# Celeritas: efficient detector simulation on GPUs for Geant4

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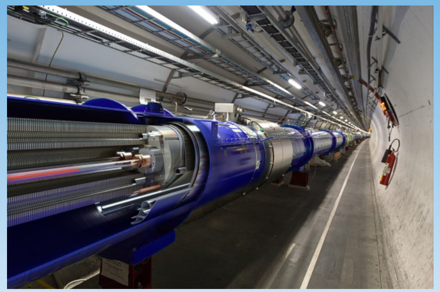
**Compute Accelerator Forum**
**11 December, 2023**

# Background
Methods
Results
Conclusions

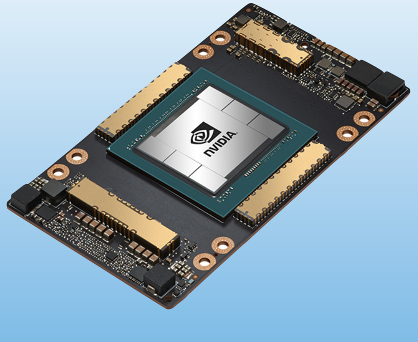
# Celeritas project goal

- **Accelerate scientific discovery** by improving LHC detector simulation throughput and energy efficiency
  - Long term goal: as much work as possible on GPU
  - Initial funding: focus on EM physics (but keep door open for more!)
- Jointly funded by US DOE ASCR and HEP
  - **Research and develop** novel algorithms for GPU-based Monte Carlo simulation in High Energy Physics
  - **Implement** production-quality code for GPU simulation
  - **Integrate** collaboratively into experiment frameworks



LHC beamline ©CERN

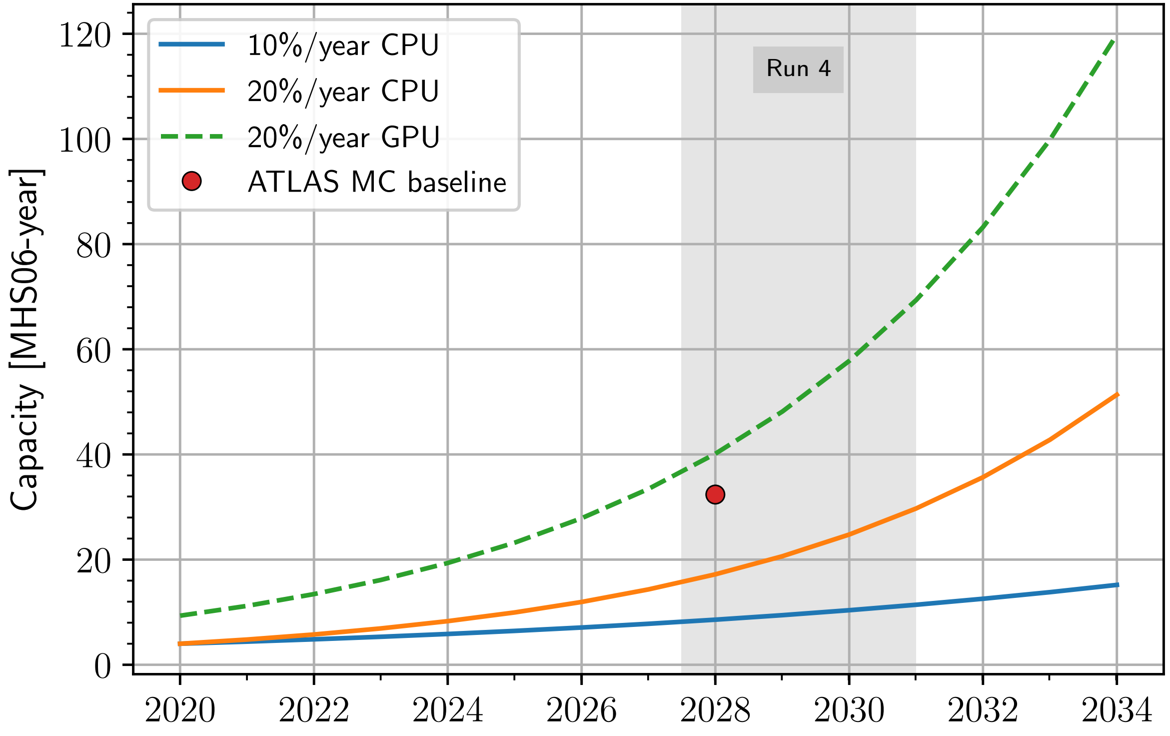
CELERITAS



Nvidia A100 GPU ©Nvidia

# Motivation 1: computational demand

- HL upgrade means 10× higher sampling rate
  - More detector data means more simulations needed
  - Tens of millions of “equivalent 2006-era CPU hours” for analysis
  - 20–25% is from full-fidelity MC
- Even AI/ML based “fast simulation” methods will need lots of training data

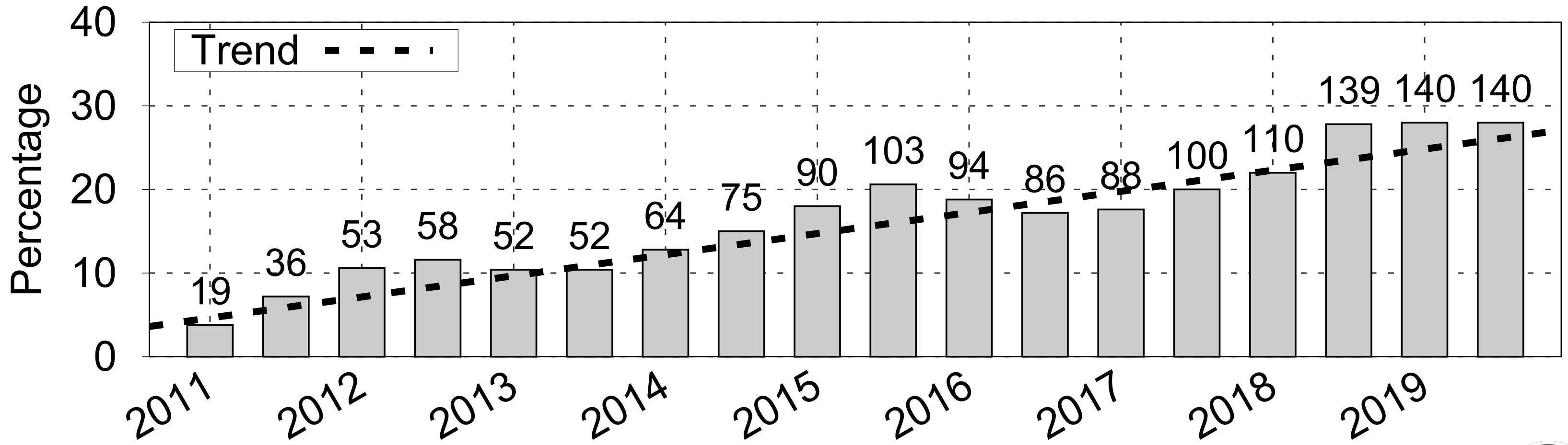



*GPU projection based on energy efficiency and speedup of ExaSMR MC code*

# Motivation 2: computational supply

- "Heterogeneous" architectures are increasingly common in high performance computing
- Scientific codes can run on GPU with much higher energy efficiency
  *e.g., Perlmutter reports 5× average: https://blogs.nvidia.com/blog/gpu-energy-efficiency-nersc/*
- Demand for AI/ML training and models ***will accelerate this trend***

Top500 supercomputers with heterogeneous architectures: >30%




Khan et al., *An Analysis of System Balance and Architectural Trends Based on Top500 Supercomputers*
Reproduced under government license. https://doi.org/10.1145/3432261.3432263

# ...but there's a catch

- Exascale Computing Project (ECP) funded a wide range of scientific libraries and applications to run efficiently on next-generation GPUs
- In *all* cases, performance on GPU requires:
  - Algorithmic restructuring *(reorganizing data, separating states, transposing loops)*
  - New numerical approaches *(targeting higher compute-to-memory ratios)*
  - Alternative physics models *(more favorable to thread-level parallelism)*
  - **Not simply porting code**

**Drastically different hardware** requires **dramatically different software**

Background

**Methods**

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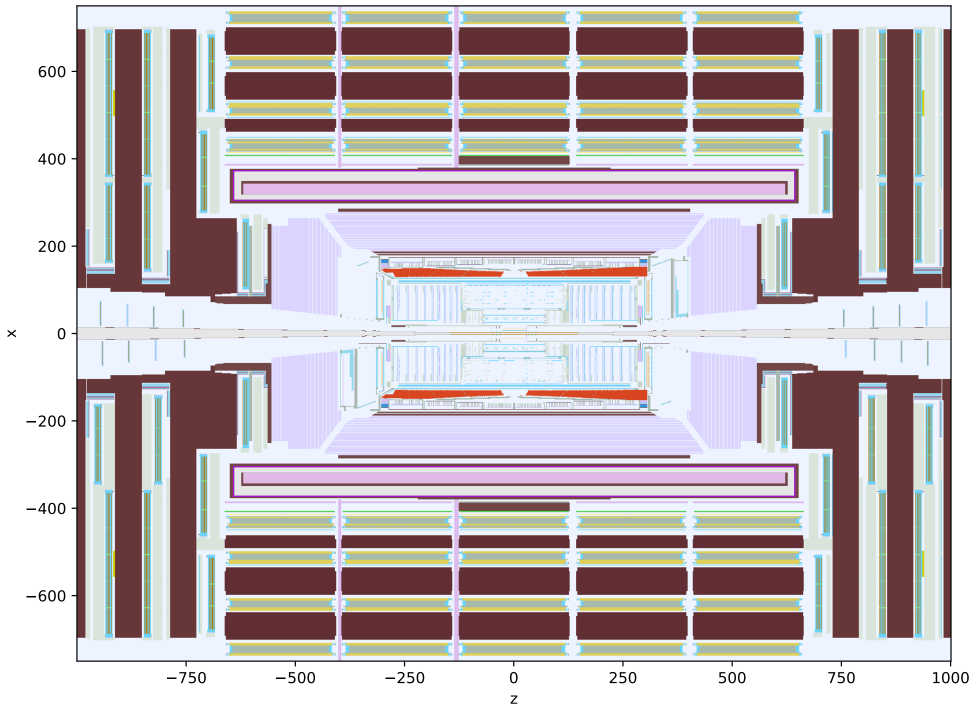
# High-level capabilities targeting LHC simulation

- Equivalent to `G4EmStandardPhysics`
  *…using Urban MSC for high-E MSC; only γ, $e^{\pm}$*
- Full-featured Geant4 detector geometries using VecGeom 1.x
- Runtime selectable processes, physics options, field definition
- Execution on CUDA (Nvidia), HIP* (AMD), ***and CPU*** devices




