Celeritas: Status and Plans

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HSF Detector Simulation Working Group Meeting

12 April, 2021

EXASCALE COMPUTING PROJECT

National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY | Office of Science

Outline

- Project Overview
- Technical Update
- 5-Year Plan

Celeritas Project

Celeritas project objective

Become the next-generation particle transport backend for LHC detector simulations

1. Why is this capability needed?
   - Current high-fidelity, time-dependent, detector energy deposition simulations will not scale to proposed 10× LHC 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

HEP/ASCR Celeritas core team

- ANL—Particle Transport Group
  - Amanda Lund
- Fermilab—Physics and Detector Simulation Group
  - Philippe Canal*, Soon Yung Jun*, Guilherme Lima*
- LBL—ATLAS Group
  - Vincent Pascuzzi*†
- ORNL—HPC Methods and Nuclear Applications Group
  - Tom Evans* (**PI**), Seth Johnson (**Code Lead**), Stefano Tognini†

- ASCR ExaSMR Team
- HEP

* Leveraged through other project funding
† Postdoc

Technical Update

Technical update: overview of first-year goals

- ✓Established initial code base with rigorous documentation, review, and testing requirements
- ✓Built technical foundation for GPU- and CPU-friendly physics development
- ✓Developed key algorithms for GPU HEP transport
- ✓Completed initial EM physics components
- ✓Characterized initial GPU/CPU performance

Source code

Language	Files	Comment	Code
C/C++ Header	300	8900	11781
C++	88	2513	5986
CMake	19	429	2048
CUDA	14	401	922
Python	5	253	387
SWIG	1	30	66
Total	**427**	**12526**	**21190**

Test code

Language	Files	Comment	Code
C++	79	1892	7401
C/C++ Header	32	637	1593
CUDA	12	237	772
Total	**123**	**2766**	**9766**

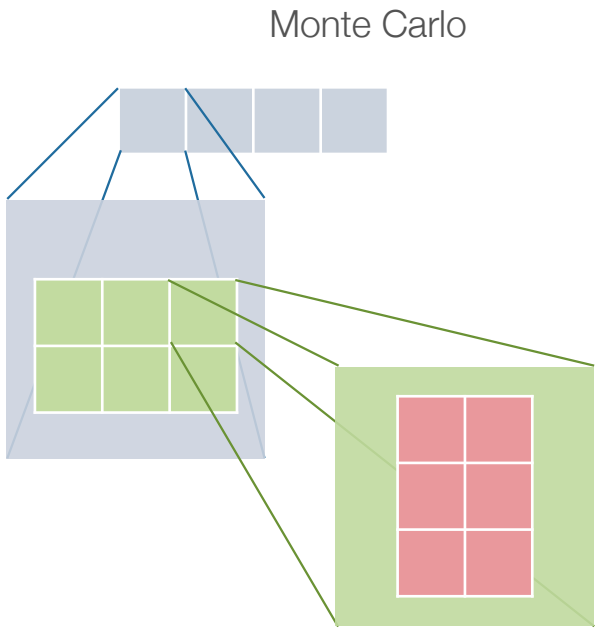
First commit: June 2020

Data model for rapid development of complex GPU physics

- Monte Carlo particle transport methods have **deep hierarchical heterogeneous data structures**
  - Material properties (Material/element/nuclide)
  - Macroscopic cross sections (Particle/material/process/energy)
  - Differential cross sections (Element/incident/exiting)
- Typical GPU algorithms designed for **wide homogeneous data**
- And can we reuse both data and execution code on both CPU and GPU?

Celeritas solution: new paradigm for GPU-friendly physics

Data model for rapid development of complex GPU physics



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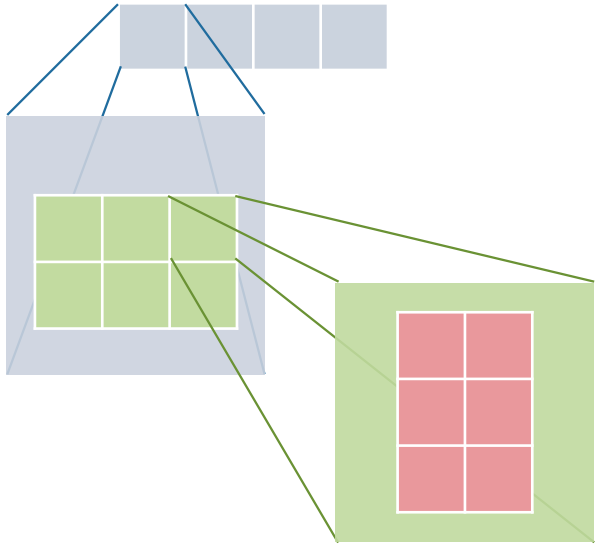
Celeritas solution: new paradigm for GPU-friendly physics

