Fermilab | U.S. DEPARTMENT OF ENERGY | Office of Science

Integration of Opticks[1] and Geant4 (an advanced example: CaTS)

Hans Wenzel

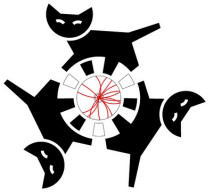
Soon Yung Jun

Krzysztof Genser

Alexei Strelchenko

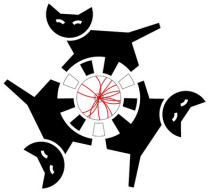
Fermilab

[1]developed by Simon Blyth
(Institute of High Energy Physics, Chinese Academy of Sciences)



Outline

- Opticks/G4Opticks/CaTS overview.
  - Opticks resources.
- CaTS:
  - Latest developments.
  - CaTS resources.
- Status of re-implementing Opticks for Optix7.
- Plans.



Opticks/G4Opticks/CaTS

Opticks is an open-source project that accelerates optical photon simulation by integrating NVIDIA GPU ray tracing, accessed via NVIDIA OptiX.

Developed by Simon Blyth:

https://bitbucket.org/simoncblyth/opticks/

CaTS: interfaces Geant4 user code with Opticks using the G4Opticks interface provided by Opticks. It defines a hybrid workflow where generation and tracing of optical photons is offloaded to Opticks (GPU), while Geant4(CPU) handles all other particles. CaTS was included in Geant4 11.0 as an advanced example:

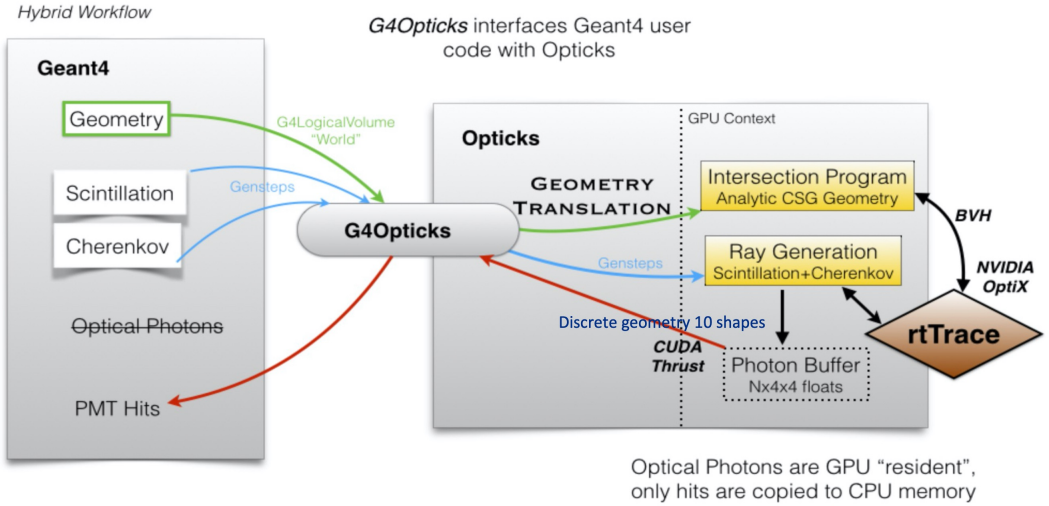
https://geant4.kek.jp/lxr/source/examples/advanced/CaTS/

Integrate NVIDIA OptiX with Geant4

Geometry Translation + **"Gensteps"**
=> entirely offload photon simulation to GPU

- upload translated geometry at initialization
- only hits need to consume CPU memory

Figure from Simon's presentation



Fermilab

Opticks resources:

https://simoncblyth.bitbucket.io/env/presentation/opticks_may2020_hsf.html

EPJ Web of Conferences **214**, 02027 (2019),
https://doi.org/10.1051/epjconf/20192140202
Simon Blyth:
"**Opticks : GPU Optical Photon Simulation for Particle Physics using NVIDIA® OptiX™ "**