*GPU-traced rasterization of CMS 2018*

**VecGeom currently requires CUDA: ORANGE navigation required for HIP*

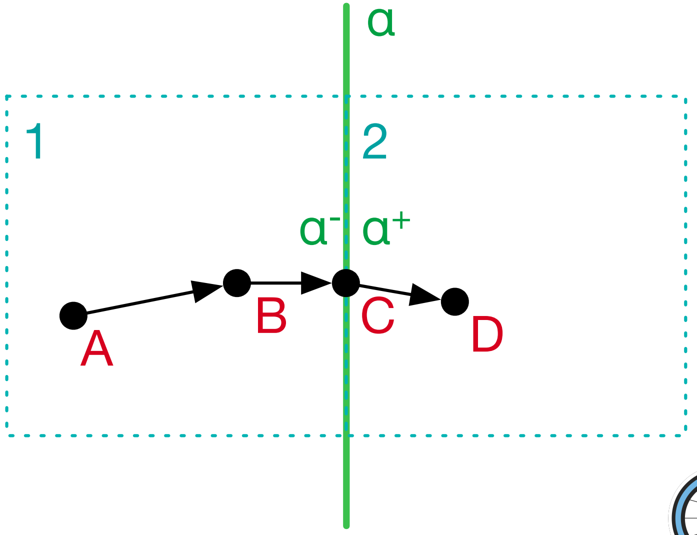
*Source:* Johnson, S.R. Geant4 Meeting 2023

# ORANGE: surface-based navigation

- Designed for deeply nested reactor models
- Portable (CUDA/HIP) geometry implementation
- Tracking based on CSG tree of surfaces comprising volumes
- Maximize run-time performance by preprocessing

| | Position | Volume | Surface+Sense |
|---|---|---|---|
| **Initialize** | A | 1 | — |
| **Find step** | A | 1 | — |
| **Move internal** | B | 1 | — |
| **Move to bdy** | C | 1 | α inside |
| **Cross bdy** | C | 2 | α outside |
| **Move internal** | D | 2 | — |

*Discrete state points (avoiding "fuzziness") is optimal for GPU*



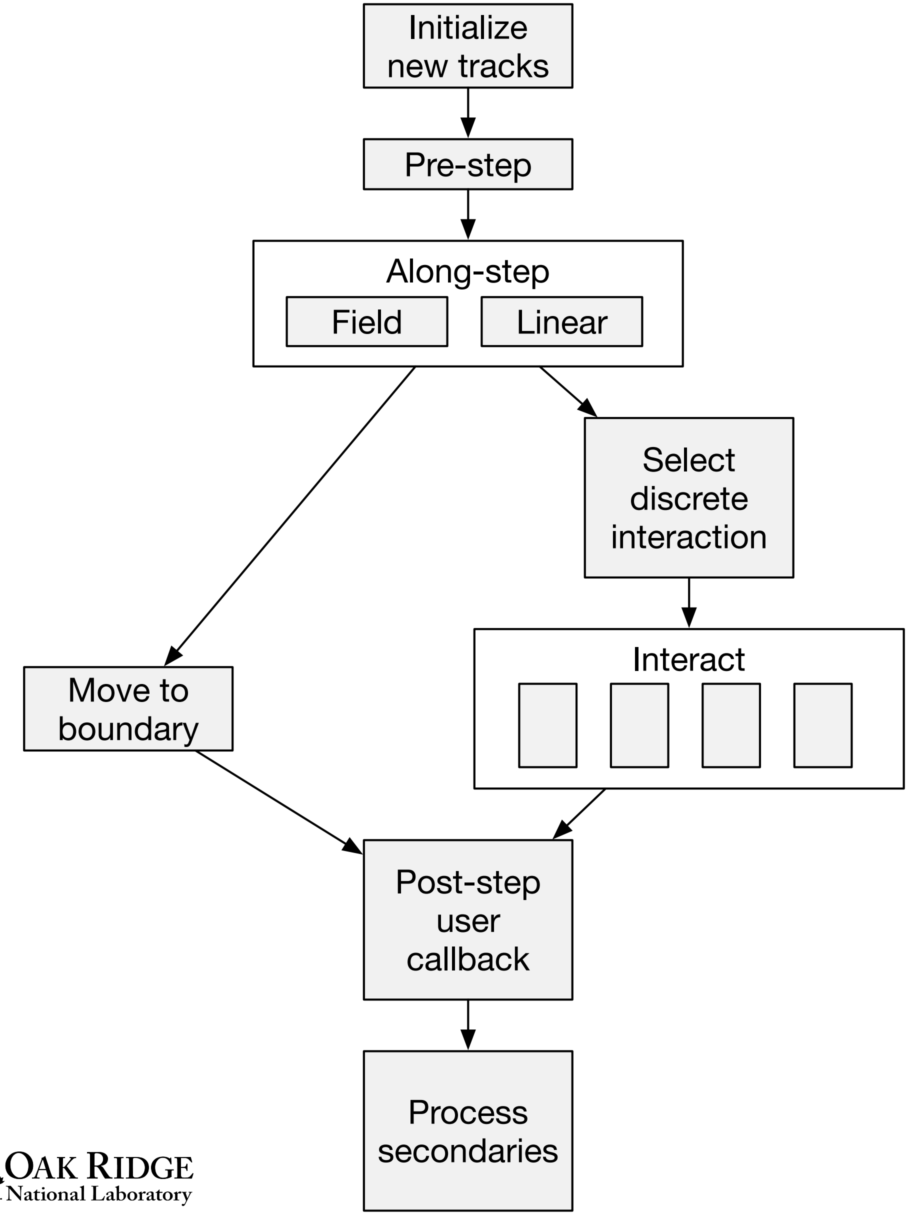
# Magnetic field propagation

- Composition based: **P○D○I○E○F**
- Templated for extensibility
  - Built-in "uniform" and "*r-z* field map"
  - Magnetic field (Lorentz) equation
  - Single driver (for now) with runtime step tolerances
  - Runge–Kutta 4 and Dormand–Prince RK5(4)7M integrators
  - Custom field propagator *without* safety evaluation*

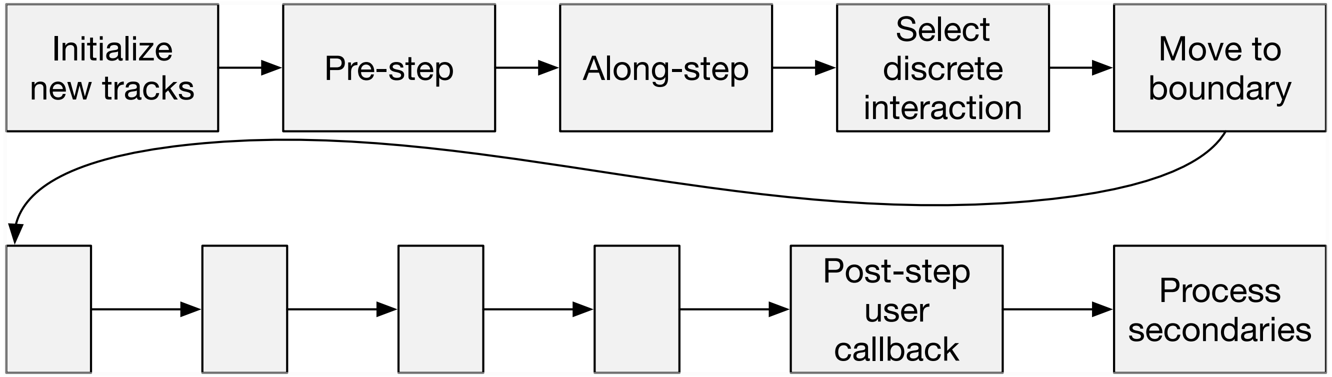
| Operator | Input | Output |
|---|---|---|
| **F**ield | $\boldsymbol{x}$ | $\boldsymbol{B}$ |
| **E**quation of motion | $\boldsymbol{x}, \boldsymbol{p}, \boldsymbol{B}$ | $\boldsymbol{x}', \boldsymbol{p}'$ |
| **I**ntegrator | $\boldsymbol{x}, \boldsymbol{p}, h$ | $\boldsymbol{x}^*, \boldsymbol{p}^*, e$ |
| **D**river | $\boldsymbol{x}, \boldsymbol{p}, s$ | $\boldsymbol{x}^*, \boldsymbol{p}^*, s^*$ |
| **P**ropagator | $\boldsymbol{x}, \boldsymbol{\Omega}, E, s$ | $\boldsymbol{x}^*, \boldsymbol{\Omega}^*, s^*$ |

**safety calculation resulted consistently in slowdown on GPU*

# Stepping loop on a GPU




*Process large batches of tracks per kernel ($10^3$–$10^6$)*




*Topological sort: a loop over kernels*

*Using many small kernels improves extensibility*





*Source:* Johnson, S.R. Geant4 Meeting 2023

# Celeritas/Geant4 integration

- **Imports** EM physics selection, cross sections, parameters
- **Converts** geometry to VecGeom model without I/O
- **Offloads** EM tracks from Geant4

  *(Via `G4UserTrackingAction`, `G4VFastSimulationModel`, or `G4VTrackingManager`)*
- **Scores** hits to user "sensitive detectors"

  *(Copies from GPU to CPU; reconstructs `G4Hit`, `G4Step`, `G4Track`; calls `Hit`)*
- **Builds** against Geant4 10.5–11.1

