Optical Modeling of Scintillation Detectors Using GATE

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Outline

1. Production and transport of optical photons
2. The UNIFIED model in GATE
3. Look-up-table based approaches (Janecek and Moses, Roncali and Cherry)
4. Optical photon analysis

Nature of Optical Photons (1-10 eV)

- Bioluminescence and fluorescence photons

  Cuplov V, Buvat I, Pain F and Jan S 2014 Extension of the gate Monte-Carlo simulation package to model bioluminescence and fluorescence imaging J. Biomed. Opt. ***19(2)****-026004*

- Cerenkov photons

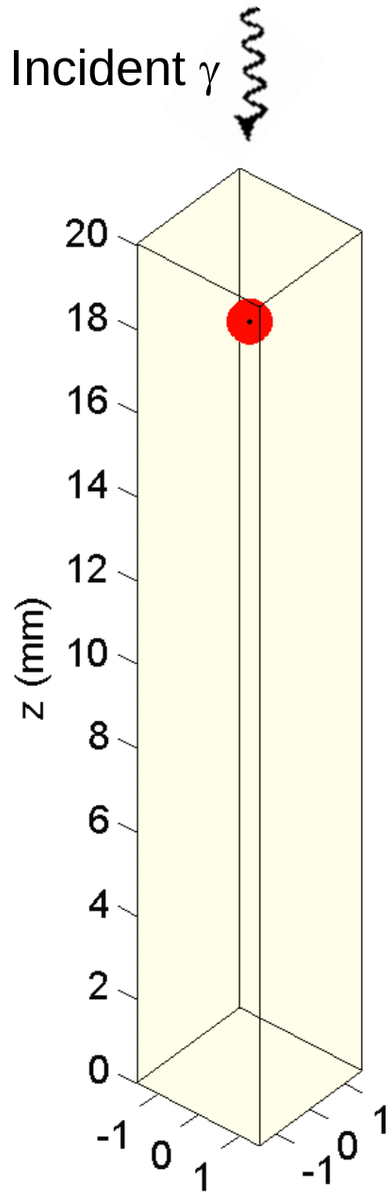
- Scintillation photons

Production of Scintillation Photons

Materials.xml

```
<material name="LSO">
<property name="SCINTILLATIONYIELD" value="30000" unit="1/MeV"/>
    <property name="RESOLUTIONSCALE" value="4.41"/>
    <property name="FASTTIMECONSTANT" value="40" unit="ns"/>
    <property name="YIELDRATIO" value="1"/>
    <propertyvector name="FASTCOMPONENT" energyunit="eV">
      <ve value energy="2.95167" value="1"/>
    </propertyvector>
    <propertyvector name="ABSLENGTH" unit="m" energyunit="eV">
      <ve value energy="1.84" value="50"/>
      <ve value energy="4.08" value="50"/>
    </propertyvector>
    <propertyvector name="RINDEX" energyunit="eV">
      <ve value energy="1.84" value="1.82"/>
      <ve value energy="4.08" value="1.82"/>
```

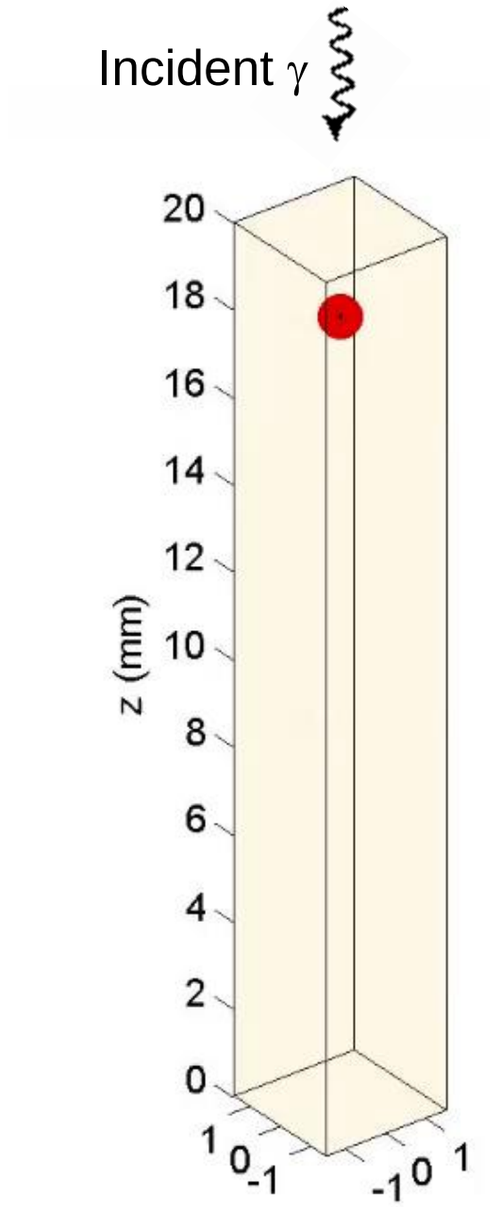
- Light yield
- Decay time
- Emission spectrum
- Absorption (μ_a)
- Index of refraction



Photodetector side

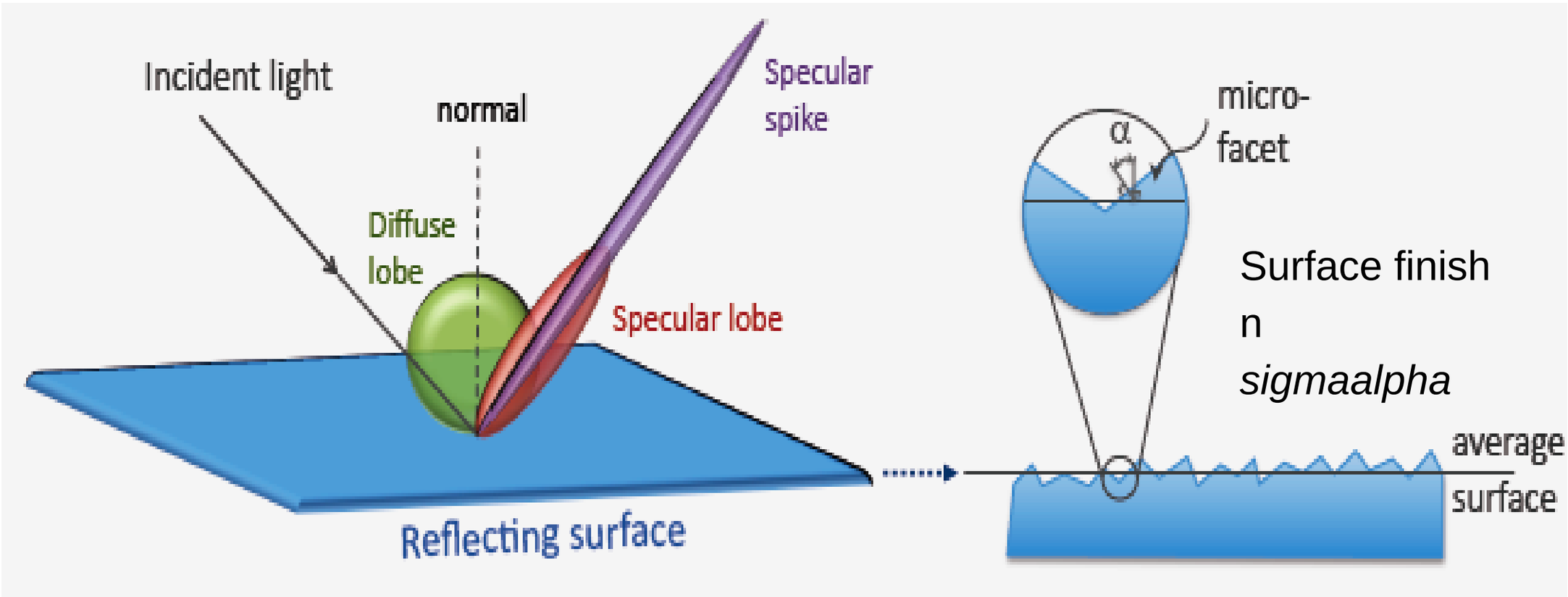
Transport of Scintillation Photons

- Bulk absorption and scattering
- Polarization (scintillation unpolarized)
- **Boundary effects**
- Transmission to photodetector



Photodetector side

GATE Default Model: *UNIFIED*



http://wiki.opengatecollaboration.org/index.php/Users_Guide_V7.0:Generating_and_tracking_optical_photons

How to Parameterize the *UNIFIED* Model

- Surface finish
- Surface type
- Roughness sigmaalpha
- Reflection probabilities
- Index of refraction
- Reflectivity
- Efficiency

