





11-13 February 2020 University of Minho Gualtar Campus, Braga https://indico.lip.pt/event/681



Optical Photon Processes

Bernardo Tomé



>The LIP competence center on Simulation and Big Data organizes the first edition of an introductory course on Geant4, a Monte Carlo simulation toolkit for particle transport widely used in fields such as high-energy physics, medical physics and material science.

Slides adapted from slides produced by : Marc Verderi,Dennis Wright, Vladimir Ivantchenko, Mihaly Novak http://cern.ch/geant4

Organizing committee:

N. Castro, P. Gonçalves, A. Lindote, R. Sarmento, B. Tomé, M. Vasilevskiy

Optical processes

- Propagation of optical photons and their interaction with materials is treated separately from regular electromagnetic processes :
 - Wavelengths are much larger than atomic spacing
 - Treated (partially) as waves; no smooth transition to gammas
 - Energy/momentum not generally conserved in G4 optics !
- Optical photons produced directly by three processes :
 - G4Cerenkov
 - G4Scintillation
 - G4TransitionRadiation

Optical photon transport

- Optical photons can undergo:
 - Refraction and reflection at boundaries
 - Wavelength shifting
 - Bulk absorption
 - Rayleigh scattering
- Material optical properties can be specified in a G4MaterialsPropertiesTable attached to G4Material
 - transmission efficiency, dielectric constants, surface properties
 - including binned wavelength/energy dependences
- Spectral properties can be also specified in G4MaterialsPropertiesTable
 - scintillation yield, time structure (fast, slow components)

Note : an optical photon will not be propagated (killed) in a material without index of refraction

Specification of material optical properties

```
const G4int NUMENTRIES = 3;
```

```
G4double ppckov[NUMENTRIES] = {2.034*eV, 3.*eV, 4.136*eV};
G4double rindex[NUMENTRIES] = {1.3435, 1.351, 1.3608};
G4double absorption[NUMENTRIES] = {344.8*cm, 850.*cm, 1450.0*cm};
```

G4MaterialPropertiesTable* MPT = **new** G4MaterialPropertiesTable();

MPT->AddConstProperty("SCINTILLATIONYIELD",100./MeV);

MPT->AddProperty("RINDEX",ppckov,rindex,NUMENTRIES}->SetSpline(true); MPT->AddProperty("ABSLENGTH",ppckov,absorption,NUMENTRIES}->SetSpline(true);

scintillator -> SetMaterialPropertiesTable(MPT);

Optical boundary processes

Refraction and reflection handled by G40pBoundaryProcess

- Boundary properties
 - dielectric-dielectric
 - dielectric-metal
 - dielectric-black material

- Surface properties
 - polished
 - ground
 - front- or back- painted

User must supply surface properties through G4OpticalSurfaceModel

Reflection and Refraction

• Geant4 reflects "particle-like" behavior – no "splitting" of tracks



- Probability for transmission/reflection computed from Fresnel's relations
- Interference effects, important in layers of thickness comparable with the wavelength, can only be accounted for by the empirical reflectivity factor for the surface

Optical bulk processes

• G4OpAbsorption

- uses photon attenuation length from material properties to get mean free path
- photon is simply killed after a selected path length
- G4OpRayleigh
 - elastic scattering including polarization of initial and final photons
 - builds its own physics table (for mean free path) using
 G4MaterialTable
 - may only be used for optical photons (a different process provided for gammas)

Optical processes : Scintillation

- In a scintillator material light is emitted when excitation energy is transferred to the material
 - isotropic emission

t0

random linear polarization





 $t0 + \Delta t$

Specification of scintillation properties

```
const G4int NUMENTRIES = 9;
G4double Scnt_PP[NUMENTRIES] = { 6.6*eV, 6.7*eV, 6.8*eV, 6.9*eV,
7.0*eV, 7.1*eV, 7.2*eV, 7.3*eV, 7.4*eV };
G4double Scnt_FAST[NUMENTRIES] = { 0.000134, 0.004432, 0.053991, 0.241971,
0.398942, 0.000134, 0.004432, 0.053991, 0.241971,
0.241971 };
G4double Scnt_SLOW[NUMENTRIES] = { 0.000010, 0.000020, 0.000030, 0.004000,
0.008000, 0.005000, 0.020000, 0.001000,
0.000010 };
```