***Celeritas has production quality interfaces to simplify user application integration***




*Source:* Johnson, S.R. Geant4 Meeting 2023

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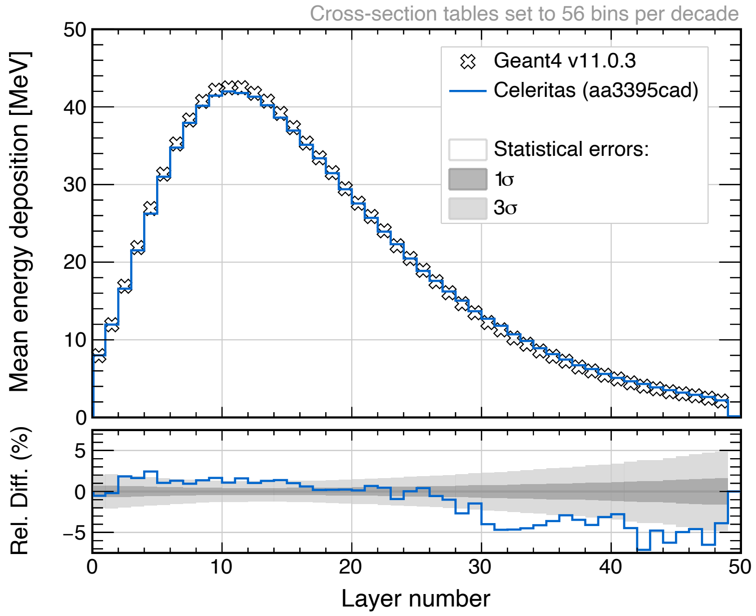
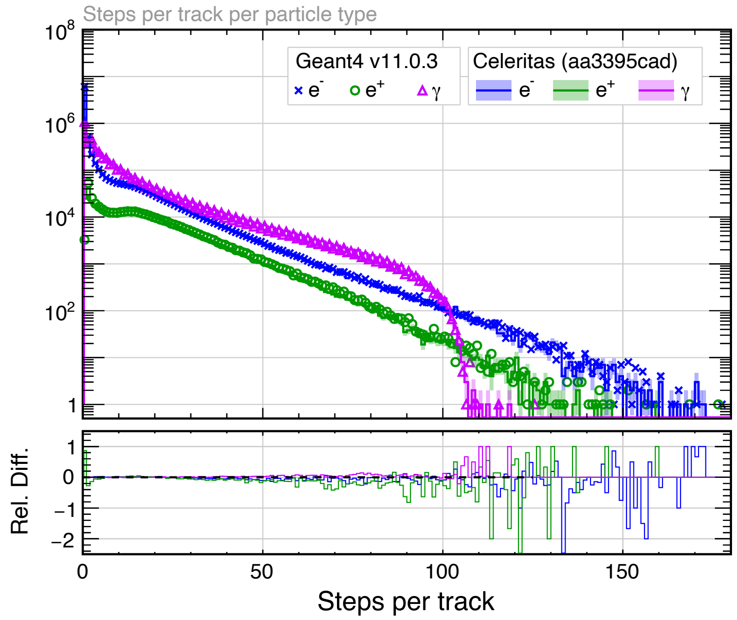
# Physics verification

- Single-model distributions
- Volume-dependent hit count and energy deposition distributions
- Step-per-track distributions
- Most significant disagreement remaining: Urban MSC





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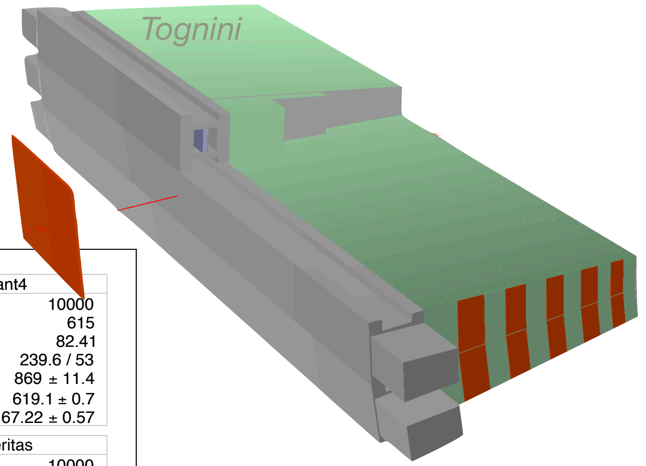
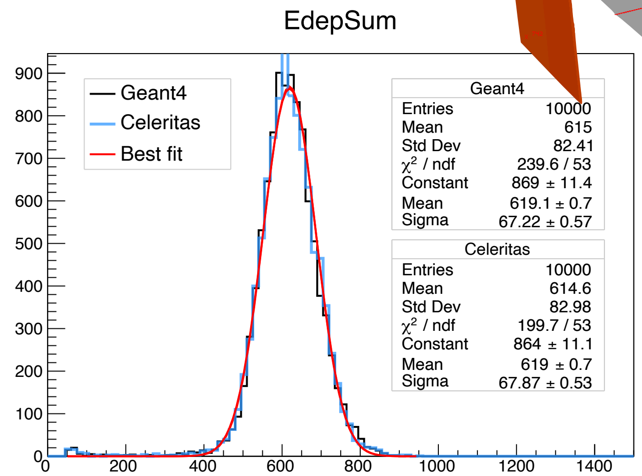
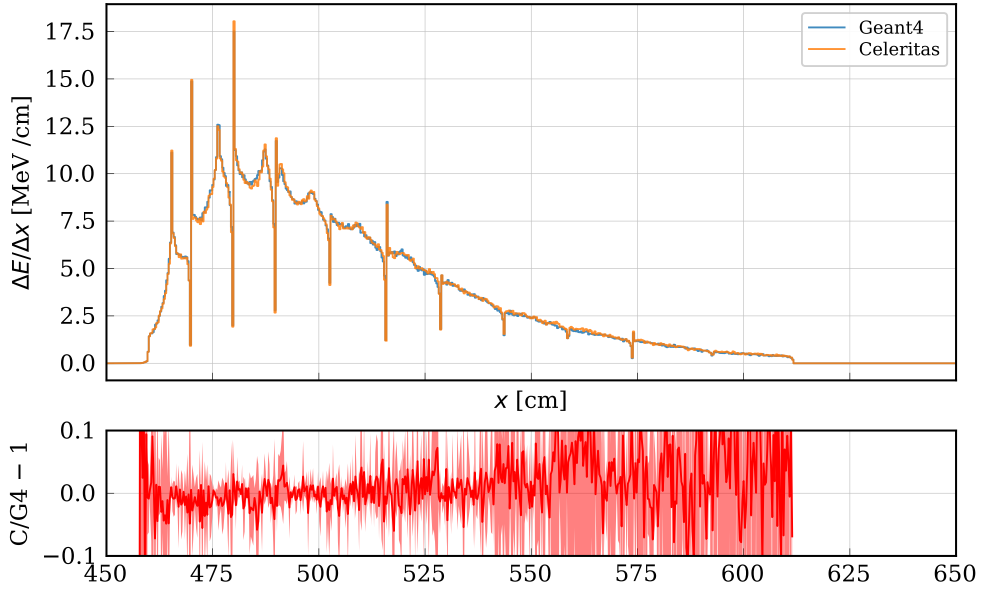
# EM offloading with FullSimLight

- ATLAS FullSimLight: hadronic tile calorimeter module segment
  - 64 segments in full ATLAS, 2 in this test beam
  - 18 GeV $\pi^+$ beam, no field
  - FTFP_BERT (default) physics list
    (includes standard EM)
- **~100 lines of code to integrate**
  - Offload $e^-$, $e^+$, $\gamma$ to Celeritas
  - Celeritas reconstructs hits and sends to user-defined `G4VSensitiveDetector`
- Good agreement in energy deposition




*yz-integrated energy deposition*

*Test problem: Lachnit, Pezzotti; FSL integration: Morgan*

*Source:* Johnson, S.R. Geant4 Meeting 2023

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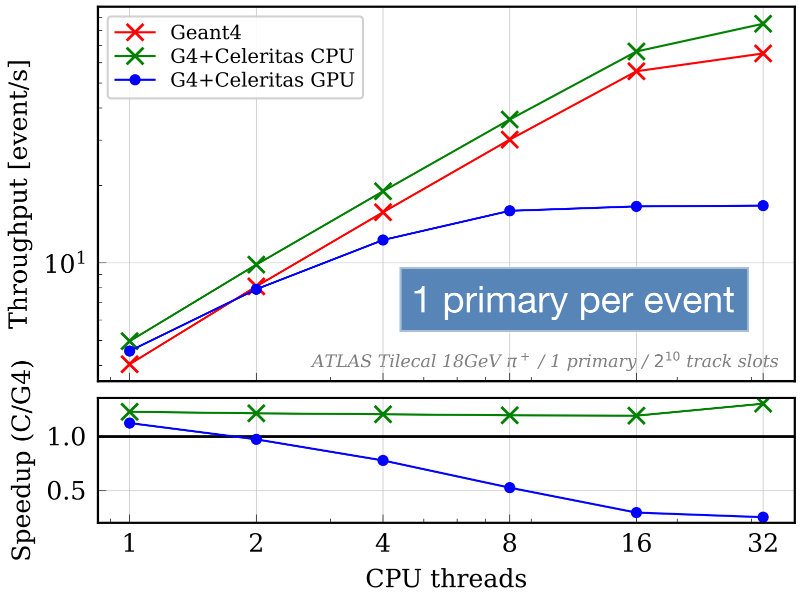
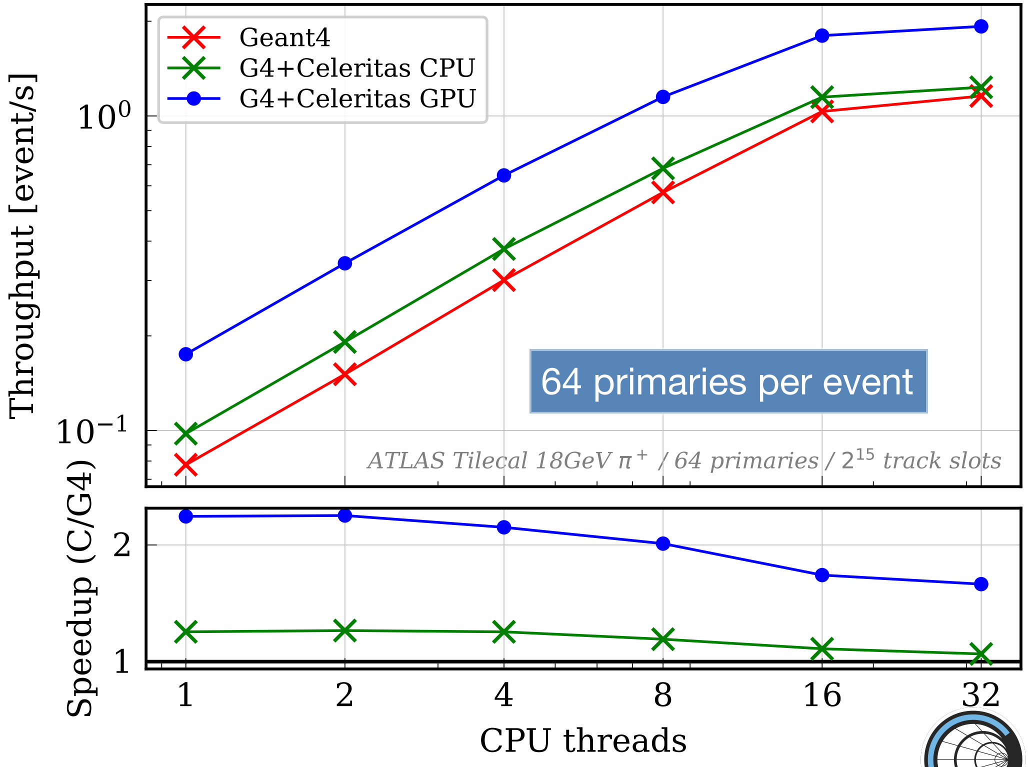
# Offload performance results

- 1/4 of a Perlmutter (NERSC) GPU node
  16 cores of AMD EPYC, 1 Nvidia A100
- Time **includes** startup overhead, Geant4 hadronic physics, track reconstruction, and SD callback
- GPU speedup: **1.7–1.9×** at full occupancy
  Using all CPU cores with a single GPU
- CPU-only speedup: **1.1–1.3×**
- LHC-scale energy per event (i.e., all 64 modules) is needed for GPU efficiency
- One fast GPU can be shared effectively by full multithreaded Geant4

