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Optical physics in Celeritas

Status of an upcoming capability

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SWIFT-HEP

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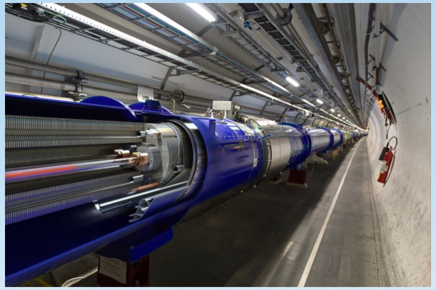
Celeritas: an overview

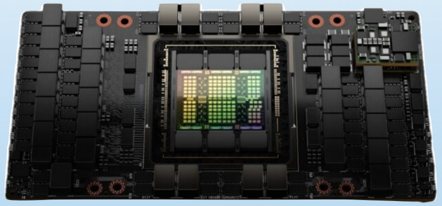
Using next-generation computing
to accelerate HEP's hardest simulations

- **GPU** optimized, CPU reproducible
- **Full-fidelity** Monte Carlo detector simulation
- **Automated** Geant4 integration (geometry, physics, SD)
- **Open source** and actively seeking collaborators



LHC beamline ©CERN

CELERITAS

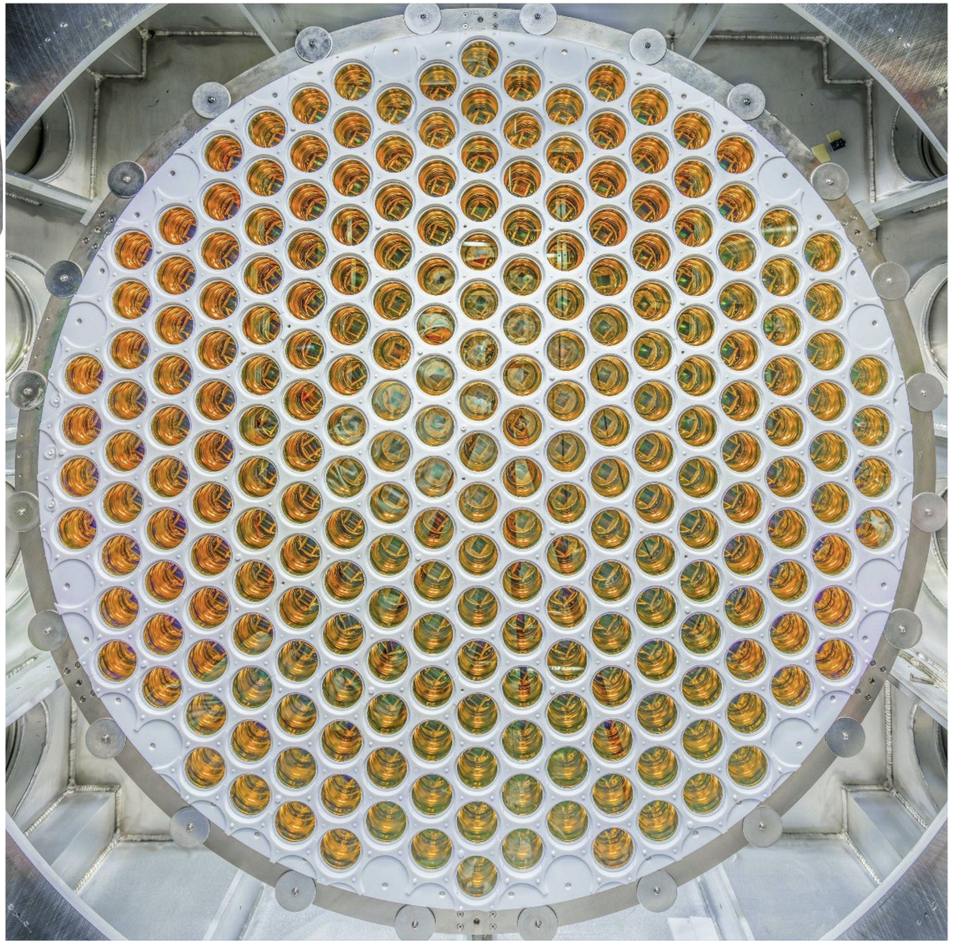


Nvidia H100 GPU @Nvidia

Informal collaborators

Optical physics for scintillation detectors

- Required for numerous experiments
  - Dark matter (LZ)
  - Neutrino physics (DUNE, SBND), LEGEND
  - R&D (Calvision)
- Thousands of Cherenkov/scintillation photons per step
- Geant4 optical physics is notoriously slow
  - Current workaround: optical “maps”
  - Future requirement: high-fidelity