Monte Carlo

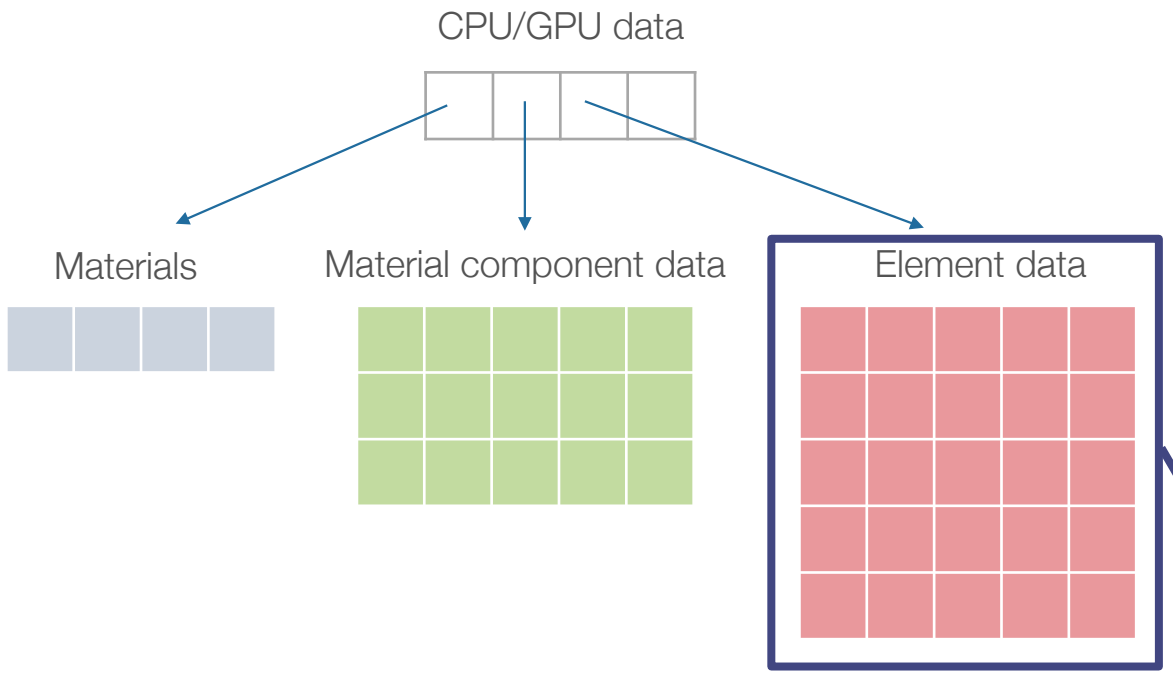


Typical GPU Application

Data model for rapid development of complex GPU physics

```
struct Element
{
    int            atomic_number;
    units::AmuMass atomic_mass;
};

struct MatElementComponent
{
    ItemId<Element> element;
    double          fraction;
};

struct Material
{
    double      number_density;
    double      temperature;
    MatterState matter_state;
    ItemRange<MatElementComponent> components;
};

template<Ownership W, MemSpace M>
struct MaterialParamsData
{
    template<class T>
    using Items = celeritas::Collection<T, W, M>;

    Items<Element>             elements;
    Items<MatElementComponent> elcomponents;
    Items<Material>            materials;
    unsigned int               max_elcomponents;

    template<Ownership W2, MemSpace M2>
    MaterialParamsData& operator=(
        const MaterialParamsData<W2, M2>& other);
}
```

Data model for rapid development of complex GPU physics

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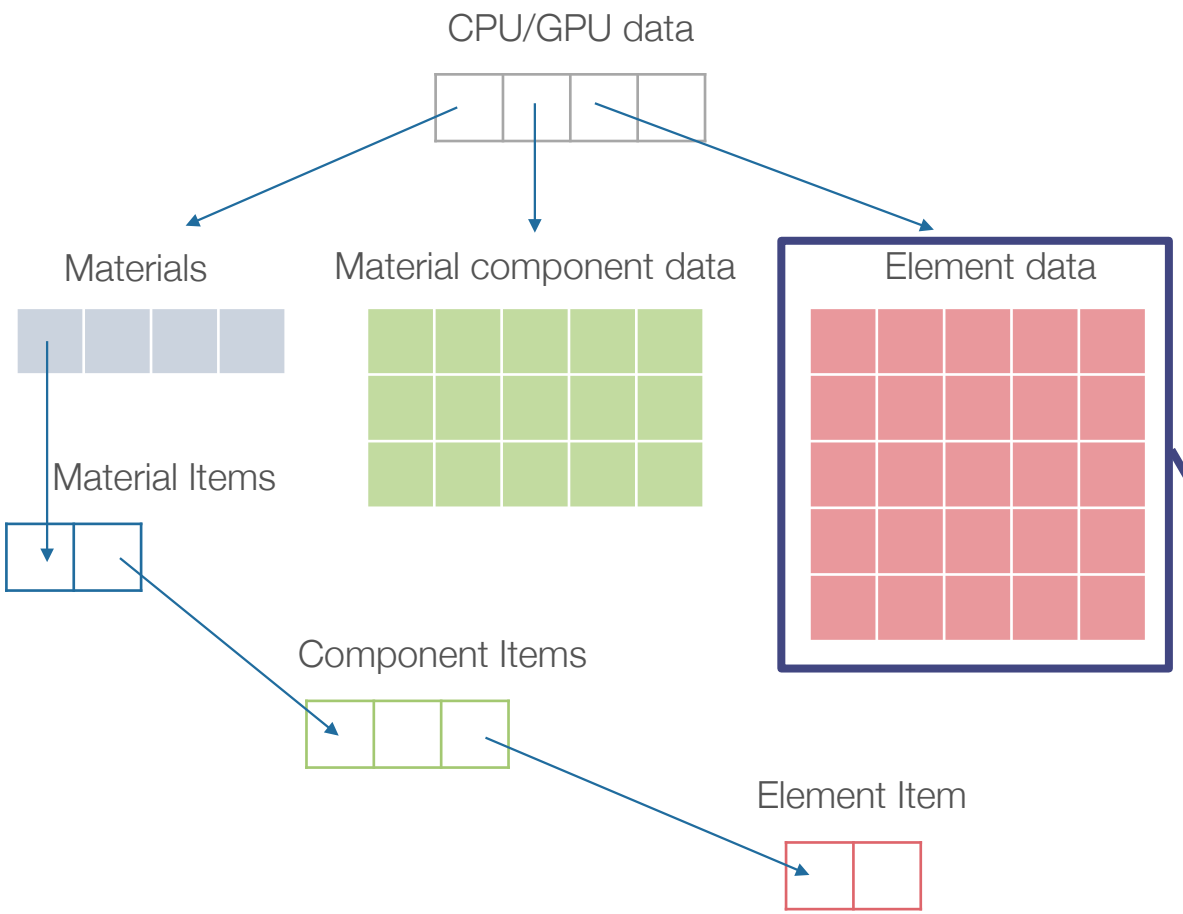