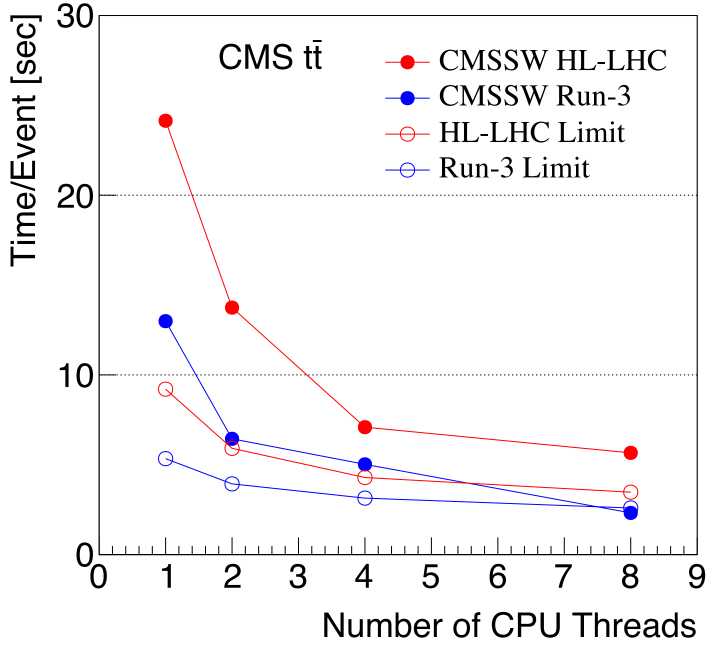


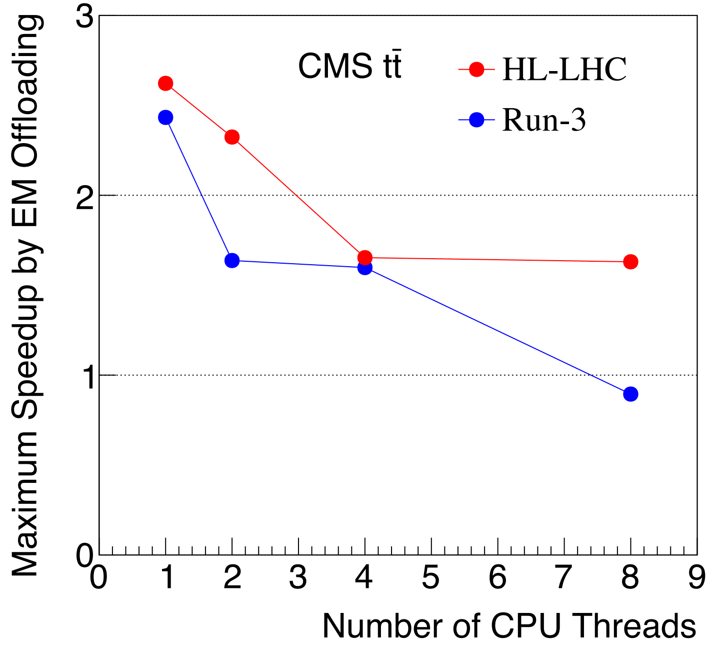




Source: Johnson, S.R. Geant4 Meeting 2023

# CMSSW integration

- Initial CMSSW integration complete
  - 500 lines of code
  - Complications from extra user track state
- Performance isn't comparable due to different physics
  - Lots of region-dependent cuts, parameter changes
  - Fast simulation bypasses transport loop
- Strong collaboration with CMS
  - **CMSSW has agreed** to integrate Celeritas as an external
  - CPU-only for now to facility software infrastructure
  - Maximum speedup for offloading EM: ~2.5×



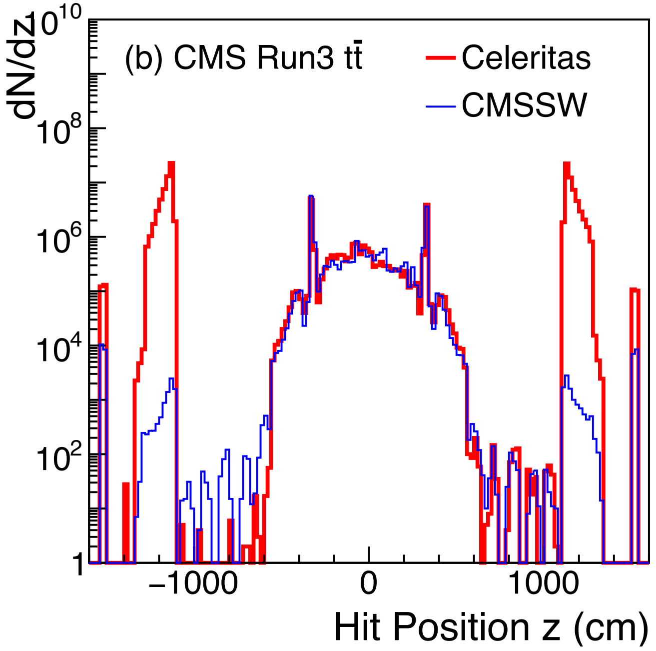



# CMS Run 3&4 Standalone Simulations

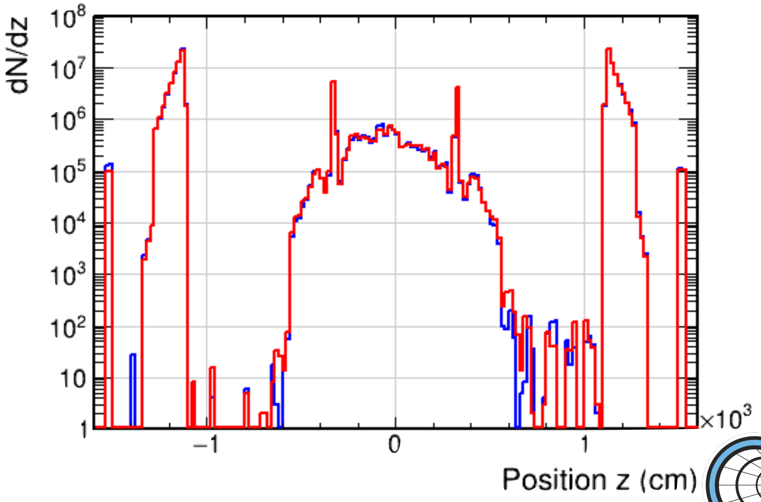
- Standalone Geant4 app `celer-g4`
- 32 $t\bar{t}$ events from Pythia
- FTFP_BERT physics
  - Geant4 simulates hadronics
  - All EM tracks offloaded to Celeritas
  - Lepto-nuclear reactions neglected
- Multiple field options
  - No magnetic field
  - Uniform 4T field
  - Discretized+interpolated RZ field (901×481 points)
- CMSSW/Geant4 throughput: **8×**

  *(we're simulating a harder problem than necessary, but we now have an equivalent test problem)*

*CMSSW Run 3 hit distribution*

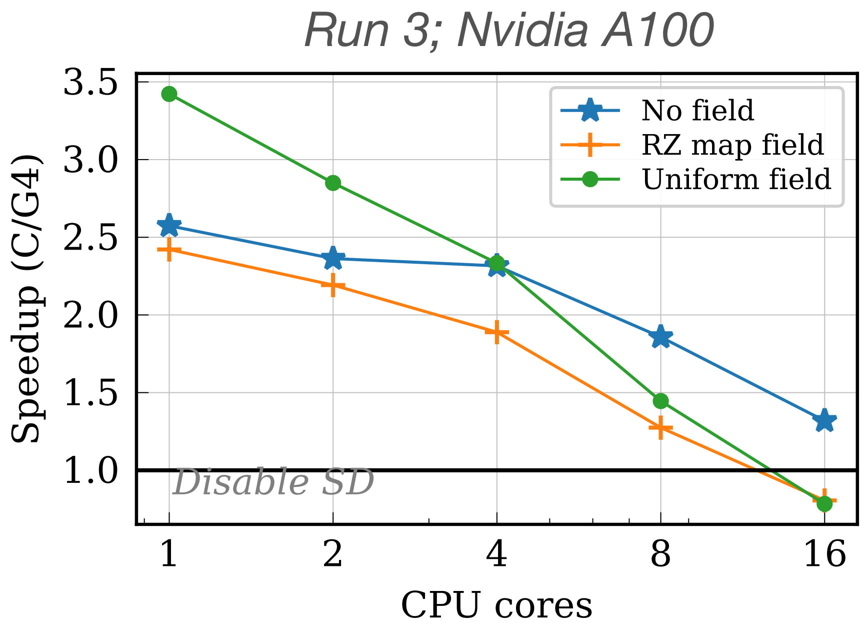


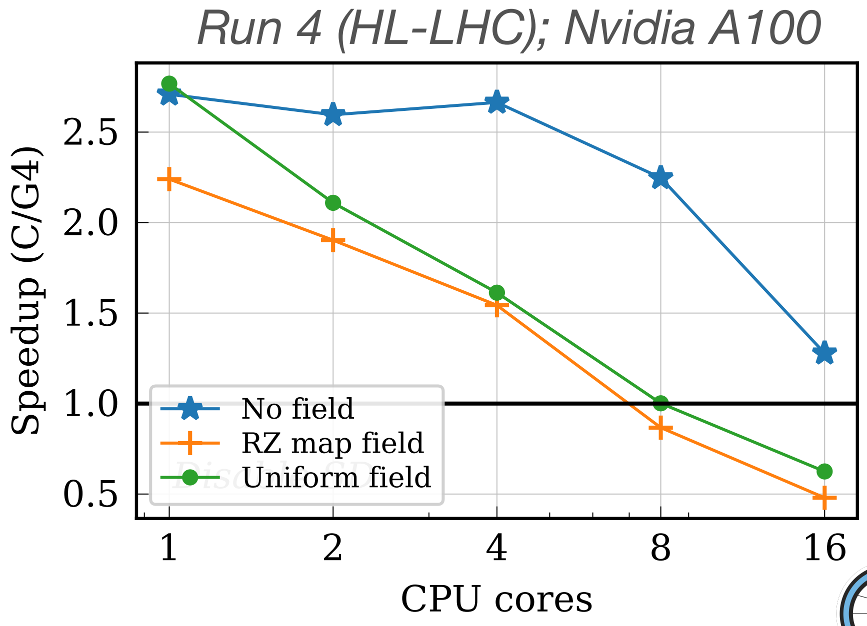

*Standalone Run 3 hit distribution*



# CMS Run 3&4 Standalone Results

- Promising performance
  - SD reconstruction adds <15% overhead
  - Initial comparison of hits shows good agreement
  - Run 3: 25%–190% improvement at 8 cores
  - With task-based framework we might see better (due to less GPU contention)
- Possible future improvements:
  - Magnetic field propagation
  - Activating track sorting to get smaller kernel grid sizes
  - Single-precision? (Especially on consumer cards)



