Simulation of Optical Properties

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Outline

> *"Bridging the gap between laboratory measurements of scintillator properties and their implementation in Geant4"*

- Simulation of optical properties is **crucial in the life cycle** of optical calorimeters, both in R&D phase and during operation
- Successful simulation of optical calorimeters needs
  - Realistic description of **optical properties** (materials, surfaces, etc.)
  - Feasible **computation time**
- Stress on CPU-time
  - What strategies are available to **speed up** simulations?

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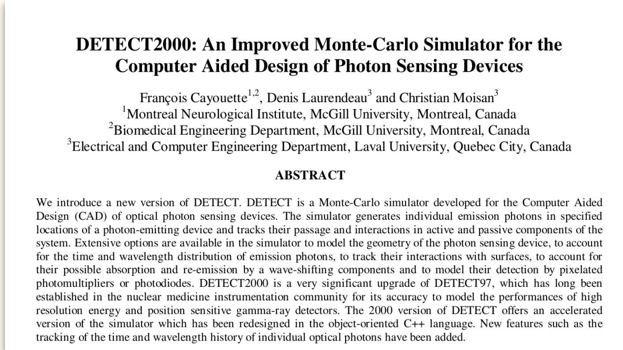
Monte Carlo simulations and optical photons

Over the years several simulation frameworks have been developed with optical photon capabilities

DETECT2000

- Designed for modeling optical properties of scintillation detectors
    - Generates photons and tracks their interaction with materials, surfaces and detectors
    - Uses the **UNIFIED model** for surface interactions
- Runs slowly for complex detector geometries
- Lack of visualization tools makes defining intricate geometries challenging



DETECT2000: An Improved Monte-Carlo Simulator for the Computer Aided Design of Photon Sensing Devices

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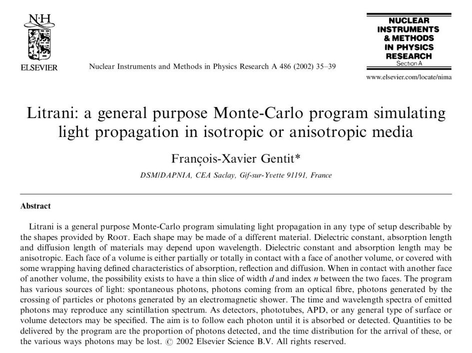
ABSTRACT

We introduce a new version of DETECT. DETECT is a Monte-Carlo simulator developed for the Computer Aided Design (CAD) of optical photon sensing devices. The simulator generates individual emission photons in specified locations of a photon-emitting device and tracks their passage and interactions in active and passive components of the system. Extensive options are available in the simulator to model the geometry of the photon sensing device, to account for the time and wavelength distribution of emission photons, to track their interactions with surfaces, to account for their possible absorption and re-emission by a wave-shifting components and to model their detection by pixelated photomultipliers or photodiodes. DETECT2000 is a very significant upgrade of DETECT97, which has long been established in the nuclear medicine instrumentation community for its accuracy to model the performances of high resolution energy and position sensitive gamma-ray detectors. The 2000 version of DETECT offers an accelerated version of the simulator which has been redesigned in the object-oriented C++ language. New features such as the tracking of the time and wavelength history of individual optical photons have been added.



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Litrani: a general purpose Monte-Carlo program simulating light propagation in isotropic or anisotropic media

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Abstract

Litrani is a general purpose Monte-Carlo program simulating light propagation in any type of setup describable by the shapes provided by ROOT. Each shape may be made of a different material. Dielectric constant, absorption length and diffusion length of materials may depend upon wavelength. Dielectric constant and absorption length may be anisotropic. Each face of a volume is either partially or totally in contact with a face of another volume, or covered with some wrapping having defined characteristics of absorption, reflection and diffusion. When in contact with another face of another volume, the possibility exists to have a thin slice of width *d* and index *n* between the two faces. The program has various sources of light: spontaneous photons, photons coming from an optical fibre, photons generated by the crossing of particles or photons generated by an electromagnetic shower. The time and wavelength spectra of emitted photons may reproduce any scintillation spectrum. As detectors, phototubes, APD, or any general type of surface or volume detectors may be specified. The aim is to follow each photon until it is absorbed or detected. Quantities to be delivered by the program are the proportion of photons detected, and the time distribution for the arrival of these, or the various ways photons may be lost.

