ORNL is managed by UT–Battelle, LLC for the US Department of Energy

Celeritas R&D Summary

Seth R Johnson

Celeritas Code Lead
Senior R&D Staff
Scalable Engineering Applications

CELERITAS

Celeritas core team:

Elliott Biondo *(ORNL),* Julien Esseiva *(LBNL),* Seth R Johnson *(ORNL),* Soon Yung Jun *(FNAL)*, Guilherme Lima *(FNAL)*, Amanda Lund *(ANL)*, Ben Morgan *(U Warwick)*, Stefano Tognini *(ORNL)*

Celeritas core advisors:

Tom Evans *(ORNL)*, Philippe Canal *(FNAL)*, Marcel Demarteau *(ORNL)*, Paul Romano *(ANL)*

U.S. DEPARTMENT OF ENERGY

Geant4 R&D Review
13 December, 2023

Background

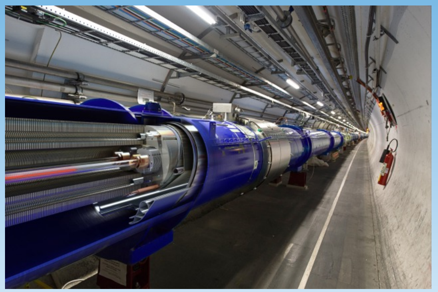
Methods

Results

Conclusions

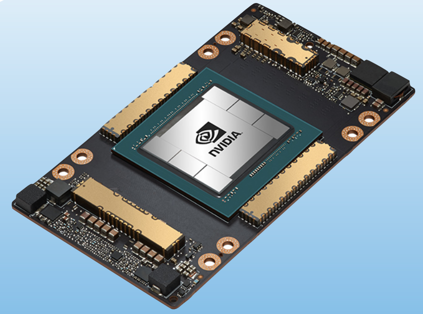
Celeritas project goal

- **Accelerate scientific discovery** by improving detector simulation throughput and energy efficiency for LHC production simulation
  - 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 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

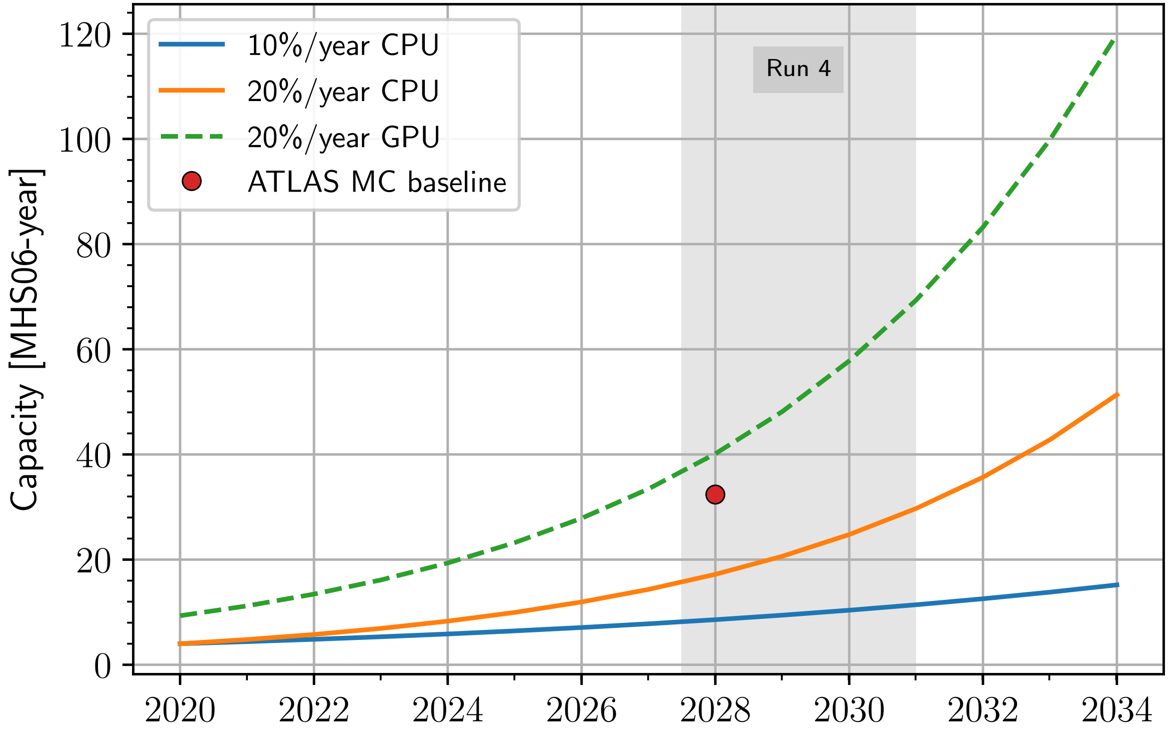
CELERITAS



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 (possibly directly via GPU)



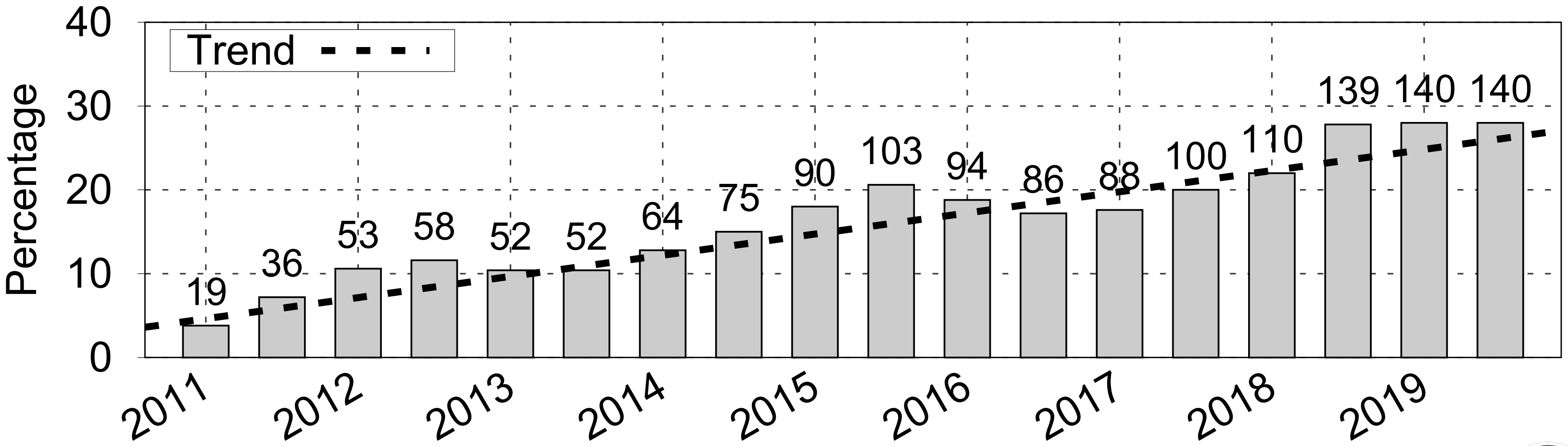
GPU projection based on energy efficiency and speedup of ExaSMR MC code

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

Celeritas team

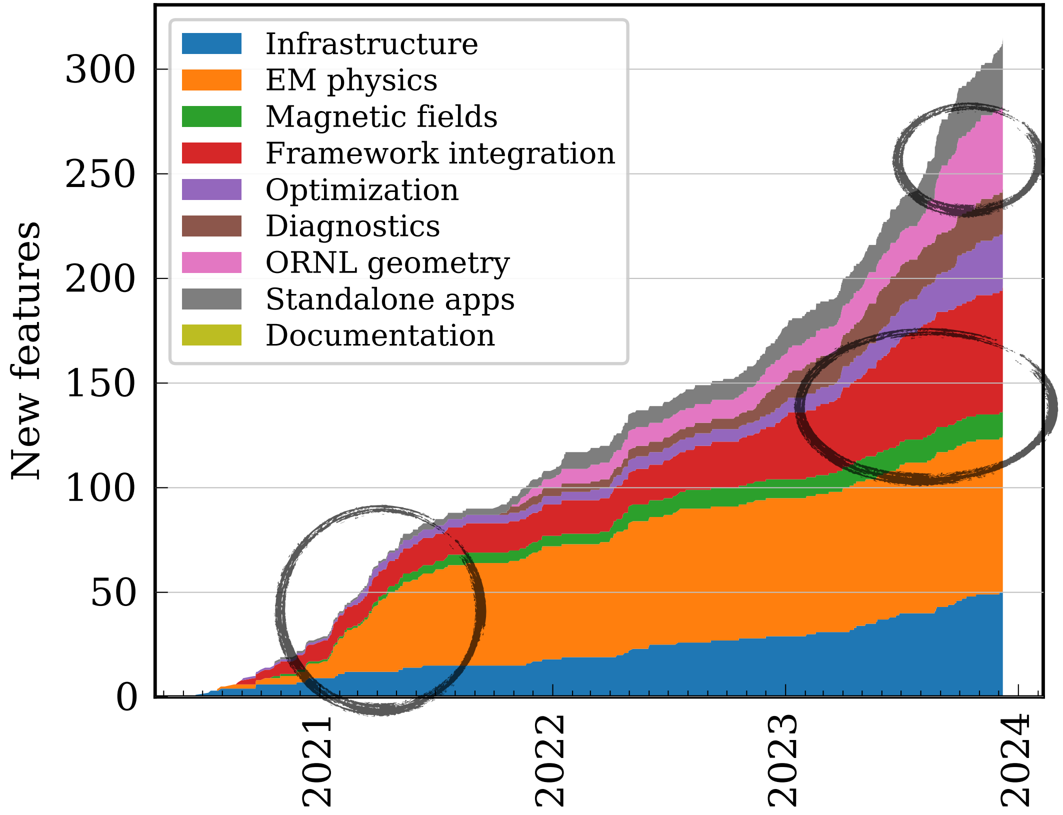
- Diverse scientific backgrounds
- Decades of combined experience managing large scientific software projects
- Multi-institution (now international)
- ***Not*** *computer scientists steamrolling physicists with mini-apps*