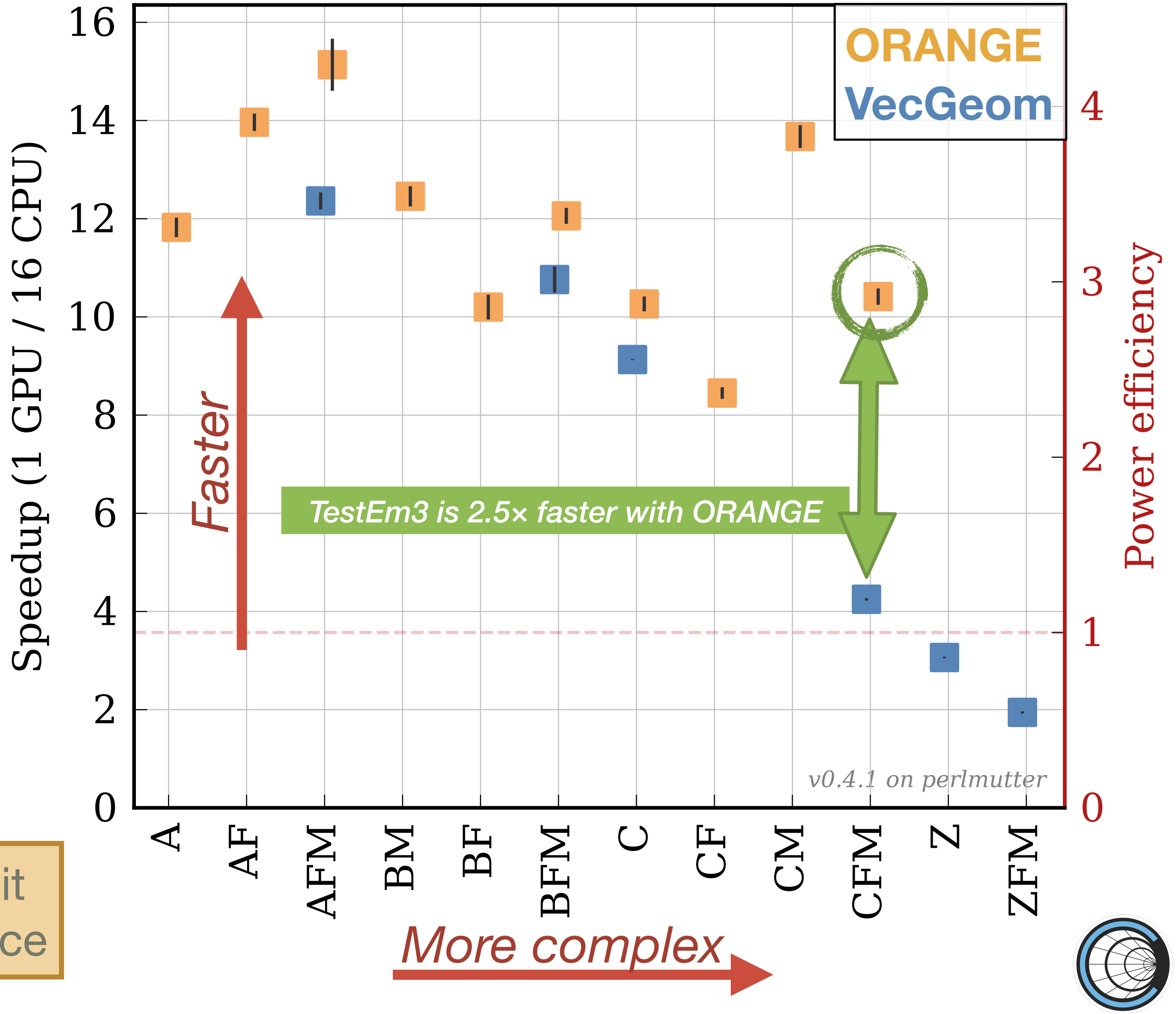

Nvidia A100 vs AMD 7532 EPYC

# Standalone EM performance

| | Problem definition |
|---|---|
| A | “infinite” medium |
| B | simple-cms |
| C | idealized calorimeter |
| Z | cms2018 |

| | Modifier |
|---|---|
| F | +field |
| M | +msc |

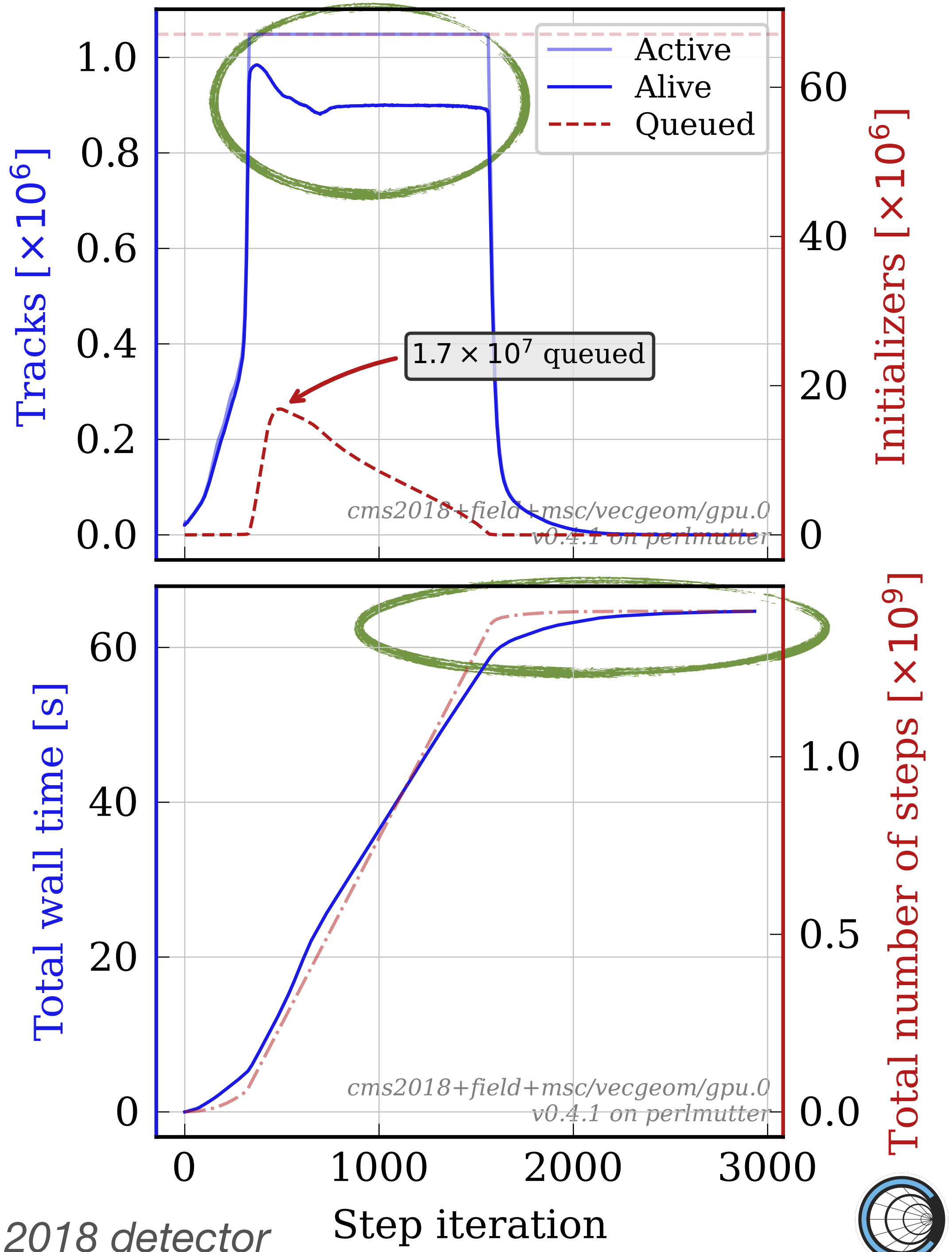
- 1300 × 10 GeV e-, 16 events
- ¼ Perlmutter node (NERSC)
  *1 × Nvidia A100 GPU, ¼ × 64-core AMD EPYC 7763*
- Celeritas GPU vs CPU
  *CUDA (1 CPU thread) vs OpenMP (16 CPU threads)*
- Key metrics favor GPU
  - *Capacity:* **50–94% loss** if GPUs are ignored
  - *Efficiency:* up to **4×** performance per watt




Previous versions of this slide used Summit which shows much worse CPU performance

# Step-dependent behavior

- Number of active particle tracks changes drastically due to EM shower
- Saturated GPU takes the most time but <50% of step iterations
  *Despite using masking instead of sorting!*
- Converting the tail of long-lived tracks does *not* kill us




*7 × 1300 × 10 GeV e⁻: CMS 2018 detector*

# Speedup with respect to Geant4

- Standalone Celeritas on CPU is ~50% faster than Geant4 for EM test suite
- GPU/G4 throughput: **2.5–20×**
- Still investigating disparity between "+G4" (offloaded from Geant4) versus standalone app