(S)Litrani

- General purpose MC designed for simulating light propagation
    - Geometry built via ROOT libraries
    - Solves Maxwell equations at boundaries, can deal with **birefringent** materials (PWO)
- Lacks proper treatment of secondary particles

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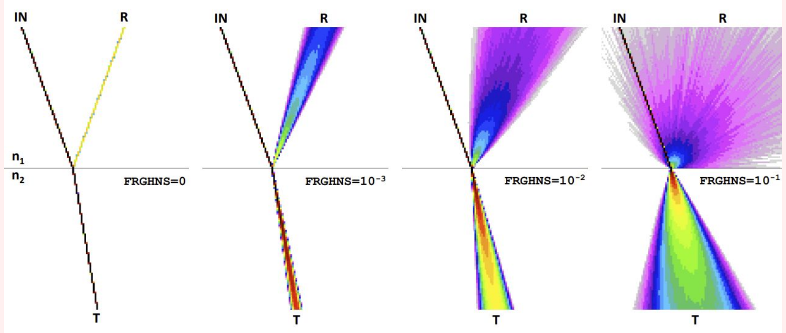
Monte Carlo simulations and optical photons

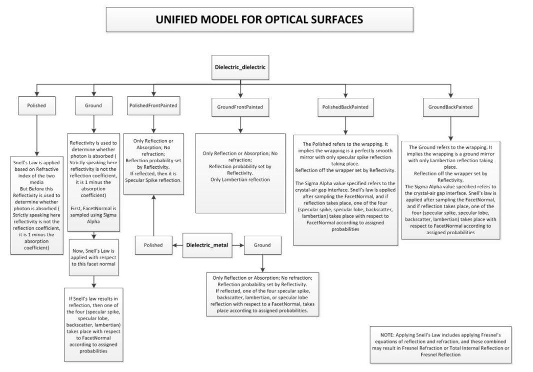
Modern general purpose Monte Carlo simulations can treat optical photons

FLUKA

- General purpose simulation for particle transport and interaction with matter
- Can generate optical photons via scintillation and Cherenkov (not transition radiation)
- **Simplified** treatment of optical surfaces



From 2023 Advanced Fluka.CERN course - Argonne Natl. Lab



Snell's Law is applied based on Refractive index of the two media But Before this Reflectivity is used to determine whether photon is absorbed (Strictly speaking here reflectivity is not the reflection coefficient, it is 1 minus the absorption coefficient)

Reflectivity is used to determine whether photon is absorbed (Strictly speaking here reflectivity is not the reflection coefficient, it is 1 minus the absorption coefficient)

First, FacetNormal is sampled using Sigma Alpha

Now, Snell's Law is applied with respect to this facet normal

If Snell's law results in reflection, then one of the four (specular spike, specular lobe, backscatter, lambertian) takes place with respect to FacetNormal according to assigned probabilities

Only Reflection or Absorption; No refraction; Reflection probability set by Reflectivity. If reflected, then it is Specular Spike reflection.

Only Reflection or Absorption; No refraction; Reflection probability set by Reflectivity. Only Lambertian reflection

The Polished refers to the wrapping. It implies the wrapping is a perfectly smooth mirror with only specular spike reflection taking place. Reflection off the wrapper set by Reflectivity.

The Sigma Alpha value specified refers to the crystal-air gap interface. Snell's law is applied after sampling the FacetNormal, and if reflection takes place, one of the four (specular spike, specular lobe, backscatter, lambertian) takes place with respect to FacetNormal according to assigned probabilities

The Ground refers to the wrapping. It implies the wrapping is a ground mirror with only Lambertian reflection taking place. Reflection off the wrapper set by Reflectivity. The Sigma Alpha value specified refers to the crystal-air gap interface. Snell's law is applied after sampling the FacetNormal, and if reflection takes place, one of the four (specular spike, specular lobe, backscatter, lambertian) takes place with respect to FacetNormal according to assigned probabilities

Only Reflection or Absorption; No refraction; Reflection probability set by Reflectivity. If reflected, one of the four specular spike, backscatter, lambertian, or specular lobe reflection with respect to a FacetNormal, takes place according to assigned probabilities.

