant4simulation_2003 _collaboration_2003 _collaboration_200$
- ${\tt geant4_2011_geant4_2006_physics_2012_reference_2008_detector_2012_scintillations_1951_recoil_1980}$

3	Energy Deposition in Polymers	
4	Matthew J. Urffer	
5	December 10, 2012	
6	Todo list	
7	Expand this section	10

8 Contents

9	1	Introduction	7
10 11 12	2	Previous Work 2.1 Spectra Measurements	
13	3	Introduction to GEANT4	10
14	Ū		10
15		3.2 GEANT4 Tracking and Secondaries	_
16	4	Methods	12
17		4.1 GEANT4 Implementation	12
18		4.1.1 Detector Geometry	12
19			13
20		4.1.3 Primary Event Generator	14
21		4.2 Sensitive Detectors and Hits	15
22		4.3 Analysis	17
23		4.4 Determination of Energy Deposition	18
24	5	Simulation Validation	21
25		5.1 Energy Deposition Validation	21
26		5.2 Spectra Validation	21
27	6	Results	23
28		6.1 Energy Deposition	23
29		6.2 Secondary Electron Energy Distribuion	23
30	7	Conclusions	24

131 List of Figures

32	1	Spectra properties as a function of film thickness	8
33	2	Gamma intrinsic efficiency (dashed lines) plotted against neutron counts (solid)	8
34	3	Single-collision energy loss spectra for electrons in water [?]	8
35	4	Average and median energy transfer in liquid water as functions of incident-electron energy [?]	9
36	5	World, Calorimeter, Layer and Absorber and Gap	13
37	6	10 Layer Detector with a simulated gamma event	13
38	7	Single Collision Energy Loss of Water	21
39	8	Gamma Simulation Agreement	22
40	9	Neutron Simulation Agreement	22
41	10	Simulated Energy Depositon for a Single Film (gammas)	23
42	11	Simulated Energy Depositon for a Single Film (neutrons)	23
43	12	Simulated kinetic energies of electrons from ⁶⁰ Co interactions	23
44	13	Comparison between average neturon and gamma energy deposition	24

$_{45}$ List of Tables

46	1	Replacement Detector Requirements [?]	7
47	2	Maximum Energy of Secondary Electrons from Compton Scattering	7

48 Listings

49	1	Tracking Example	1
50	2	World Physical Volume	2
51	3	Calorimeter Volume	2
52	4	Layer Volume	3
53	5	Absorber and Gap Volumes	
54	6	Implemented Physics List	4
55	7	Implemented Physics List	4
56	8	Primary Event Generator	4
57	9	Generate Primaries	ļ
58	10	Calorimeter Hit	ļ
59	11	Sensitive Detector	.(
60	12	Creating Sensitive Detectors	7
61	13	Event Action	7
62	14	Run Action	8
63	15	Process Hit Collection	8
64	16	Run Macro	ç

$_{\scriptscriptstyle{5}}$ 1 Introduction

A typical day in 2011 saw 932,456 people enter into the U.S. (258,191 by air 48,073 by sea, and 621,874 by land) in addition to 64,483 truck, rail and sea containers and 253,821 privately-owned vehicles [?]. Any one of these could be a pathway of special nuclear material to enter the U.S. The interdiction of special nuclear material is desirable before the materials enters into the transportation infrastructure of the U.S. and interdiction becomes more complex. Radiation Portal Monitors (RPMs) are passive radiation detection systems implemented at over a thousand border crossings designed to determine if cargo contains any nuclear material in a safe, nondestructive and effective manner[?]. The Department of Homeland Security (DHS) continues to fund research through the Domestic Nuclear Detection Office (DNDO) in order to develop replacement technologies for the current ³He RPMs as ³He cannot be economically replaced. There are several alternatives to ³He being considered, and all, with the exception of gas filled proportional detectors, involve the detection of neutrons from scintillation events of the energy deposited in the material from the neutron absorption reaction. These detectors (among other requirements outline in Table 1) must be able to effectively discriminate between gamma (which can occur in medical isotopes) and neutrons (indictive of special nuclear material).

Table 1: Replacement Detector Requirements [?]

Parameter	Specification
Absolute neutron detection efficiency	$2.5 \text{ cps/ng of } ^{252}\text{Cf}$
Intrinsic gamma-neutron detection efficiency	$\epsilon_{int,\gamma n} \le 10^{-6}$
Gamma absolute rejection ratio for neutrons	$0.9 \leq \text{ GARRn } \leq 1.1 \text{ at } 10 \text{ mR/h exposure}$
(GARRn)	
Cost	\$ 30,000 per system

Neutron detectors often utilize a material doped with an isotope of large thermal cross section for absorption such as ⁶Li or ¹⁰B. When these materials absorb a neutron the nucleus of the isotope becomes unstable and fissions into reaction products. These reaction products (having an initial kinetic energy from the Q-value of the neutron absorption reaction) travel through the material, transferring their kinetic energy to the material. Photon interactions in the detector occur when a photon scatters off a single electron in a Compton scattering event (Table 2). This Compton electron then produces a cascade of secondary electrons in the material, which, depending upon the energy, may or may not deposit a majority of its energy in the detector. The difference in the transfer of kinetic energy from charged particle to electrons and from photon interactions (Compton scattering) to electrons introduces an opportunity to exploit the difference in energy deposition in order to maximize the discrimination between neutron and photon interactions in a detector.