PMT array ©LZ

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Celeritas optical physics strategy

- Platform portable (CPU, Nvidia, AMD) *always*
- Separate tracking loop from main particles
  - Vast numbers of tracks, often few steps per track
  - Physics and detectors at surface crossings
  - Reuse core Celeritas components: geometry, etc.
- Progressive integration complexity
  1. Emit via Cherenkov/scintillation from Celeritas EM loop
  2. Standalone "optical map" application
  3. Offload photons produced from Geant4 optical physics
  4. Replace Geant4 optical physics processes

Supported platforms

	CPU	Nvidia	AMD
Geant4	✅	❌	❌
OptiX	❌	✅	❌
Celeritas	✅	✅	✅
Mitsuba3	✅	✅	❌

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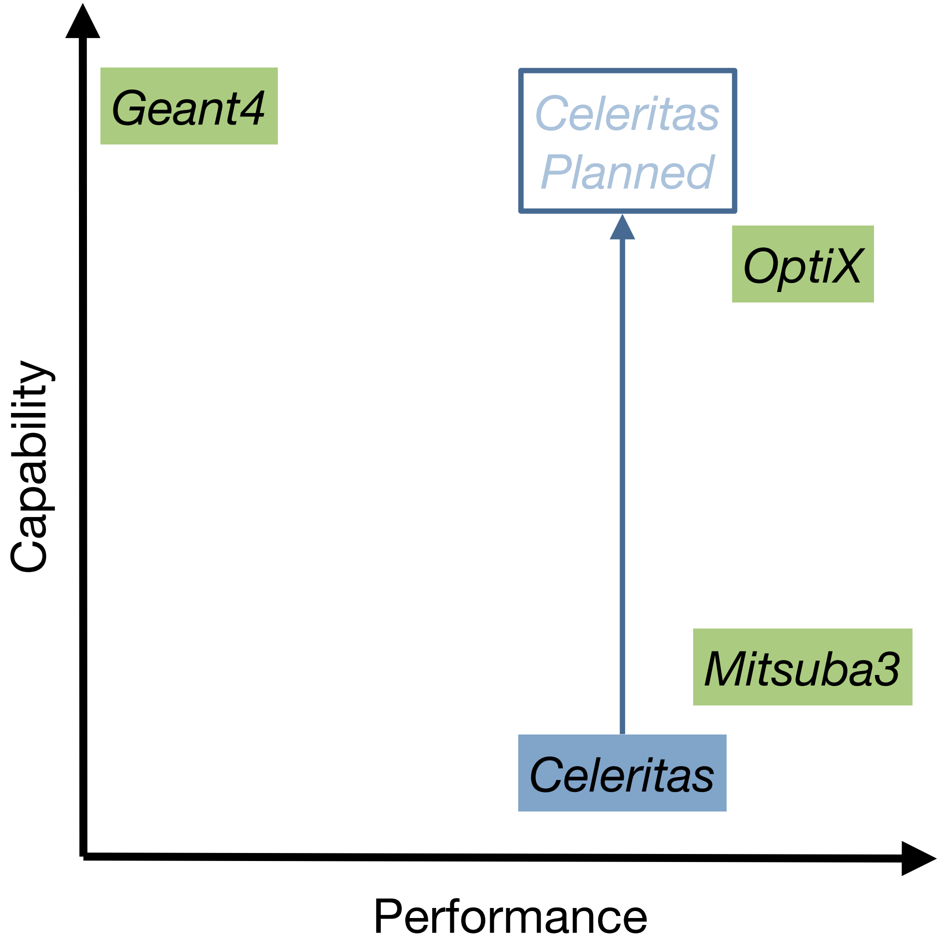
Planned physics capabilities

✓ Optical generation
  ✓ Cherenkov emission
  ✓ Scintillation
- Volumetric optical physics
  ✓ Absorption
  ✓ Rayleigh scattering
  ▪ Wavelength shifting
- Surface optical physics



