Celeritas: toward GPU-based particle transport for detector simulations in HEP experiments

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U.S. DEPARTMENT OF ENERGY | Office of Science

Celeritas Project

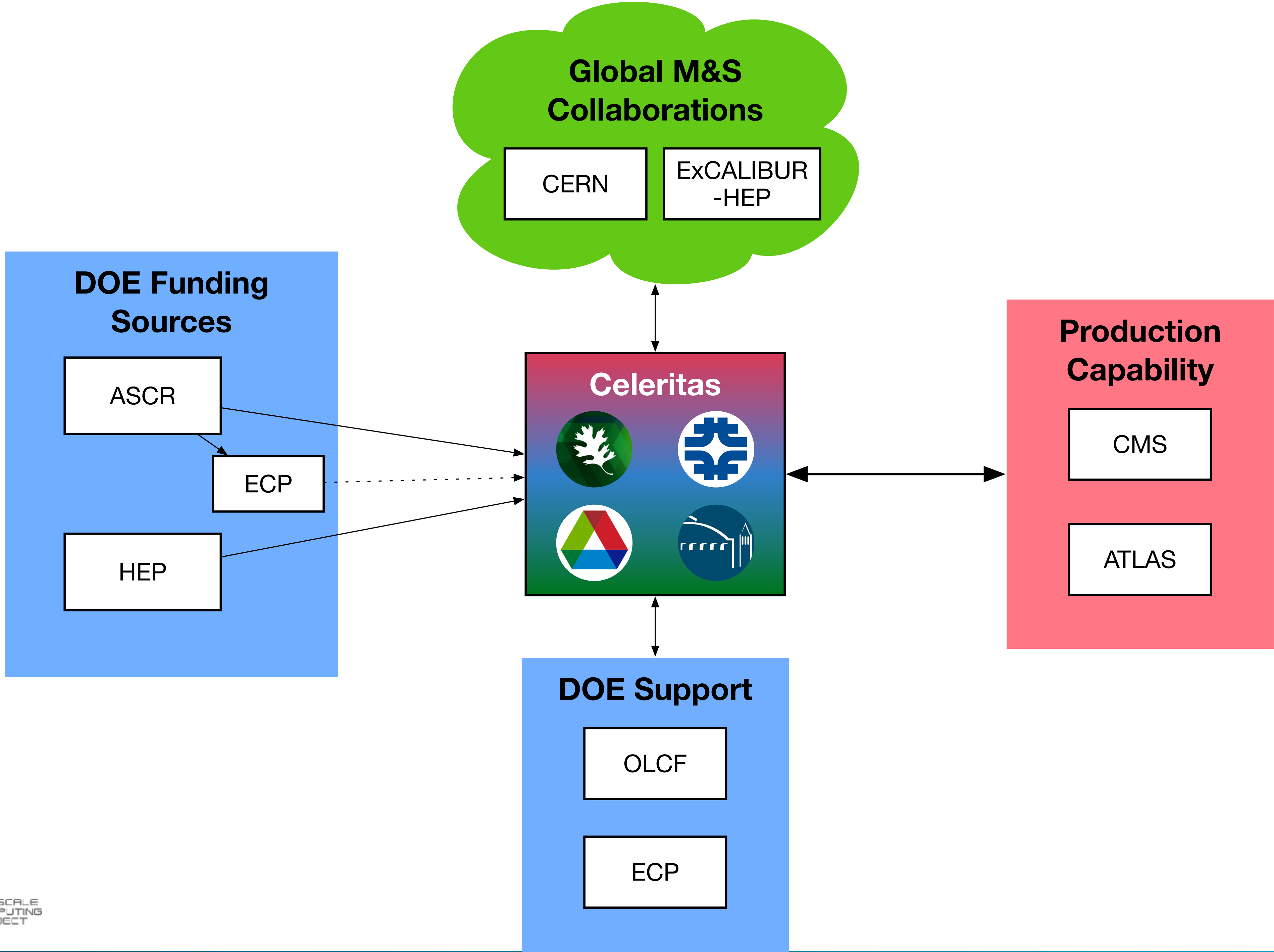
Project objective

Deliver a GPU-accelerated particle transport application for HEP detector simulations