G4Material* Scnt; G4MaterialPropertiesTable* Scnt_MPT = new G4MaterialPropertiesTable();

```
Scnt_MPT->AddProperty("FASTCOMPONENT", Scnt_PP, Scnt_FAST, NUMENTRIES);
Scnt_MPT->AddProperty("SLOWCOMPONENT", Scnt_PP, Scnt_SLOW, NUMENTRIES);
```

```
Scnt_MPT->AddConstProperty("SCINTILLATIONYIELD", 5000./MeV);
Scnt_MPT->AddConstProperty("RESOLUTIONSCALE", 2.0);
Scnt_MPT->AddConstProperty("FASTTIMECONSTANT", 1.*ns);
Scnt_MPT->AddConstProperty("SLOWTIMECONSTANT", 10.*ns);
Scnt MPT->AddConstProperty("YIELDRATIO", 0.8);
```

Scnt->SetMaterialPropertiesTable(Scnt_MPT);

Optical processes : Wavelength Shifting

- In a WLS material light is absorbed and reemitted with a longer wavelength
 - isotropic emission
 - random linear polarization
- Handled by G40pWLS process
 - initial photon is killed, one with new wavelength is created
- User must supply :
 - absorption length in function of photon energy
 - emission spectra parameters as function of energy
 - time delay between absorption and reemission





Specification of WLS properties

```
const G4int nEntries = 9:
G4double PhotonEnergy[nEntries] = { 6.6 \times eV, 6.7 \times eV, 6.8 \times eV, 6.9 \times eV,
                                    7.0*eV, 7.1*eV, 7.2*eV, 7.3*eV, 7.4*eV };
G4double RIndexFiber[nEntries] =
          \{ 1.60, 1.60, 1.60, 1.60, 1.60, 1.60, 1.60, 1.60, 1.60, 1.60 \};
G4double AbsFiber[nEntries] =
          {0.1*mm, 0.2*mm, 0.3*mm, 0.4*cm, 1.0*cm, 10*cm, 1.0*m, 10.0*m, 10.0*m};
G4double EmissionFiber[nEntries] =
          \{0.0, 0.0, 0.0, 0.1, 0.5, 1.0, 5.0, 10.0, 10.0\};
 G4Material* WLSFiber:
 G4MaterialPropertiesTable* MPTFiber = new G4MaterialPropertiesTable();
 MPTFiber->AddProperty("RINDEX", PhotonEnergy, RIndexFiber, nEntries);
 MPTFiber->AddProperty("WLSABSLENGTH", PhotonEnergy, AbsFiber, nEntries);
 MPTFiber->AddProperty("WLSCOMPONENT", PhotonEnergy, EmissionFiber, nEntries);
 MPTFiber->AddConstProperty("WLSTIMECONSTANT", 0.5*ns);
```

```
WLSFiber->SetMaterialPropertiesTable(MPTFiber);
```

Boundary processes : The Unified model

- Applies to dielectric-dielectric and dielectric-metal interfaces and tries to provide a realistic simulation, dealing with many aspects of surface finish and reflector coating :
 - surface may be assumed as smooth and covered with a metalized coating representing a specular reflector with given reflection coefficient
 - painted with a diffuse reflecting material where Lambertian reflection occurs.
 - surfaces may or may not be in optical contact with another component
 - a rough surface made up of micro-facets with normal vectors that follow given distributions around the nominal normal for the volume at the impact point.

Boundary processes : The Unified model

Provides for a range of different reflection mechanisms.



- a) specular lobe constant : reflection probability about the normal of a micro facet
- b) specular spike constant : the probability of reflection about the average surface normal.
- c) diffuse lobe constant is for the probability of internal Lambertian reflection
- d) back-scatter spike constant : several reflections within a deep groove with the ultimate result of exact back-scattering

Surface finishes



http://geant4-userdoc.web.cern.ch/geant4-userdoc/UsersGuides/ForApplicationDeveloper/html/TrackingAndPhysics/physicsProcess.html#optical-photon-processes

Example of specification of dielectric-dielectric surface properties

G4VPhysicalVolume* volume1; G4VPhysicalVolume* volume2;