Table 2: Maximum Energy of Secondary Electrons from Compton Scattering

	Photon Energy (MeV)	Maximum Compton Energy (MeV)
$^{-137}\mathrm{Cs}$	0.662	0.478
$^{60}\mathrm{Co}$	1.17, 1.33	0.960, 1160

This document is organized as follows. A brief overview of the interaction of charged particles in matter will be provided in Section 2, as well as some preliminary experiments demonstrating the range of secondary electrons in neutron-gamma discrimination. The GEANT4 toolkit was used for the modeling of the energy deposition. Section 3 will provide an overview of the GEANT4 toolkit. Section 4 will provide details on how the GEANT4 toolkit was implemented for this particular simulation, as well as providing validation of the calculations performed by the GEANT4 toolkit in Section 5. In Section 6 the results of this model applied to a single film will demonstrate the enhanced ability of neutron-gamma discrimination through secondary electrons.

$_{ iny 98}$ 2 Previous Work

Previous work on the energy deposition of thin films focused on spectra measurements from fabricated films along with single collision energy loss spectra for physical insights. A sequence of 10% 6 LiF, 5% PPO-POPOF films in a PS matrix cast to thickness between 15 and 600 μ m were fabricated and the response was measured from a gamma source as well as a neutron source. These experiment results are shown in 2.1. The single collision energy loss spectra was investigated for electrons in water in order to provide insight on the amount of energy an electron loses in a collision. These results are discussed in Section 2.2.

2.1 Spectra Measurements

Evidence that the secondary electrons contribute to energy loss can be seen in Figure 1 where there is an increase in the endpoint of the spectra as films become thicker. This increase in the spectra endpoint is indicative of the film producing more light, and as the light collection geometry remained constant, the increase in the endpoint is attributed to a larger energy deposition in the 50 μ m film compared to the 15 μ m or 25 μ m film. Figure 2 shows the intrinsic efficiency of these film from spectra obtained from a ⁶⁰Co

(a) Beta (³⁶Cl) Spectra Endpoints for PS films (b) Gamma (⁶⁰Co) Spectra Averages for PS films

Figure 1: Spectra properties as a function of film thickness

source. As the film thickness increases the pulse height discriminator at which an intrinsic efficiency of one in a million ($\epsilon_{int,\gamma} \leq 10^{-6}$) is reached also increases. The neutron spectra (shown in the solid lines) does not increase in light yield with increasing thickness, further providing an indication that the thickness of the films can be optimized to maximize the neutron count rates¹ while minimizing the response of the detector to photons.

Figure 2: Gamma intrinsic efficiency (dashed lines) plotted against neutron counts (solid)

2.2 Single Collision Energy Loss

Single collision energy loss spectra provides the probability that that a given collision will result in an energy loss. Provided a spectra of secondary electrons from either the Compton scattered electron or the ⁶Li reaction products it is then possible to determine the average energy loss per collision. A single collision energy loss spectra for water is shown in Figure 3. For low electron energies (< 50 eV) it is very probable that the electron will lose a majority of its energy in a single collision. More energetic electrons, however, tend to lose a lower fraction of there total energy. A Compton scattered photon, with an energy in the 100's of keV range, will then lose far less energy per collision than an electron in the low keV range liberated from the passage of a neutron reaction product through the material. When the average and median energy transfer are plotted

Figure 3: Single-collision energy loss spectra for electrons in water [?]

as a function of incident electron energy (Figure 4) the difference in the energy loss spectra becomes more apparent. For low energies (up to an incident electron energy of 100 eV) the average and median energy transfer are roughly equal to each other, about half of the incident electron. Past 100 eV average energy increases faster than the median energy transfer implying that while a few collisions result in large energy transfers most of the collisions do not. It is also interesting to note that the average and median do not increase linearly with the incident energy past 100 eV (the ordinate axis is a log scale). In fact, the average

¹The neutron count rate is increased with thickness by the increased mass of the detector

energy transferred per collision is mostly bounded by 60 eV even for incident electron energies of 10 keV. This is significant because it implies that high energy electrons from photon events will deposit a small fraction of their energy in the material.

Figure 4: Average and median energy transfer in liquid water as functions of incident-electron energy [?]

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3 Introduction to GEANT4

GEANT4 (GEomentry ANd Tracking) is a free, open source, Monte Carlo based physics simulation toolkit 135 developed and maintained at CERN widely used in the physics community [?, ?, ?]. It is based off of 136 the existing FORTRAN based GEANT3, but updated to an object-oriented C++ environment based on 137 an initiative started in 1993. The initiative grew to become an international collaboration of researchers 138 participating in a range of high-energy physics experiments in Europe, Japan, Canada and the United States. 139 As GEANT4 is a toolkit primarily developed for high energy physics, particles are designated according 140 the PDG (Particle Data Group) encoding. In addition, the physics processes are referenced according to the 141 standard model. In the standard model particles are divided into two families, bosons (the force carriers such 142 as photons) and fermions (matter). The fermions consist of both hadrons and leptons. Hadrons are particles 143 composed of quarks which are divided into two classes: baryons (three quarks) and mesons (two quarks).h 144 Typical baryons include the neutron and the proton, while an example of a meson is the pion. An example of a lepton is the electron. 146

₇ 3.1 Organization of the GEANT4 Toolkit

8 The GEANT4 toolkit is divided into eight class categories:

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- Run and Event generation of events and secondary particles.
- Tracking and Track transport of a particle by analyzing the factors limiting the step size and by applying the relevant physics models.
- Geometry and Magnetic Field the geometrical definition of a detector (including the computation of the distances to solids) as wells as the management of magnetic fields.
- Particle Definition and Matter definition of particles and matter.
- Hits and Digitization the creation of hits and their use for digitization in order to model a detector's readout response.
 - Visualization the visualization of a simulation including the solid geometry, trajectories and hits.
 - Interface the interactions between the toolkit and graphical user interfaces and well as external software.

There are then three classes which must be implemented by the user in order use the toolkit. These classes are:

- G4VUserDetectorConstruction which defines the geometry of the simulation,
- G4VUserPhysicsList which defines the physics of the simulation, and
- G4VUserPriamryGeneratorAction which defines the generation of primary events.