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

GEANT4

- General purpose simulation for particle transport and interaction with matter
- Can generate optical photons via scintillation, Cherenkov and transition radiation
- Can use both GLISUR and **UNIFIED** models for optical surfaces

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General aspects of optical simulations

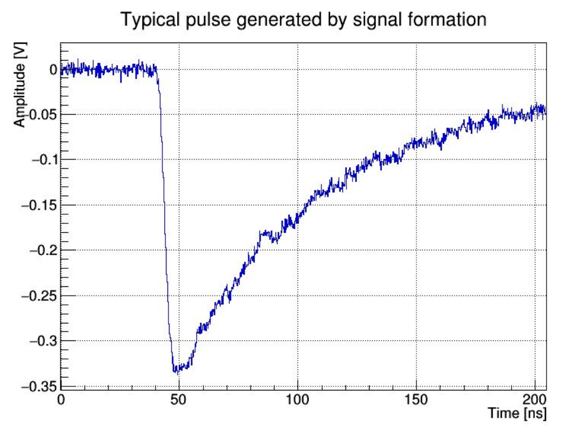
Essential features common to any Monte Carlo that deals with optical photons

- **Material** properties
  - Chemical composition, density
  - Refractive index
  - Absorption length, diffusion length
  - Scintillation properties (light yield, emission spectrum, time constants…)
  - WLS properties
  - Surface state (polished, ground…)
  - Birk’s coefficients

Require accurate inputs from **measurements** of material and detector characteristics!

- Photon **generation** and **propagation**
  - Scintillation, Cherenkov, Transition radiation
  - Navigation through geometry

- Photon **detection**
  - Photons will be propagated until absorbed or detected
  - Some modeling of photo-detector is needed



Typical pulse generated by signal formation

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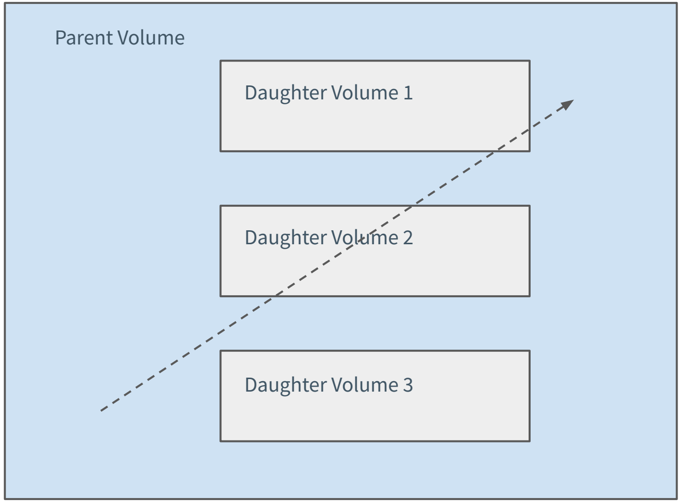
Geometry and track propagation in Geant4

Geant4 utilizes a parametric 3D **solid-based modeling** along with a **tree structure**

- A scene is composed of **primitive solids** defined by parameters
    - Sphere, cubes, etc.
    - Can be displaced, rotated and combined (boolean operations)
- All volumes need to implement classes to **answer questions** like:
    - Is a point inside?
    - Does a ray intersect the surface?
    - What's the normal vector on the surface at point x?



- Solids are organized in a **hierarchical tree structure**:
    - World volume at the top contains other volumes
    - Daughter volumes subtracts their space from the parent

- When tracking a particle, a ray in the direction of travel must be checked for intersection with the containing volume, plus all of the immediate daughter volumes (although other optimizations are in place, e.g. pixelization)
- As a result, the **number of sibling volumes** at a given node is a strong indicator of the tracking performance

The most computationally demanding aspect of photon propagation is the **calculation of intersection** positions of rays representing photons with the detector geometry