Surfaces.xml

```
<surface finish="“groundbackpainted" sigmaalpha="“18 deg" type="dielectric_dielectric
" name="“ground_teflon">
      <propertyvector name="SPECULARLOBECONSTANT" energyunit="eV">
          <ve value="“1" energy="3.0261"/>
          <ve value="“1" energy="3.265"/></propertyvector>
      <propertyvector name="SPECULARSPIKECONSTANT" energyunit="eV">
          <ve value="“0" energy="3.0261"/>
          <ve value="“0" energy="3.265"/>
</propertyvector>
<propertyvector name="BACKSCATTERCONSTANT" energyunit="eV">
          <ve value="0" energy="3.0261"/>
          <ve value="0" energy="3.265"/>
</propertyvector>
<propertyvector name="RINDEX" energyunit="eV">
          <ve value="“1" energy="3.0261"/>
          <ve value="“1" energy="3.265"/>
</propertyvector>
<propertyvector name="REFLECTIVITY" energyunit="eV">
          <ve value="0.99" energy="3.0261"/>
          <ve value="0.99" energy="3.265"/>
</propertyvector>
<propertyvector name="EFFICIENCY" energyunit="eV">
          <ve value="0" energy="3.0261"/>
          <ve value="0" energy="3.265"/>
```

LUT-based Approaches

- Measured Reflectance look-up-table (LUT) versus *UNIFIED*:
  - \+ More realistic, computationally efficient, no complex input parameters
  - \+ Crystal and reflector integrated in single optical surface
  - \- Specific to one material and surface finish
  - \- Needs to be provided in database or enabled through user interface

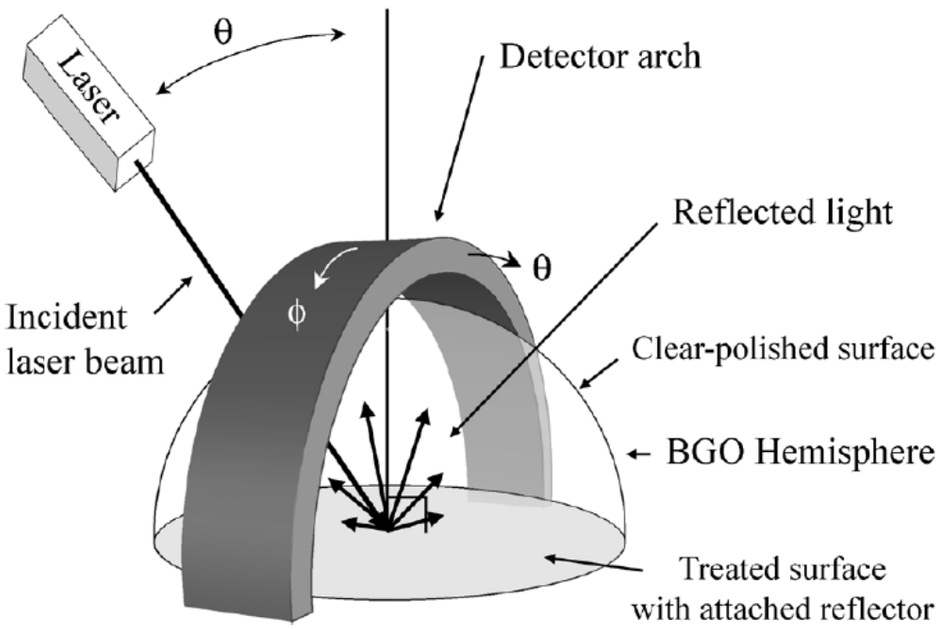
- Approach from Janecek and Moses* implemented in Geant4 (February 2016)

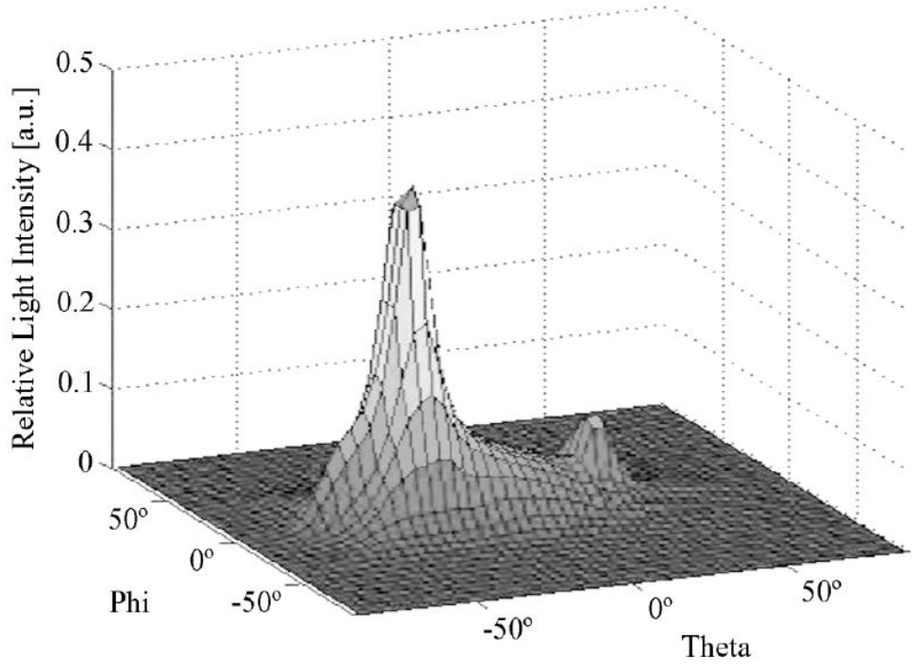
- Approach from Roncali and Cherry** validated in Matlab and being implemented in GATE (available in future release 2017)

Janecek M and Moses W W 2010. Simulating scintillator light collection using measured optical reflectance IEEE Trans . Nucl. Sci.* ***57* *964-70*
***Roncali E and Cherry S R 2013. Simulation of light transport in scintillators based on 3D characterization of crystal surfaces Phys. Med. Biol. 58 2185-98*

Reflectance LUT from Janecek and Moses

- Measure angular distribution of reflected light using laser and photodiodes*
- Hemispherical crystal eliminates internal reflections and refractions
- Probability of reflection and reflected light distribution stored in LUT **for incidence 0°−90°** to be used in simulation





Etched BGO with Lumirror at 26 °

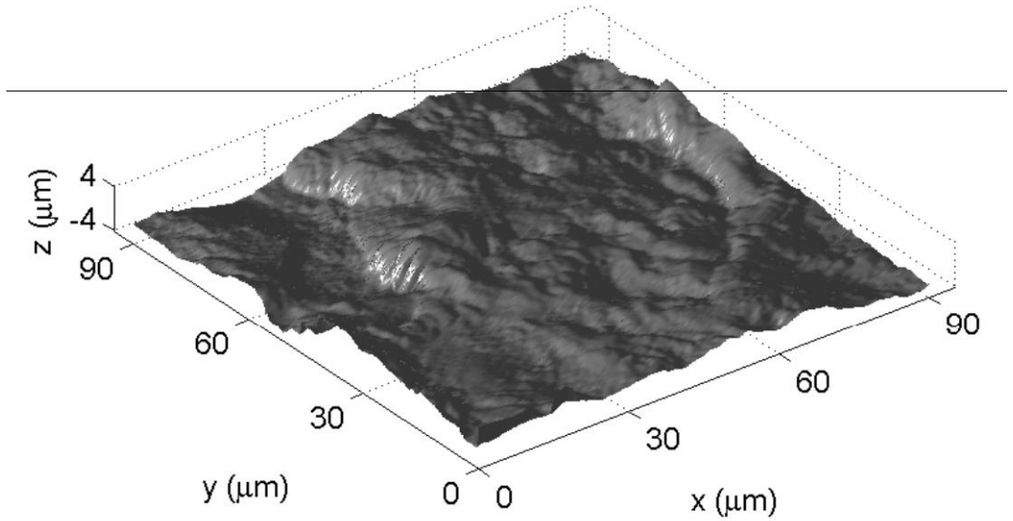
** Janecek M and Moses W W 2010 Simulating scintillator light collection using measured optical reflectance IEEE Trans. Nucl. Sci.* ***57*** *964-70*

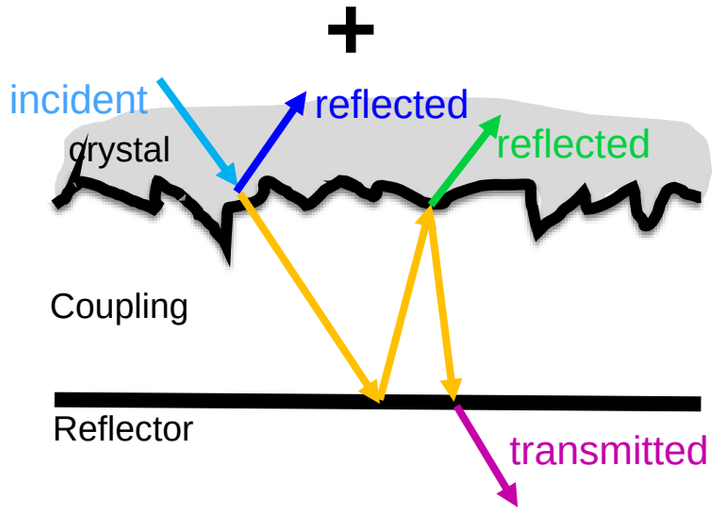
G4surface.cc modifications for MJ's model

```
// if found create the optical surface
surface = new G4OpticalSurface(name);
// model is always the unified model
// PMJ - adding one more model - the LUT model
G4String model = doc->GetProperty("model");
if (model=="LUT") surface->SetModel(LUT);
else if (model=="DAVIS") surface->SetModel(DAVIS);
else surface->SetModel(unified);
// set the type
G4String type = doc->GetProperty("type");
if (type=="dielectric_dielectric") surface->SetType(dielectric_dielectric);
else if (type=="dielectric_metal") surface->SetType(dielectric_metal);
else if (type=="dielectric_LUT") surface->SetType(dielectric_LUT);
else if (type=="dielectric_LUTDavis") surface->SetType(dielectric_LUTDavis);
```