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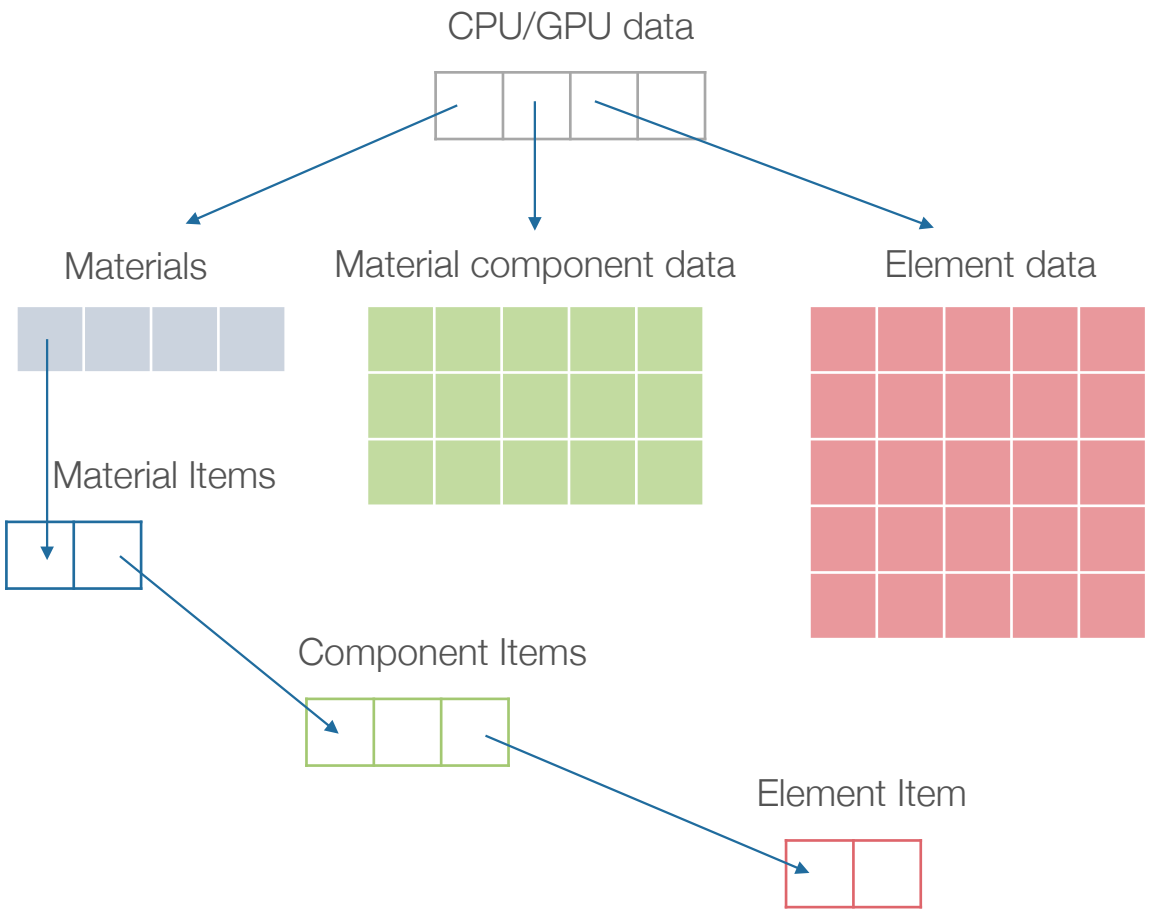


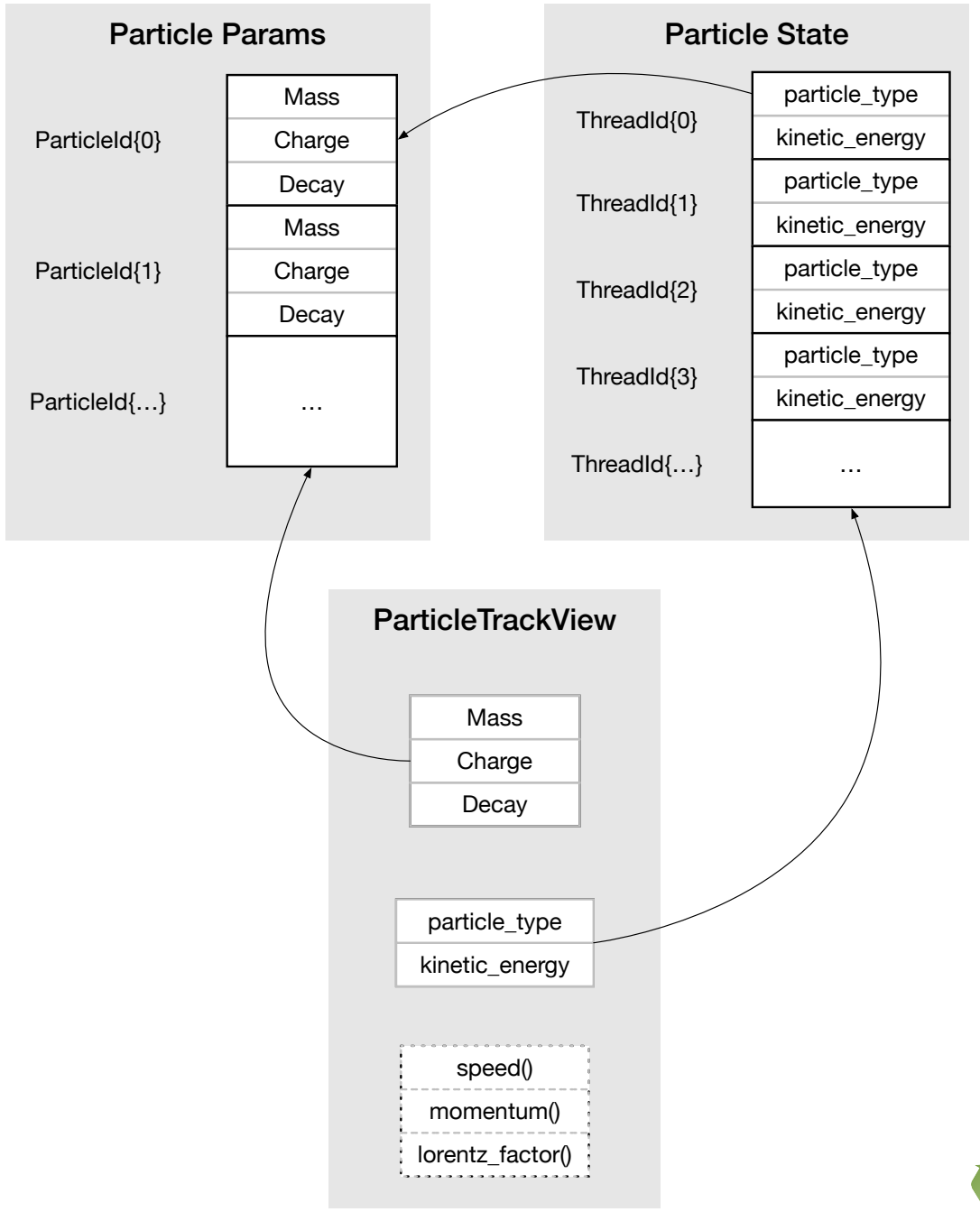
- Easily assemble data on CPU
- Define data structures *once*
- Data and execution on both CPU and GPU
- **Payoff:** safe and effective framework for physicists to implement and test GPU-compatible physics