Educational background of core+advisors

	Bachelor	Master	Doctorate
Physics	7	5	5
Engineering	3	3	3
Computer science	1	3	
Mathematics	2	1	

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*

Background

Methods

Results

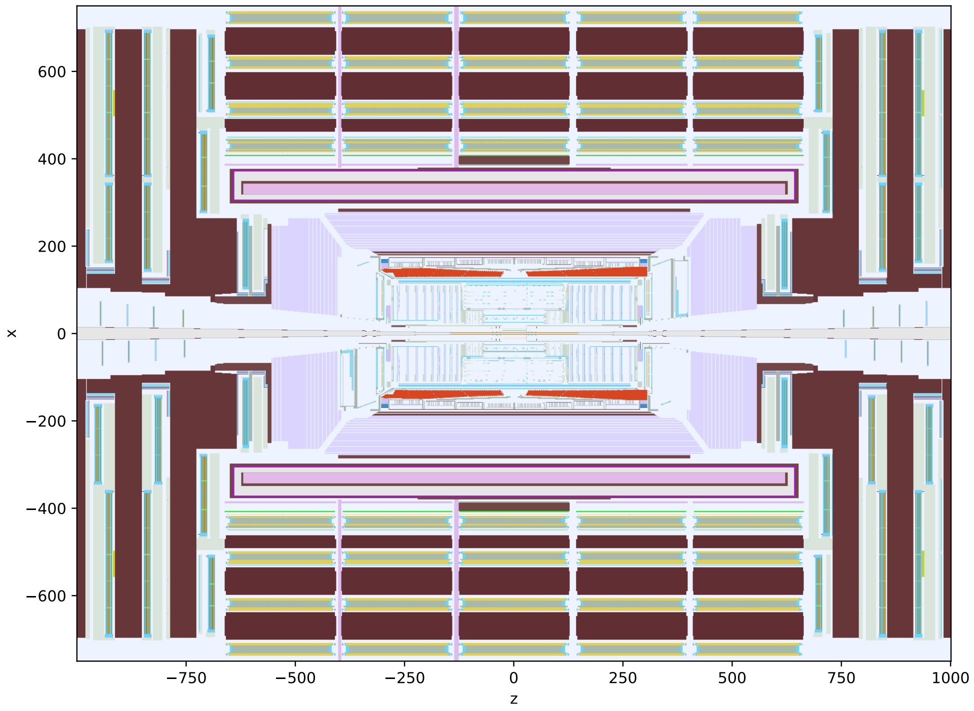
Conclusions

Core design philosophy

- Algorithms and structure *will* need to change due to:
  - Increasing complexity of new physics added
  - Unexpected 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

High-level capabilities targeting LHC simulation

- Equivalent to `G4EmStandardPhysics`
  …using Urban MSC for high-E MSC; only γ, e±
- 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 AMD*

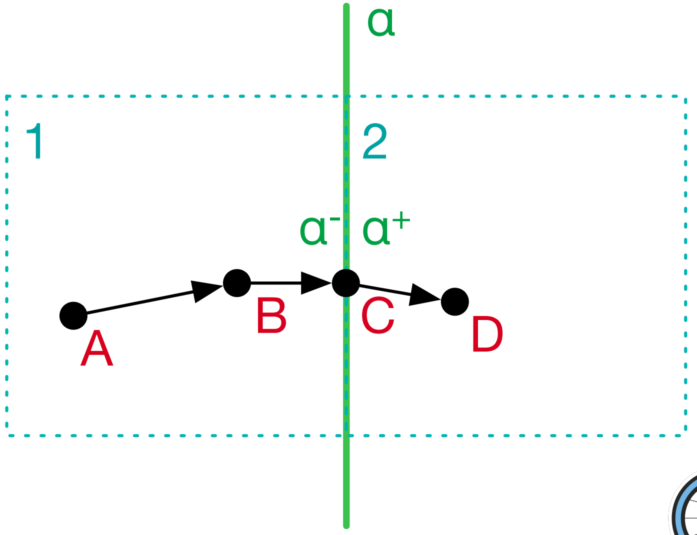
Source: Johnson, S.R. Geant4 Meeting 2023

ORANGE: surface-based navigation

- Designed for deeply nested reactor models
- Portable (CUDA/HIP) geometry implementation
- Tracking based on CSG tree of surfaces **constructed from volumes**
- Maximize run-time performance and robustness 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”) are optimal for GPU



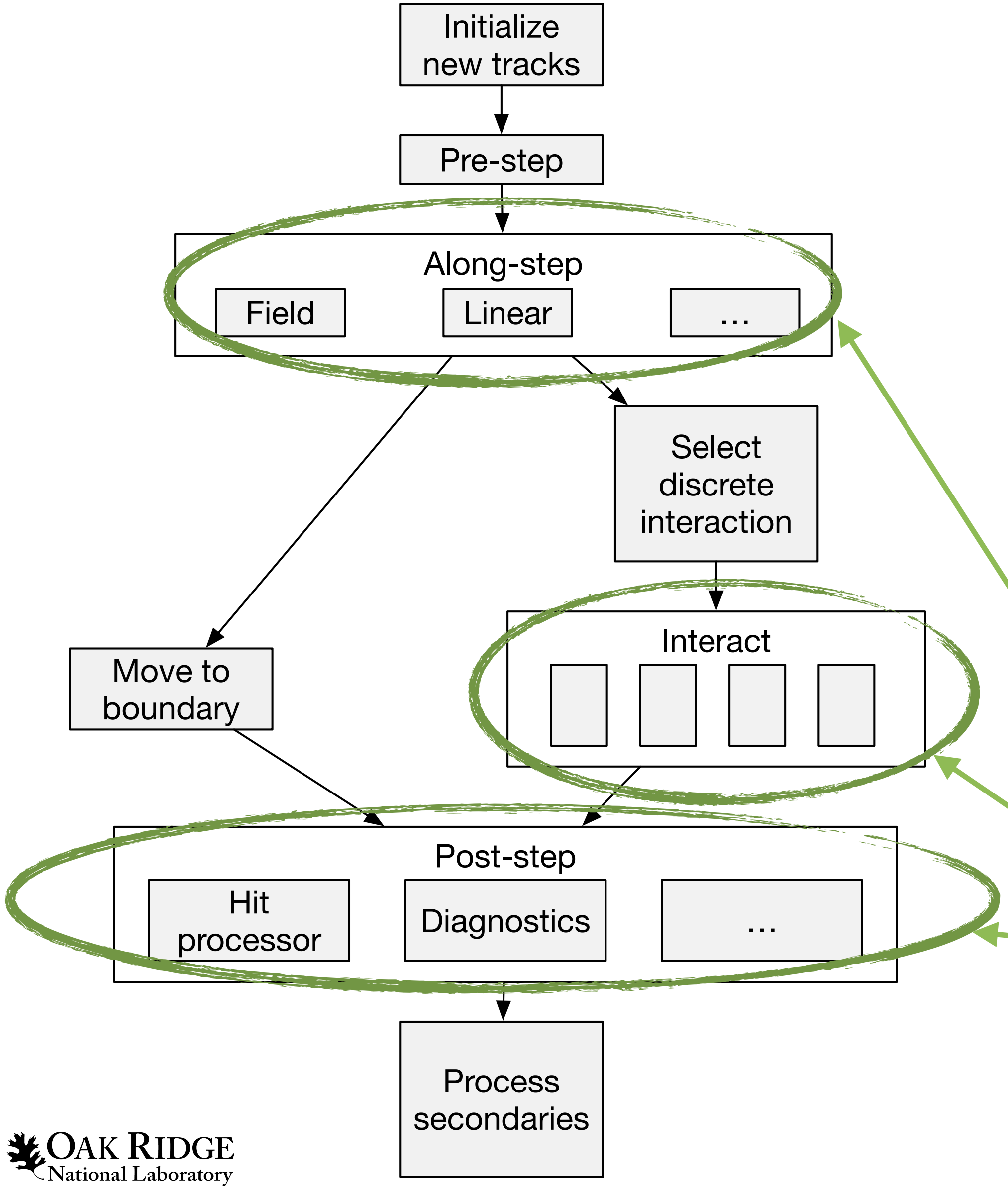
Magnetic field propagation

- 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*

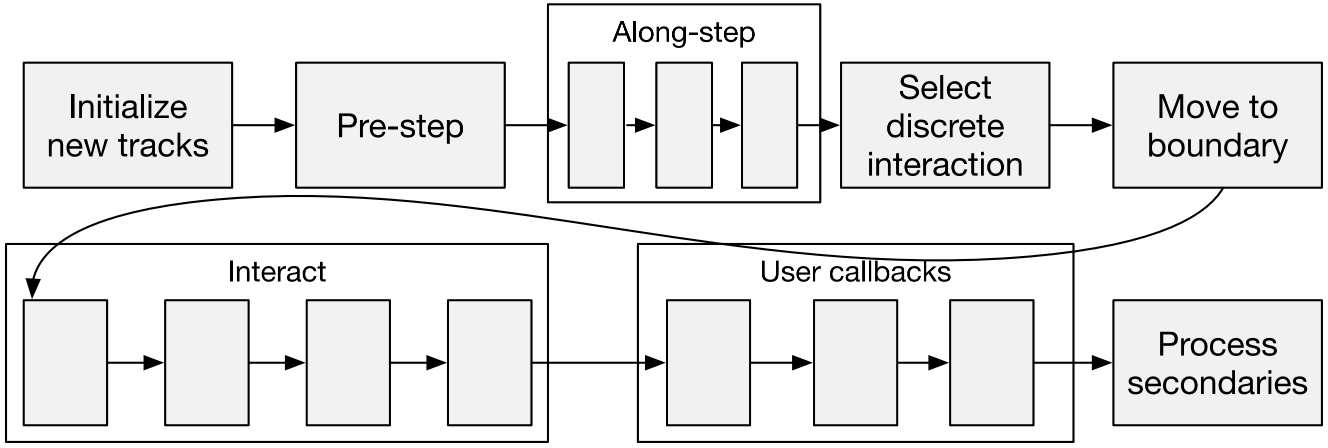
Operator	Input	Output
Field	$\mathbf{x}$	$\mathbf{B}$
Equation of motion	$\mathbf{x}$, $\mathbf{p}$, $\mathbf{B}$	$\mathbf{x}'$, $\mathbf{p}'$
Integrator	$\mathbf{x}$, $\mathbf{p}$, h	$\mathbf{x}^*$, $\mathbf{p}^*$, e
Driver	$\mathbf{x}$, $\mathbf{p}$, s	$\mathbf{x}^*$, $\mathbf{p}^*$, s^*
Propagator	$\mathbf{x}$, $\boldsymbol{\Omega}$, E, s	$\mathbf{x}^*$, $\boldsymbol{\Omega}^*$, s^*