Reflectance LUT from Roncali and Cherry

- Measure crystal topography in 3D with SEM, or AFM (resolution ~100 nm)
- Compute reflected rays **for incidence 0°−90°** using virtual illumination*
- Store in LUT and use in simulation





Roncali E and Cherry S R 2013. Simulation of light transport in scintillators based on 3D characterization of crystal surfaces Phys. Med. Biol. 58 2185-98

Use Reflectance LUT-DAVIS in GATE (preliminary)

- First version will be available in GATE with LUTs for different surface/reflector combinations

Surfaces.xml

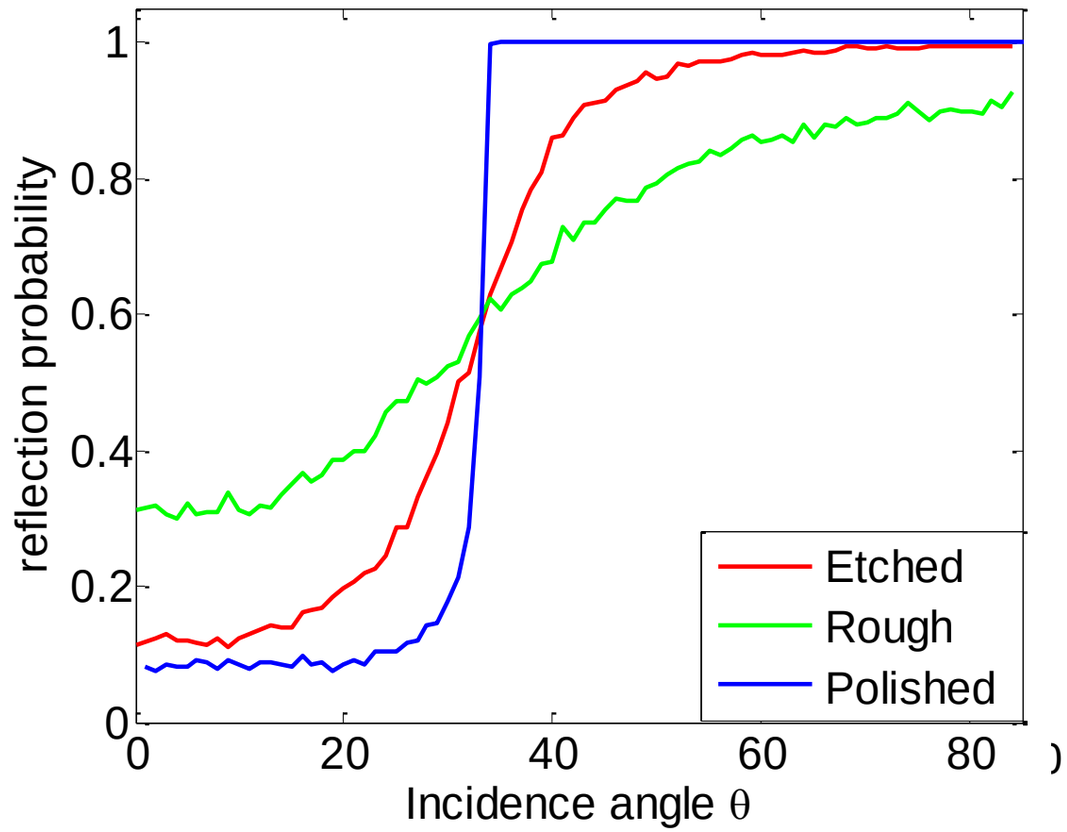
```
surface finish=" ground_LUT type="dielectric_LUTDAVIS" name="ground_LUT" model="DAVIS">
```

- Next version will include an interface for users to generate their own LUTs from their surface data or reflector parameters