Five additional classes are available for further control over the simulation:

Expand this section

• G4UserRunAction which allows for user actions

3.2 GEANT4 Tracking and Secondaries

A GEANT4 simulation starts with a run which contains a set number of events. An event is particular process of interest to the user, such as shooting a single particle at a detector. Typical usage might be to have a run firing 1,000 neutrons at a detector, where each neutron is a single event. Each particle transported in GEANT4 is assigned a unique track ID and a parent ID. The particle that initiates the event is given a parent ID of 0 and a track ID of 1. If the parent particle has a collision, and produces a secondary particle, this secondary particle is then given a parent ID of 1 (corresponding to the first secondary) and a track ID of

2. Secondaries are tracked in GEANT4 utilizing a stack in which the most recent secondary (and its cascade) is tracked first.

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Listing 1 provides an example from the verbose output of GEANT4 of the tracking. The initial particle in the event is the neutron because it has a parent ID of 0. The alpha and triton are the secondaries produced by this collision. The alpha is assigned a parent ID of 1 (corresponding to the first generation) with a track ID of 3. The triton is also assigned a parent ID of 1, but with a track ID of 2.

Listing 1: Tracking Example 180 181 182 * G4Track Information: formation: Particle = neutron, Track ID = 1, Parent ID = 0 $Parent\ ID\ =\ 0$ 183 184 $\begin{array}{ccc} Z\,(mm) & \text{Kin}\,E\,(\text{MeV}) \\ -6.59 & 2.5\,e\,-08 \\ -3.64 & 0 \end{array}$ $\begin{array}{ccc} \mathrm{dE}\,(\mathrm{MeV}) & \mathrm{StepLeng} & \mathrm{TrackLeng} \\ 0 & 0 & 0 \end{array}$ NextVolumeAbsorber Absorber 186 2.95 2.95 187 NeutronInelastic #SpawnInStep= -3.64 2.73 -3.64 2.05 2(Rest= 0, Along= 0, Post= 2), triton 190 alpha 191 EndOf2ndaries Info -192 193 Particle = alpha 194 * G4Track Information: Track ID = 3, Parent ID = 1 195 196 197 dE(MeV) StepLeng TrackLeng Step# X(mm) Y(mm) Z(mm) KinE(MeV) NextVolume ProcName -3.64 -3.64 -3.642.05 2.01 1.93 Absorber initStep Absorber ionIoni Absorber ionIoni 198 $\begin{smallmatrix} 0.0491 & 0.000266 \\ 0.0705 & 0.000381 \end{smallmatrix}$ 0.000266 0.000647 202 * G4Track Information: Particle = triton Track ID = 2, Parent ID = 2030 204 2052 $Z (mm) \quad \text{KinE} (MeV) \\ -3.64 \quad 2.73 \\ -3.64 \quad 2.7$ dE(MeV) StepLeng TrackLeng 206 X(mm) $Y\left(mm\right)$ NextVolume ProcName 0 0 1 0.000339 Absorber initStep Absorber hIoni -0.0002150.0116 0.000447 0.000447 388

Methods 4 210

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A discussion of the steps necessary to implement the simulation of energy deposition in GEANT4 follows. 211 This involved writing the code for the simulation, as well as correctly interpreting the output. As such, this 212 section is organized by first examining the process of setting up the simulation and then will go into the 213 analysis of the results from the toolkit. 214

4.1 **GEANT4** Implementation

A large focus of this work was on creating a working simulation of the GEANT4 toolkit. Preliminary attempts were made to install GEANT4 on a Windows based machine linking to Microsoft Visual Studio. While these attempts were successful, a larger scale computing environment was desired. GEANT4 was then installed on the University of Tennessee's nuclear engineering computing cluster, along with 219 the necessary visualization drivers and data files. Brief documentation on compiling simple examples on the cluster are available at the necluster wiki ². For convenience a subversion repository was created to manage the developed code base, and all source code is available by anonymous checkout from http://www.murphs-code-repository.googlecode.com/svn/trunk/layeredPolymerTracking. Revision 360 was the code base used to generate the results shown. The following section provides implementation specific details of the code base used to simulate the energy deposition in thin films. It is organized according to the three base classes that a user must implement in GEANT4, namely G4VUserDetectorConstruction, G4VUserPhysicsList, and G4VUserPrimaryGeneratorAction.

4.1.1**Detector Geometry**

A detector geometry in GEANT4 is made up of a number of volumes. The largest volume is the world volume which contains all other volumes in the detector geometry. Each volume (an instance of G4VPhysicalVolume) is created by assigning a position, a pointer to the mother volume and a pointer to its mother volume (or NULL if it is the world volume). A volume's shape is described by G4VSolid, which has a shape and the specific values for each dimension. A volume's full properties is described by a logical volume. A G4LogicalVolume includes a pointer to the geometrical properties of the volume (the solid) along with physical characteristics including:

- the material of the volume,
- sensitive detectors of the volume and,
- any magnetic fields.