Current hierarchical physics data in Celeritas

- Material: materials→element components→elements
- Physics: particles→processes→{tables→materials→grids, models}
- Livermore PE: elements→{grids, subshells→{grids, params}}
- Seltzer–Berger tables: elements→2D grids
- Rayleigh parameters: elements→params

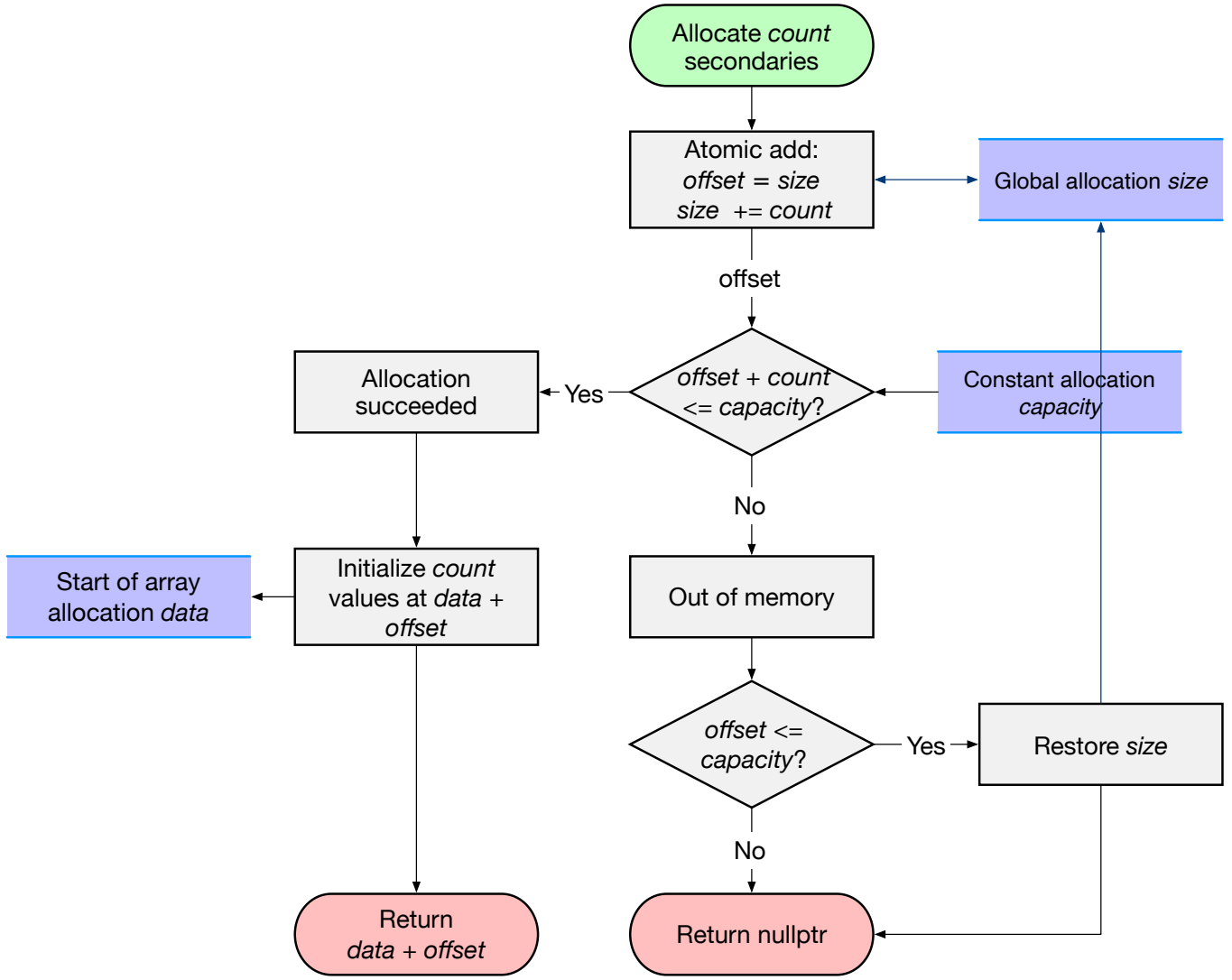
Software abstractions for portability

- 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



Stack allocator for fast on-device secondary/hit construction

- Novel algorithm for satisfying **performance** and **reproducibility** requirements
- Unknown number of tracks (running in parallel, one per thread) creating unknown number of secondaries per track
- Finite amount of GPU memory preallocated
- Failure to allocate secondaries for a thread *must* result in graceful failure to avoid advancing RNG (random number generator) state



Physics capabilities (GPU)