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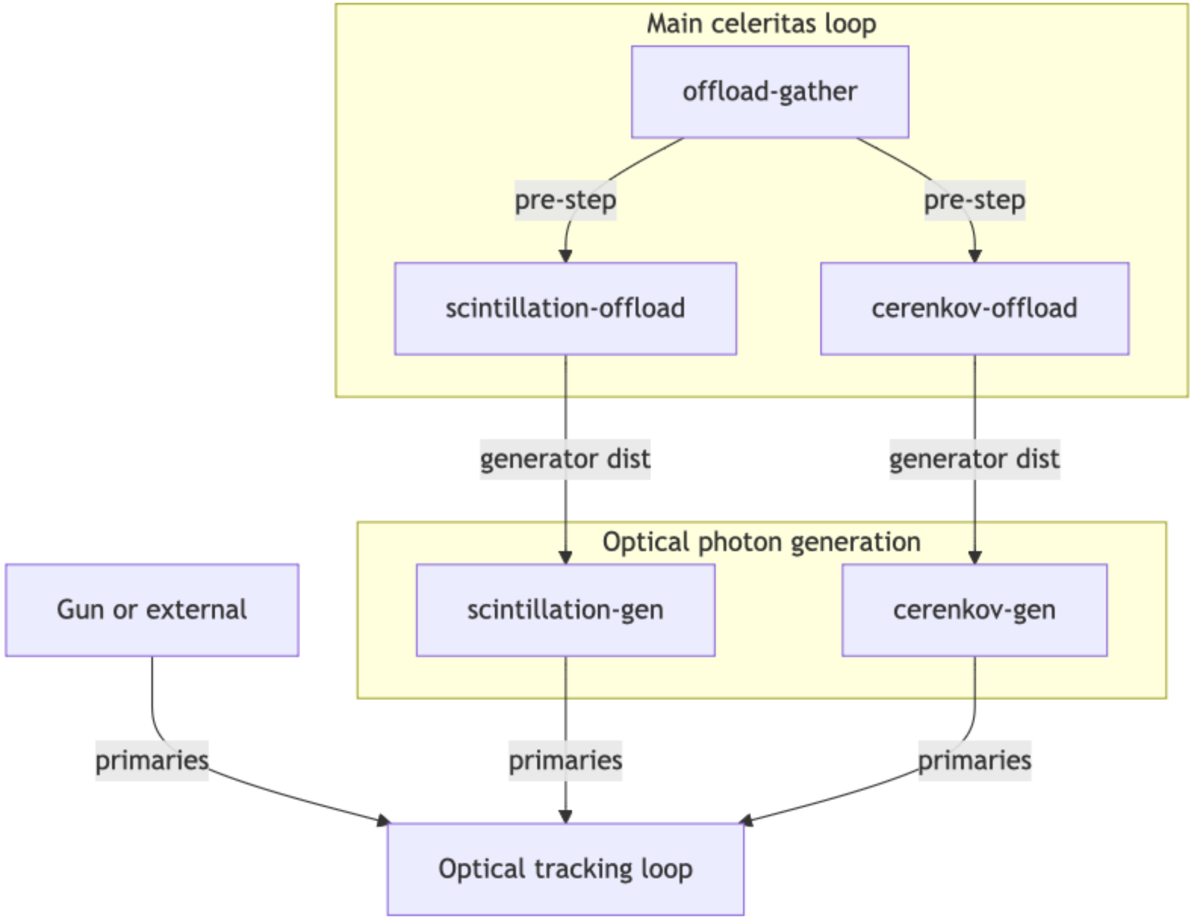
Optical loop structure

- Steps generate "distributions"
  - Currently, Cherenkov and scintillation
  - Small struct with all data needed to sample optical photons (number of photons, time, step length, material…)
  - More efficient than generating and transferring many individual tracks
- Distributions generate tracks
  - Distributions transfer to device/optical loop
  - Generate photon tracks from distributions
  - Transport optical photons
  - Collect and send back hits



Optical material/model properties

- Imported from Geant4 material properties
  - Photon-creating process data: scintillation spectra
  - Photon model data: Rayleigh, wavelength shifting (WLS)
  - Energy-dependent mean free path (MFP)
  - Material data: index of refraction
- Future work: open source material database

```
/*!
 * Store basic properties for different scintillation
 *
 * Fast/intermediate/slow/etc scintillation components
 * particle- and material-dependent spectra, as well a
 */
struct ImportScintComponent
{
    double yield_frac{};  //!< Fraction of total scint
    double lambda_mean{};  //!< Mean wavelength [len]
    double lambda_sigma{};  //!< Standard deviation of
    double rise_time{};  //!< Rise time [time]
    double fall_time{};  //!< Decay time [time]
};
```