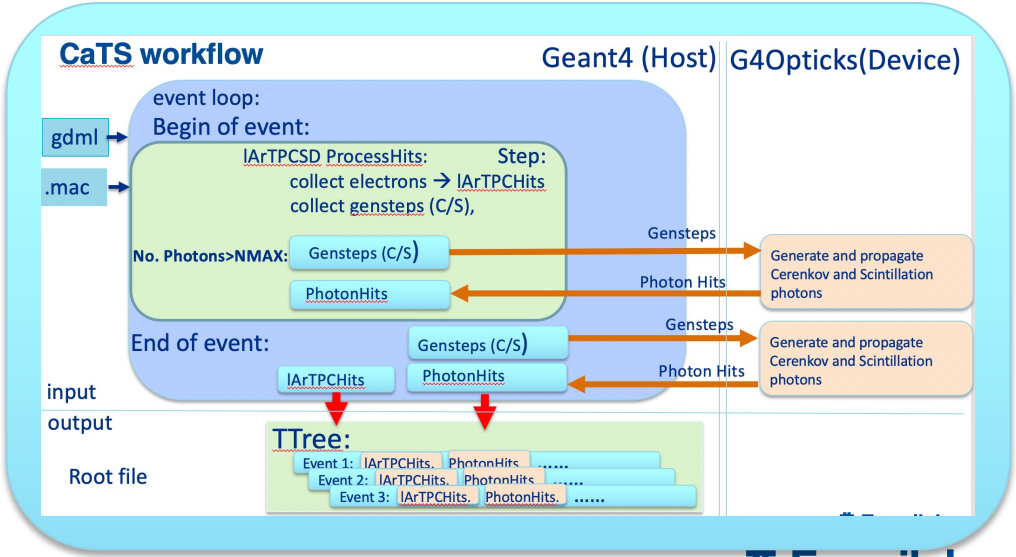
Detector geometry in Opticks: https://indico.cern.ch/event/975008/
Documentation: https://simoncblyth.bitbucket.io/opticks/index.html

Code repositories:
https://bitbucket.org/simoncblyth/opticks/ : main development repository
https://github.com/simoncblyth/opticks : used for snapshots and tagged releases.
The most recent tag is https://github.com/simoncblyth/opticks/releases/tag/v0.1.7
→ Starting point from 'our' github fork.

CaTS: advanced Geant4 example

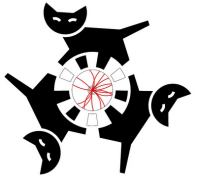
- Uses Geant4 to collect Scintillation and Cerenkov Gensteps. A Genstep collects all the data necessary to generate Cerenkov/Scintillation photons on the GPU. The harvesting is done in Sensitive Detectors(SD) (RadiatorSD/lArTPCSD). The number of photons to be generated is calculated by Geant4 and constrained to be identical whether one uses the Geant4 optical physics or G4Opticks.
- Use of G4Opticks is both a build and runt-time option.
- The PhotonHits collected by the PhotonSD sensitive detector have the same content whether Geant4 or G4Opticks is used.
- Uses GDML with extensions for flexible Detector construction and to provide optical properties at runtime. The gdml extensions include:
  - Assigning Sensitive Detectors to logical Volumes.
    Available:
    - **RadiatorSD**, **lArTPCSD**, **PhotonSD.**
    - TrackerSD, CalorimeterSD, DRCalorimeterSD, ...
  - Assigning step-limits to logical Volumes.
  - Assigning production Cuts by regions.
  - Assigning visualization attributes.
  - Note there are Opticks specific keywords!
- Uses G4PhysListFactoryAlt to define and configure physics.
- Uses Root IO to provide persistency for Hits.

Achieved speed up in the order of a few times 10^2, depends strongly on detector geometry, hardware and settings.