Courtesy Mariele Stockhoff

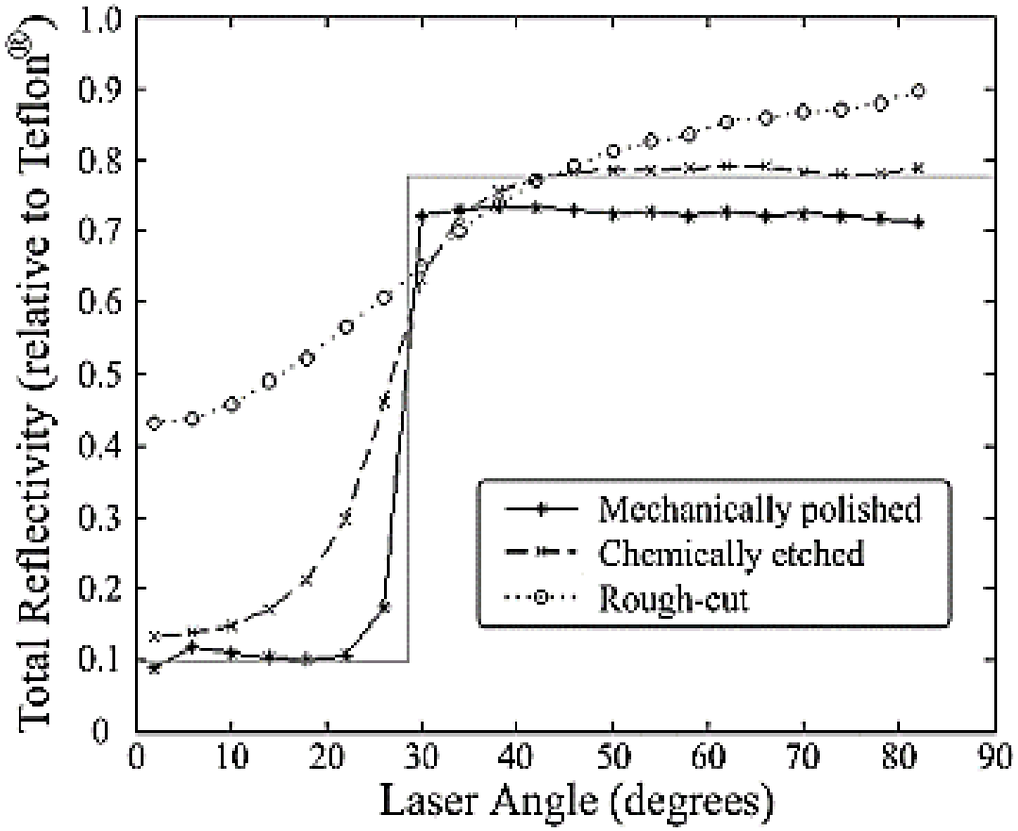
Comparison of Reflectance LUTs

Roncali et. al



Reflectance probability

Janecek et. al



Reflected rays

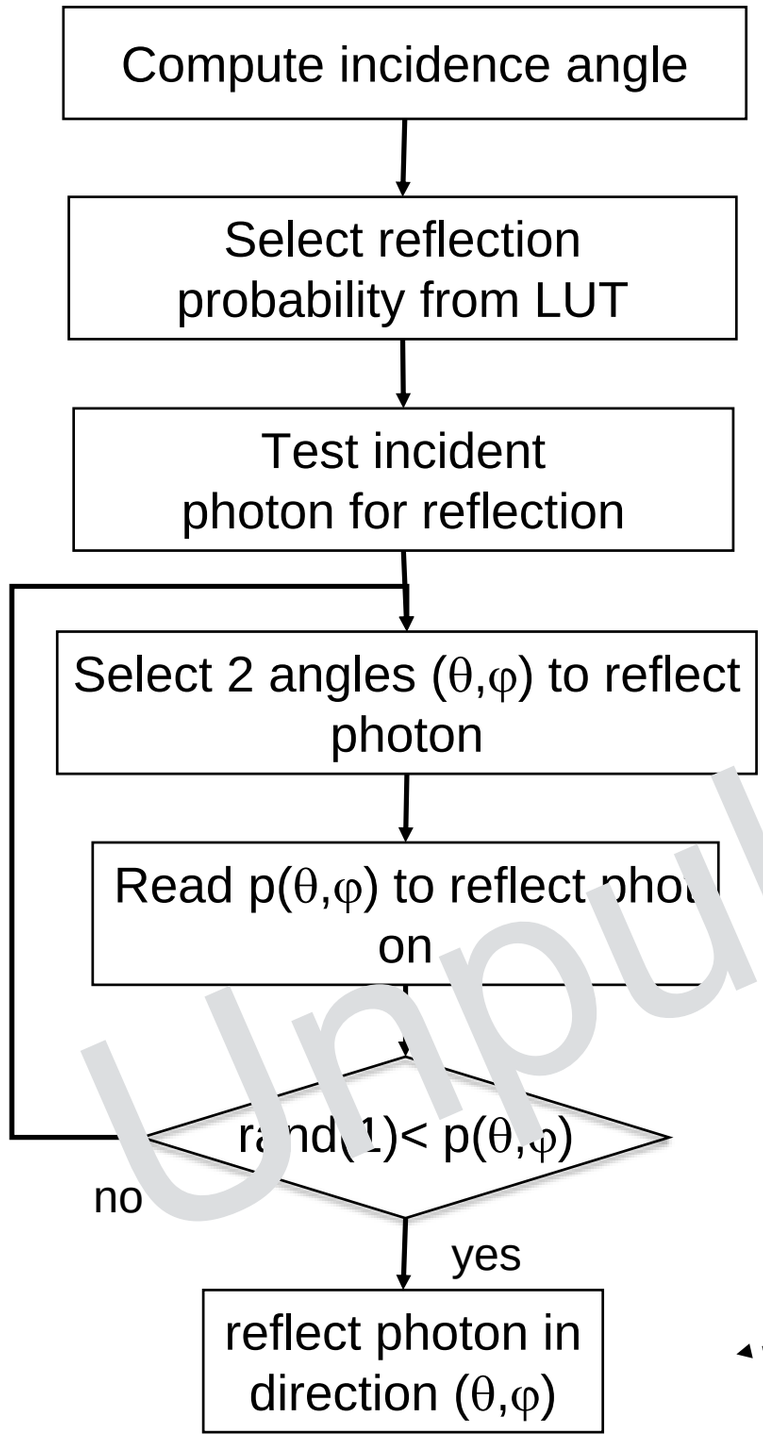
Use Reflectance LUT (Janecek and Moses) from Geant4

- Can be enabled in GATE by changing source code Gatesurface.cc, and recompiling
- Geant4 needs to be compiled with the LUTs by downloading the RealSurface 1.0 module (http://geant4.web.cern.ch/geant4/support/download.shtml)
- LUTs available for BGO only with different finishes, reflectors

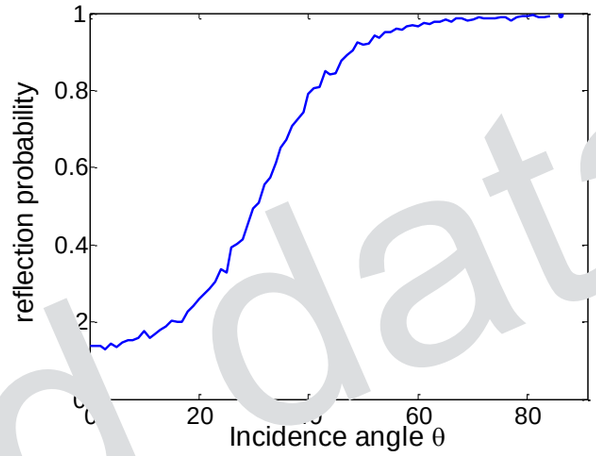
Surfaces.xml

```
<surface finish="groundlumirrorair" sigmaalpha="0.1" type="dielectric_LUT"
name="ground_lumirror_LUT" model="LUT">
    <propertyvector name="RINDEX" energyunit="eV">
        <ve value="1" energy="4.08"/>
        <ve value="1" energy="1.84"/>
    </propertyvector>
    <propertyvector name="REFLECTIVITY" energyunit="eV">
        <ve value="0.980" energy="4.08"/>
        <ve value="0.980" energy="1.84"/>
    </propertyvector>
    <propertyvector name="EFFICIENCY" energyunit="eV">
        <ve value="0" energy="4.08"/>
        <ve value="0" energy="1.84"/>
```

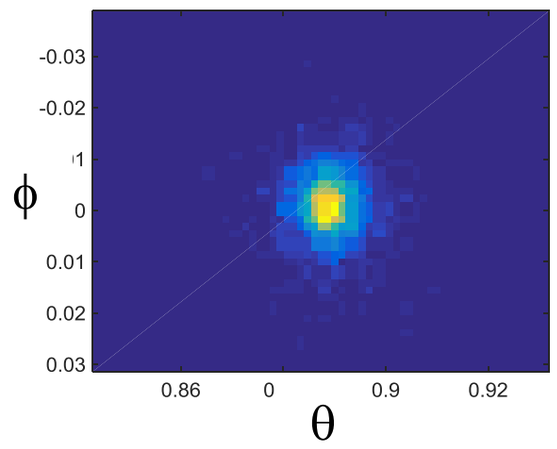
Use LUT to Track Optical Photons

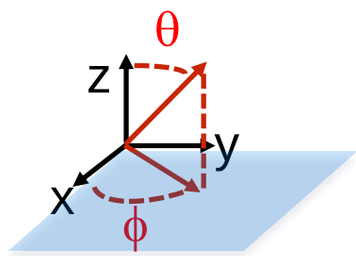


Reflection probability



Probability of reflection in direction (θ,ϕ): p(θ,φ)





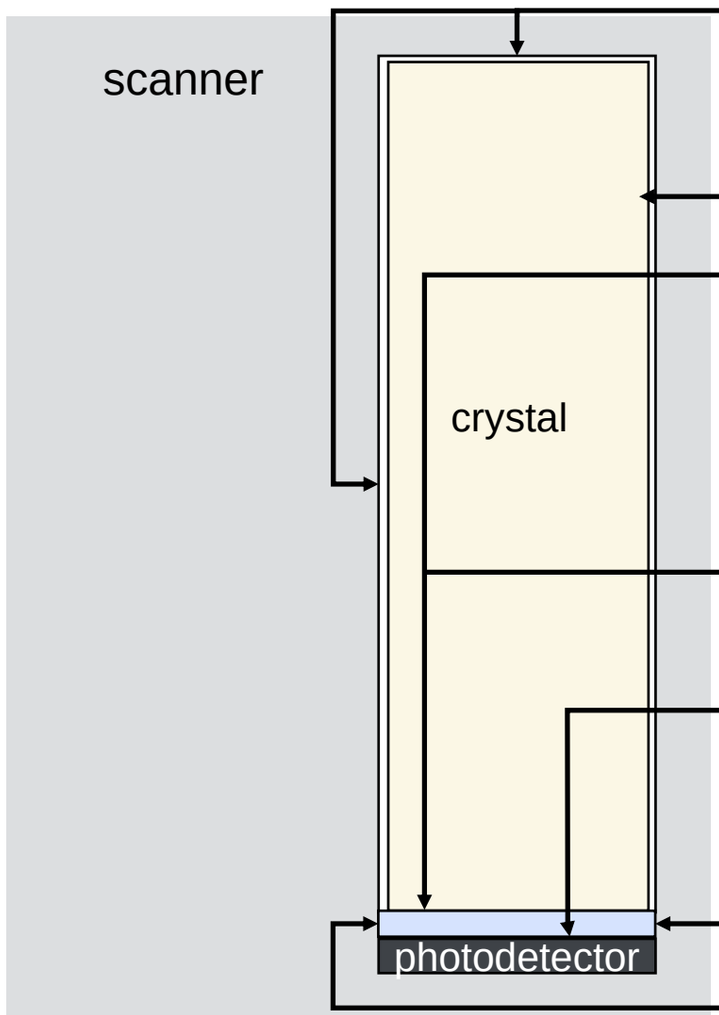
Enable Optical Simulation in GATE

Turn on **GATE_USE_OPTICAL** in ccmake process

```
                                                                Page 1 of 1
BUILD_TESTING                                OFF
CMAKE_BACKWARDS_COMPATIBILITY                2.4
CMAKE_BUILD_TYPE                             Release
CMAKE_INSTALL_PREFIX                         /PATH_TO/gate_v7.2-install
EXECUTABLE_OUTPUT_PATH
GATE_ALLOW_MT_GEANT4                         OFF
GATE_DOWNLOAD_BENCHMARKS_DATA                OFF
GATE_DOWNLOAD_EXAMPLES_DATA                  OFF
GATE_USE_ECAT7                               OFF
GATE_USE_GEANT4_UIVIS                        ON
GATE_USE_GPU                                 OFF
GATE_USE_ITK                                 OFF
GATE_USE_LMF                                 OFF
GATE_USE_OPTICAL                             OFF
GATE_USE_RTK                                 OFF
GATE_USE_STDC11                              OFF
GATE_USE_SYSTEM_CLHEP                        OFF
Geant4_DIR                                   /PATH_TO/geant4.10.02-install/lib/Geant4-10.2.0
LIBRARY_OUTPUT_PATH
ROOTCINT_EXECUTABLE                          /PATH_TO/root_v5.34/bin/rootcint
```