1. Why is this capability needed?
   - Current high-fidelity, time-dependent, detector energy deposition simulations will not scale to proposed 10× luminosity increase in 2025-2026
2. What are the technical capabilities and opportunities needed for breakthroughs in the detector mod-sim area?
   - Efficiently use leadership class hardware (GPUs) to increase particle tracking throughput with concurrent improvements in I/O and post-processing analysis
3. How is the current project different from previous efforts and how will it enable those breakthroughs?
   - Accelerator technology (GPUs) has reached maturity
   - Monte Carlo transport applications have demonstrated performance on these architectures in ECP (exascaleproject.org) and CASL (casl.gov) for science campaign level simulations
   - Through ECP, we have access to a complete ecosystem of high performance libraries and tools
4. What is the long-term strategy for integration with Geant4?
   - Use Celeritas to offload EM physics in a standard Geant4-constructed application
   - Use Celeritas as part of a broader LHC workflow for complete detector simulation
   - Combinations of both approaches should be possible

Requirements

- Utilize modern heterogeneous (CPU + GPU) architectures at all scales (laptop to exa)
- Read events from HEP community event generators (Pythia/HEPMC3, etc)
- Use community Geant4 geometry models (VecGeom/GDML)
- Include (ultimately) complete physics models for HEP detector simulation in Geant4
  - Preliminary focus is on high-energy EM physics
- Target most compute-intensive component of HEP detector simulation workflow: time-dependent, detector energy deposition (hit generation)
  - Complements and is part of standard Geant-driven LHC simulation workflow



Global M&S Collaborations
CERN
ExCALIBUR -HEP
DOE Funding Sources
ASCR
ECP
HEP
Celeritas
Production Capability
CMS
ATLAS
DOE Support
OLCF
ECP
EXASCALE COMPUTING PROJECT

Celeritas Code

Development approach

- Bottom-up development approach
- Parallelize effort over individual components
- Integration guided by weekly group meetings
- Modularity will enable restructuring for performance
- Demo mini-app progression for integrating components

Source code

Language	Files	Comment	Code
C/C++ Header	182	4537	5974
C++	45	1180	2494
CMake	17	344	1609
Bourne Shell	14	96	381
CUDA	7	202	358
Python	4	473	320
Total	**269**	**6832**	**11136**

Test code

Language	Files	Comment	Code
C++	49	1037	3172
C/C++ Header	22	394	1021
CUDA	8	159	510
Total	**79**	**1590**	**4703**