*Problem definition*

| | |
|---|---|
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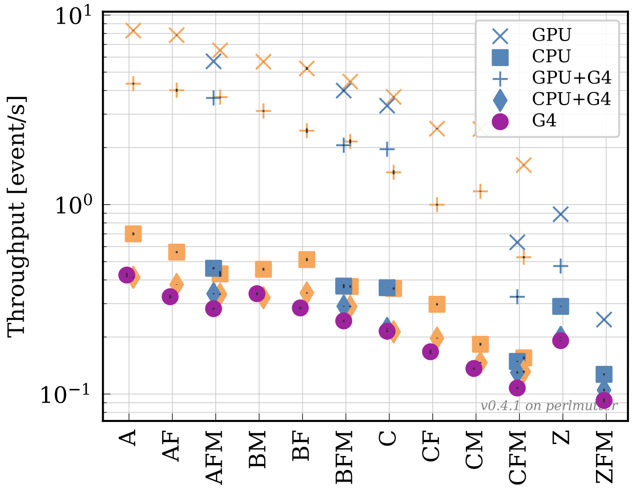
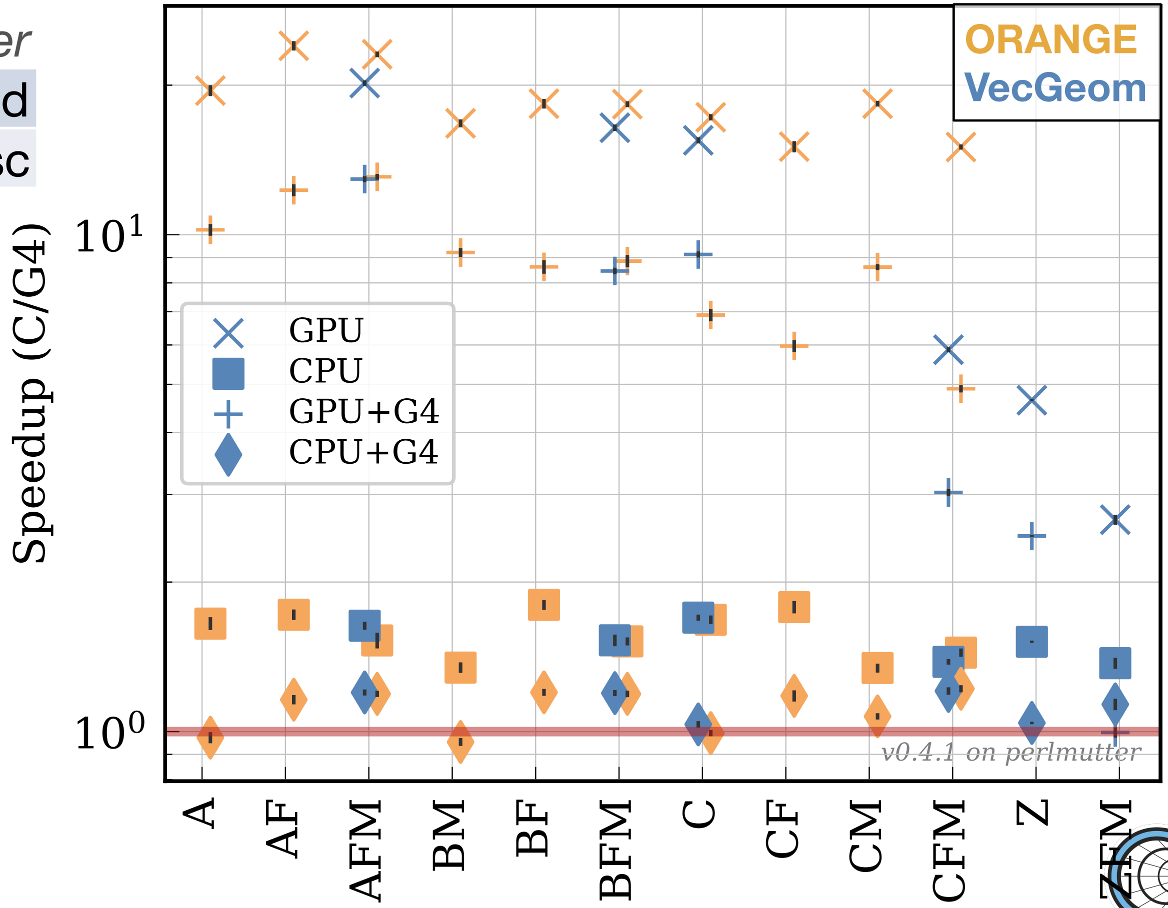
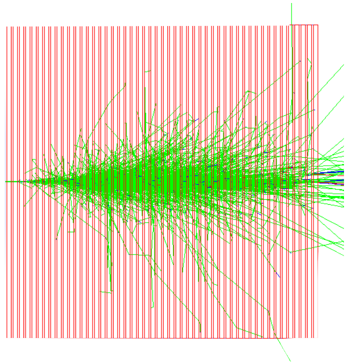
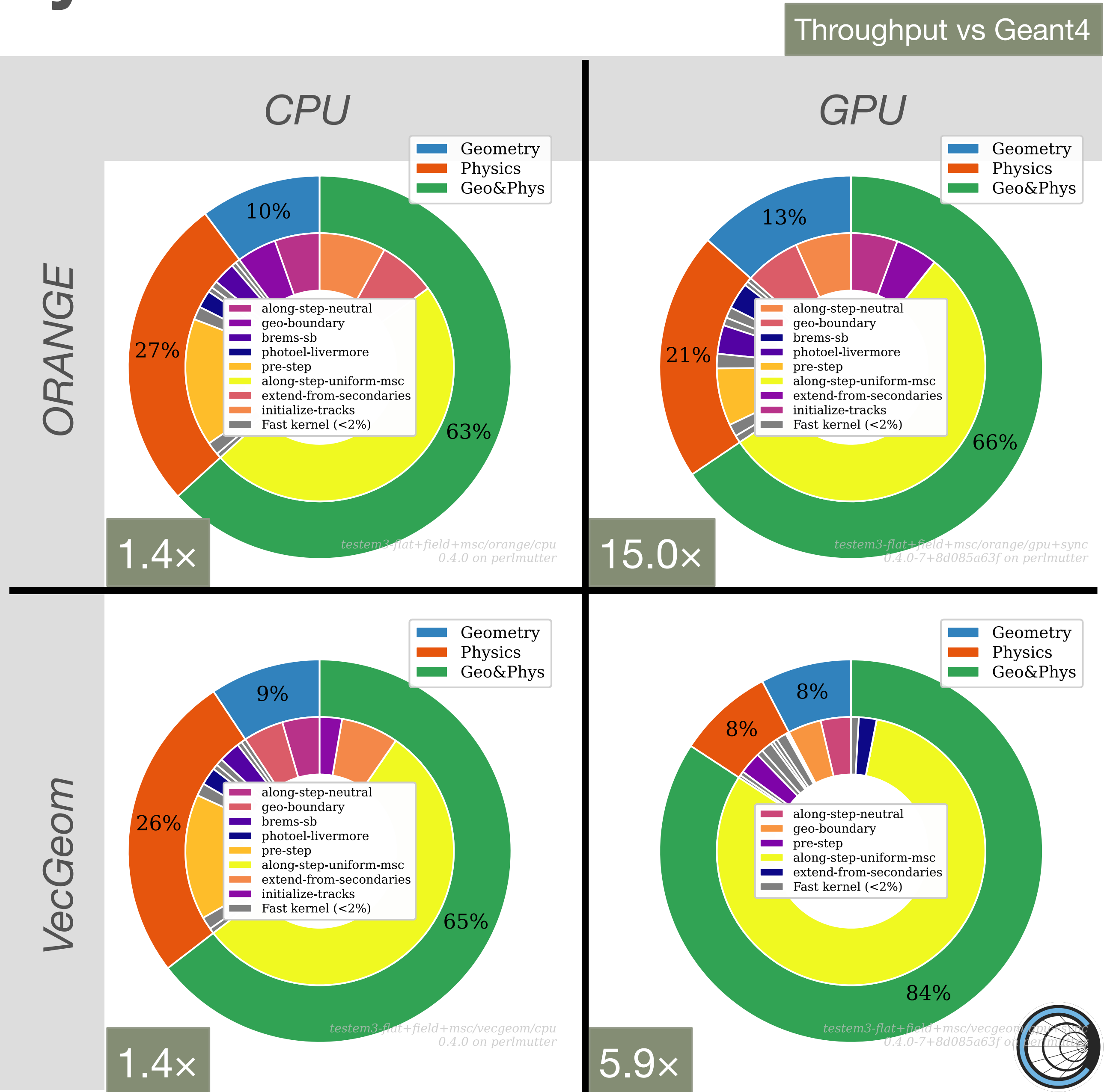


# TestEM3 performance disparity

- “No” divergence (all boxes)
- Performance parity on CPU
- *Physics* time parity on GPU
- Step counts are equivalent
- ORANGE faster on GPU
  - Neutral propagation: 1.4×
  - Field propagation: 3.6×
  - Boundary crossing: 1.5×



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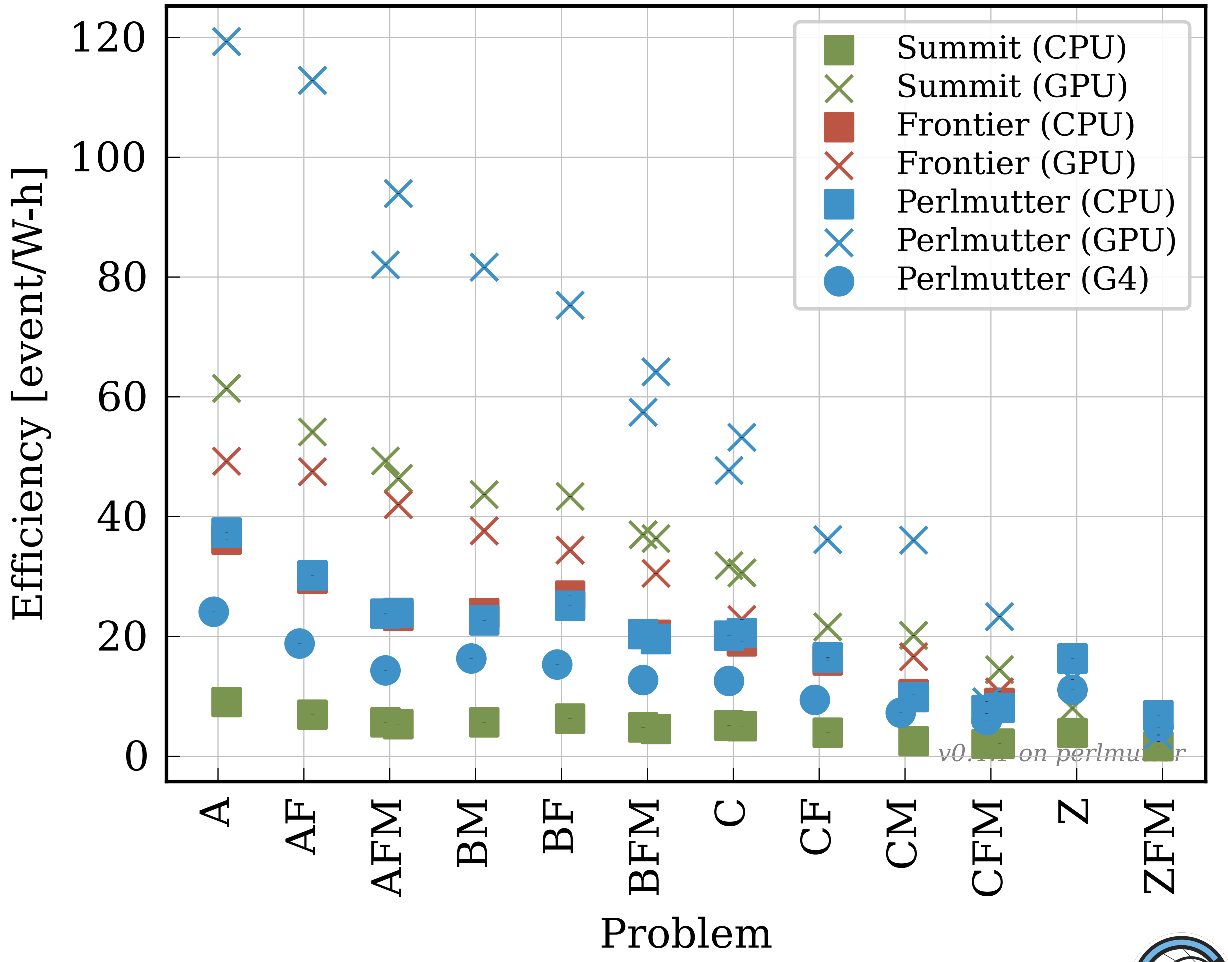
# Power efficiency

| Machine | GPU | CPU |
| --- | --- | --- |
| Summit | Nvidia V100 | IBM Power9 |
| Perlmutter | Nvidia A100 | AMD EPYC 7763 |
| Frontier | AMD MI250x | AMD EPYC 7453 |