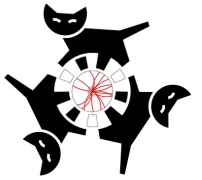


Fermilab

Latest developments:



- For the Geant4 advanced example:
  - Lots of code and cmake cleanup, make use of C++17 features, follow Geant4 code conventions added visual code configuration.
- More examples: (e.g. scintillation crystals, WLS examples, …).
- Help users getting started with CaTS.
- Ensure that gdml examples are compatible with Geant4 10/11 and Opticks.
- Various optimizations.
- Changes to RootIO.
- Allow for Geant4 event-level multi-threading for offloading Opticks– autolock for G4Opticks call (generate and propagate Photons). But poor scaling due to mutex (as expected as kernels calls are sequential).



Hardware: Nvidia RTX3090, Core i9-10900k@ 3.7Ghz 10 CPU cores, results are very preliminary.

Number of threads	Geant4 [sec/evt]	Opticks [sec/evt]	Gain
1	330	1.8	189
2	175	1.8	101
4	105	1.8	59
8	45	1.9	24
16	36.5	2.	18

CaTS/Opticks resources

- https://github.com/hanswenzel/opticks, our fork to work on Opticks with Optix 6.5.

  Changes include:
  - Changes to make it compatible with the Geant4 11 API.
  - Bulk reemission process during photon propagation disabled. If reemission is necessary, it can be expressed as WLS process where Scintillation and WLS share the same PDF.
  - Extract properties relevant to WLS.
- Main git repository: https://github.com/hanswenzel/CaTS/ :used for development.
- Instructions how to build and run CaTS: https://github.com/hanswenzel/CaTS/blob/master/README.md
- Instructions how to build Opticks and how to install all necessary software: https://github.com/hanswenzel/CaTS/blob/master/Instructions.md
- Instruction how to run various CaTS examples (examples consist of: gdml file, Geant4 macro and an application that makes histograms from the hits collections): https://github.com/hanswenzel/CaTS/blob/master/Examples.md
- https://gitlab.cern.ch/geant4/geant4 : will be used for snapshots and tagged releases

Status of re-implementing Opticks for Optix 7[1].

Huge change unavoidable from new OptiX API → So profit from rethink of simulation code → **2nd implementation advantage**. Goals of re-implementation : flexible, modular GPU simulation, easily testable, less code:

- COMPLETED: Full Simulation re-implementation for OptiX 7 API, but new workflow not ready for testing yet.
- Many packages were removed or are planned to be removed.
- Move code that doesn't require Optix or Cuda out of GPU context (SYSRap, not QUDARap).
- Rather monolithic .cu was replaced by many small GPU+CPU headers many GPU+CPU headers.

1) Extracted from status report by Simon Blyth for more details see:
https://simoncblyth.bitbucket.io/env/presentation/opticks_20220718_towards_production_use_juno_collab_meeting.html

Plans

G4Opticks/Opticks:

- Add opticks to the framework used by the liquid Argon TPC community. That requires Cuda, Optix, Opticks … being packaged in the way required by these frameworks (ups/upd, spack).
- Try out the new Opticks as soon as Simon gives the go-ahead.
- Use the same implementation of the scintillation process on CPU and GPU, use the same optical properties/keywords.
- Implement Wavelength shifting process (WLS).
- Have a look at simplifying cmake, e.g., get rid of obsolete modules.

CaTS:

- Achieve true concurrency by using G4Tasking. Allow to fully utilize GPU resources like vram, cpu cores, multiple GPU's.
- Change to use Root TBufferMerger for RootIO instead of using separates file and merging them when in multithreaded mode.
- Provide benchmarking and physics validation results with realistic (including WLS) liquid Argon TPC geometry.

Geant4:

- Move the harvesting of Gensteps to the Geant4 optical producer processes (G4Cerenkov, G4Scintillation)→ general interface to external ray tracing programs like Opticks. Trigger the G4Opticks from UserSteppingAction whenever sufficient photons/gensteps are collected for efficient processing on GPU.