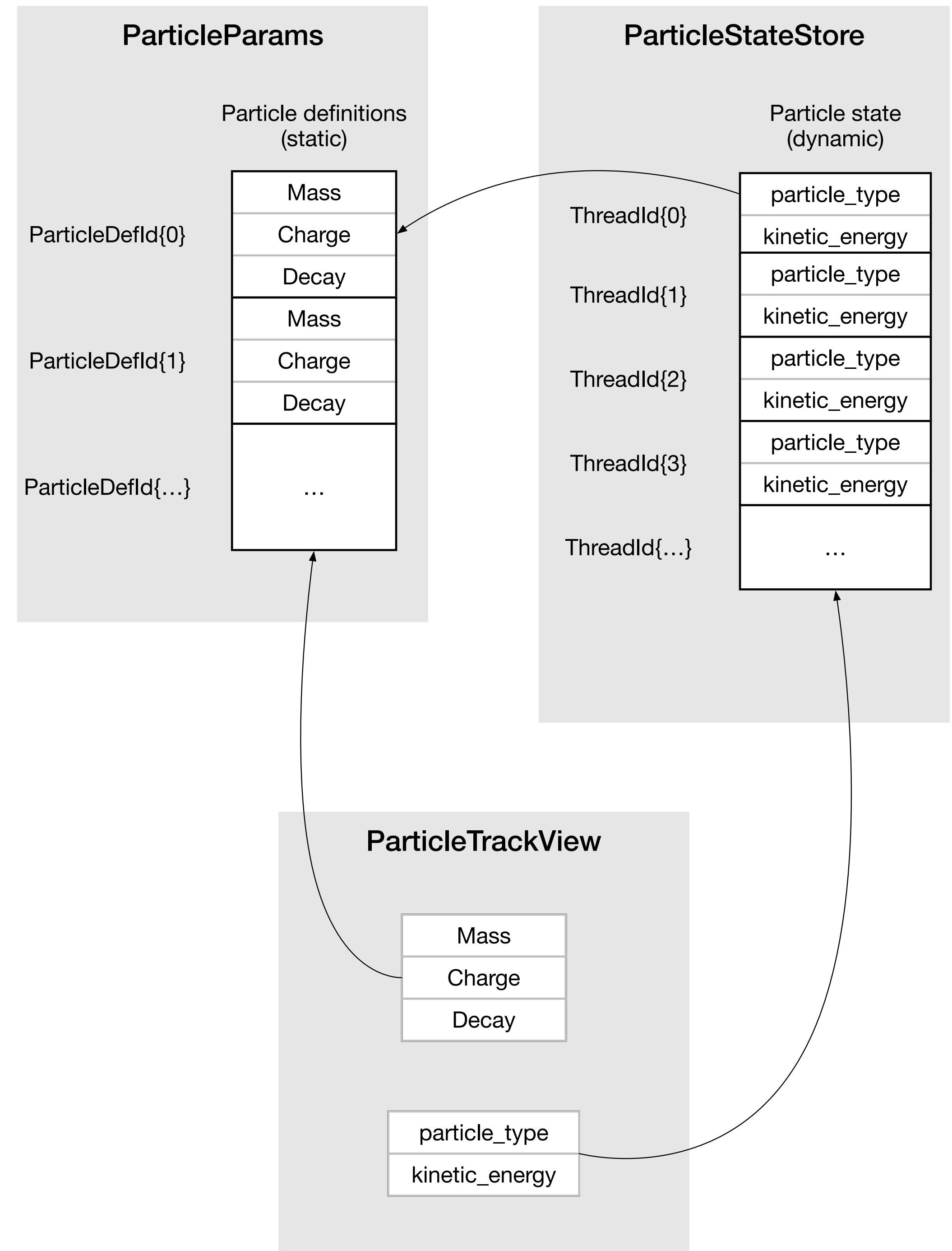
Celeritas code base statistics

Current development focus areas

- **Infrastructure**
  - Cohesive framework (GitHub wiki)
  - Import GPU algorithms from Shift GPU code
- **Physics**
  - Leverage Geant4 physics implementations and documentation
  - Export preprocessed Geant4 data where possible
- **Geometry**
  - Interface with VecGeom CUDA library

Software abstractions for portability

- Kernel code is separate from memory management and memory layout
    - Enables development, testing, and debugging on CPU