- Estimated using reported Thermal Design Power (TDP) and Celeritas throughput
- GPU consistently shows higher energy efficiency 🌱
- A100/EPYC price: ~4× 💸




*EM only, no SDs*

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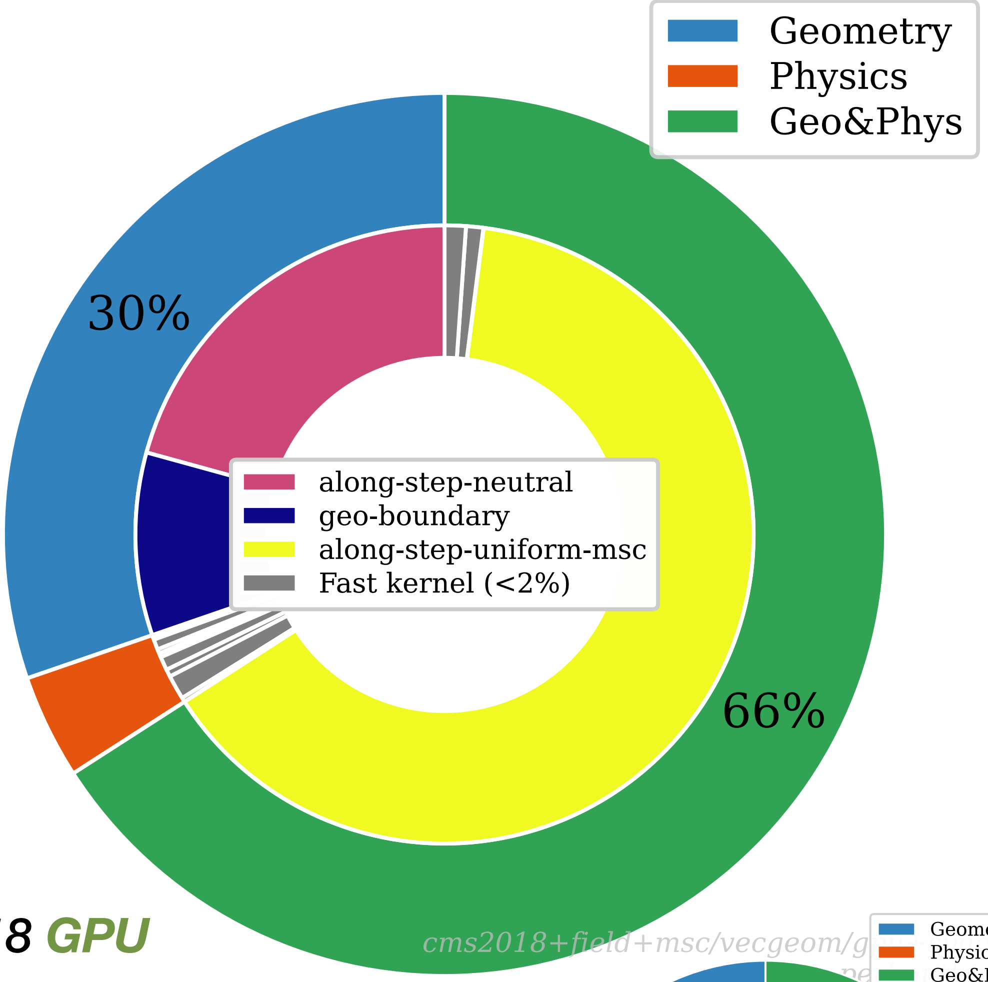
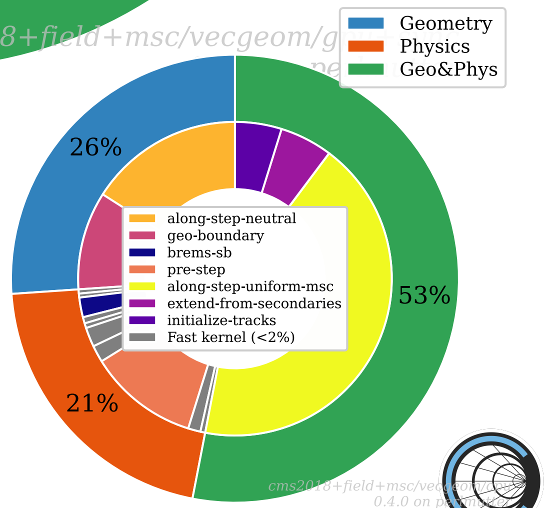
# Ongoing work

- Collaboration & integration
  - CMSSW
  - Athena (ATLAS) framework
  - Student projects
- Verification & validation
  - EM test problems
  - CMSSW workflow
- Optimization and geometry
  - **96%** of standalone runtime in CMS2018 is in geometry routines
  - GPU native sensitive detectors
  - ORANGE navigation
  - Track sorting




*CMS2018 GPU*




*CMS2018 CPU*



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# Celeritas future

- Designed for **easy integration**
  - Potentially incorporate into Geant4 as an accelerator for certain HEP applications
  - Continue integration into HEP experiment frameworks
- Designed for **extensibility**
  - Optical photon simulation to be funded starting next year
  - Incremental addition of HEP physics for GPU offloading
- Designed for **performance**
  - Still have many avenues to investigate (without change to external interface!)
  - Surface-based geometry predicted to be much faster for complex applications
  - Works well on CPU, better on GPU

# Summary: by the numbers

| | | |
|---|---|---|
| **100** | **lines of code** | to integrate Celeritas into a FullSimLight tile calorimeter test application, with no modifications to Geant4 |
| **1.8×** | **full-simulation speedup** | including hadronics and SD hits, by using 1 Nvidia A100 with 16 AMD EPYC cores for the ATLAS test beam application *[NERSC Perlmutter]* |
| **2–20×** | **throughput** | when using Celeritas on GPU (compared to Geant4 MT CPU) for EM test problems *[NERSC Perlmutter]* |
| **4×** | **performance per watt** | for TestEM3 (ORANGE geometry) using Celeritas GPU instead of Geant4 CPU *[NERSC Perlmutter]* |

*Celeritas v0.4: https://celeritas-project.github.io/celeritas/*

# Acknowledgments

*Celeritas v0.4 code contributors:*

- Elliott Biondo (@elliottbiondo)
- Philippe Canal (@pcanal)
- Julien Esseiva (@esseivaju)
- Tom Evans (@tmdelellis)
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- Soon Yung Jun (@whokion)
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- Vincent R Pascuzzi (@vrpascuzzi)
- Paul Romano (@paulromano)

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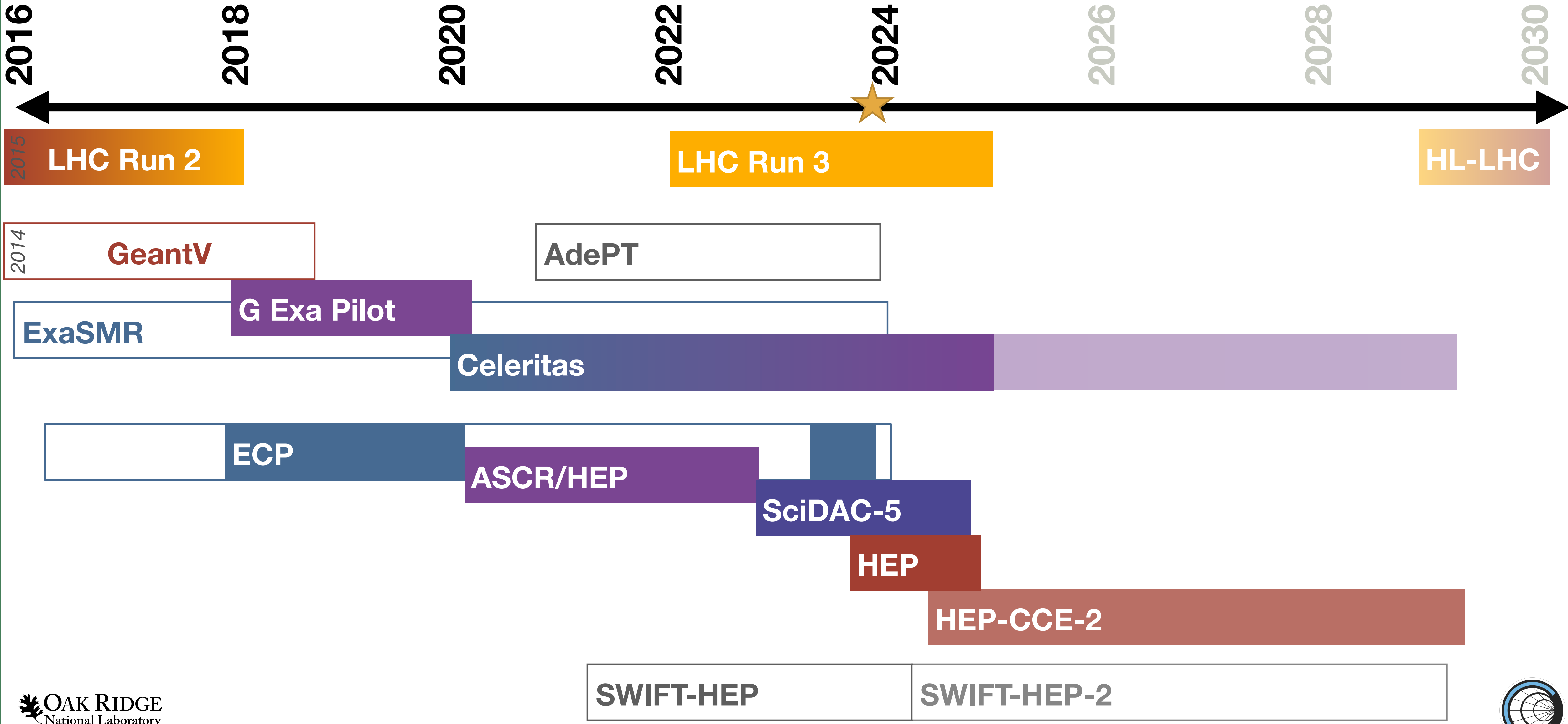
https://github.com/celeritas-project/celeritas