Listing 2 provides the implementation of the world physical volume. The geometry was set up such that it is 230 possible to define multiple layers of detectors, as shown in Figure 6. 240

```
Listing 2: World Physical Volume
        // World
242
        worldS = new G4Box("World", worldSizeXY, worldSizeXY, worldSizeZ*0.5);
243
        worldLV = new G4LogicalVolume(worldS, defaultMaterial, "World");
244
                  new G4PVPlacement(0,G4ThreeVector(),worldLV,"World",0,false,0,fCheckOverlaps);
345
```

The detector was described by creating creating a single layer of neutron absorber and gap material and 247 placing it in another volume (the calorimeter). The containing volume (calorimeter) was placed inside of the 248 the physical world (Listing 3).

```
Listing 3: Calorimeter Volume
250
           Calorimeter (gap material)
        caloS = new G4Tubs("Calorimeter", iRadius, oRadius, caloThickness/2, startAngle, spanAngle);
252
```

²It should be noted that this example uses the CMAKE build system (as per the GEANT4 recommendation) but a large majority of the examples still use GNUMake for building. This can be accomplished by adding source /opt/geant4/geant4-9.5p1/share/Geant4-9.5.1/geant4make/geant4make.sh to the user's .bashrc.

```
caloLV = new G4LogicalVolume(caloS,gapMaterial, "Calorimeter");
caloPV = new G4PVPlacement(0,G4ThreeVector(),caloLV, "Calorimeter",worldLV,false,0,
fCheckOverlaps);
```

The calorimeter was the mother volume for each layer. The code was developed such that the simulation of multiple layers can be easily set at compile time or by utilizing a run macro through the DetectorMessenger class. Multiple repeated volume can be achieved in GEANT4 through G4PVReplica or G4PVParameterised. As each of the layers had the same geometry, G4PVReplica was chosen as the implementation (Listing 4).

```
Listing 4: Layer Volume
261
        // Layer (Consists of Absorber and Gap)
262
        layerS = new G4Tubs("Layer", iRadius, oRadius, layerThickness/2, startAngle, spanAngle);
263
        layerLV = new G4LogicalVolume(layerS, defaultMaterial, "Layer");
264
        if (nofLayers > 1){
265
            layerPV = new G4PVReplica("Layer",layerLV,caloLV,kZAxis,nofLayers,layerThickness,-
266
                 caloThickness/2);
267
268
            layerPV = new G4PVPlacement(0,G4ThreeVector(0.0,0.0,0.0),layerLV,"Layer",caloLV,
269
                 false,0,fCheckOverlaps);
271
```

Finally, the neutron absorber and gap material were defined as single cylinders which were then placed in the layer mother volume (Listing 5). The size of these solids (and the materials) could be set either at compile time through DetectorConstruction constructor or by using the DetectorMessenger in the run macro. Figure 6 shows a rendering of the 10 layers of the detector with the trajectories from a gamma event.

```
Listing 5: Absorber and Gap Volumes
277
278
        // Absorber
        absS = new G4Tubs("Abso", iRadius, oRadius, absThickness/2, startAngle, spanAngle);
279
        absLV = new G4LogicalVolume(absS,absMaterial,"Absorber",0);
280
        absPV = new G4PVPlacement(0,G4ThreeVector(0.0,0.0,-gapThickness/2),absLV,"Absorber",
281
282
            layerLV, false, 0, fCheckOverlaps);
283
        // Gap
284
285
        gapS = new G4Tubs("Gap",iRadius,oRadius,gapThickness/2,startAngle,spanAngle);
        gapLV = new G4LogicalVolume(gapS,gapMaterial,"Gap",0);
286
        gapPV = new G4PVPlacement(0,G4ThreeVector(0.0,0.0,absThickness/2),gapLV,"Gap",layerLV,
287
            false.0.fCheckOverlaps):
388
```

Figure 5: World, Calorimeter, Layer and Absorber and Gap

Figure 6: 10 Layer Detector with a simulated gamma event

4.1.2 Physics Lists

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The user of the GEANT4 toolkit is responsible for selecting the proper physics processes to model in the PhysicsList. This is unlike other transport codes (such as MCNPX) where basic physics are enabled by default and the user only has select the appropriate cards. However, GEANT4 does provide examples of implemented PhysicsLists as well as modular physics lists which provide a way to construct a physics list by combing physics list. Thus, extensive use of G4ModularPhysicsList was employed to handle the assigning of the physics processes to each particle in the correct order. The physics lists chosen for this simulation are listed below:

• G4EmStandardPhysics The electromagnetic physics defines the electrons, muons, and taus along with their corresponding neutrinos. For electrons, the primary concern of this simulation, multiple scattering,

electron ionization, and electron bremsstrahlung processes were assigned. In addition the positron is defined and the multiple scattering process, electron ionization process, electron bremsstrahlung process and positron annihilation is assigned [?].

- G4EmLivermorePhysics The Livermore physics process extend the EMStandardPhysics down to low (250 eV) energies. Even lower energies can be reached by including G4DNAPhysics. The physics processes extended with G4EmLivermorePhysics are the photo-electric effect, Compton scattering, Rayleigh scattering, gamma conversion, Ionisation and Bremsstrahlung[?].
- HadronPhysicsQGSP_BERT_HP Hadronic physics are included to model the nuclear interactions. The chosen list is a Quark Gluon String Model for energies in the 5-25 GeV range, with a Bertini cascade model until 20 MeV. Once a hadron has an energy of 20 MeV the high precision cross section driven models are applied[?].
- G4IonPhysics Finally, to handle the transport of the charged ions resulting from an $^6\text{Li}(n,\alpha)^3\text{H}$ interaction the G4IonPhysics list was used.

```
313
314
     * PhysicsList
315
316
317
       Constructs the physics of the simulation
318
    PhysicsList::PhysicsList() : G4VModularPhysicsList() {
319
        currentDefaultCut
320
                             = 10*nm;
321
322
        // Adding Physics List
        //RegisterPhysics( new G4EmDNAPhysics());
323
324
        RegisterPhysics( new G4EmStandardPhysics());
        RegisterPhysics( new G4EmLivermorePhysics());
325
        RegisterPhysics( new HadronPhysicsQGSP_BERT_HP());
        RegisterPhysics( new G4IonPhysics());
327
328
```

Finally, the default cut range was decreased from 1 cm to 1 nm in SetCuts() (Listing 7)

```
Listing 7: Implemented Physics List

331
332 1
void PhysicsList::SetCuts() {
SetDefaultCutValue(10*nm);
}

333
336 3
}
```