    - Allows isolated experimentation with data layouts to optimize GPU performance
    - Could enable (for example) Kokkos data management
- Kernels are plain C++ with annotations
    - Macros to enable CUDA device code, extensible to HIP and other performance abstraction layers
    - Runtime initialization code is host-only



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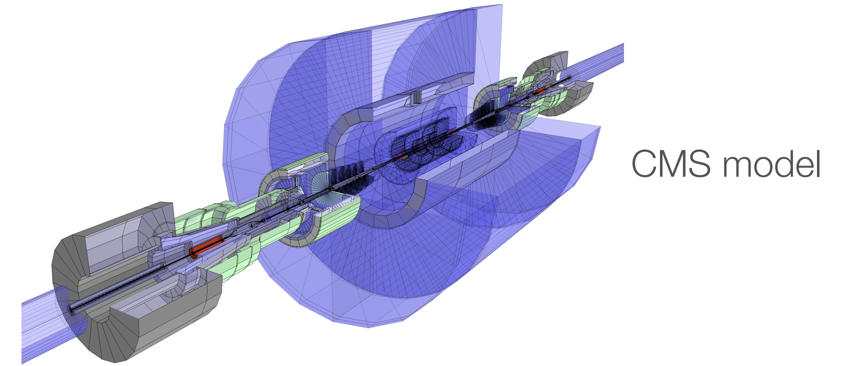
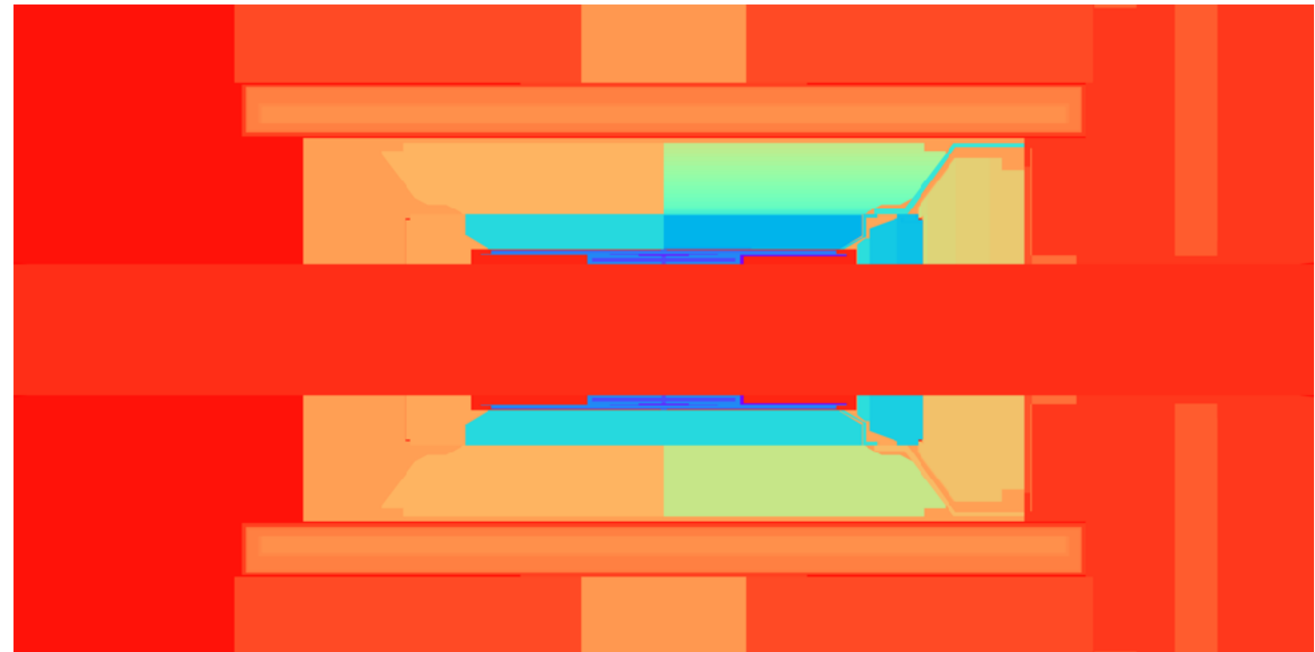
Geometry mini-app: CMS ray trace