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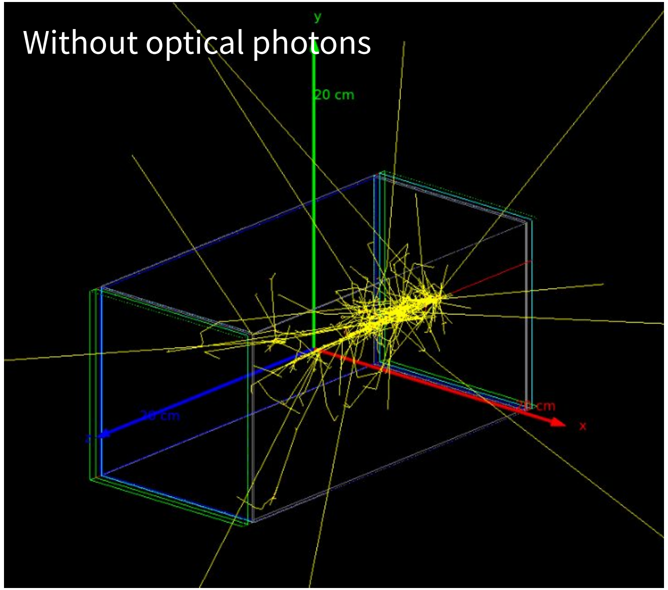
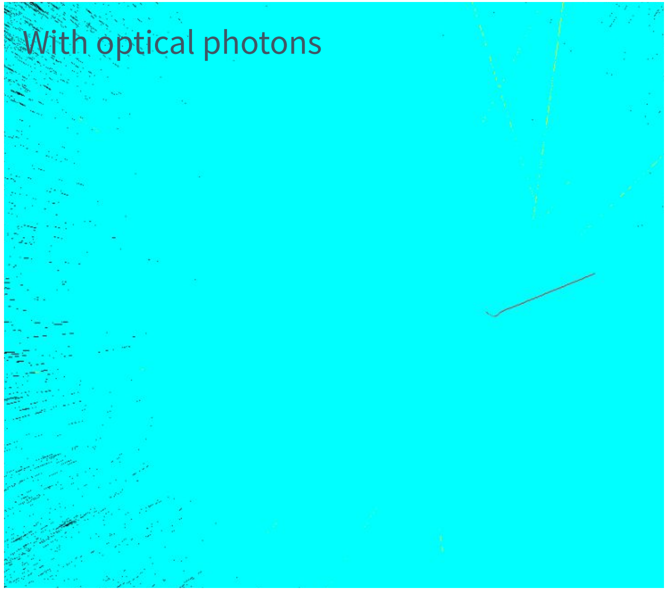
Number of tracks and optical photons

When optical photons are involved, the number of particles to propagate through the geometry greatly increases



Without optical photons



With optical photons

- Homogeneous **PWO crystal** (120x120x250 mm^3) hit by a single **1 GeV electron**:
  - On the left, only em shower particles → **2.5k tracks**
  - On the right, adding optical photons → **100k tracks**
- Remember that PWO has a low light yield (100 Ph/MeV), typical scintillators have in the order of 10kPh/MeV

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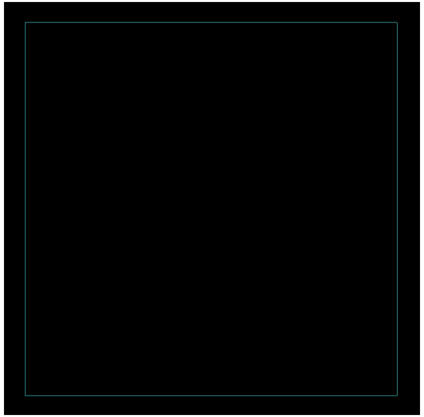
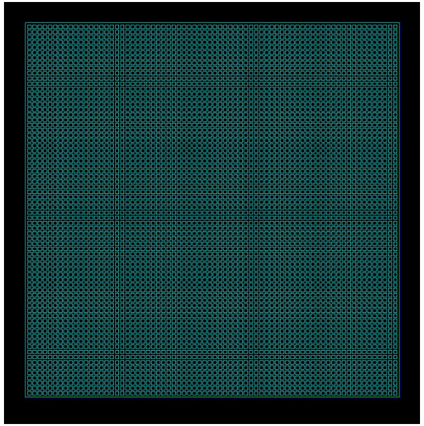
CPU time and optical photons

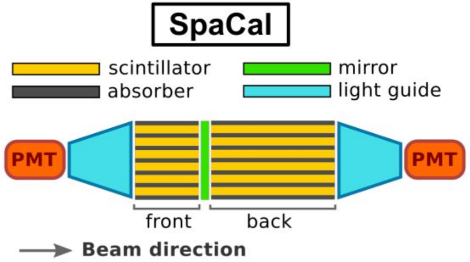
Simple test performed with Geant4.11 on 2 different configurations, on local PC



- **Homogeneous** PWO crystal (120x120x250 mm^3):
  - No optical photons → **0.06s** per GeV of primary electron
  - With optical photons → **3.2s** per GeV of primary electron
- About **50x slower** with optical photons
  - 1 crystal 120x120x250 mm^3
  - PWO light yield 100 Ph/MeV



- **SpaCal** module made of W and Polystyrene (120x120x200 mm^3):
  - No optical photons → **0.25s** per GeV of primary electron
  - With optical photons → **633s** per GeV of primary electron
- About **2500x slower** with optical photons
  - 5184 crystals, each 1x1x200 mm^3
  - Sampling fraction about 5%
  - Polystyrene light yield 10000 Ph/MeV