4.1.3 Primary Event Generator

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The user is responsible for telling the simulation toolkit the primary event to generate. While there is great flexibility to generate any source distribution, a particle gun was chosen for simplicity. G4ParticleGun generates primary particle(s) with a given momentum and position without any randomization. The implementation of this is shown in Listing 8.

```
341
                  {\tt Primary Generator Action:: Primary Generator Action(): G4VU ser Primary Generator Action(), and a series of the series of t
                                     fParticleGun(0) {
343
344
                           G4int nofParticles = 1;
                           fParticleGun = new G4ParticleGun(nofParticles);
345
346
347
                            // default particle kinematic
                           G4ParticleDefinition* particleDefinition = G4ParticleTable::GetParticleTable()->
348
349
                                               FindParticle("e-");
                           fParticleGun -> SetParticlePosition(G4ThreeVector(0.,0.,0.0));
350
351
                           fParticleGun -> SetParticleDefinition (particleDefinition);
                           fParticleGun -> SetParticleMomentumDirection (G4ThreeVector (0.,0.,1.));
352
```

```
fParticleGun->SetParticleEnergy(50.*MeV);
}
```

Actual primary particles are generated with GeneratePrimaries, which uses the G4ParticleGun to determine the vertex of the primary event.

```
Listing 9: Generate Primaries
   void PrimaryGeneratorAction::GeneratePrimaries(G4Event* anEvent)
359
360
      // This function is called at the begining of event
361
362
      // In order to avoid dependence of PrimaryGeneratorAction
363
      // on DetectorConstruction class we get world volume
364
      // from G4LogicalVolumeStore
365
      G4double worldZHalfLength = 0;
366
      G4LogicalVolume* worlLV = G4LogicalVolumeStore::GetInstance()->GetVolume("World");
367
368
      G4Box* worldBox = 0;
      if ( worlLV) worldBox = dynamic_cast < G4Box*>(worlLV->GetSolid());
369
370
      if ( worldBox ) {
        worldZHalfLength = worldBox->GetZHalfLength();
371
372
373
      else
        G4cerr << "World volume of box not found." << G4endl;
374
        G4cerr << "Perhaps you have changed geometry." << G4endl;
375
        G4cerr << "The gun will be place in the center." << G4endl;
376
377
3782
      // Set gun position
379
3802
      fParticleGun->SetParticlePosition(G4ThreeVector(0., 0., -worldZHalfLength+1*cm));
      fParticleGun -> GeneratePrimaryVertex(anEvent);
381
382
```

4.2 Sensitive Detectors and Hits

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GEANT4 offers a myriad of different ways to output the results of a simulation. It is possible to write out every track with the Verbose = 1 option, create MultiFunctionalDetector and G4VPrimitiveScorer, or implement a hit and readout based approach [?]. Previous GEANT4 experience included G4VHit and G4VSensitiveDetector, so this approach was used in this simulation. A hit is defined to be a snapshot of the physical interaction of a track in a sensitive region of a detector. As the user is responsible for implementing G4VHit the hit can contain any information about the step, including:

- the position and time of the step,
- the momentum and energy of the track,
- the energy deposition of the step,
- or information about the geometry.

For this simulation any information about the particle that could be recorded was recorded. This included the energy deposition, position of the hit, momentum, kinetic energy, track ID, parent ID, particle definition, volume and copy number (Listing 10).

```
Listing 10: Calorimeter Hit
398
399
    * @brief - Hit: a snapshot of the physcial interaction of a track in the sensitive region
400
         of a detector
401
402
       Contians:
403
404
        - Particle Information (type and rank (primary, secondary, tertiary ...))
        - Positon and time
405
        - momentum and kinetic energy
406
```

```
- deposition in volume
407 8
408
          geometric information
409
410
    class CaloHit : public G4VHit {
411.2
      public:
        CaloHit(const G4int layer);
412
413
        ~CaloHit():
414
        inline void* operator new(size_t);
415
        inline void operator delete(void*);
416
        void Print();
417
418
      private:
41920
        G4double edep;
                                          /* Energy Deposited at the Hit */
420
        G4ThreeVector pos;
                                            /* Position of the hit */
42122
        G4double stepLength;
                                            /* Step Length */
422
        G4ThreeVector momentum;
                                              /* Momentrum of the step */
4230
        G4double kEnergy;
                                                /* Kinetic Energy of the particle */
424
        G4int trackID;
                                          /* Track ID */
4252
        G4int parentID;
                                                /* Parent ID */
426
4272
            G4ParticleDefinition* particle;
                                                    /* Particle Definition */
                                                /* Primary, Secondary, etc */
        G4int particleRank;
428
        G4VPhysicalVolume* volume;
                                            /* Physical Volume */
42930
                                                /* Copy Number of Layer */
430
        G4int layerNumber;
43B2
432
        // Setter and Getters
4338
434
43586
    typedef G4THitsCollection < CaloHit > CaloHitsCollection;
436
    extern G4Allocator < CaloHit > HitAllocator;
4373
438
    inline void* CaloHit::operator new(size_t){
43910
      void *aHit;
440
      aHit = (void *) HitAllocator.MallocSingle();
44142
442
      return aHit;
44314
444
   inline void CaloHit::operator delete(void *aHit){
44516
446
      HitAllocator.FreeSingle((CaloHit*) aHit);
   }
447
```