CMS model

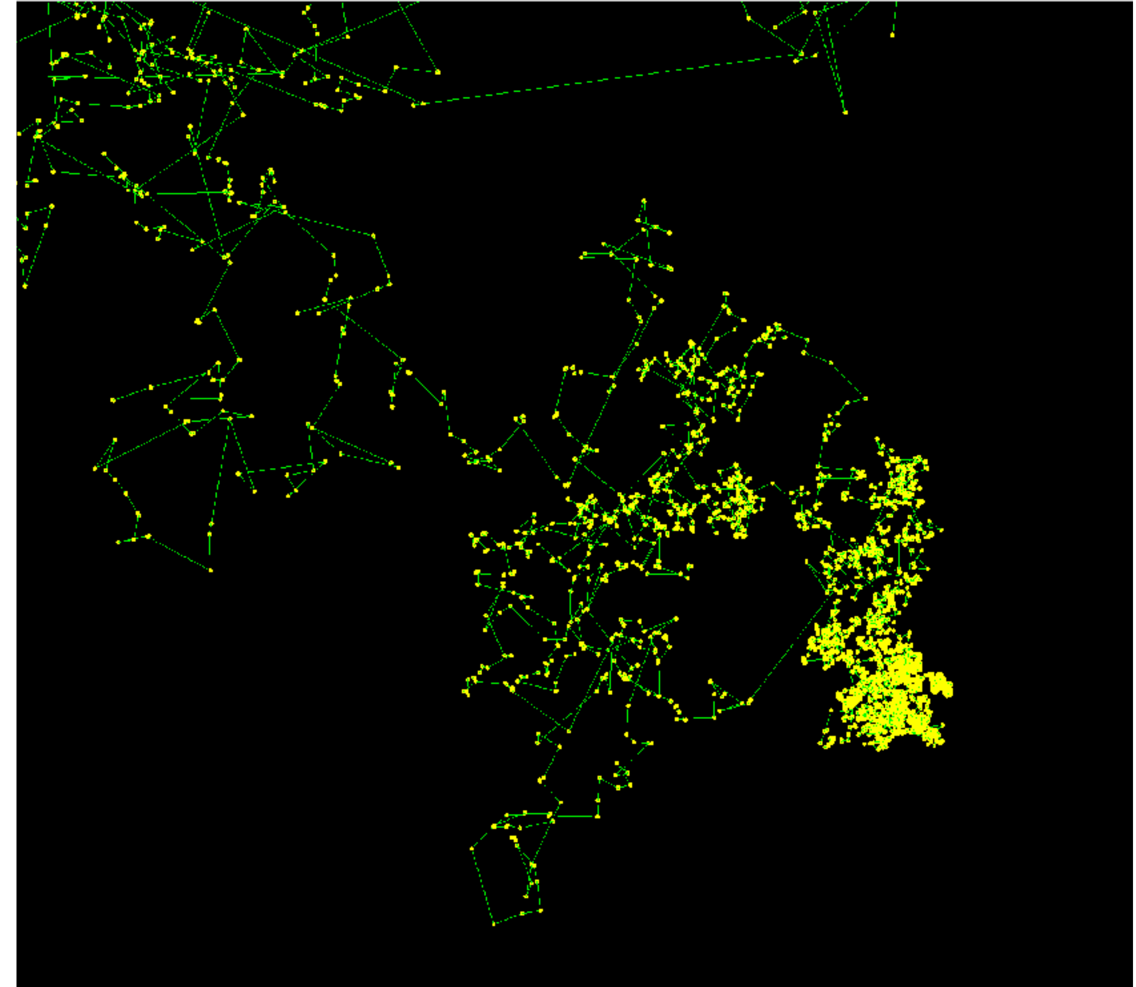
- VecGeom linked into Celeritas externally
  - CUDA device object library/separable compilation for GPU support
  - Invaluable support from VecGeom liasons
- Raytrace mini-app
  - Integration test of VecGeom interface, LinearPropagator, MaterialTrackView
  - Each horizontal line is a CUDA thread