**safety calculation resulted consistently in slowdown on GPU*

Stepping loop on a GPU



Process large batches of tracks through all kernels (10^3–10^6)



Topological sort: a loop over kernels

Using many small kernels improves extensibility

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 with no patches required

Celeritas has production quality interfaces to simplify user application integration

Source: Johnson, S.R. Geant4 Meeting 2023

Background

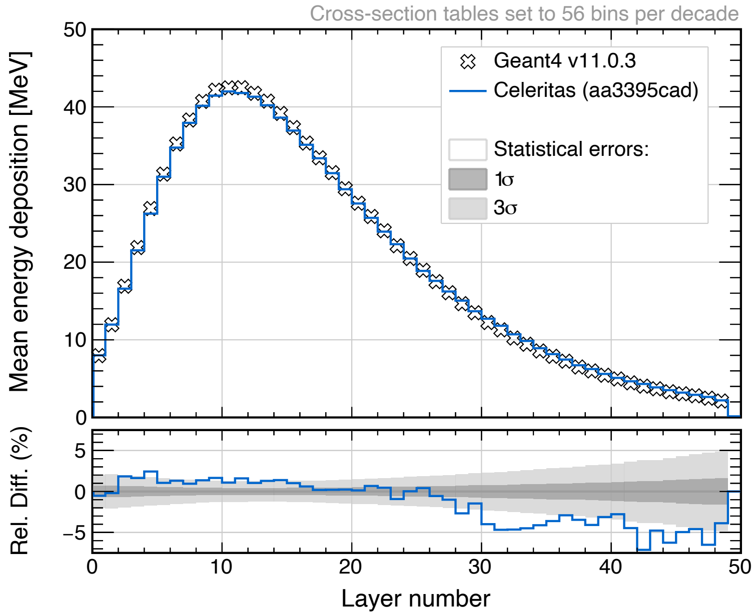
Methods

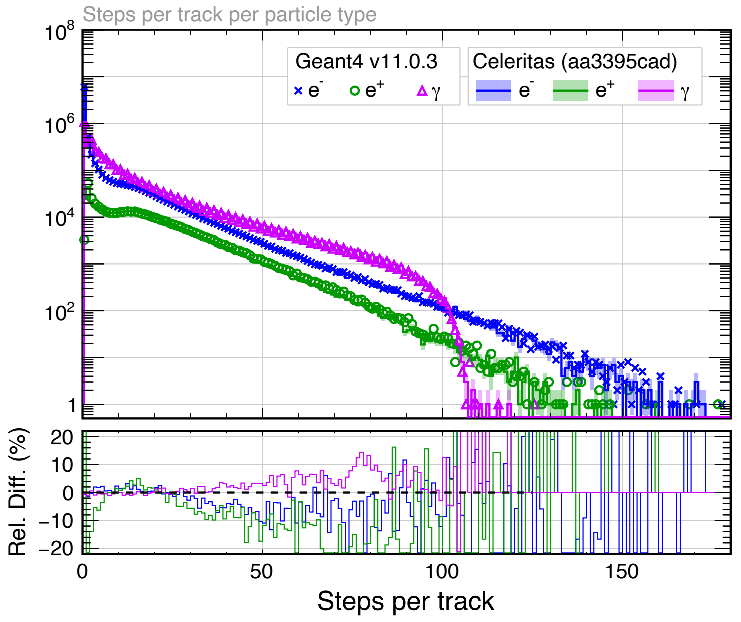
Results

Conclusions

Physics verification

- Single-model distributions
- Volume-dependent hit count and energy deposition distributions
- Step-per-track distributions (same total steps to within half a percent)
- Most significant disagreement remaining: Urban MSC

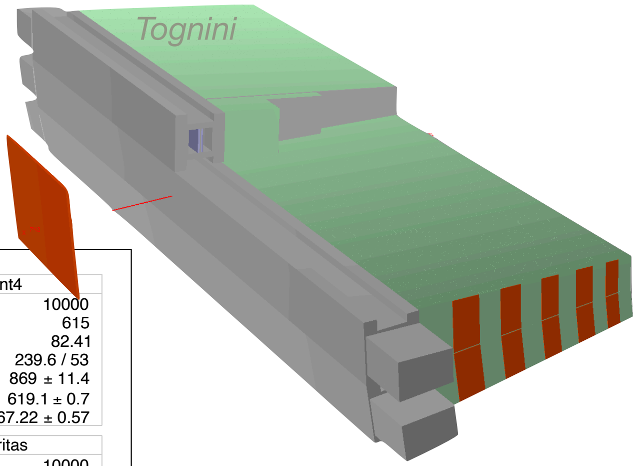


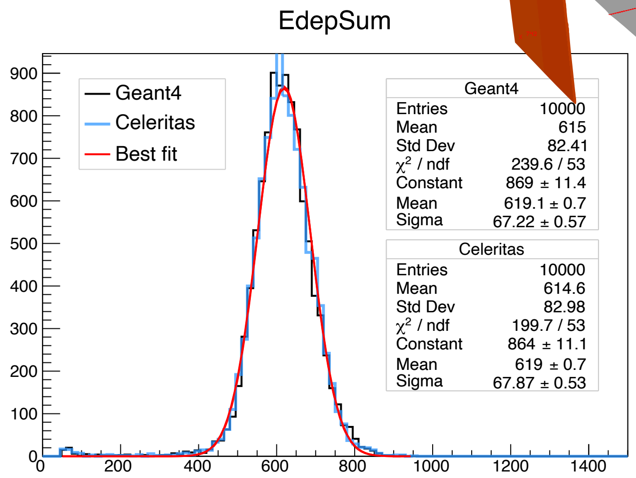


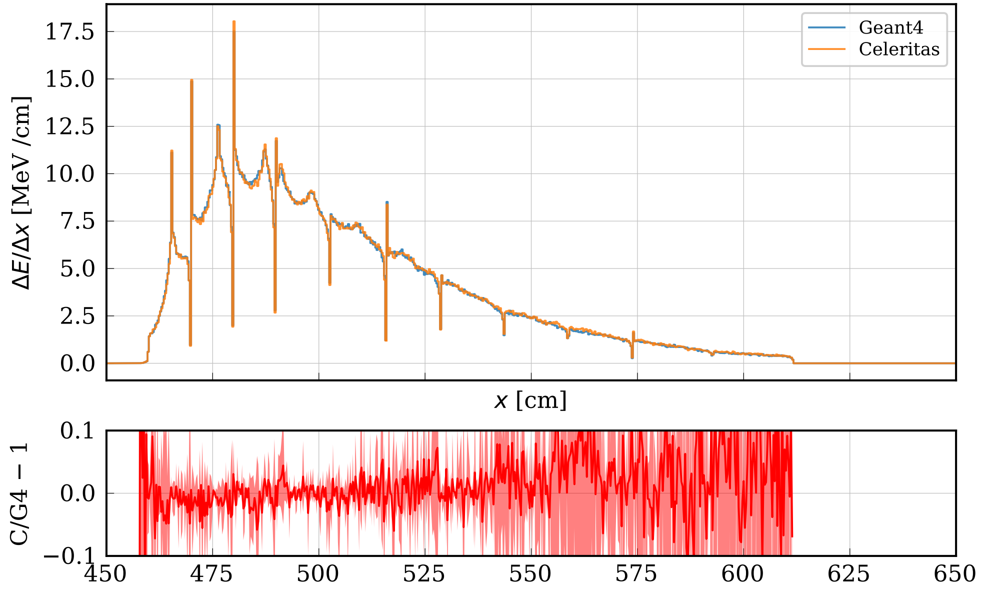
OAK RIDGE National Laboratory

EM offloading with FullSimLight

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







yz-integrated energy deposition

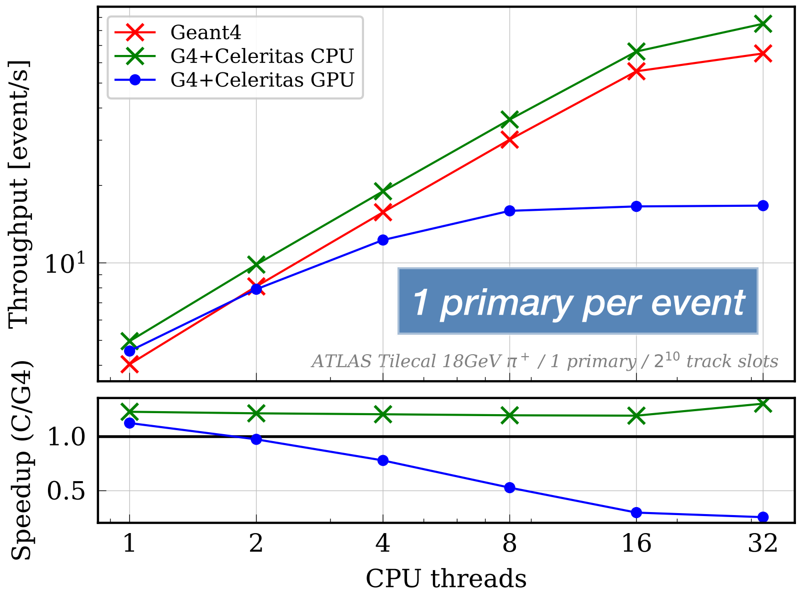
Test problem: Lachnit, Pezzotti; FSL integration: Morgan