The G4VSensitiveDetector is attached to a logical volume and is responsible for filling the hit collection.
This is accomplished in ProcessHits of CaloSensitiveDetector (Listing 11).

```
Listing 11: Sensitive Detector
451
    * ProcessHits
453
454
    * Adds a hit to the sensitive detector, depending on the step
455
456
   G4bool CaloSensitiveDetector::ProcessHits(G4Step* aStep,G4TouchableHistory*){
457
458
        G4double edep = aStep->GetTotalEnergyDeposit();
459
        G4double stepLength = aStep->GetStepLength();
460
461
        // Getting the copy number
462
        G4TouchableHistory* touchable = (G4TouchableHistory*)
463
464
             (aStep->GetPreStepPoint()->GetTouchable());
        G4int layerIndex = touchable -> GetReplicaNumber(1);
465
466
        // Creating the hit
467
        CaloHit* newHit = new CaloHit(layerIndex);
468
        newHit->SetTrackID(aStep->GetTrack()->GetTrackID());
469
        newHit->SetParentID(aStep->GetTrack()->GetParentID());
470
471<sup>2</sup>
        newHit ->SetEdep(edep);
        newHit ->SetStepLength(stepLength);
472
```

```
newHit->SetPosition(aStep->GetPreStepPoint()->GetPosition());
47322
        newHit->SetLayerNumber(layerIndex);
474
        newHit->SetMomentum(aStep->GetPreStepPoint()->GetMomentum());
475
476
        newHit->SetKineticEnergy (aStep->GetPreStepPoint()->GetKineticEnergy());
        newHit->SetParticle(aStep->GetTrack()->GetDefinition());
4772
        newHit->SetVolume(aStep->GetTrack()->GetVolume());
478
479
        // Adding the hit to the collection
480
        hitCollection -> insert( newHit );
4813
482
        return true;
4838
   }
484
```

The simulation was designed so that a separate sensitive detector was assigned to the gap and absorber. While this is not strictly necessary as the geometric position determines what layer of the gap or absorber the hit occurred in, this made the analysis code easier to write. A separate method was written in DetectorConstruction to create the sensitive detectors and assign them to the proper logical volumes (Listing 12) SetSensitiveDetectors() is called from the the constructor of DetectorConstruction.

```
Listing 12: Creating Sensitive Detectors
491
492
     * SetSensitiveDetectors
493
494
495
       Setting the Sensitive Detectors of the Detector
496
    void DetectorConstruction::SetSensitiveDetectors(){
497
        G4SDManager* SDman = G4SDManager::GetSDMpointer();
498
499
        absSD = new CaloSensitiveDetector("SD/AbsSD", "AbsHitCollection");
        SDman -> AddNewDetector(absSD);
500
        absLV->SetSensitiveDetector(absSD);
501
502
        gapSD = new CaloSensitiveDetector("SD/GapSD", "GapHitCollection");
503
        SDman -> AddNewDetector(gapSD);
504
505
        gapLV->SetSensitiveDetector(gapSD);
589
```

4.3 Analysis

Analysis of hit collection was preformed with ROOT. Once again there are other options (notably Open-Scientist) but previous experience was why ROOT was selected as the base for the Analysis framework. A singleton class was written for the analysis which processed the hit collections, assigning the various results to root histograms. User action classes EventAction and RunAction are called at the beginning and end of each run and event, respectively (Listing 13,14). These classes allowed for the analysis code to be independent of the simulation.

```
EventAction::EventAction() : G4UserEventAction(){
516
        // Nothing to be Done Here
517
518
519
520
     * BeginOfEventAction
521
522
       @param const G4Event* event - event to be processed
523
      At the begining of an event we want to clear all the event
525
       accumulation variables.
526
527
   void EventAction::BeginOfEventAction(const G4Event* event){
528
        Analysis::GetInstance()->PrepareNewEvent(event);
529
530
531
```

```
532
     * EndOfEventAction
533
534
535
       @param const G4Event* event - event to be processed
5362
       At the end of an event we want to call analysis to proccess
537
5382
      this event, and record the useful information.
539
    void EventAction::EndOfEventAction(const G4Event* event){
5402
        Analysis::GetInstance()->EndOfEvent(event);
541
   }
543
```

```
Listing 14: Run Action
    RunAction::RunAction() : G4UserRunAction(){ }
545
546
    void RunAction::BeginOfRunAction(const G4Run* run){
547
      G4cout << "Starting run: " << run->GetRunID() << G4endl;
548
549
        Analysis::GetInstance()->PrepareNewRun(run);
550
551
    void RunAction::EndOfRunAction(const G4Run* aRun){
552
553
        Analysis::GetInstance()->EndOfRun(aRun);
554
```

₆ 4.4 Determination of Energy Deposition

559

The energy deposition of an event is calculated by the sum of all of the energy deposited by individual hits in the sensitive detector (Equation 1). While it is possible to break down the energy deposition by which physics process caused the deposition, this was not implemented in order to avoid over complication.

$$E_{\text{dep,event}} = \sum E_{\text{dep,hit}}$$
 (1)

ProcessHitCollection is called at the end of each event (Listing 15). Each hit is accessed and the layer at which it occurs is determined³. In addition the name of the volume is determined, and the energy deposition of the hit is added to the energy deposition of the event. If the hit occurred in the absorber layer and the particle is an electron the kinetic energy of that hit is also recorded.

```
561
     * ProcessHitCollection
563
564
       @param G4VHitsCollection *hc
565
566
    void Analysis::ProcessHitCollection(G4VHitsCollection *hc,G4int eventID){
567
568
        // Looping through the hit collection
569
        G4double hitColEDepTot_Abs[NUMLAYERS+1];
                                                       // Total EDep (abs) for Hit Collection
570
                                                       // Total EDep (gap) for Hit Collection
        G4double hitColEDepTot_Gap[NUMLAYERS+1];
571
        G4int PID;
                                                       // Parent ID
572
        for(int i= 0; i < NUMLAYERS+1; i++){</pre>
573
574
            hitColEDepTot_Abs[i] = 0.0;
            hitColEDepTot_Gap[i] = 0.0;
575
576
577
        // Energy Deposition of the event
578
        for(G4int i = 0; i < hc->GetSize(); i++){
579
            CaloHit* hit = (CaloHit*) hc->GetHit(i);
580
581
            G4double eDep = hit->GetEdep();
582
```