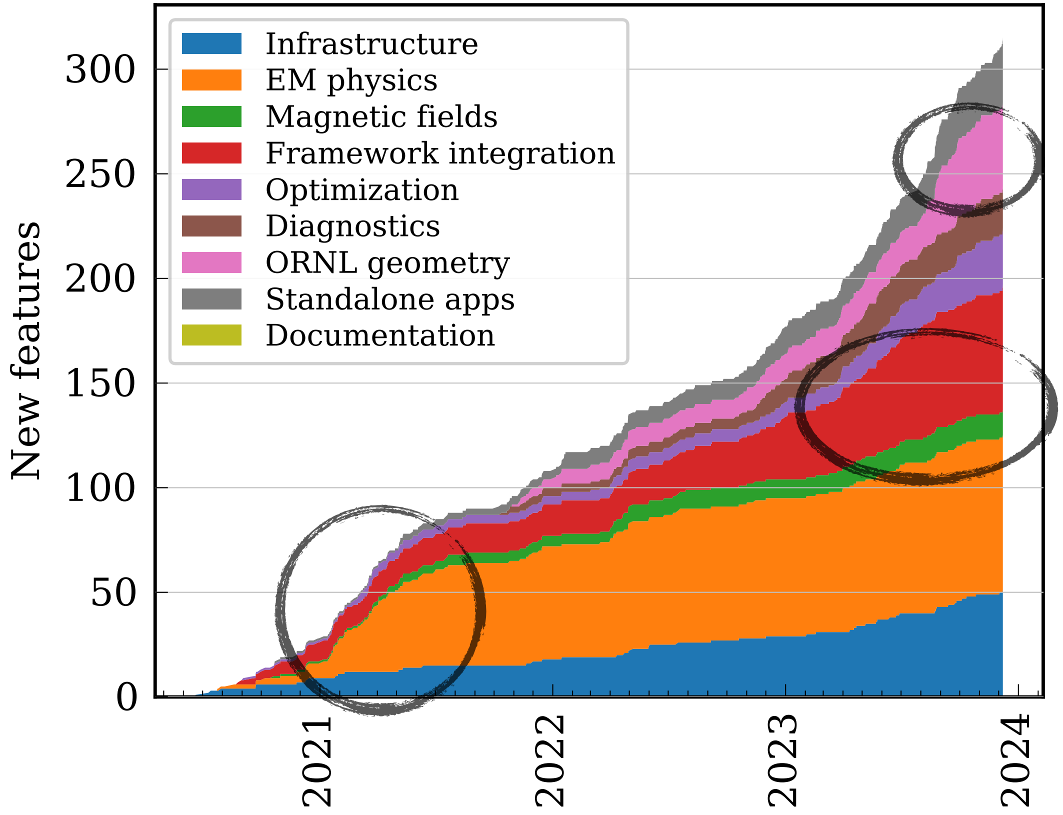
# Backup slides

# Historical context



# Code development

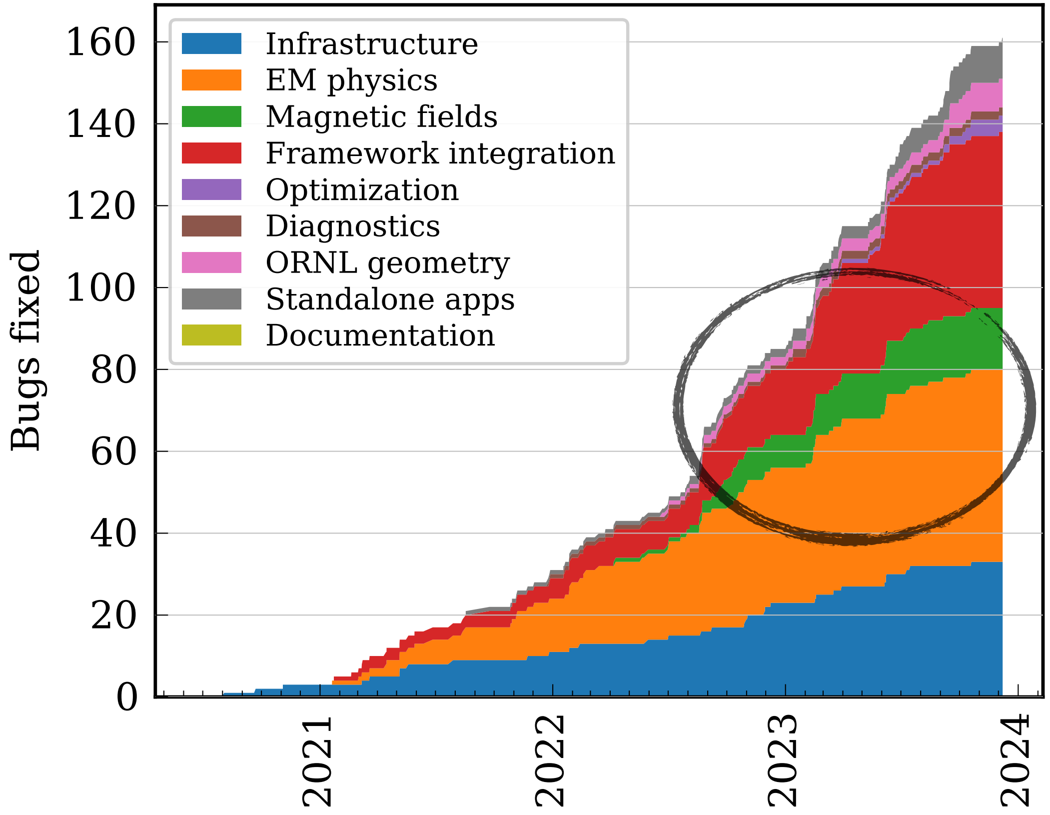
- Production-focused scientific software
  - **90%** of source code is reusable library code
  - **1:2** ratio of lines of documentation to code
  - **50k** lines of test code
- Early push for EM physics
- Last year's focus:
  - Integration with Geant4
  - Optimization on GPU (and CPU)
  - ORANGE features for ExaSMR reactor simulation




***Enhancement** pull requests*

# Code development (flip side)

- 1 fix for every 2 enhancements
- Integration campaigns critical for finding bugs/issues
  - ATLAS integration at LBL, Feb. 2023
  - CMS integration at ORNL, June 2023
- Bug fix rate is decreasing though!
  - Most fixes are for new features
  - Each PR requires a new unit test that fails without the fix and passes after




***Bug fix** pull requests*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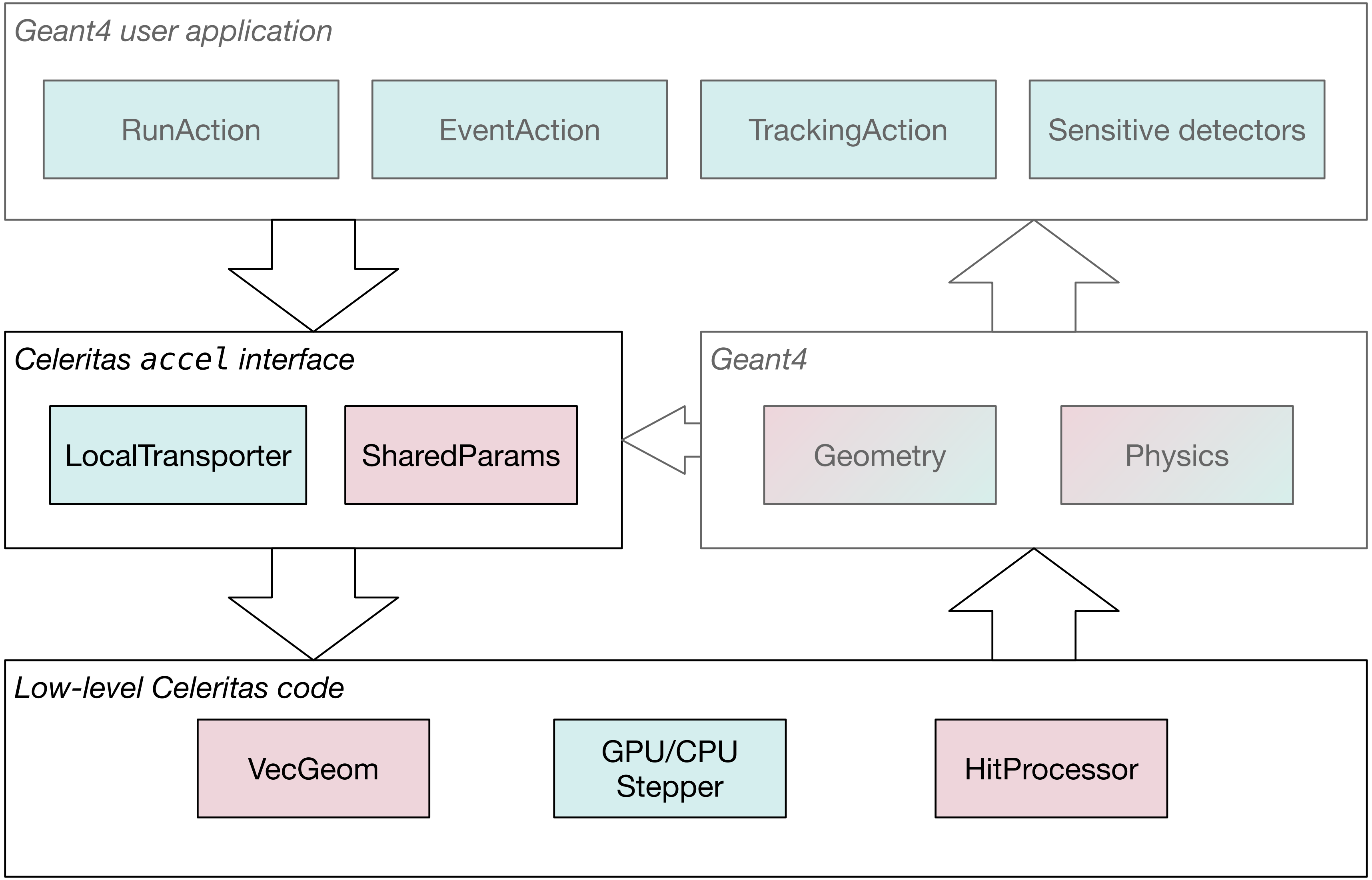
# Core design philosophy

- Algorithms and structure *will* need to change due to:
  - Increasing complexity of new physics added
  - Design requirements from downstream integration
  - Performance bottlenecks found during analysis
- Therefore code needs to be amenable to refactoring
  - Heavy use of composition rather than inheritance or massive functions
  - Data-oriented to allow the same data to be reused in multiple functions
  - Template-friendly interfaces hide underlying data structures

# Geant4 interface library




*Thread-local*
*Shared*

https://celeritas-project.github.io/celeritas/user/index.html

# Performance per step

- Large variation in timing for early steps
  *possibly due to "looping" low-energy particles in vacuum*
- For same number of active tracks, end of simulation is 50–80% slower per step
  *likely due to geometry divergence*