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Speedup strategies

At least to my knowledge, the main strategies to reduce computation time with Geant4 fall into 3 categories

Parameterization

Skipping the optical photon propagation entirely, reproducing the effects in a parameterized way

- Can be very CPU-efficient
- Applicability is highly application dependent
- Can result in loss of information

Ray tracing on GPU

Moving the ray tracing classes of Geant4 on GPU

- Few physics processes need to be implemented on GPU
- Little data transfer CPU-GPU
- Minimal communication between threads
- Can benefit from available efficient algorithms and hardware (NVIDIA CUDA, NVIDIA OptiX)

Rendering technologies on GPU

Performing the propagation of optical photons outside Geant4, using rendering technologies

- Active development, often used in animated movies
- Can be performed on GPUs as well

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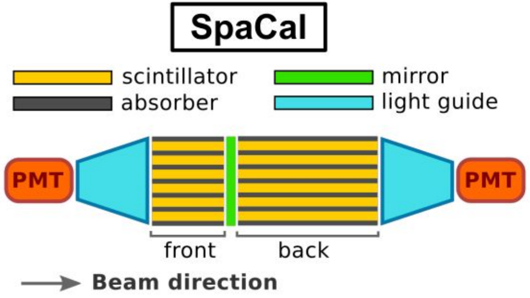
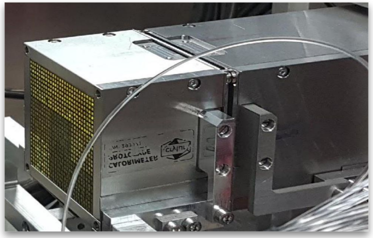
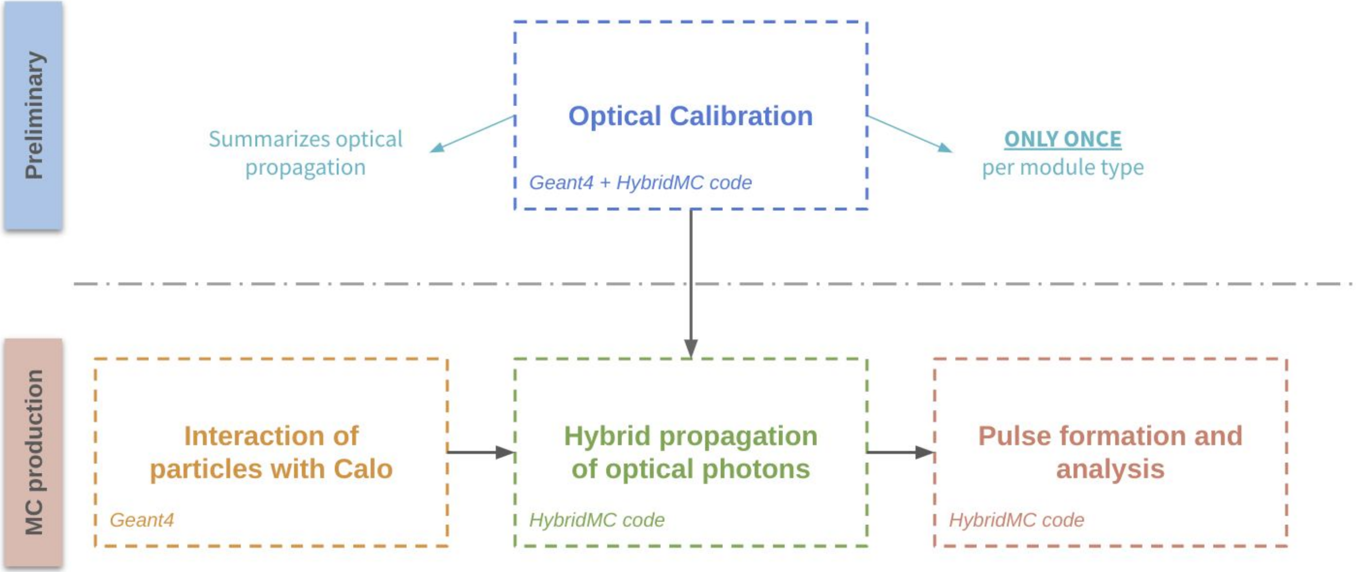
LHCb PicoCal: the HybridMC concept

Developed for detailed simulation of SpaCal and Shashlik technologies, moving transport of optical photons **outside of Geant4**