✓Discrete process interactions including dynamic allocation of secondaries

✓Continuous slowing-down energy loss

✓Multiple competing processes

✓Multiple materials

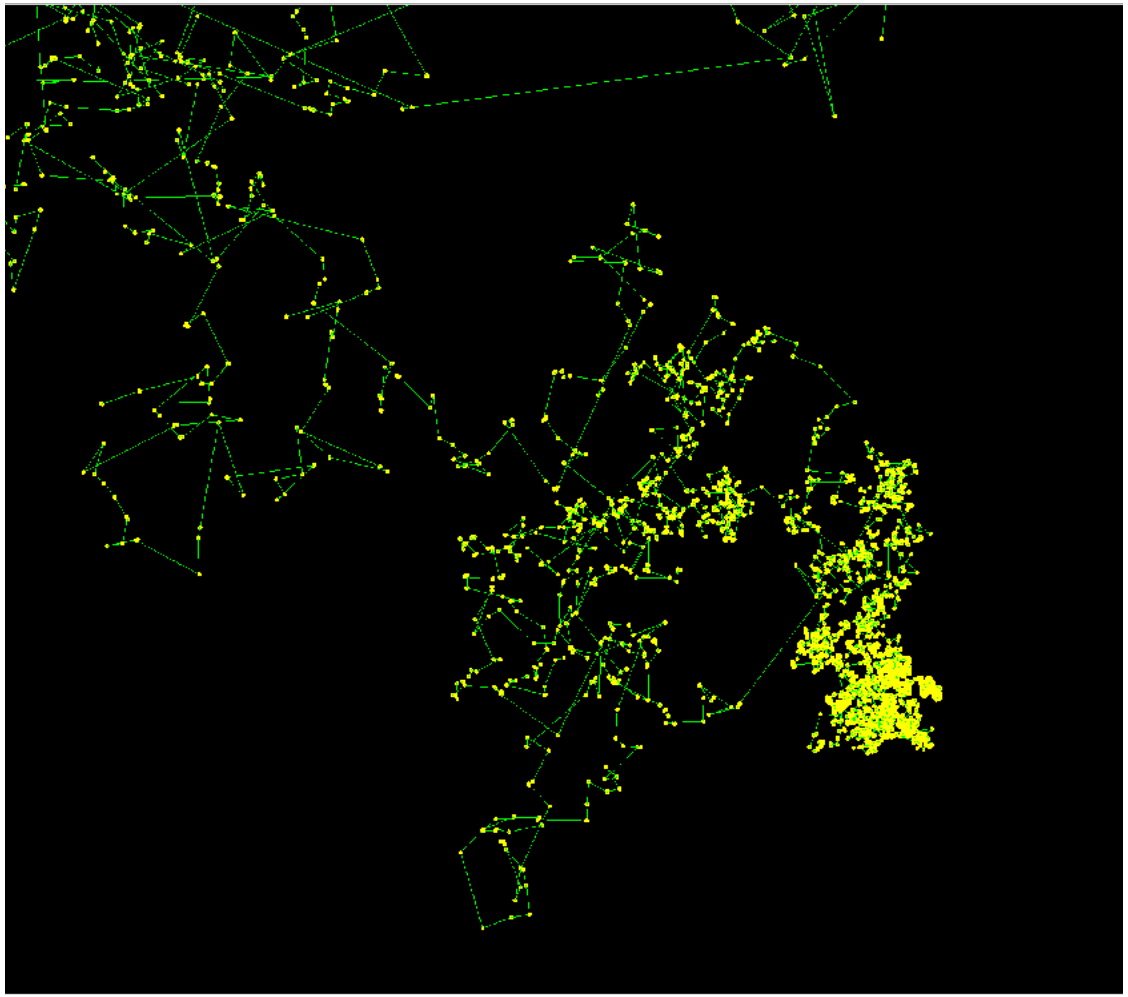
→Uniform magnetic field

→Integrated stepping loop

	Process (Model)	Status
γ	Conversion (Bethe-Heitler)	Implemented
	Compton scattering (Klein-Nishina)	Verified
	Photoelectric (Livermore)	Implemented
	Rayleigh scattering (Livermore)	In progress
e	Ionization (Møller-Bhabha)	Implemented
	Bremsstrahlung (Seltzer-Berger)	In progress
	Multiple scattering	Deferred
μ		Deferred

Physics mini-app: Klein–Nishina photon transport (Nov. 2020)

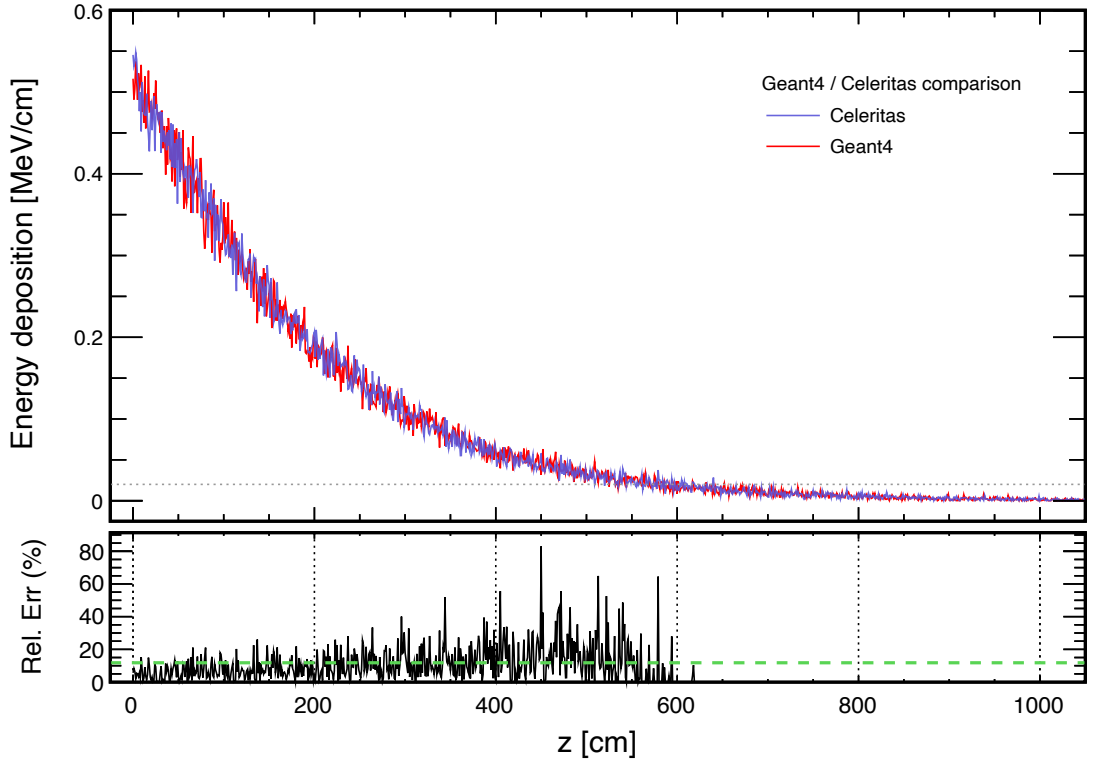
- Simplest **physical** simulation we can run
  - Photon-only transport (electrons created but immediately killed and locally deposited)
  - Single process (inelastic scattering neglecting binding energy)
  - Single infinite material (aluminum)
  - 100 MeV monodirectional point source
- Celeritas (GPU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