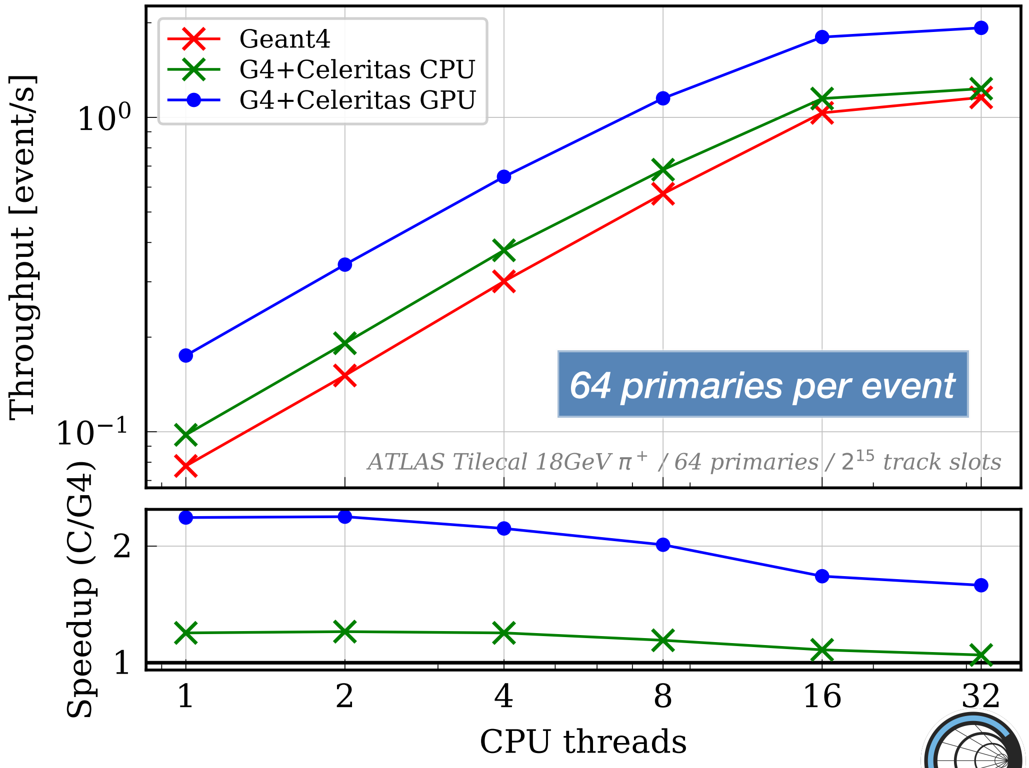
Source: Johnson, S.R. Geant4 Meeting 2023

OAK RIDGE National Laboratory

Offload performance results

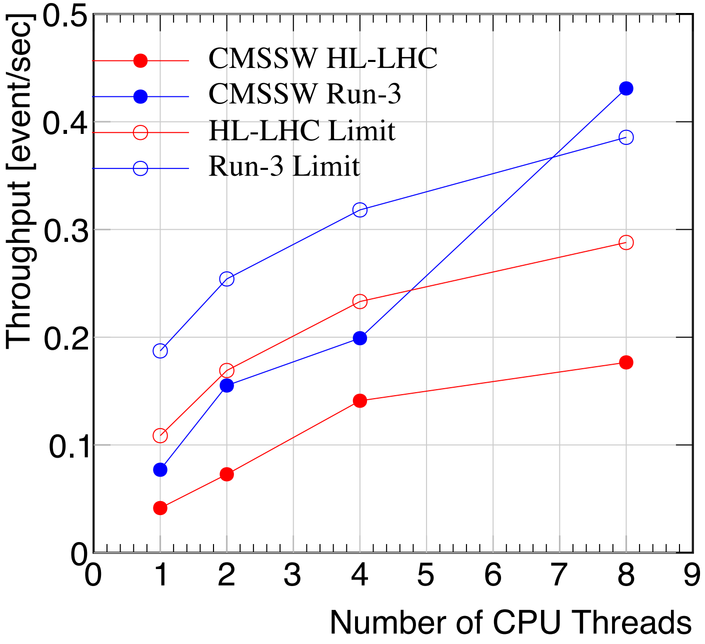
- 1/4 of a Perlmutter (NERSC) GPU node
  16 cores of AMD EPYC, 1 Nvidia A100
- Time includes startup overhead, Geant4 hadronic physics, track reconstruction, and SD callback
- GPU speedup: **1.7×** at full occupancy
  Using all CPU cores with a single GPU
- CPU-only speedup: **1.1–1.3×**
- Theoretical maximum speedup: **2.2–2.5×**
  Instantly killing e-, e+, γ when born
- **LHC-scale energy per event (>1 TeV) is needed for GPU to be effective**
- **One GPU is effective with many-CPU Geant4**