CMS raytrace, tracks initialized on CPU and traced on GPU

https://github.com/celeritas-project/celeritas/pull/40

Physics mini-app: Klein–Nishina photon transport

- Simplest **physical** simulation we can run
  - Photon-only transport (electrons created but immediately killed and locally deposited)
  - Single process (inelastic scattering neglecting binding energy)
  - Single infinite material (aluminum)
  - 100 MeV monodirectional point source
- Celeritas (GPU and CPU-only versions), Geant4
- Verification: axial energy deposition



https://github.com/celeritas-project/celeritas/pull/51

Physics mini-app: features

- Stepping kernel is parallel over tracks (one launch per step)
  - Interaction length sampling with (uniform-in-energy) cross section calculation
  - Movement and direction updates
  - Full Klein–Nishina Compton scattering (neglecting binding energy)
  - Allocation and construction of secondary particle
  - Detector hit allocation and assignment (energy, position, direction, time, event)
- Tallying kernel to process “hit list” into bins
- Reduction kernel for termination criteria and diagnostics

```
//---------------------------------------------------------------------------/
/*!
 * Perform a single interaction per particle track.
 *
 * The interaction:
 * - Clears the energy deposition
 * - Samples the KN interaction
 * - Allocates and emits a secondary
 * - Kills the secondary, depositing its local energy
 * - Applies the interaction (updating track direction and energy)
 */
__global__ void iterate_kn(ParamPointers const             params,
                           StatePointers const             states,
                           SecondaryAllocatorPointers const secondaries,
                           DetectorPointers const          detector)
{
    SecondaryAllocatorView allocate_secondaries(secondaries);
    DetectorView           detector_hit(detector);
    PhysicsArrayCalculator calc_xs(params.xs);

    for (int tid = blockIdx.x * blockDim.x + threadIdx.x;
         tid < static_cast<int>(states.size());
         tid += blockDim.x * gridDim.x)
    {
        // Skip loop if already dead
        if (!states.alive[tid])
        {
            continue;
        }

        // Construct particle accessor from immutable and thread-local data
        ParticleTrackView particle(
            params.particle, states.particle, ThreadId(tid));
        RngEngine rng(states.rng, ThreadId(tid));

        // Move to collision
        {
            // Calculate cross section at the particle's energy
            real_type                          sigma = calc_xs(particle);
            ExponentialDistribution<real_type> sample_distance(sigma);
            // Sample distance-to-collision
            real_type distance = sample_distance(rng);
            // Move particle
            axpy(distance, states.direction[tid], &states.position[tid]);
            // Update time
            states.time[tid] += distance * unit_cast(particle.speed());
        }

        Hit h;
        h.pos    = states.position[tid];
        h.thread = ThreadId(tid);
        h.time   = states.time[tid];

        if (particle.energy() < KleinNishinaInteractor::min_incident_energy())
        {
            // Particle is below interaction energy
            h.dir              = states.direction[tid];
            h.energy_deposited = particle.energy();

            // Deposit energy and kill
            detector_hit(h);
            states.alive[tid] = false;
            continue;
        }

        // Construct RNG and interaction interfaces
        KleinNishinaInteractor interact(params.kn_interactor,
                                        particle,
                                        states.direction[tid],
                                        allocate_secondaries);

        // Perform interaction: should emit a single particle (an electron)
        Interaction interaction = interact(rng);
        CHECK(interaction);
        CHECK(interaction.secondaries.size() == 1);

        // Deposit energy from the secondary (effectively, an infinite energy
        // cutoff)
        {
            const auto& secondary = interaction.secondaries.front();
            h.dir                 = secondary.direction;
            h.energy_deposited    = secondary.energy;
            detector_hit(h);
        }

        // Update post-interaction state (apply interaction)
        states.direction[tid] = interaction.direction;
        particle.energy(interaction.energy);
    }
}
```