Define Optical Surfaces

EACH optical interface = TWO surfaces in geometry macro



geometry.mac

```
# === Optical surfaces ===
### Scanner - Crystal
/gate/crystal/surfaces/name                    teflonsurf
/gate/crystal/surfaces/insert                  scanner
/gate/crystal/surfaces/teflonsurf/setSurface teflon

### COUPLING - Crystal
/gate/coupling/surfaces/name                    coupling_crystal
/gate/coupling/surfaces/insert                  crystal
/gate/coupling/surfaces/coupling_crystal/setSurface polish

/gate/crystal/surfaces/name                   crystal_coupling
/gate/crystal/surfaces/insert                 coupling
/gate/crystal/surfaces/crystal_coupling/setSurface polish

### COUPLING - Photodetector
/gate/coupling/surfaces/name                    SiPM_coupling
/gate/coupling/surfaces/insert                  SiPM
/gate/coupling/surfaces/SiPM_coupling/setSurface
Photodetector

### COUPLING - Scanner
/gate/scanner/surfaces/name                   coupling_Scanner
/gate/scanner/surfaces/insert                 coupling
/gate/scanner/surfaces/coupling_Scanner/setSurface polish
```

Define Physics and Optical Digitizer

Physics.mac

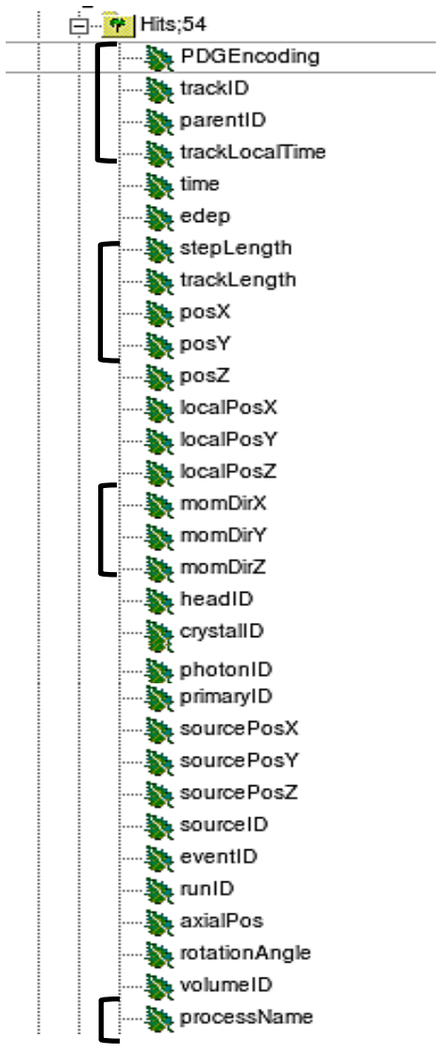
```
#
#       P H Y S I C S
#

/gate/physics/addProcess PhotoElectric
/gate/physics/processes/PhotoElectric/setModel StandardModel

/gate/physics/addProcess Compton
/gate/physics/processes/Compton/setModel StandardModel

/gate/physics/addProcess OpticalAbsorption
/gate/physics/addProcess OpticalRayleigh
/gate/physics/addProcess OpticalBoundary
```

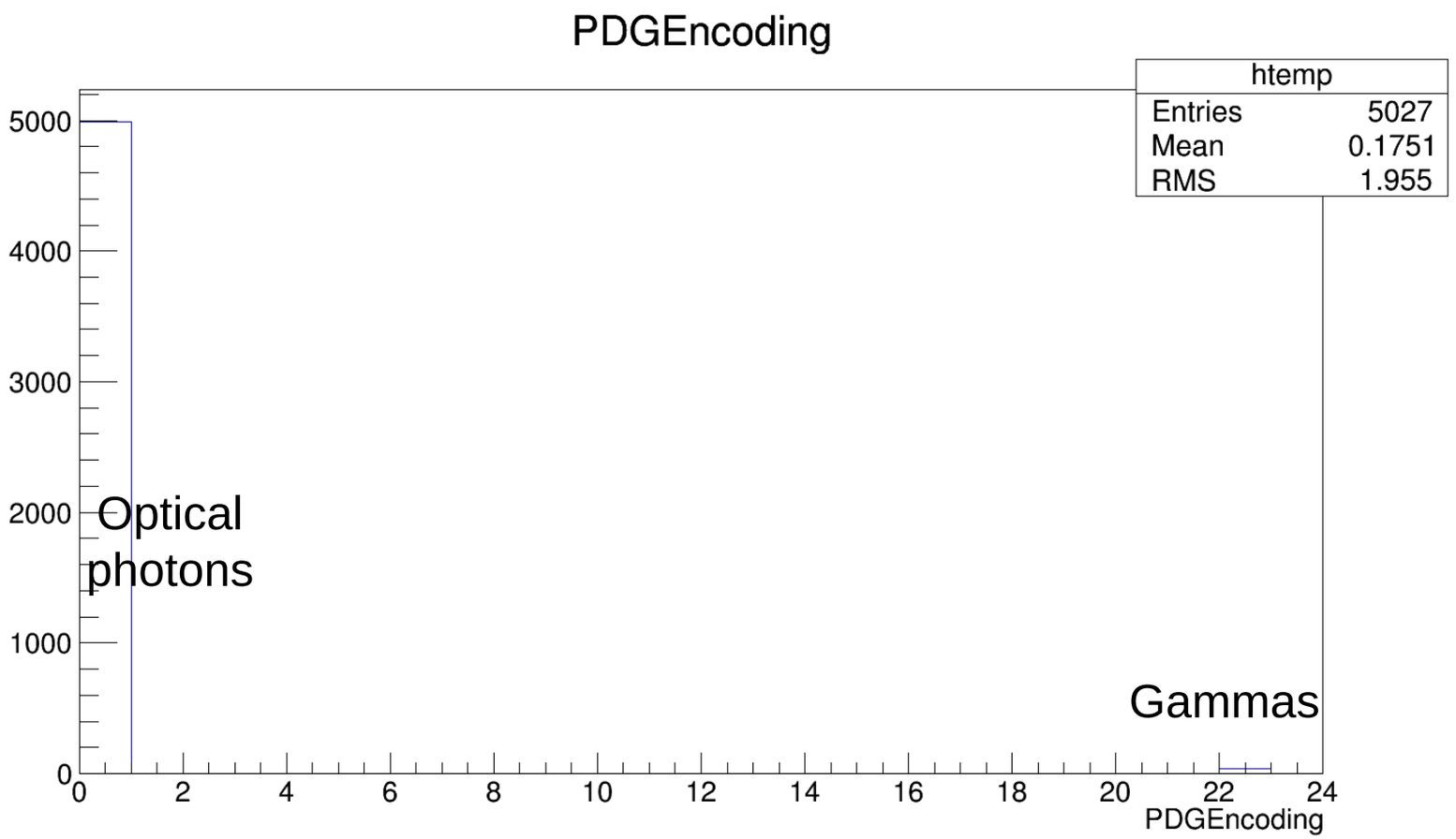
geometry.mac

```
/gate/digitizer/Singles/insert opticaladder
/gate/digitizer/Singles/insert readout
/gate/digitizer/Singles/readout/setDepth detector level
```

Optical Output for Scintillation Detectors

- Crystal is sensitive detector
- Root: use Hits tree and not OpticalData tree





Courtesy Mariele Stockhoff

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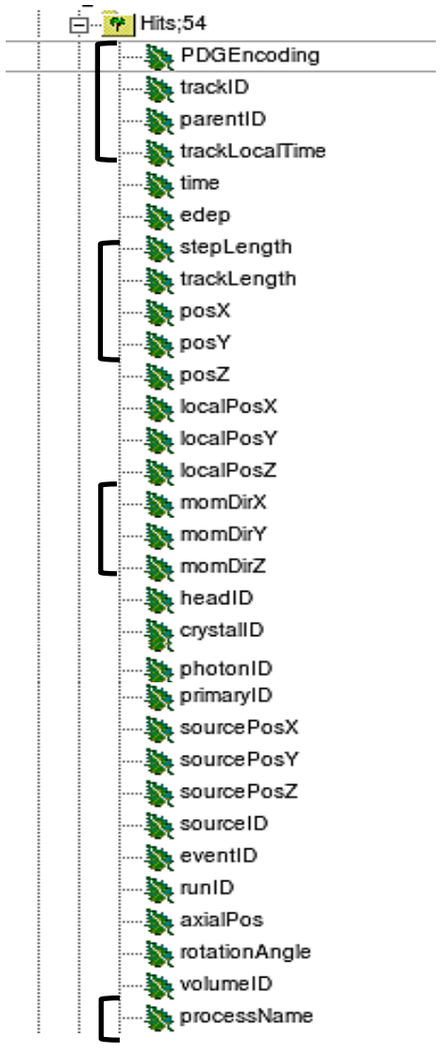