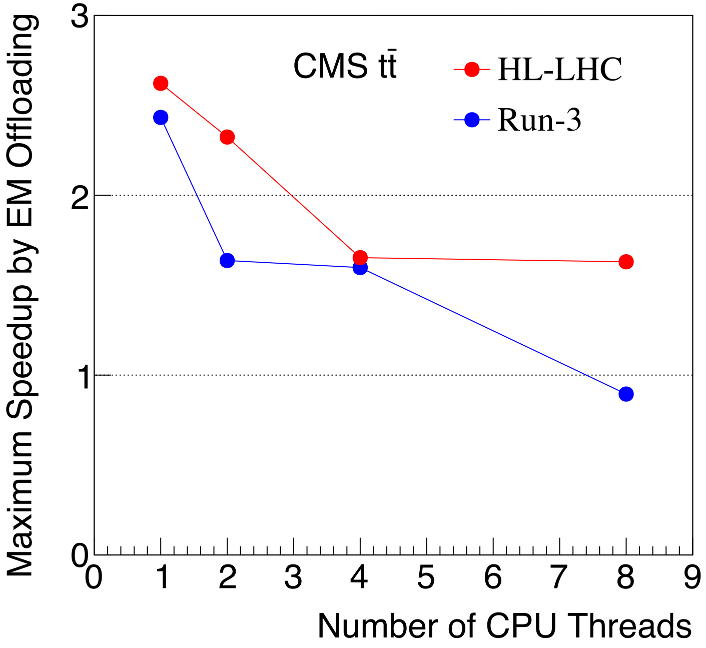




CMSSW integration

- 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×**



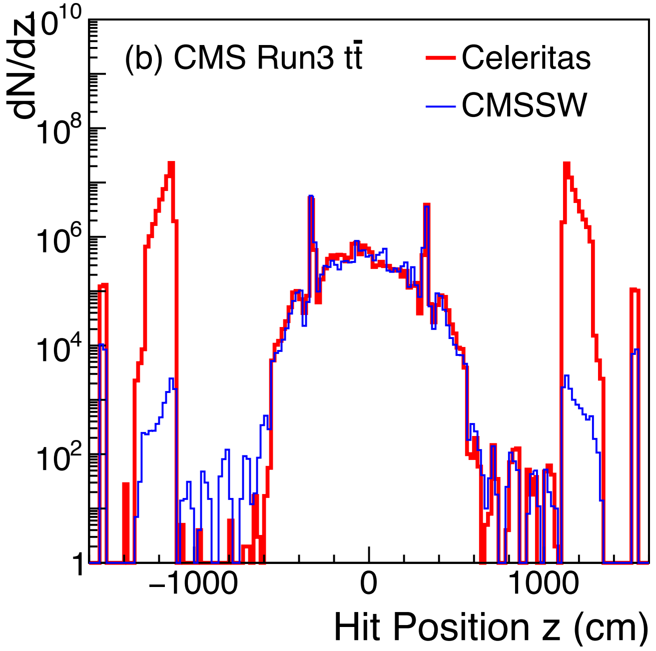


Oak Ridge National Laboratory

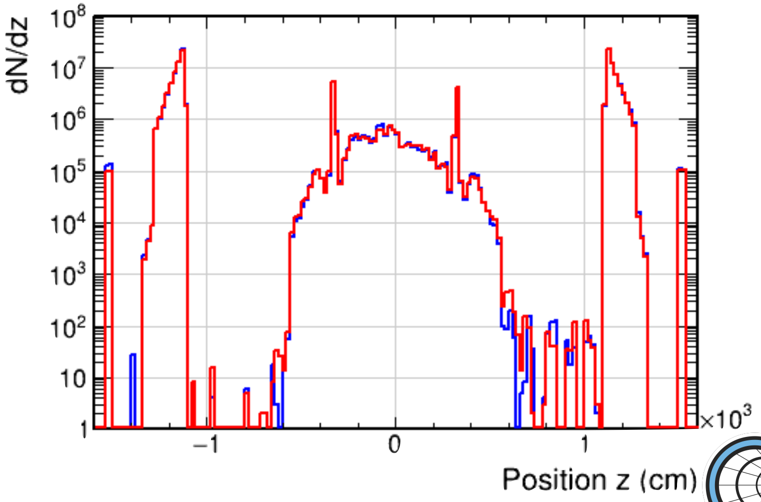
CMS Run 3&4 Standalone Simulations

- 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

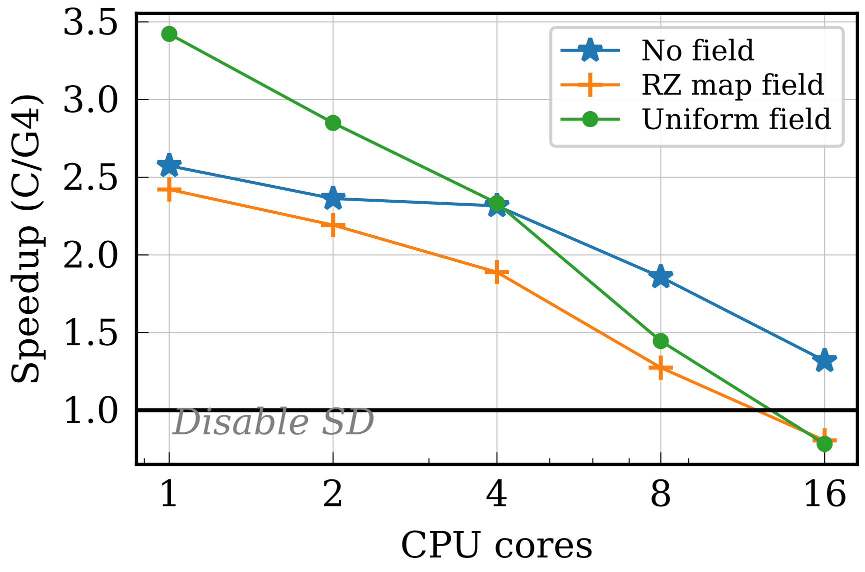


Oak Ridge National Laboratory

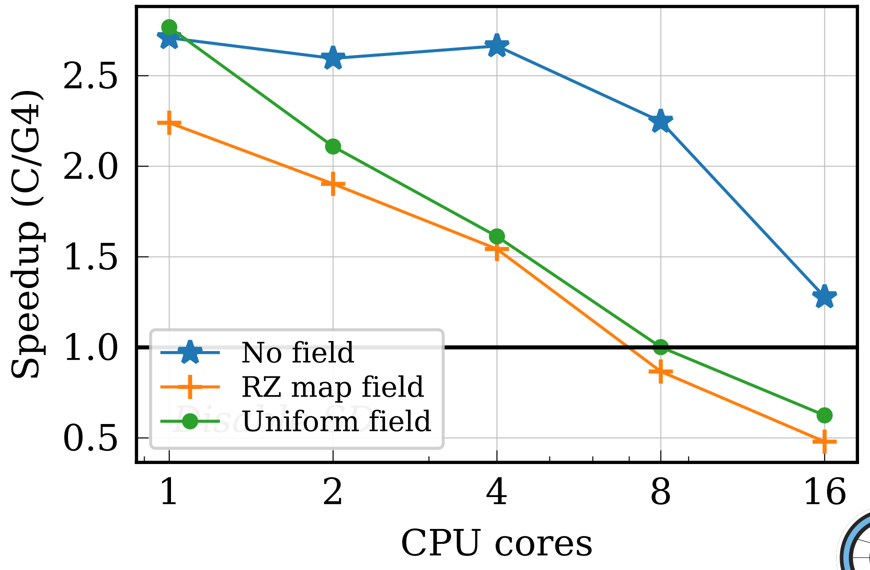
CMS Run 3&4 Standalone Results

- 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)

Run 3; Nvidia A100



Run 4 (HL-LHC); Nvidia A100



Nvidia A100 vs AMD 7532 EPYC

Standalone EM performance

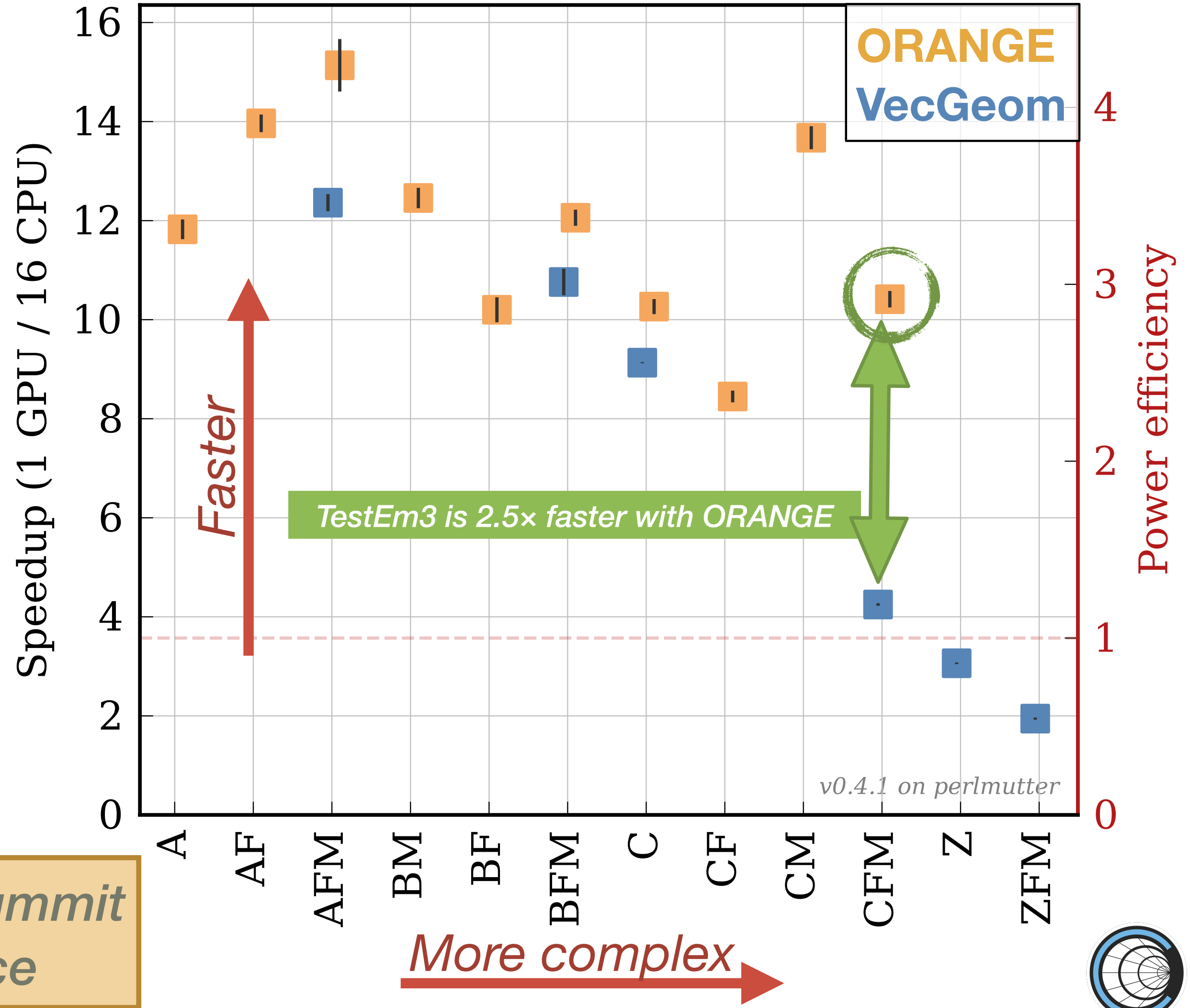
	Problem definition
A	“infinite” medium
B	simple-cms
C	idealized calorimeter
Z	cms2018

	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 has slower CPU performance

Speedup with respect to Geant4

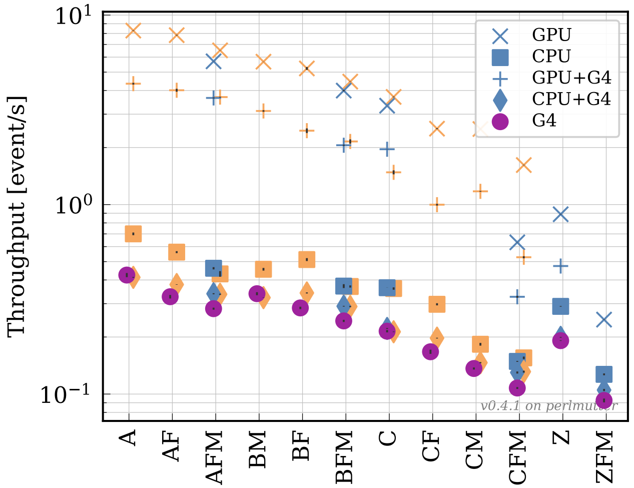
- Standalone Celeritas on CPU is ~50% faster than Geant4 for EM test suite
- GPU/G4 throughput: **2.5–20×**
- Still investigating disparity between "+G4" (offloaded from Geant4) versus standalone app