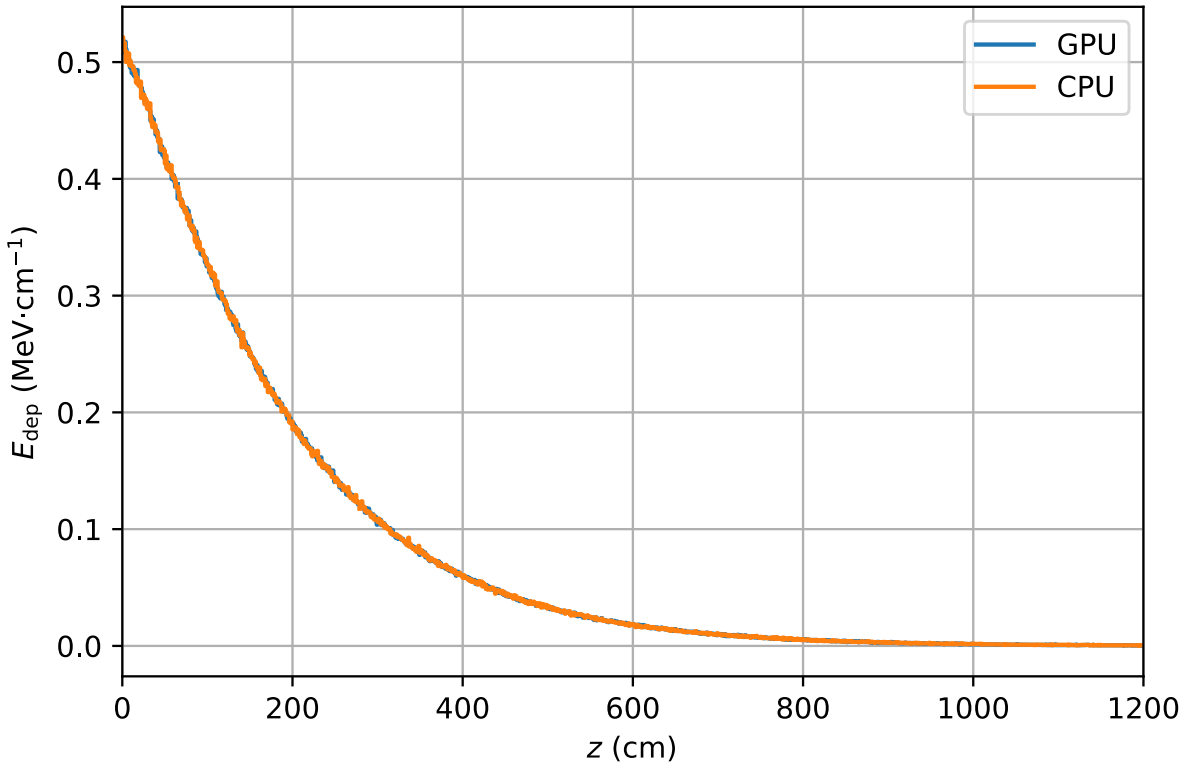
https://github.com/celeritas-project/celeritas/pull/51

Celeritas reproduces Geant4 physics results (Nov. 2020)

Celeritas GPU vs Geant4 (64K tracks)