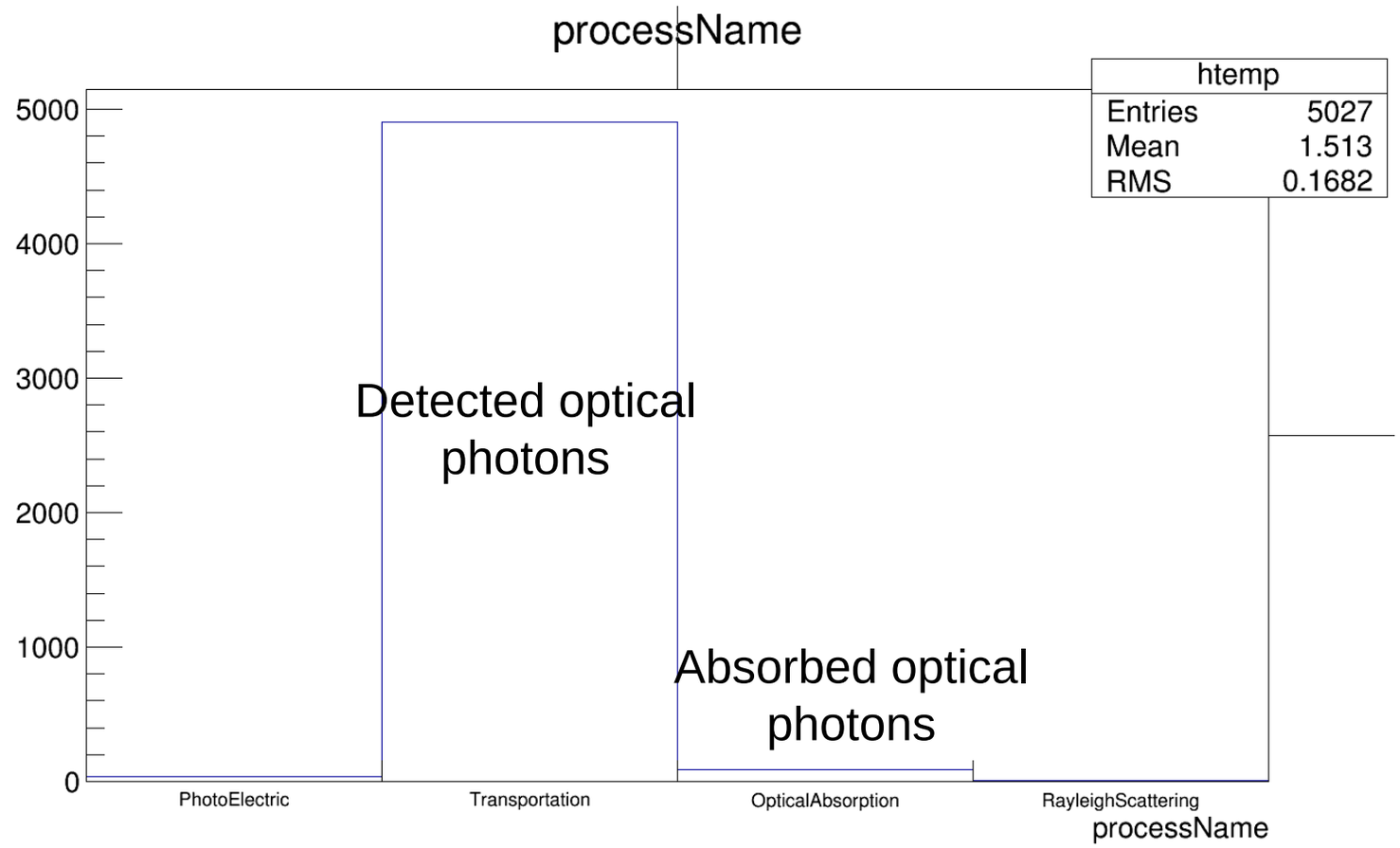

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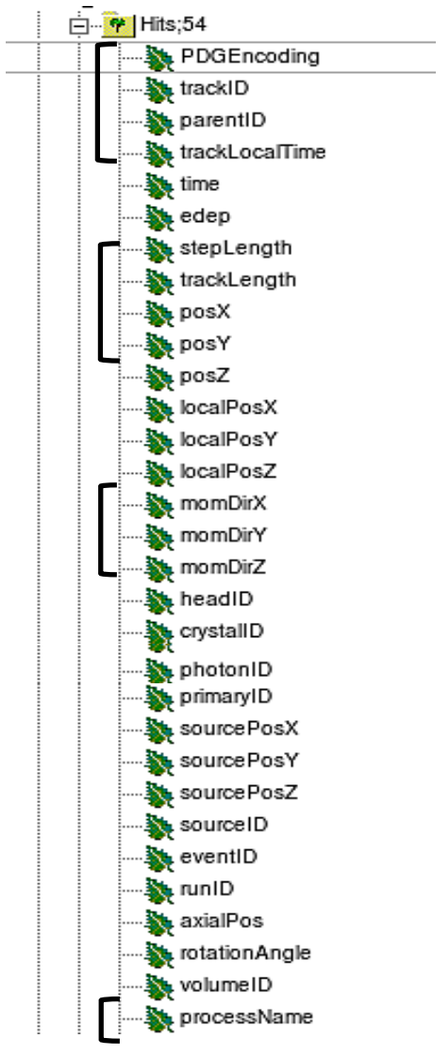