Geometry for photon transport

- **ORANGE**: *Oak Ridge Advanced Nested Geometry*
  - Originally developed for reactor engineering applications
  - Ported to GPU (Nvidia, AMD, CPU) in 2021
  - Represents volumes as quadric surfaces + CSG
- GPU-optimized: low divergence
- Automatic conversion of Geant4 geometry
- Biggest shortcoming (no inherent "safety distance") doesn't matter for photons

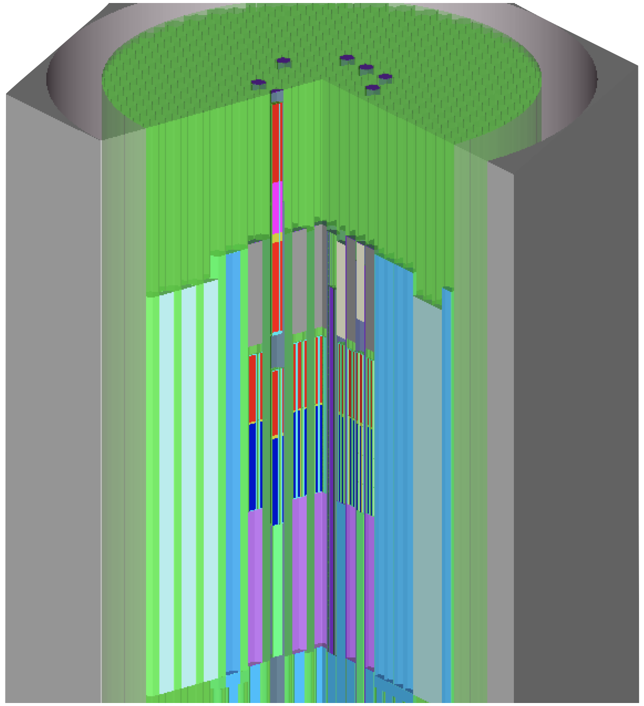
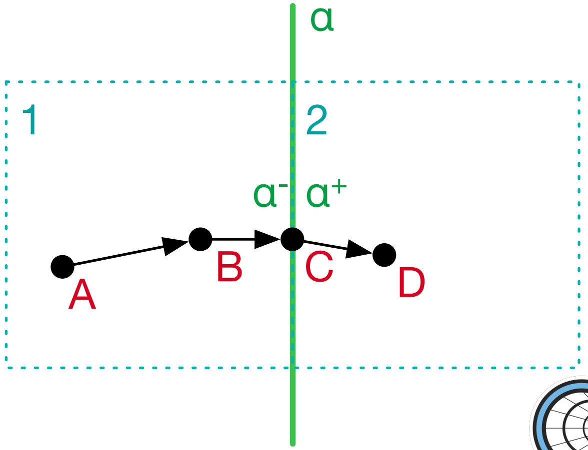


Image credit: Steve Skutnik (ORNL)



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Proof-of-concept performance: photon generation

- Single 10 MeV electron primary in a LAr sphere
  - Roughly **300 million** optical photons total
  - AMD EPYC 7532 (32 core) vs Nvidia A100
- Only **generating** optical (scintillation + Cherenkov) photons, not tracking
  - `celer-sim` (standalone Celeritas): kill the optical photons immediately
  - `celer-g4` (Geant4 front end): immediately kill optical photons via user tracking action

	CPU threads	Runtime (s)
Geant4	1	204.5
Celeritas CPU	1	99.3
Celeritas CPU (OMP)*	64	5.7
Celeritas GPU	1	1.3

**OpenMP track-level parallelism*

150 CPU : 1 GPU performance tracks with previous results

Conclusions and future work

- Celeritas has lofty goals
  - High performance
  - Platform portable
  - Feature parity with Geant4 (and beyond)
- Still a work in progress
- Performance results are promising
- Initial volumetric physics by end-of-year
- Full surface physics by mid-2025

Acknowledgments

Celeritas v0.5 code contributors:

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Code

Documentation

Publication