Preliminary

Optical Calibration

Geant4 + HybridMC code

Summarizes optical propagation

ONLY ONCE per module type

MC production

Interaction of particles with Calo

Geant4

Hybrid propagation of optical photons

HybridMC code

Pulse formation and analysis

HybridMC code

- Preliminary characterization with a special full ray-tracing run → **optical calibration**
  - Optical photons produced over a grid of points, propagated and collected at the exit of the modules
  - Histograms of the extracted photons are recorded
- Fundamental features of optical transport are **encoded in the histograms** (extraction efficiency, time distribution)
- Optical calibration needs to be performed **only once per module type** (so CPU time doesn't matter)

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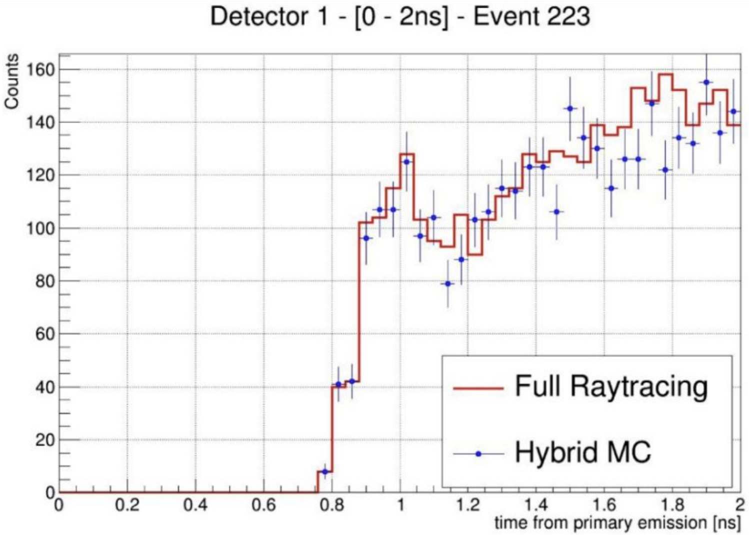
HybridMC: validation and CPU speedup



Technology	Type	Full ray-tracing *[s/GeV] of $e^{\pm}/\gamma$*	HybridMC *[s/GeV] of $e^{\pm}/\gamma$*	Gain
SpaCal	*W-GAGG*	990 ± 20	9.4 ± 0.1	~100
	Pb-Polystyrene	3600 ± 100	2.28 ± 0.04	~1500
	W-Polystyrene	1070 ± 20	2.88 ± 0.04	~400
Shashlik	–	1800 ± 30	3.83 ± 0.09	~500

- The HybridMC parameterized propagation is in **excellent agreement** with standard full ray tracing
- Substantial **gain in computation time**: from **100x** to **1500x** times faster
  - Allows to perform physics benchmark studies at LHC Run5 conditions in reasonable time
- Good agreement also with **experimental measurements** obtained in test beam on several SpaCal and Shashlik prototypes
  - Crucial for the R&D phase of LHCb PicoCal

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Opticks in Geant4

- Opticks is an open-source project that **accelerates optical photon simulation in Geant4** by:
    - Translating the Geant4 geometry to NVIDIA OptiX without approximation
    - Implementing the Geant4 optical processes on the GPU
    - Integrating NVIDIA GPU ray tracing

- Geant4 handles on CPU all particles but optical photons
- Information on Cherenkov and Scintillation photons stored
- Generation and tracing of optical photons is **offloaded to Opticks** and performed on GPU

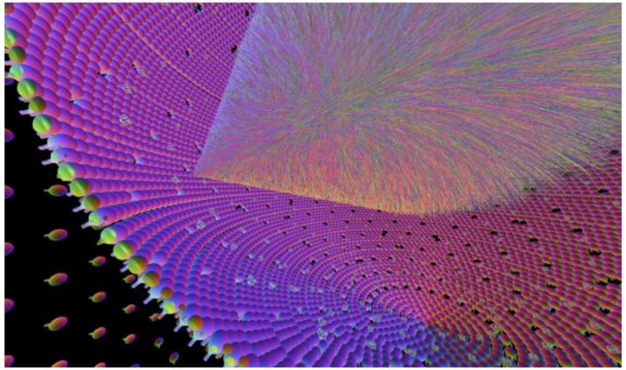
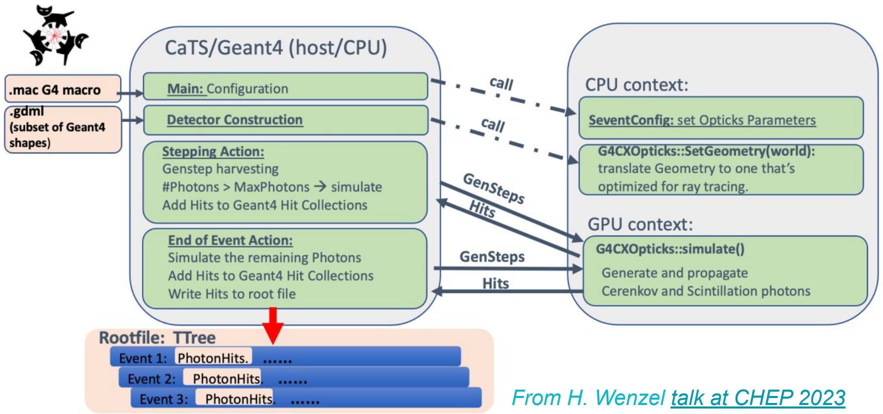