³C arrays start at 0, so memory is allocated for one more than the total number of layers. This allows for NUMLAYERS+1 to be used an index into the histogram for the total of all layers in the material (either gap or absorber).

```
G4int layerNum = hit->GetLayerNumber();
583
            if (strcmp(hit->GetVolume()->GetName(), "Gap")){
584
                 // Hit occured in the Gap
585
5862
                 hitColEDepTot_Gap[layerNum] += eDep;
                 (hHitTotEDepGap[layerNum]) -> Fill(eDep);
587
            }else if(strcmp(hit->GetVolume()->GetName(), "Absorber")){
588
                 // Hit occured in the Abs
589
                 hitColEDepTot_Abs[layerNum] += eDep;
59Œ
                 (hHitTotEDepAbs[layerNum]) -> Fill(eDep);
591
5928
                 /* Is this a secondary electron of the event? */
593
                 if(hit->GetParticle()->GetPDGEncoding() == 11){
5943
                     PID = hit->GetParentID();
595
                     if (PID < NUMPID){</pre>
5963
                          (hSecElecKinAbs[layerNum][PID]) -> Fill(hit->GetKineticEnergy());
597
598
                 }
599
            }
6003
            else{
601
                 G4cout << "ERROR - Unkown Volume for sensitive detector" << G4end1;
602
603
        }
604
605
        // Adding this Hit collection's energy deposited to event total
606
        for (int i = 0; i < NUMLAYERS; i++){</pre>
607
            // Incrementing each individual bin
608
            eventEDepTot_Abs[i] += hitColEDepTot_Abs[i];
609
             eventEDepTot_Gap[i] += hitColEDepTot_Gap[i];
610
611
            // Last bin is Calorimter Total (all Abs layers and all Gap layers)
6125
            eventEDepTot_Abs[NUMLAYERS] += hitColEDepTot_Abs[i];
            eventEDepTot_Gap[NUMLAYERS] += hitColEDepTot_Gap[i];
6145
        }
615
   }
819
```

Finally, a run macro was written to control the entire run (Listing 16). The material and thickness of the detector are declared (made possible by the use of DetectorMessenger), and then the detector is dynamically updated. A ⁶⁰Co source is simulated by shooting photons of the 1.1732 MeV and 1.3325 MeV. The source particle is then changed to a neutron, and thermal (0.025 eV) neutrons are shot at the detector. The thickness of the absorber is then increased, the geometry updated, and the entire process repeated. As these runs tend to take a large amount of time, GEANT4 was parallelized for use with MPI to take advantage of the cluster computing power.

618

620

622

623

624

```
Listing 16: Run Macro
625
626
    /tracking/verbose 0
627
628
   # Setting up the detector
629
630
    /PolymerTransport/det/setAbsMat PS_Detector
631
    /PolymerTransport/det/setGapMat G4_POLYSTYRENE
632
    /PolymerTransport/det/setGapThick 0.3175 cm
633
634
    /PolymerTransport/det/setAbsThick 15 um
635
636
   /PolymerTransport/det/update
    # Cobalt 60
637
   /gun/particle gamma
638
   /gun/direction 0 0 1
639
   /gun/energy 1.1732 MeV
    /run/beamOn 500000000 # 500 Million
641
    /gun/energy 1.3325 MeV
642
    /run/beamOn 500000000 # 500 Million
643
   # Neutron
644.9
   /gun/particle neutron
   /gun/energy 0.025 eV
64621
   /run/beamOn 1000000 # 1 Million
```

```
648:3 # /PolymerTransport/det/setAbsThick 25 um /FolymerTransport/det/update /FolymerTransport/det/update
```

5 Simulation Validation

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GEANT4 is a toolkit implemented by the user so extensive efforts were completed in order to validate the results and ensure no bugs exists. First steps were taken (for small runs) to compute the energy deposition for small runs by hand in order to make sure they agreeded with the analysis code. In addition the reaction products of the $^6\text{Li}(n,\alpha)^3\text{H}$ were checked to make sure that they agreeded with the published values 4 . The GEANT4 simulation was validated by comparing the single collision energy loss spectra in water and by comparing the simulation energy deposition to that of a measured spectra.

5.1 Energy Deposition Validation

The energy deposition was tested by reproducing the single collision energy loss spectra in water⁵. The PhysicsList was extended to include G4DNAPhysics and the detector material was set to the NIST definition contained in the toolkit with G4Material* H2O = man->FindOrBuildMaterial("G4_WATER"). In general there was excellent agreement between the simulated energy spectra and a previously published spectra[?]. The simulated spectra had much better resolution at fine energies (corresponding to discrete states) of which Turners did not.

(b) Single-collision energy loss spectra for electrons in water [?]

(a) Simulated

(c) Published

Figure 7: Single Collision Energy Loss of Water

5.2 Spectra Validation

The simulated energy deposition is not the directly equivilant to light collected on the PMT because the scintillation process and light collection is not modeled. However, it is well known that scintillation follows the energy deposition[?]. Thus, up to scaling contants, the energy deposition can be considered equivilant to the scintillation and representative of the measured spectra. Rather than attempting to back out these scaling contants the weighted average of spectra were used in which integration and normalization removes these fudge factors. The simulation was validated by computing the weighted average of the energy deposition 2 and comparing it to the spectra average defined in 3. There is excellent agreement between the measured gamma weighted average (right ordinate axis) and the average energy deposition from a 60 Co source (left ordinate axis). Non-linearity is observed for films less than 200 μ m, this is evidance that the cascade electrons from the Compton electron are energetic enough that the range of the electrons is much greater than the thickness of the film and leave the film without colliding to an energy in which the energy deposition is linear (Figure 4).