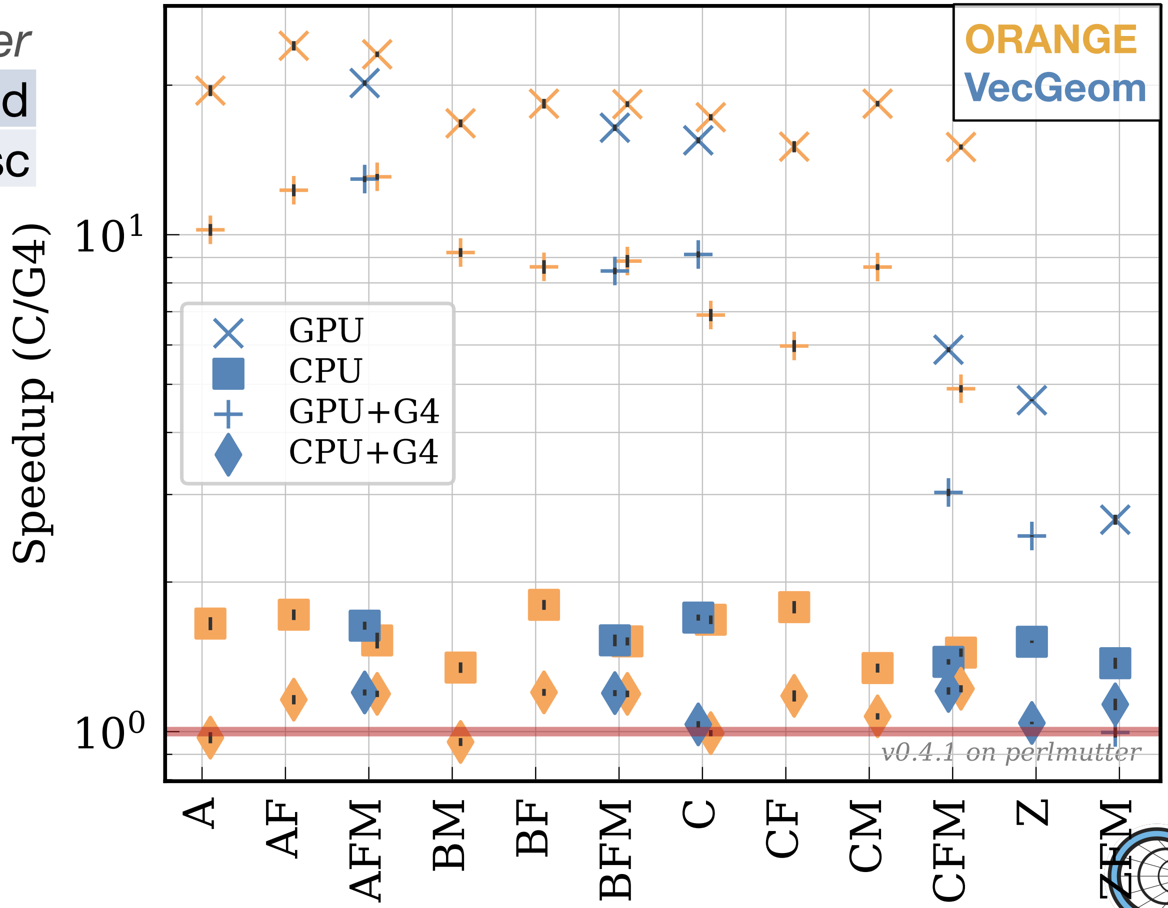
Problem definition

A	"infinite" medium
B	simple-cms
C	idealized calorimeter
Z	cms2018

Modifier

F	+field
M	+msc

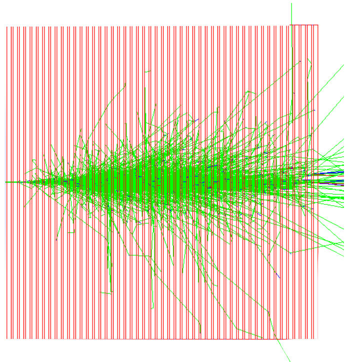




Oak Ridge National Laboratory

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×



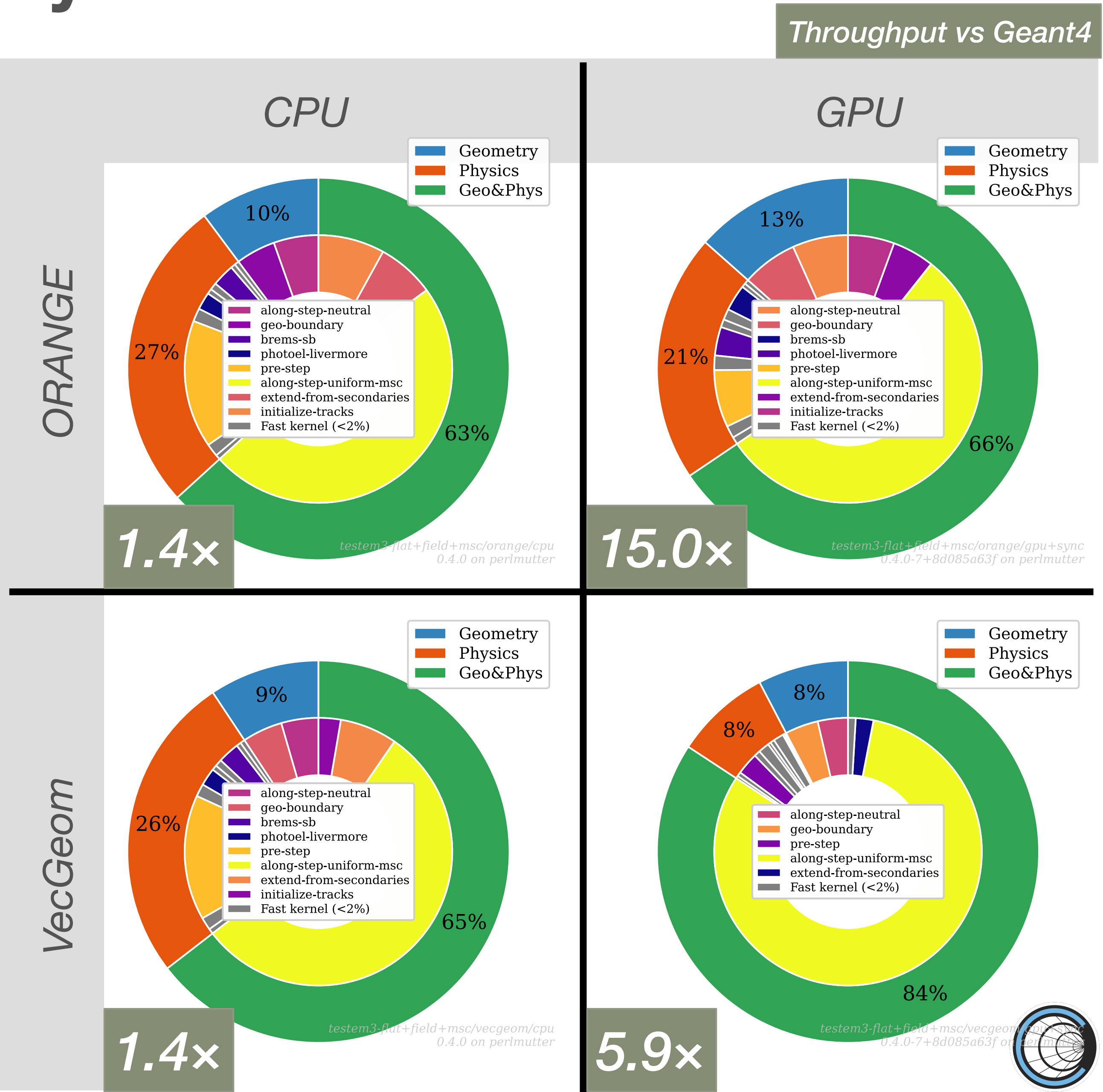
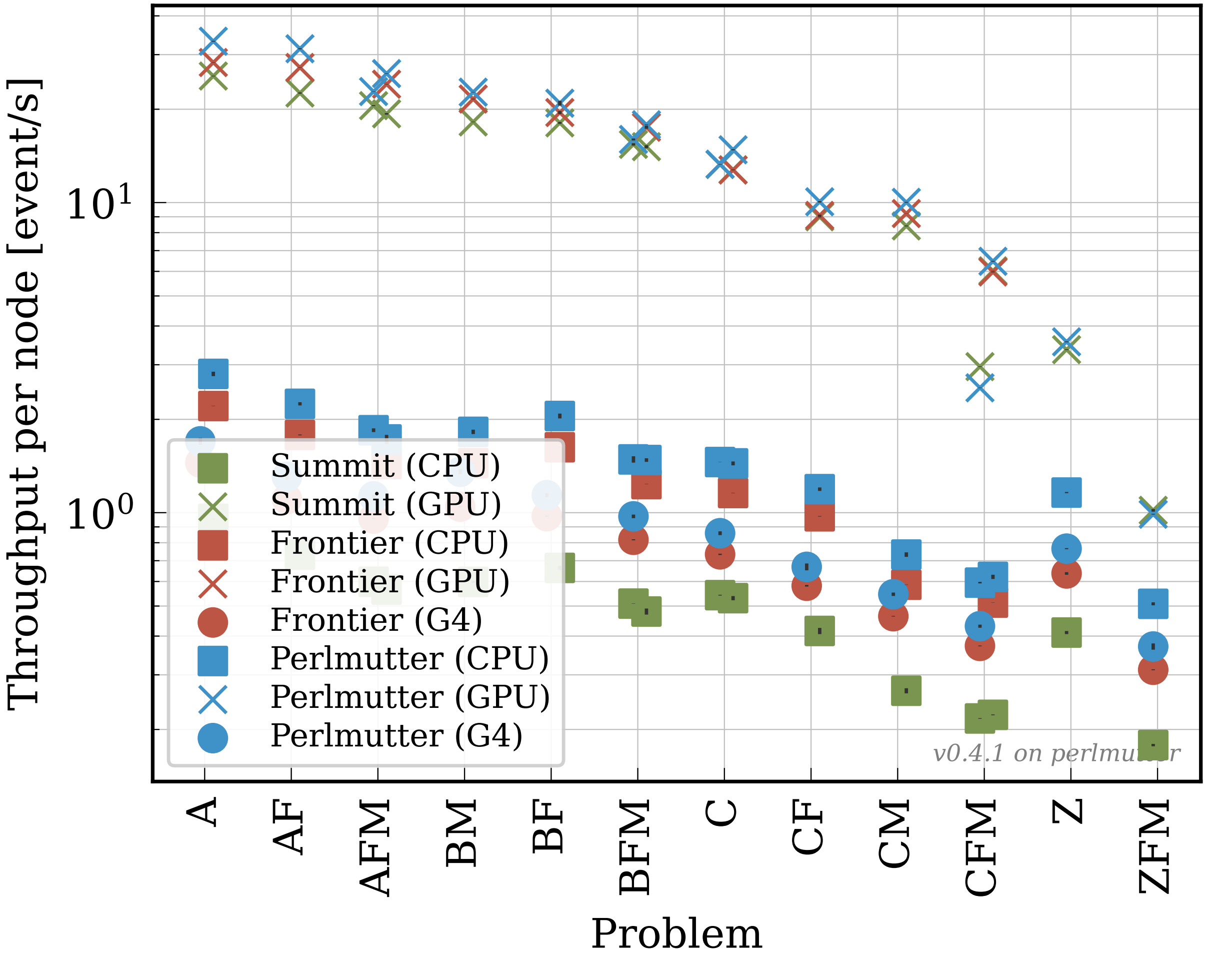