Figure 1. Cutaway OpenGL rendering of millions of simulated optical photons from a 200 GeV muon crossing the JUNO liquid scintillator. Each line corresponds to a single photon with line colors representing the polarization direction. Primary particles are simulated by Geant4, scintillation and Cherenkov "gensteps" are uploaded to the GPU and photons are generated, propagated and visualized all on the GPU. Representations of some of the many thousands of photomultiplier tubes that instrument the liquid scintillator are visible. The acrylic vessel that contains the liquid scintillator is not shown.

S. Blyth, Integration of JUNO simulation framework with Opticks: GPU accelerated optical propagation via NVIDIA OptiX

- Primarily developed for simulation of the JUNO detector
    - Demonstrated **speedup factor up to 1500x** using a single NVIDIA Quadro RTX 8000 GPU compared to a single threaded Geant4 simulation

- Example using Opticks is **available in Geant4.11**:
    - **CaTS**: Calorimeter and Tracking Simulation
    - Demonstrated speedup of a factor about 200x



From H. Wenzel talk at CHEP 2023

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Mitsuba3 and Geant4

- Mitsuba3 is a **physics-based renderer** developed by Realistic Graphics Lab at EPFL:
  - Supports the use of NVIDIA CUDA and NVIDIA OptiX
  - Also supports parallel processing on CPUs using LLVM

- Prototype workflow recently developed for propagation of Cherenkov photons in LHCb Rich
  - Hybrid approach that **offloads optical photons to the Mitsuba3 renderer**

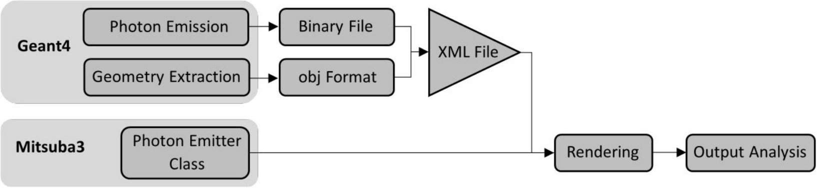
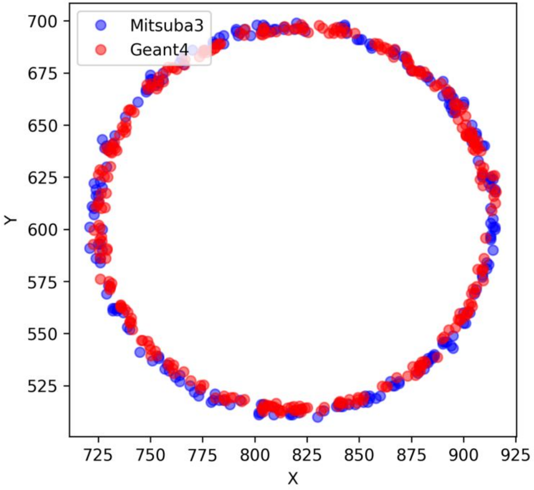
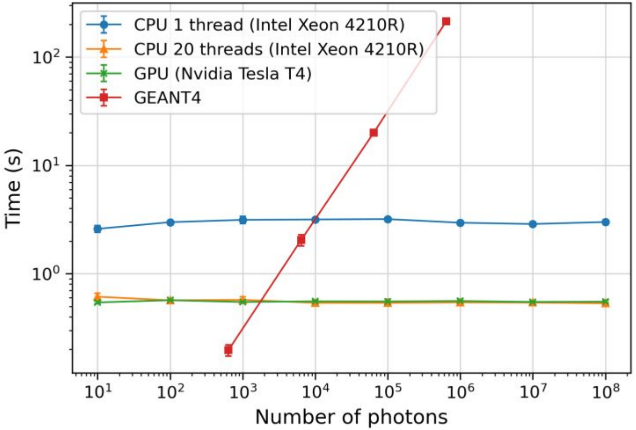


Fig. 1. Prototype workflow of the incorporation of MITSUBA3 within the GEANT4 framework. Each step was designed to be replaceable by a memory-resident implementation.