$$\langle E \rangle = \frac{\int_0^\infty \phi(E)EdE}{\int_0^\infty \phi(E)dE}$$
 where (2)

$$<\mu> = \frac{\int_0^\infty f(x)xdx}{\int_0^\infty x(x)dx}$$
 where (3)

The comparison between the average energy deposition and measured channel allows for the a relationship to be drawn between the energy deposited and the channel number. This is completed by an taking an average

⁴GEANT4 4.9.2.p01 contains an error in which extra photons are generated, This has been fixed in the release used, 4.9.5p1
⁵An analysis class was not written for this simulation. Instead the verbosity of the simulation was set to verbose=1 in the run macro. The first ionisation collision (e-_G4DNAIonisation) was then extracted with sed -n '/ParentID = 0/,/e-_-G4DNAIonisation/p' G4OutputFileName.txt| grep "e-_G4DNAIonisatioin" | awk '\${print \$5}' '

Figure 8: Gamma Simulation Agreement

Figure 9: Neutron Simulation Agreement

of the ratio between the average channel number (Equation 3 and the average energy deposition (Equation 2). This ratio is defined in Equation 4. This quantity is defined separately for neturons and gammas.

$$\eta = \sum_{t} \frac{\langle E \rangle}{\langle \mu} \tag{4}$$

$_{58}$ 6 Results

6.1 Energy Deposition

The energy deposition was calcutated for neutron and gamma events for films of thickness of 15 μ m, 25 μ m, 50 μ m, 300 μ m, 600 μ m, 1 mm and 1 cm (Figure 10, 11).

Photons have a very low probability of interacting in the film due to polymer film being a low z-material. This is reflected in the majority of the events not interacting at all; about 1 in 10,000 of the events deposit energy in the film as seen in Figure 10. Several classic features of the spectra are apparent on the 1 cm thick thin. These included the photo-peak in which all of the incident energy of the 60 Co is deposited in the film, as well as the individual Compton edges of the two photons from 60 Co. These features are not visiable on the measured spectra due to the poor energy resolution of these films. There is also physical evidance of a lack of a Compton edge on the thinner films, but the films greater than 150 μ mthick show some feature around 0.2 MeV. Films thinner than 150 μ mshow a very small amount of energy deposition that quickly tails off for higher energies, indicating that when a photon interaction occurs in the film the electrons from that interaction leave the film and the only energy deposition occurs from small ionizations as the highly energetic electron leaves the film material. It is also observed that the thinnest film (15 μ m) has an average energy deposition of around 10 keV, while the 1 cm film has an average energy deposition of around 150 keV. The simulated energy deposition for neutron interactions in thin films is shown in Figure

Figure 10: Simulated Energy Depositon for a Single Film (gammas)

11. Several features of the spectra can be immediately noted. For thick films (1 cm) there is a very high probability that a given event will deposit all of its energy in the film (as expected). Thinner films have a smaller probability of depositing all of their energy, but this is overshawded by the thick samples when plotted. It is also intresting to note that it is possible to observe the comparative effects of the the α and ³H in the neutron energy deposition spectra. The triton has a much shorter range ($\tilde{1}0 \mu \text{min PS}$ [?]) than the α ($\tilde{6}0 \mu \text{m}$) so it has a higher probability of depositing all of its energy. Thus, for energies above 2.73 MeV (the energy of the triton) there is a higher probability of energy energy deposition (by about a factor of 10). These events are still very infrequent compared to the probability of depositing all of the reaction product energy. Even for the 15 μ mthe average energy deposition was above 50% of the total Q-value of the reaction, and by 200 μ mthis average energy deposited approaches 95% of the total 4.78 MeV.

Figure 11: Simulated Energy Depositon for a Single Film (neutrons)

6.2 Secondary Electron Energy Distribuion

The distribution of secondary electrons from photon interactions are plotted in Figure 12. From these results it can be concluded that the it is unlikely (around 1 in 10,000) that an electron will be scattered with the maximum Compton scattering kinetic energy, but rather have an energy somewhat lower than that. The distribution of secondary electrons from photon interactions is actually very flat, implying that it is likely for the electron from a Compton scattering event to have an energy in the 100's of keV. The distribution of the next generation of electrons was also calculated, and this distribution was also quite entergetic (with a maximum energy corresponding to 0.55 MeV) but with a much large probability of having a collision that produces and electron with a much lower energy.

(a) First Secondary Electron

(b) Second Secondary Electron

Figure 12: Simulated kinetic energies of electrons from ⁶⁰Co interactions

7 Conclusions

GEANT4 has been employed to simulate the energy spectra of electrons and energy deposition from thermal neutrons and 60 Co gammas. A versitile implemenation of the geometry was used in which it is possible to dynamically set the materials, thickness, and number of layers between runs. In addition, analysis methods have been written to aid in the reporting of the results. This simulation was verified by reproducting the single collision energy loss spectra for water, and also by comparing the average energy deposited to the measured average channel number for film ranging from 15μ mto 600μ m.

The energy deposition of the films were calculated and plotted in Figure 11 and Figure 10. It is then observable that the gamma interactions have a very low probability of depositing a majority of the energy from a 60 Co photon into the material, while neturons tend to deposit over 50% of their energy in the material for a 15 μ mfilm, and increasing to 96% for a 1 cm thick film. Figure 13 shows the average energy deposition as a function of thickness for neturons and gammas, along with the calculated channel number (according to Equation 4). At thickness of less than 200 μ mthere is significant seperation between the average energy deposited by neutron events compared to gamma events. As the thickness of the films increased the average neturon energy approached the asymptotic limit of 4.78 MeV, while the average gamma energy increased. This creates less seperation between the two, and provides less of an ability for neutron-gamma discrimination based on pulse height.

(a) Energy Deposition

(b) Esimated Channel Number

Figure 13: Comparison between average neturon and gamma energy deposition

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