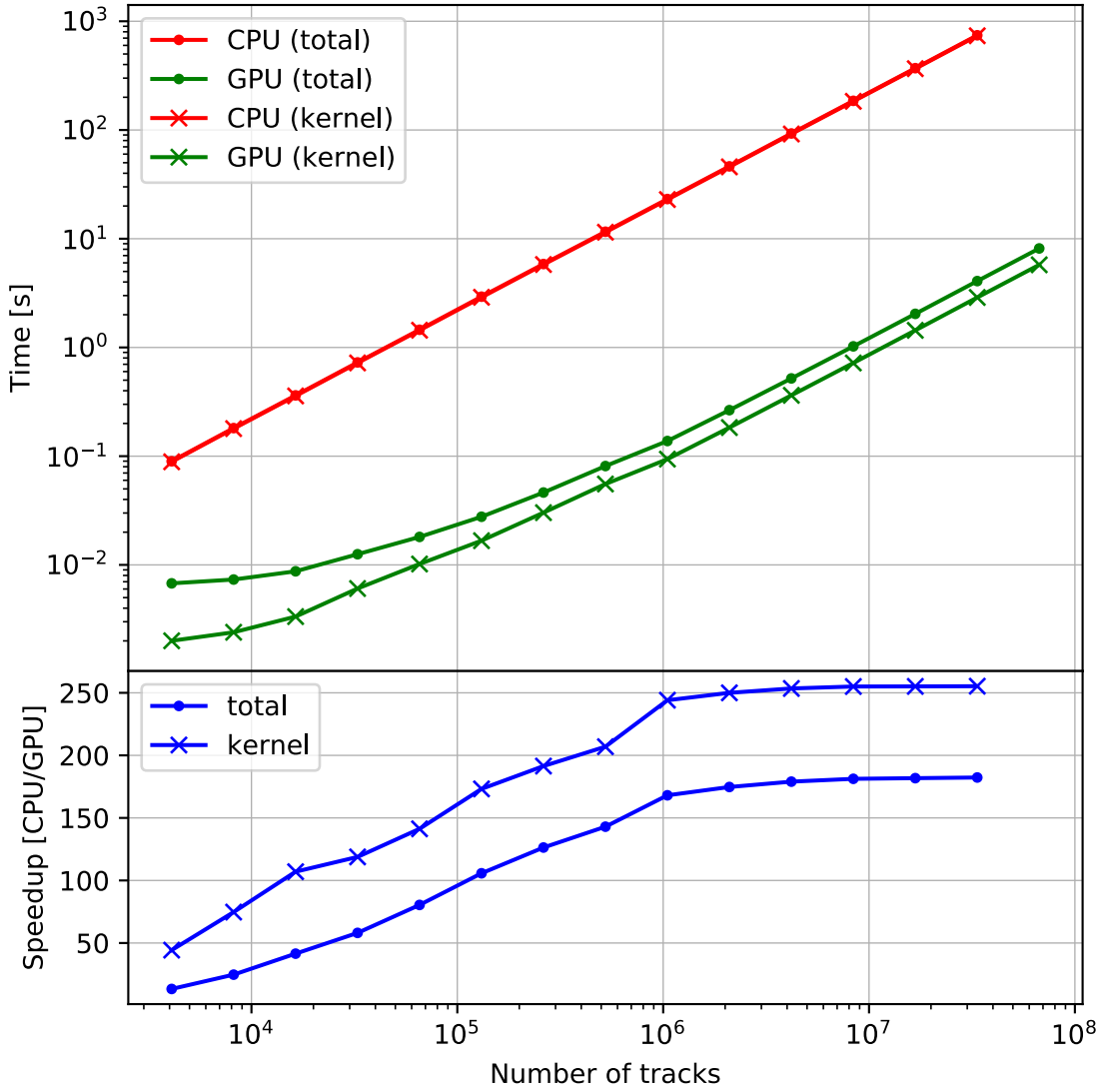
Celeritas GPU vs CPU (4M tracks)



First successful verification of Celeritas physics

Initial mini-app CPU/GPU results (Nov. 2020)

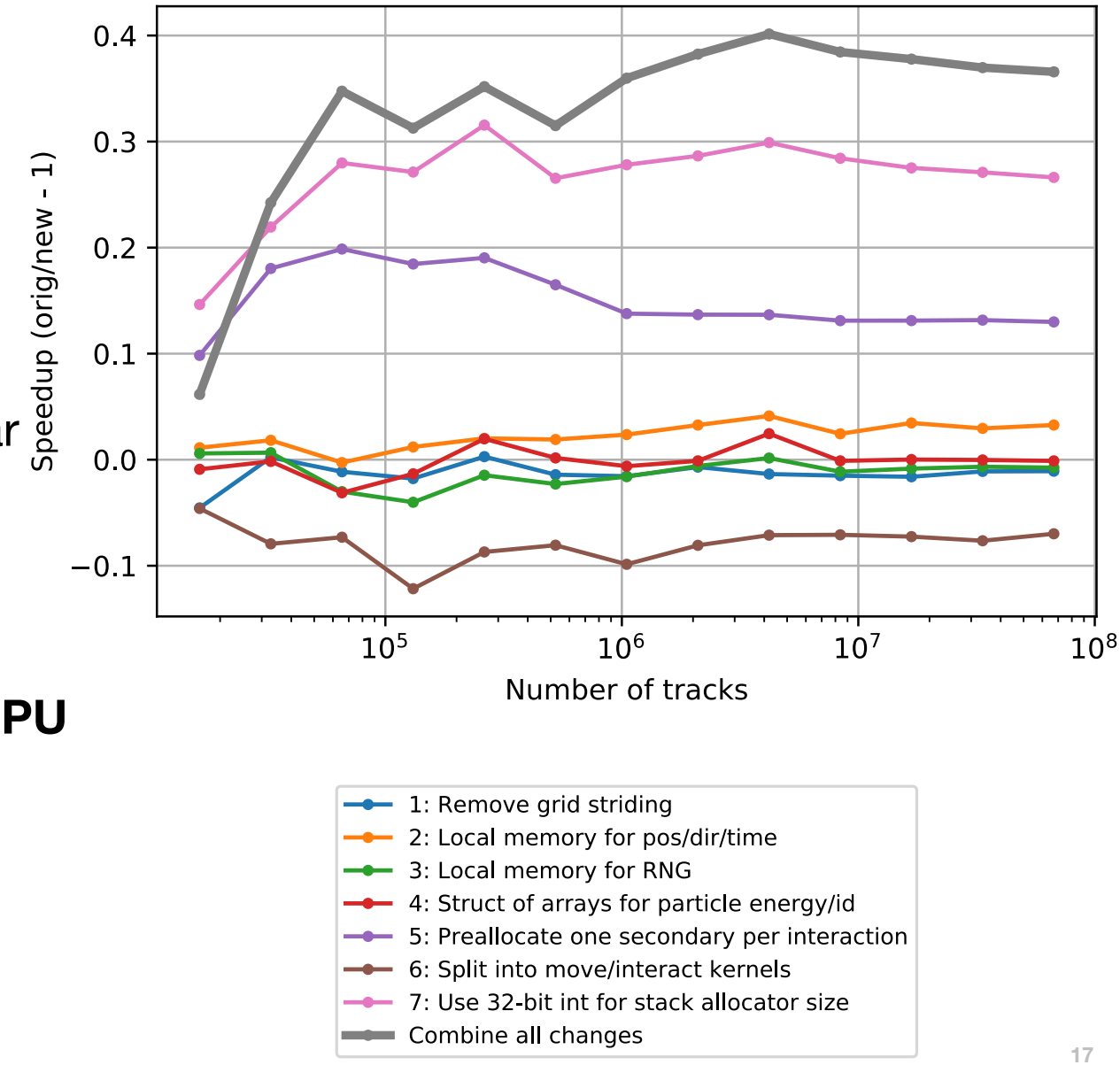
- Shared Celeritas physics code
- Sequential events on CPU and parallel events on GPU
- Primary GPU kernel is an entire “step”
- Single core of Intel “Cascade Lake” Xeon (2.3 GHz) vs single Nvidia Tesla V100 (1.53 GHz)
- **~150×** overall speedup for 1M tracks in parallel