G4OpticalSurface* OpSurface = **new** G4OpticalSurface("name");

G4LogicalBorderSurface* Surface = new
G4LogicalBorderSurface("name",volume1,volume2,OpSurface);

```
G4double sigma_alpha = 0.1;
```

```
OpSurface->SetType(dielectric_dielectric);
OpSurface->SetModel(unified);
OpSurface->SetFinish(groundbackpainted);
OpSurface->SetSigmaAlpha(sigma_alpha);
```

const G4int NUM = 2;

```
G4double pp[NUM] = {2.038*eV, 4.144*eV};
G4double specularlobe[NUM] = {0.3, 0.3};
G4double specularspike[NUM] = {0.2, 0.2};
G4double backscatter[NUM] = {0.1, 0.1};
G4double rindex[NUM] = {1.35, 1.40};
G4double reflectivity[NUM] = {0.3, 0.5};
G4double efficiency[NUM] = {0.8, 0.1};
```

Physical volume 2

Physical volume 1

C_aR

C alR

C ...R

A.A.nl

Ground backpainted

 $C_{bs}R$

G4MaterialPropertiesTable* SMPT = **new** G4MaterialPropertiesTable();

SMPT->AddProperty("RINDEX",pp,rindex,NUM); SMPT->AddProperty("SPECULARLOBECONSTANT",pp,specularlobe,NUM); SMPT->AddProperty("SPECULARSPIKECONSTANT",pp,specularspike,NUM); SMPT->AddProperty("BACKSCATTERCONSTANT",pp,backscatter,NUM); SMPT->AddProperty("REFLECTIVITY",pp,reflectivity,NUM); SMPT->AddProperty("EFFICIENCY",pp,efficiency,NUM);

OpSurface->SetMaterialPropertiesTable(SMPT);

Surface finishes

GroundBackPainted







NOTE: Applying Snell's Law includes applying Fresnel's uations of reflection and refraction, and these combined result in Fresnel Refraction or Total Internal Reflection or Fresnel Reflection

Hands-On Optical Physics Processes

- We will use a new branch where part of the needed code is already inserted;
- Start by committing the modifications you inserted : git commit -am "My new code"
- Fetch the new branch :

git checkout step6-optics-0

Let's make the crystal shine

- We are going to use the personalised modular physics list (class PhysicsList) to include the optical physics processes category; modify the code as appropriate to use this class and include the optical physics category;
- In the DetectorConstruction() inspect the function
 SetMaterialOpticalProperties(); it defines the optical properties table to be set to the Nal crystal,
- Choose a light yield such that a few (~ 10 100) photons will be emitted for the typical energies of the radioactive sources being simulated.
- Run the simulation with the visualisation and the macro gamma.mac
- For a small number of gammas shot, you should see several photon tracks inside the crystal; if yes proceed to the next slide

Detecting the optical photons

We will assume that a photon is detected if it arrives at the back of the crystal :

- In the SteppingAction class check if a step occurred inside your volume of interest and if the particle is an opticalphoton;
- Additionally use the Pre or PostStep points as needed to check if the photon detection condition is met;
- Increment a variable in the EventAction to count the number of detected photons; kill the optical photon afterwards;
- At the end of the event, write the total number of detected photons (together with the already existing true and smeared energies) to the output file;
- Increase the crystal light yield (L.Y.) to about 3 photons / keV (of the order of the Nal L.Y. (1 photon / 26 eV) times a 10% overall efficiency;

Detecting the optical photons

- Run the program for a few thousands of events using gamma.mac;
- Plot the distribution for the number of detected photons;
- What do you think about the result ?

Improving the light collection

We will now wrap the Nal crystal with a white diffuser

- In the DetectorConstruction class the function SetSurfaceOpticalProperties() is used to set the optical properties of the wrapping material;
- At the end of the **Construct()** function you can find the placeholders to use the **G4LogicalBorderSurface constructor** to set the optical properties of the surface of the crystal;

Detecting the optical photons

- Run the program for a few thousands of events using gamma.mac;
- Plot the distribution for the number of detected photons;
- Try to fit a gaussian distribution to the total absorption peak and extract the resolution of our spectroscopy setup;
- Now run the macros with the isotopes and compare the results with what was obtained yesterday using the true energy deposition;