Stepping kernel

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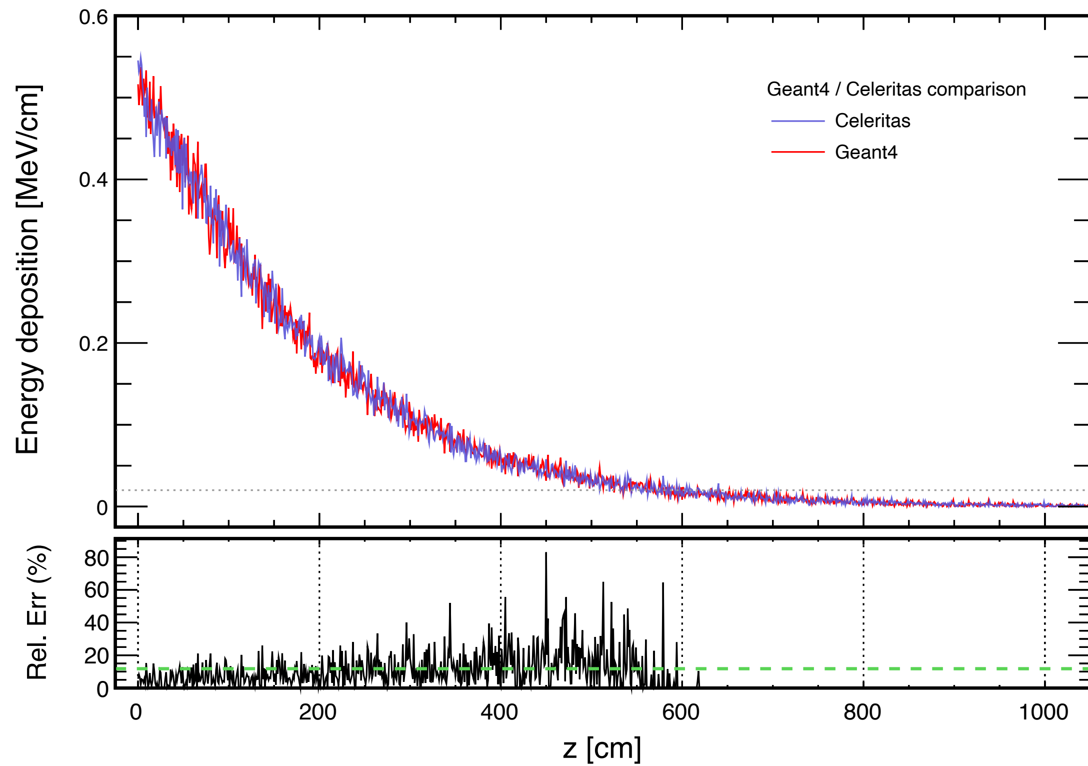
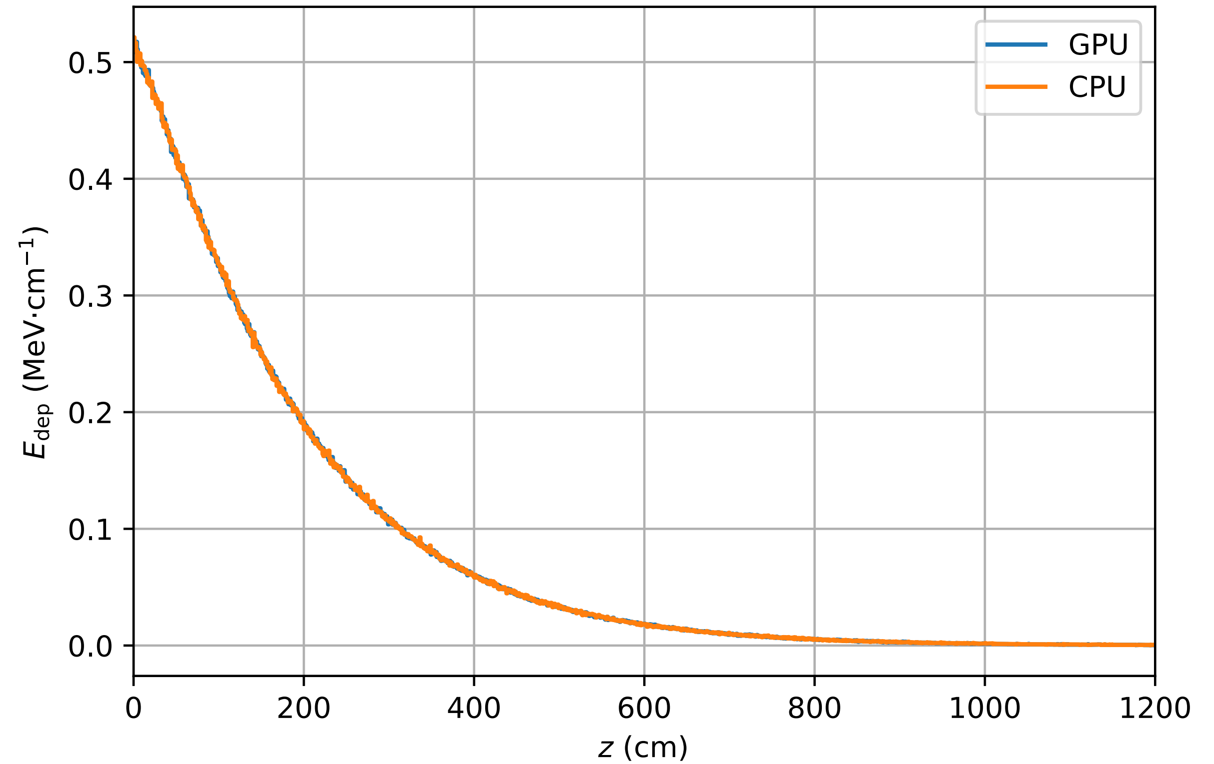
Celeritas reproduces Geant4 physics results (so far...)