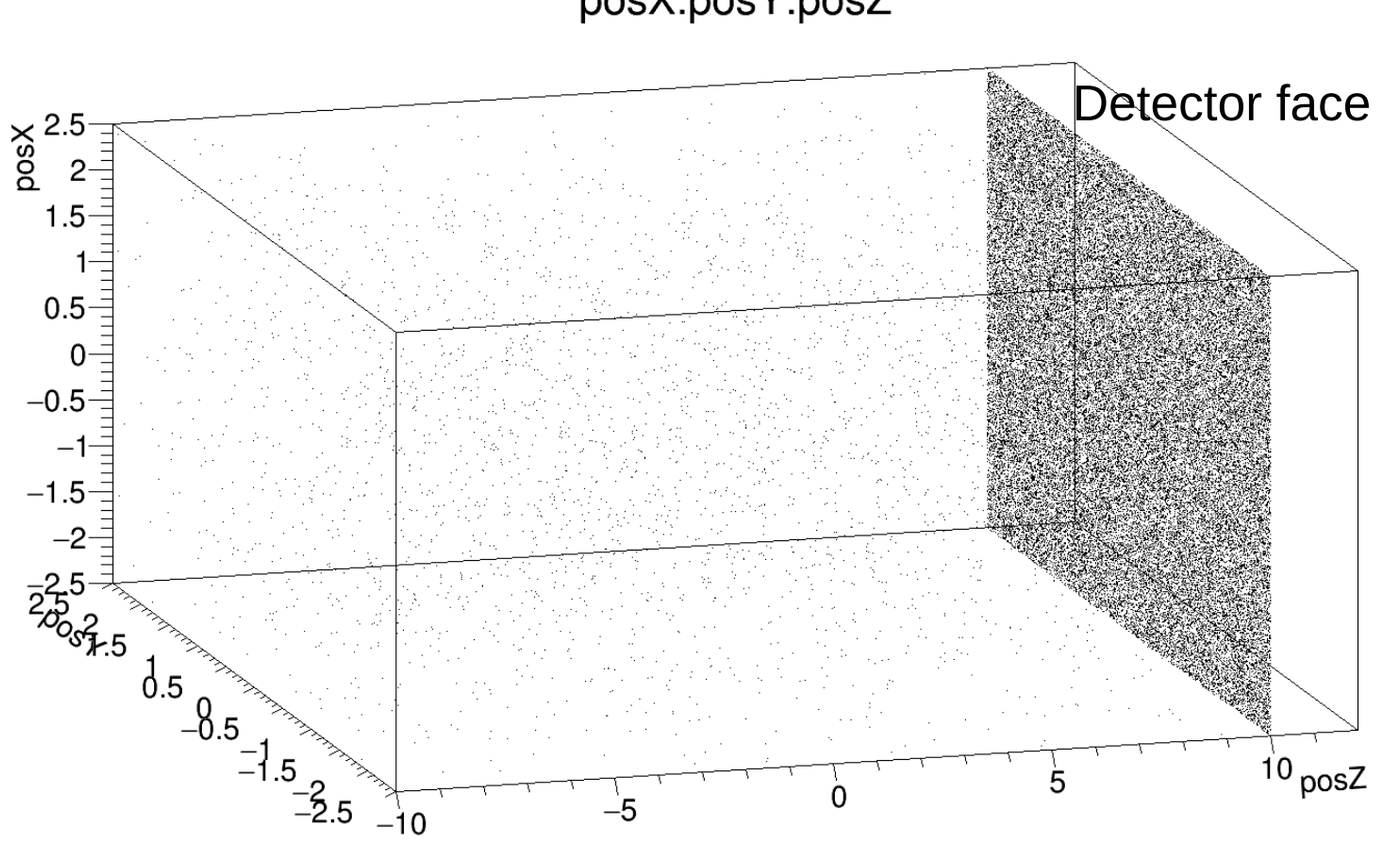

Courtesy Mariele Stockhoff

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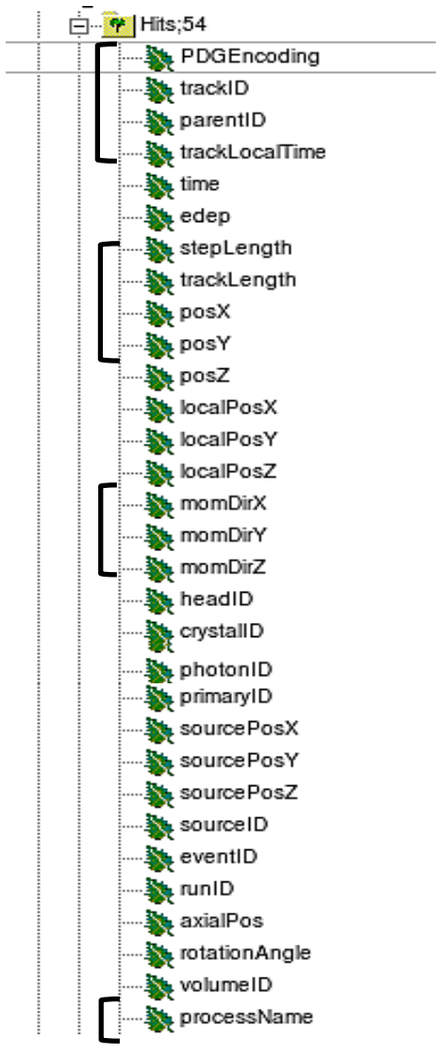
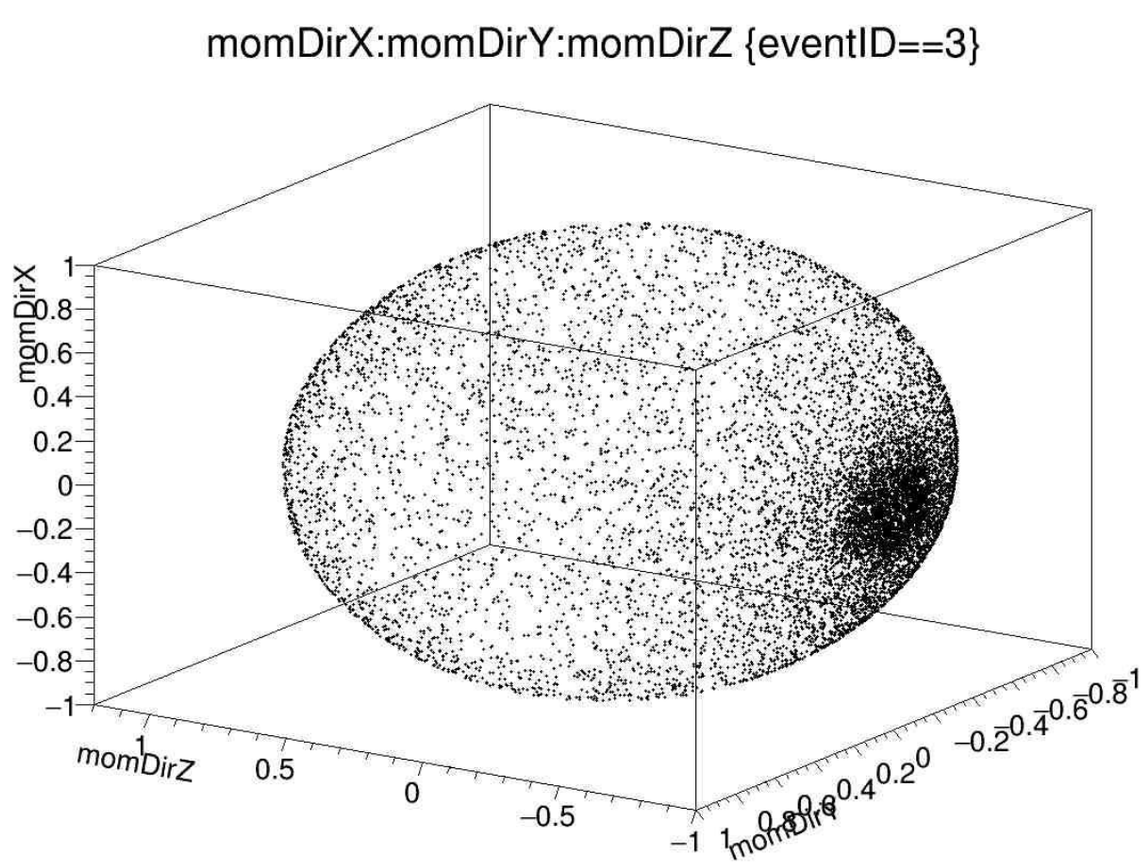


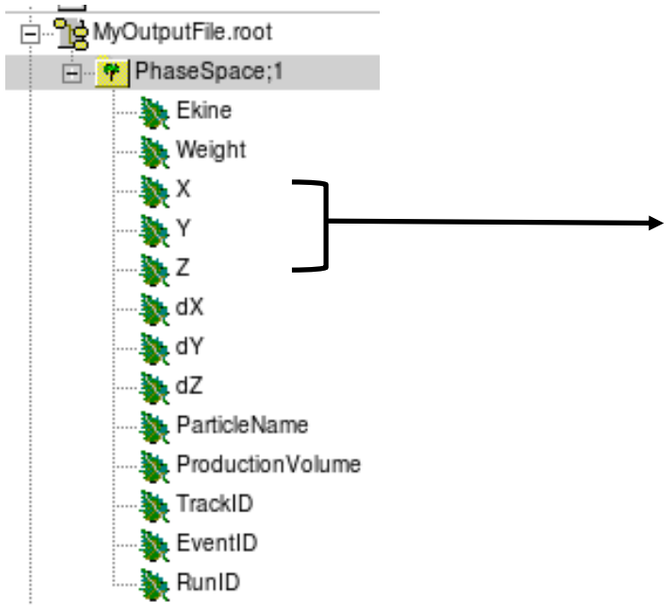


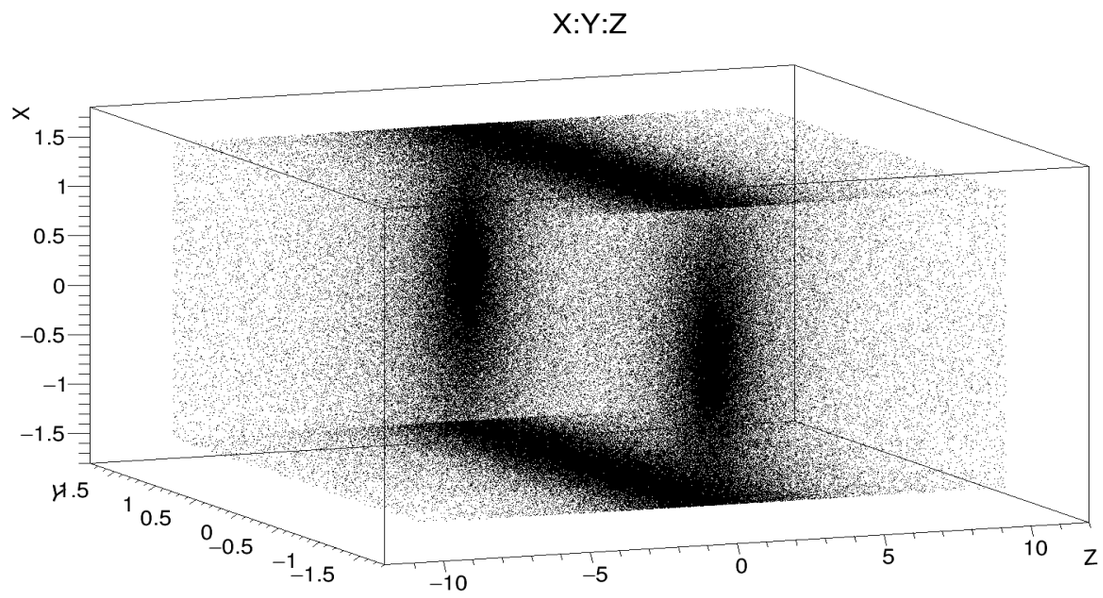
Courtesy Mariele Stockhoff

Use PhaseSpace Actor in Optical Simulations

PhaseSpaceActor.mac

```
/gate/actor/addActor PhaseSpaceActor MyActor
/gate/actor/MyActor/save MyOutputFile.root
/gate/actor/MyActor/attachTo crystal
/gate/actor/MyActor/enableProductionProcess false
/gate/actor/MyActor/storeOutgoingParticles true # Store exiting particles
```