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

Performance enhancements (Feb. 2021)

- Code structure facilitates performance exploration
- “Non-traditional” bottlenecks: atomics and irregular memory access
- Combining different “tweaks”: **38%** GPU speedup in mini-app
- **~220× overall mini-app speedup compared to CPU**

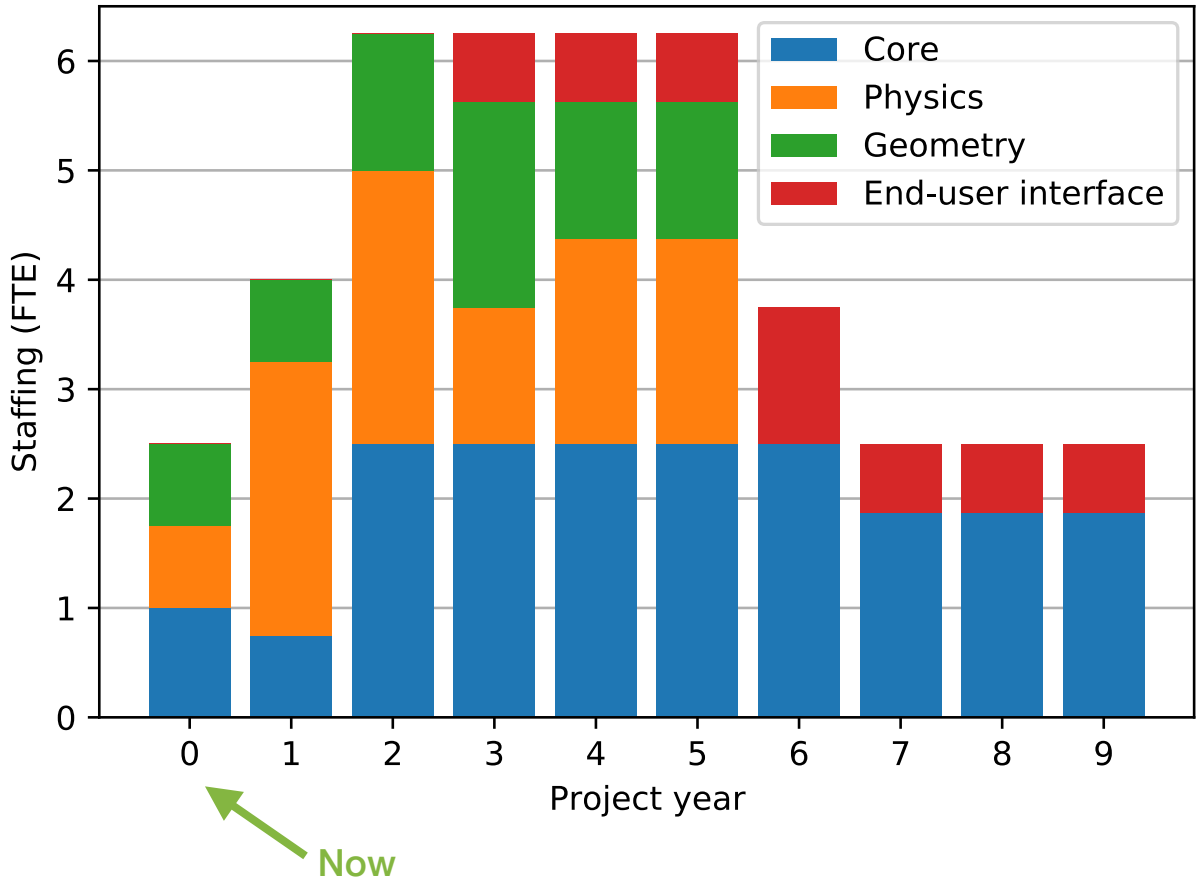


5-Year Plan

5-Year Celeritas Plan

- Period until July 1, 2021
  - Form core team and primary collaborations
  - Integrate into Geant/HEP community
  - Implement fundamental infrastructure
- 3-year plan (July 1, 2021–July 1, 2024)
  - Incorporate Celeritas EM physics into HEP experimental workflows
- 2-year continuation (through 2026)
  - Celeritas user app/framework with complete standard high-energy physics

Proposed project staffing and milestones



Year	Principal milestone
0	Start-up and application demonstration
1	Complete EM physics
2	EM physics integration into experimental workflows
3	Validation of EM physics
4	Hadronic physics for LHC
5	Validation of LHC physics
6+	Transition to operations; integration into federated networks

Principal milestones per year

July 1, 2021 — July 1, 2022

- Prototype performance portability
  - Gather requirements for performance portability
  - Kokkos/HIP/SYCL
  - Performance portable geometry
- Complete EM physics
- Integration with experimental detector output post-processing
  - Client-defined scoring regions

July 1, 2022 — July 1, 2023

- Baselining EM physics simulation runtime performance
  - 32-bit (fast) vs 64-bit
- Validation of EM physics
  - Benchmarks
  - CMS or other experiments
- Integrated Celeritas + Geant4 workflow for EM Physics

July 1, 2023 — July 1, 2024

- Integration of expanded physics to support experimental campaigns
  - e.g. hadronic physics
- Demonstration of full event simulation in Celeritas
- Integration as a training data generator
  - Support external AI/ML fast simulations

QUESTIONS?