Celeritas GPU vs Geant4 (64K tracks)



Celeritas GPU vs CPU (4M tracks)

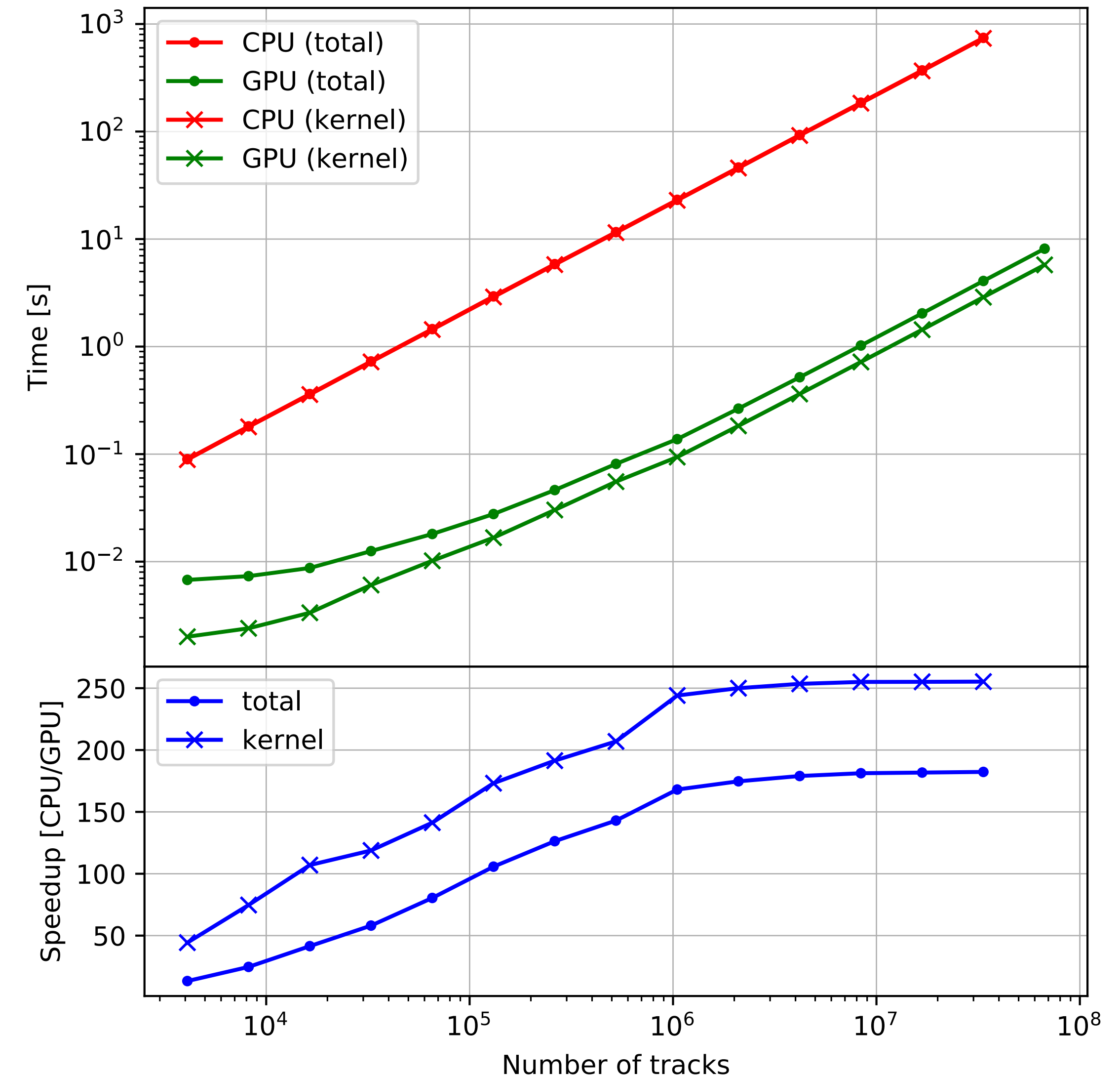


Successful verification of Celeritas physics

Celeritas CPU/GPU comparison

- Identical kernels, sequential events on CPU and parallel events on GPU
- Primary GPU kernel is an entire "step"
- Single core of Intel "Cascade Lake" Xeon (2.3 GHz)
  vs single Nvidia Tesla V100 (1.53 GHz)
- **~150×** overall speedup for 1M tracks in parallel

Likely a representative upper bound for raw performance



CUDA 10.1: `-O3 --use_fast_math`
GCC 8.3: `-O3 -march=skylake-avx512 -mtune=skylake-avx512`

Summary and Future Work

Summary of accomplishments *(first code commit: June 16, 2020)*

- Infrastructure
  - ✓ Established code base, procedures, and project tracking: https://github.com/celeritas-project
  - ✓ Extensible build system that supports unit testing and Continuous Integration (CI) using modern CMake
- Geometry
  - ✓ CUDA-enabled VecGeom integrated and distributed as a Spack package
  - ✓ Track initialization ported to device
  - ✓ Ray-tracing tests and application driver developed
- Physics
  - ✓ Integrated ability to source events from common HEP event-generators (HEPMC3, Pythia)
  - ✓ Built device memory pool allocators for efficient generation of secondary particles in device memory
  - ✓ Built, tested, and profiled simple event loop (Klein–Nishina interactions) on device
  - ✓ Built infrastructure and interactors for EM physics models

Work plan for next 3 months

- Work on full set of standard EM physics models is proceeding
  - Cross section tables
  - Physical materials
  - EM physics interaction models
- Integration of geometry tracker into transport app
- Implementation of multi-process transport loop
  - Scheduler for full process loop
  - Device-side optimization
- Background EM field integration

Target delivery: February 1

- Base:
  - Multi-process EM physics
  - Integrated geometry with material definitions
- Stretch:
  - Constant EM field integrator

July 1 milestone: EM Physics hit-generation application

- Features:
  - Functionally representative EM Physics list
  - Constant background EM field integration
  - Full VecGeom integration
  - Sensitive detector hit-scoring
- Objective:
  - Perform detailed performance analysis of transport loop on device
  - Establish baseline Figure-of-Merit in events simulated per wall-clock-time
  - Identify risks to performance and robustness