Figure of merit: throughput

- GPUs *cannot* be ignored if present
- AI/ML "revolution" guarantees more coprocessors at all scales

Per-node stats for DOE supercomputers

Machine	Arch	Card	TDP (W)	Cores*	Cards
Summit	CPU	IBM Power9	190	‡22	2
	GPU	Nvidia V100	250	80	6
Perlmutter	CPU	AMD EPYC 7763	280	64	1
	GPU	Nvidia A100	250	108	4
Frontier	CPU	AMD EPYC 7453	225	‡64	1
	GPU	AMD MI250x	500	220	†4



EM only, no SDs

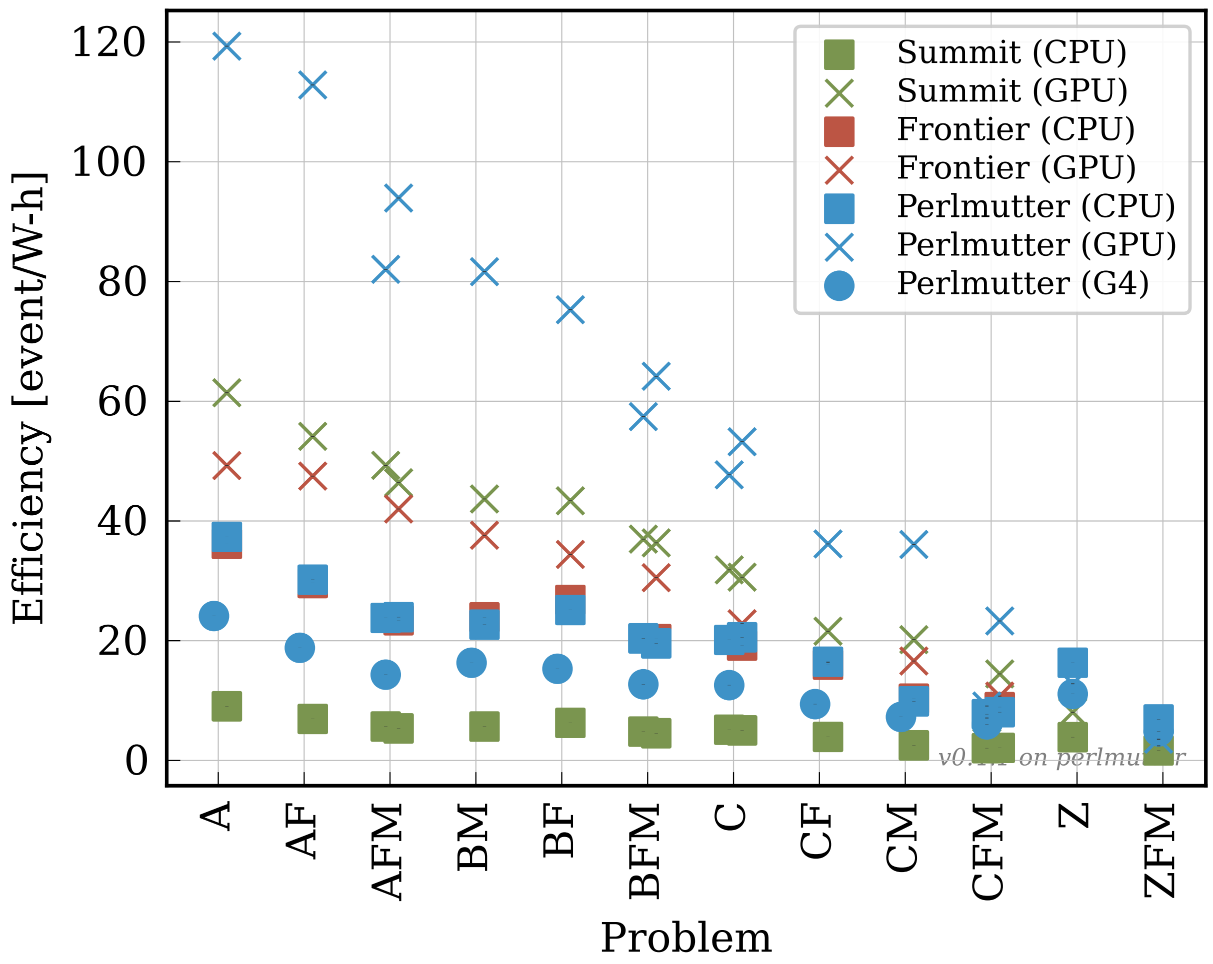
*or SMs;

†Each card has 2 GPUs

‡One core reserved per GPU

Figure of merit: efficiency

- Estimated using reported Thermal Design Power (TDP)* and Celeritas throughput
- GPU consistently shows higher energy efficiency 🌱
  - Reduced operating costs
  - Higher compute density (fewer nodes, smaller data centers)
- A100:EPYC price is ~4× 💸



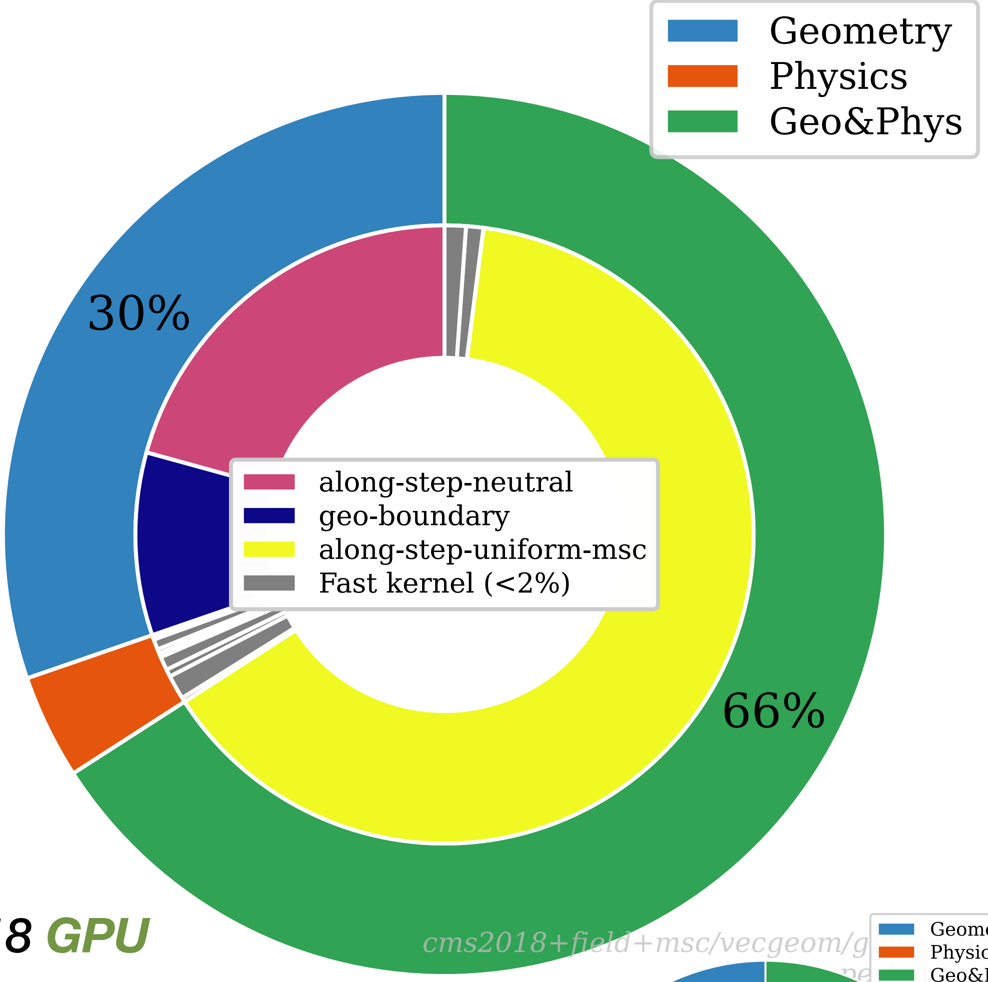
*May be conservative based on nvidia-smi readings

EM only, no SDs

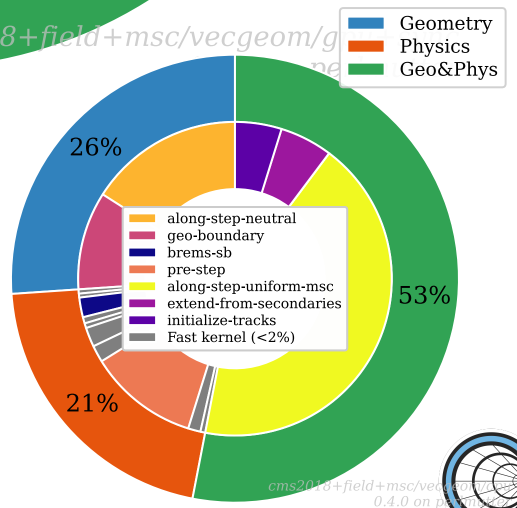
Background
Methods
Results
Conclusions

Ongoing work

- Integration
  - CMSSW
  - Athena (ATLAS) framework
  - ...and more!
- 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