A. Davis et al., Optical Photon Simulation with Mitsuba3





- **Comparable physical results** between Mitsuba3 and Geant4 (ring center and radius)
- Contrary to Geant4, Mitsuba3 implementation **does not scale with number of optical photons**
- Code generation time limits the GPU performance in this first test, but can be further optimized

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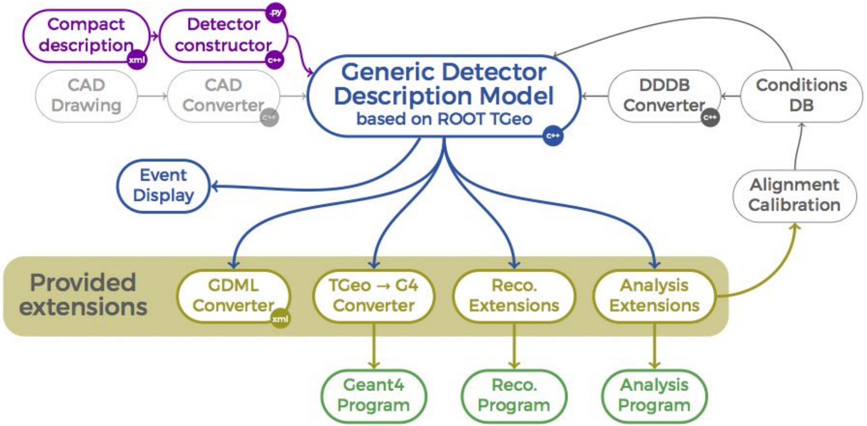
Reminder: DD4Hep

A toolkit developed to provide a **comprehensive detector description** for HEP

- Experience from HEP experiments points to the advantages of having a **single source of detector description** for
  - Simulation
  - Reconstruction
  - Analysis

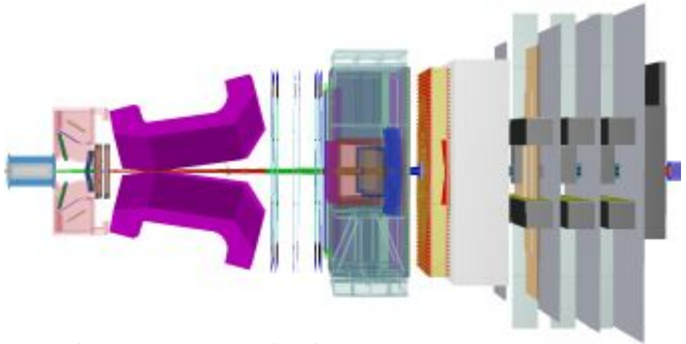
- DD4Hep developed to support **full life cycle** of an experiment:
  - Detector concept development
  - Detector optimization
  - Construction and operation
  - Extendible for future use cases

- Designed based on the experience of LHCb experiment and developments in the Linear Collider community:
  - Combines pre-existing widely used software in a **coherent generic detector description** (ROOT, Geant4…)
  - Actively used by CMS and LHCb among others



Compact description
Detector constructor
CAD Drawing
CAD Converter
Generic Detector Description Model
based on ROOT TGeo
DDDB Converter
Conditions DB
Event Display
Alignment Calibration
Provided extensions
GDML Converter
TGeo → G4 Converter
Reco. Extensions
Analysis Extensions
Geant4 Program
Reco. Program
Analysis Program

From DD4Hep website



Current description of LHCb Run4-5 geometry in DD4Hep

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Conclusions

- Simulation of optical properties is **crucial** in the life cycle of optical calorimeters

- Realistic **description of optical properties** is fundamental for the success of simulations
  - As the development of new materials and detectors (scintillators, absorbers, PMTs etc) is central in the R&D of optical calorimeters, it is difficult to imagine standardized libraries

- **Computation time** quickly becomes infeasible for full ray-tracing of optical photons
- Different speedup **strategies implemented**
  - Parameterizations have been developed, highly experiment-dependent
  - Benefits of massive parallel computing on GPUs have been demonstrated

Thank you for your attention!

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