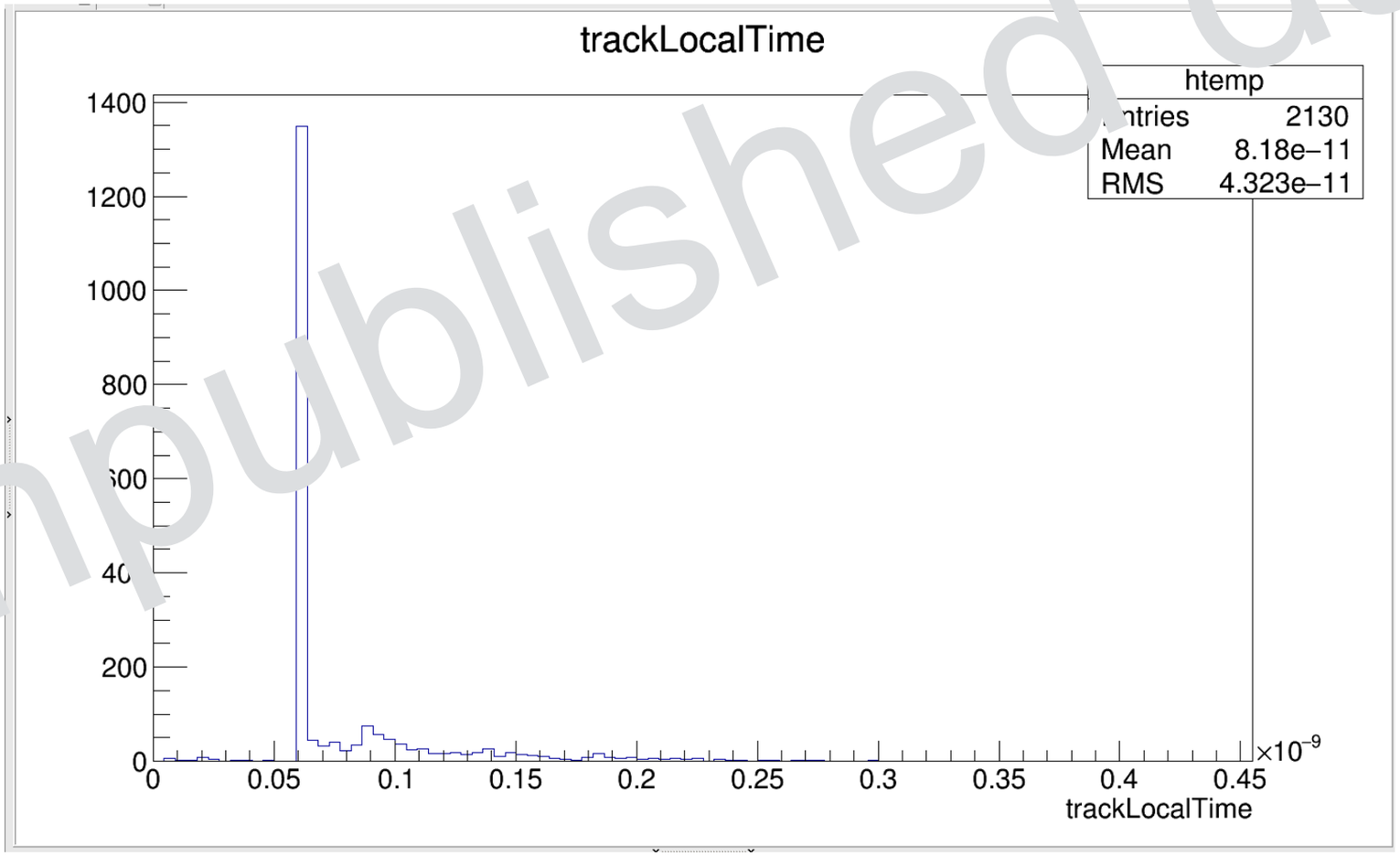


Escape scintillation photons for gamma interaction at z=0

Courtesy Mariele Stockhoff

Optical Output: Timing Properties

- Track transit time and length of photons is possible
- **BUT** accuracy limited by accuracy of reflectance model!



Courtesy Mariele Stockhoff

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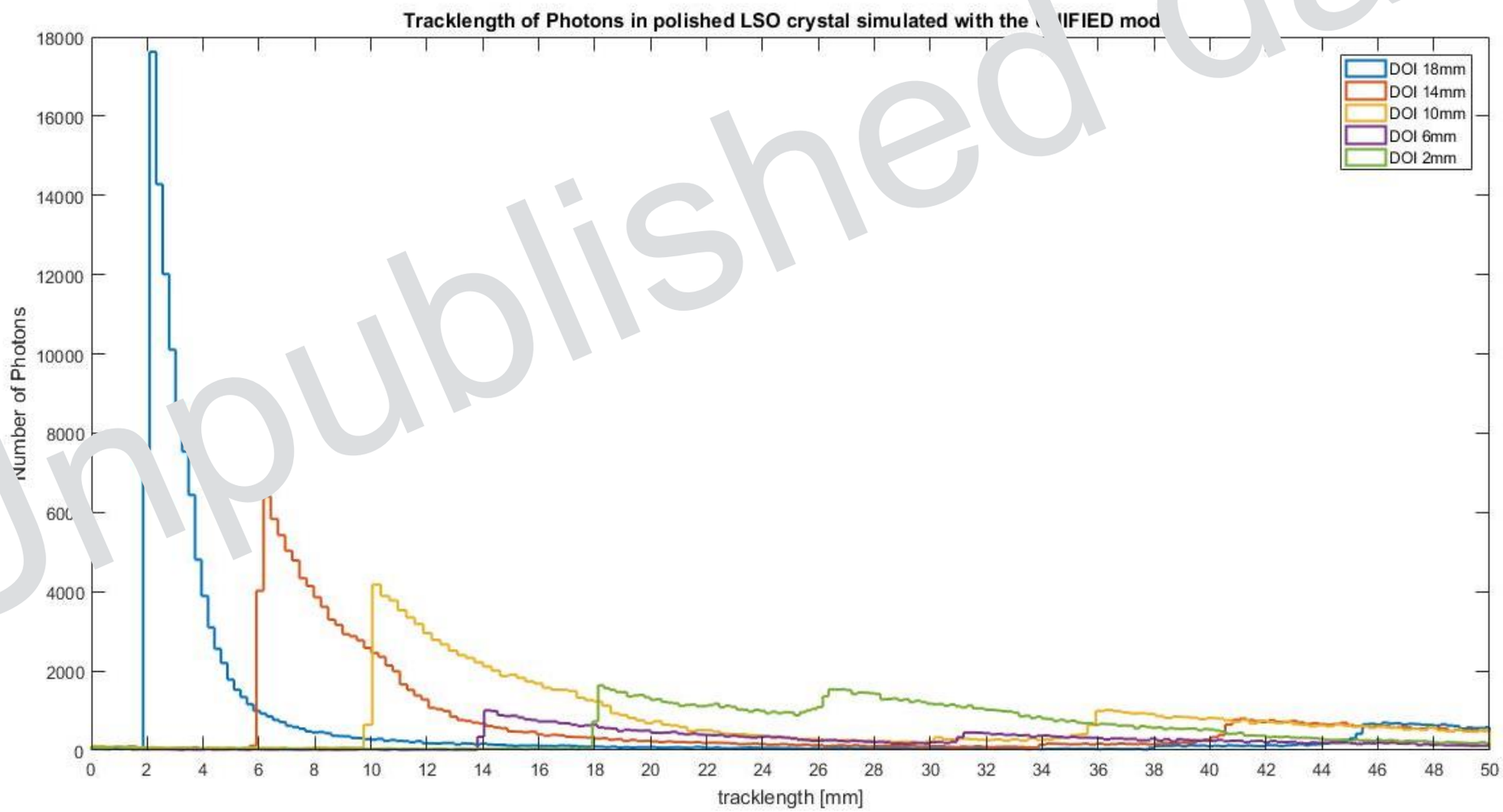

Courtesy Mariele Stockhoff

Conclusions

- UNIFIED model well established, but presents challenges with rough surfaces
- Reflectance models have been developed
- LUTs from Janecek and Roncali will be available, with the possibility of using custom surfaces (Roncali and Cherry)
- Timing information can be obtained to conduct timing studies
- phaseActor can provide information on photons that escaped

Questions?

eroncali@ucdavis.edu,

mstockhoff@ucdavis.edu

http://wiki.opengatecollaboration.org/index.php/Users_Guide_V7.2:Generating_and_tracking_optical_photons

http://wiki.opengatecollaboration.org/index.php/Users_Guide_V7.2:Phase_space_concept