Funding outlook over next 2–3 years

- **Current**
  - 2 FTE* extension for optical physics
  - ¾ FTE through SWIFT-HEP
- **Future** (high probability)
  - 2 FTEs/year from HEP-CCE 2 for 5 years
    - Cross-cutting geometry for HEP
    - Optical photon transport
  - ½ FTE/year SciDAC extension for 3 years
    - Neutron physics
- Future (possibility):
  - 1 FTE for muon physics

- **Previous funding**
  - Primary SciDAC 5 almost expended (3–4 FTE)
    - EM physics and Geant4 integration
    - Performance goals: 2× per watt vs CPU (efficiency), 160× CPU:GPU (capacity)
  - ECP money expended (3–4 FTE)
    - Initial Geant Exascale Pilot work
    - Celeritas prototype
    - LBL/NERSC funding
    - Recent ORANGE work targeting ExaSMR

Increasing support from DOE and interest from experiments

P5 recommendations ($9M) align with further Celeritas development

**Full Time Equivalent (approximately 1 full person-year)*

Future avenues for Geant4/AdePT integration

- Share common dependencies but leave integration to users
- Include offloading as an “example” in Geant4
  - Separate Celeritas example (CPU/HIP/CUDA; VecGeom required)
  - Combined AdePT/Celeritas interface being developed this week (CUDA+VG required)
- Enable as an optional library in Geant4 for installation
  - Add high-level Geant4 offload library for directly exposing AdePT/Celeritas
  - Convenient options for dedicated fast sim or tracking manager

Stronger coupling

Both Celeritas and Geant4 benefit from increased collaboration

Conclusion: 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)
- Hayden Hollenbeck (@hhollenb)
- Seth R Johnson (@sethrj)
- Soon Yung Jun (@whokion)
- Guilherme Lima (@mrguilima)
- Amanda Lund (@amandalund)
- Ben Morgan (@drbenmorgan)
- Stefano C Tognini (@stognini)

Past code contributors:

- Doaa Deeb (@DoaaDeeb)
- Vincent R Pascuzzi (@vrpascuzzi)
- Paul Romano (@paulromano)

OLCF: This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

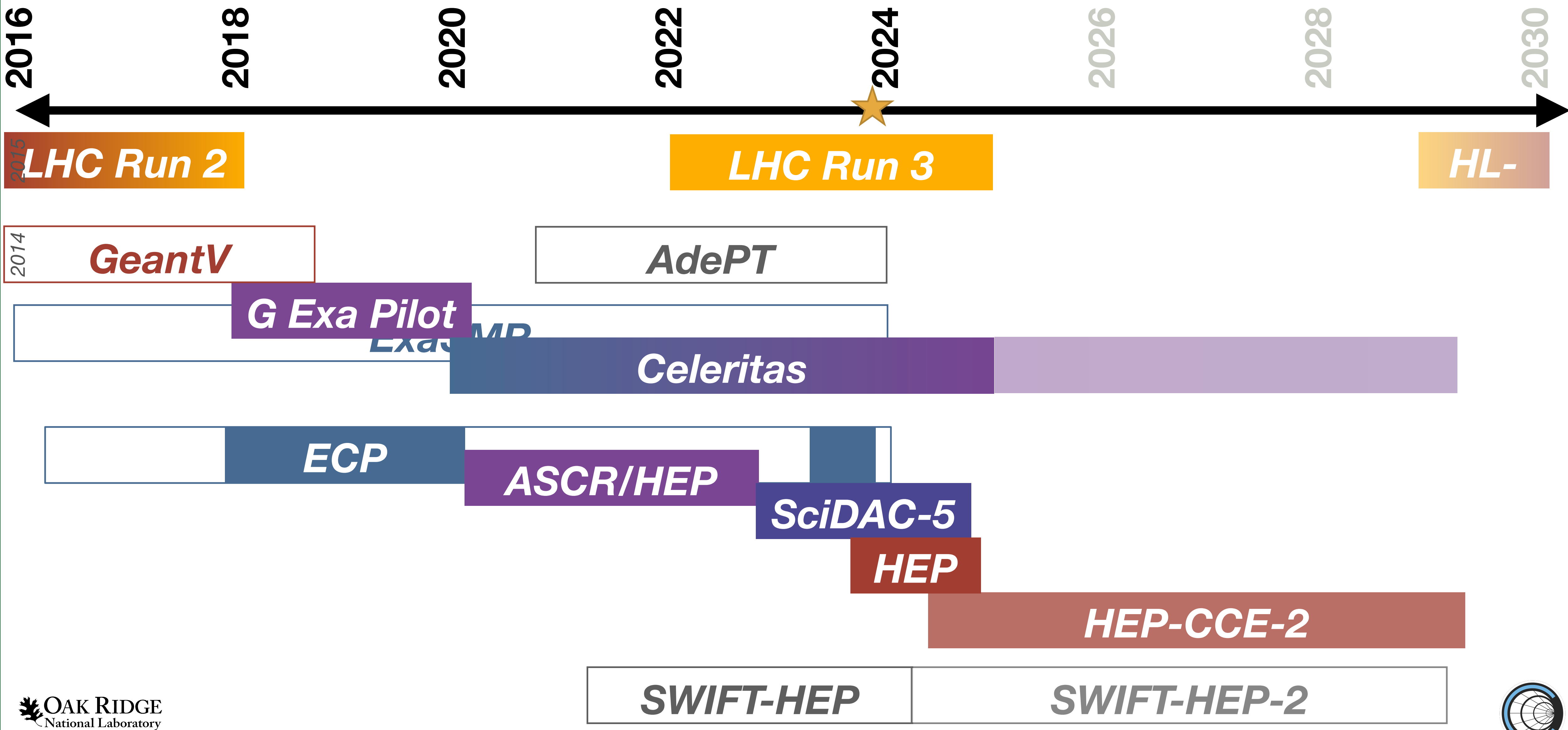
SciDAC: This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research and Office of High Energy Physics, Scientific Discovery through Advanced Computing (SciDAC) program.

NERSC: This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award HEP-ERCAP-0023868.

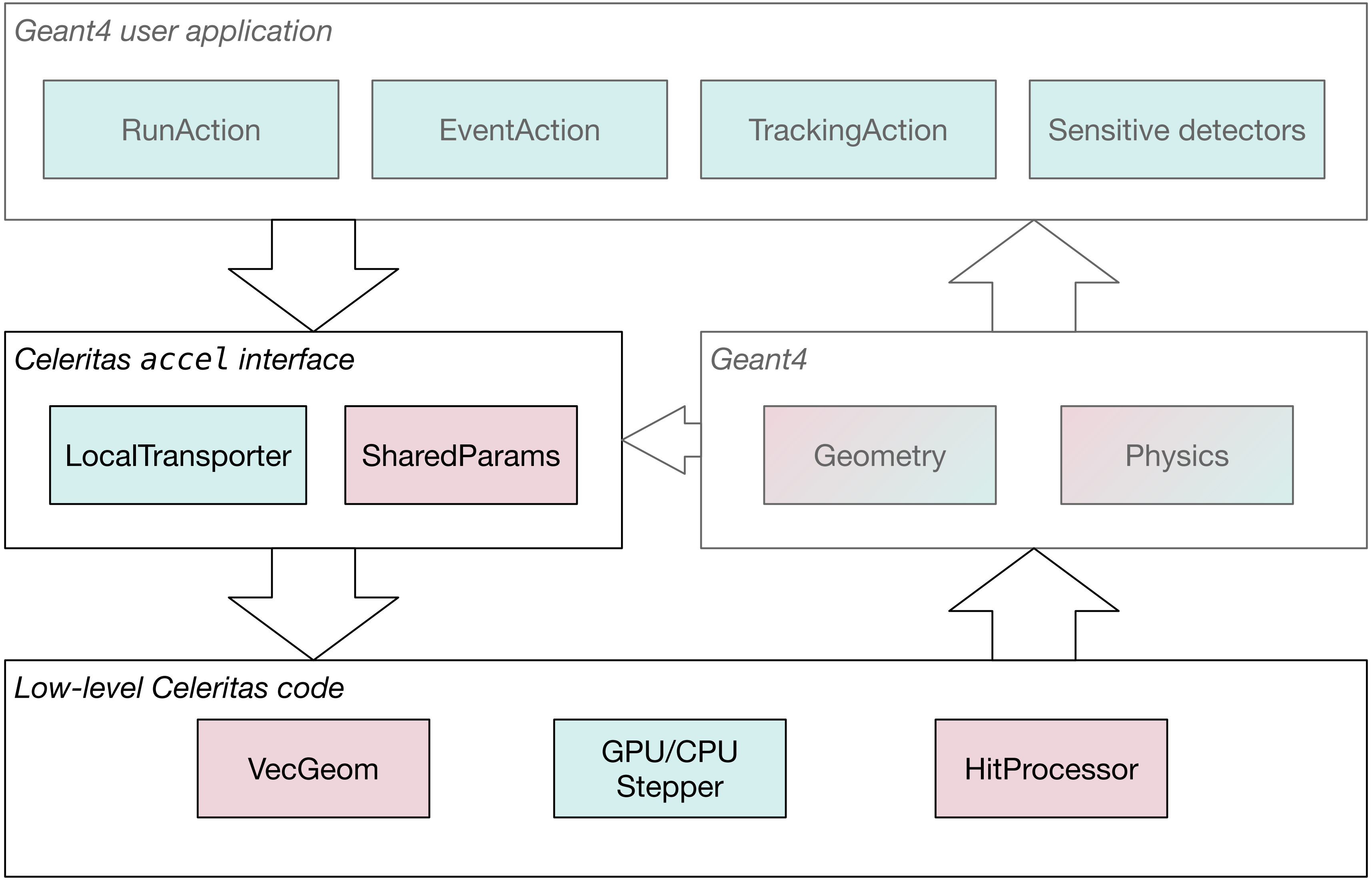
https://github.com/celeritas-project/celeritas

Backup slides

Historical context



Geant4 interface library

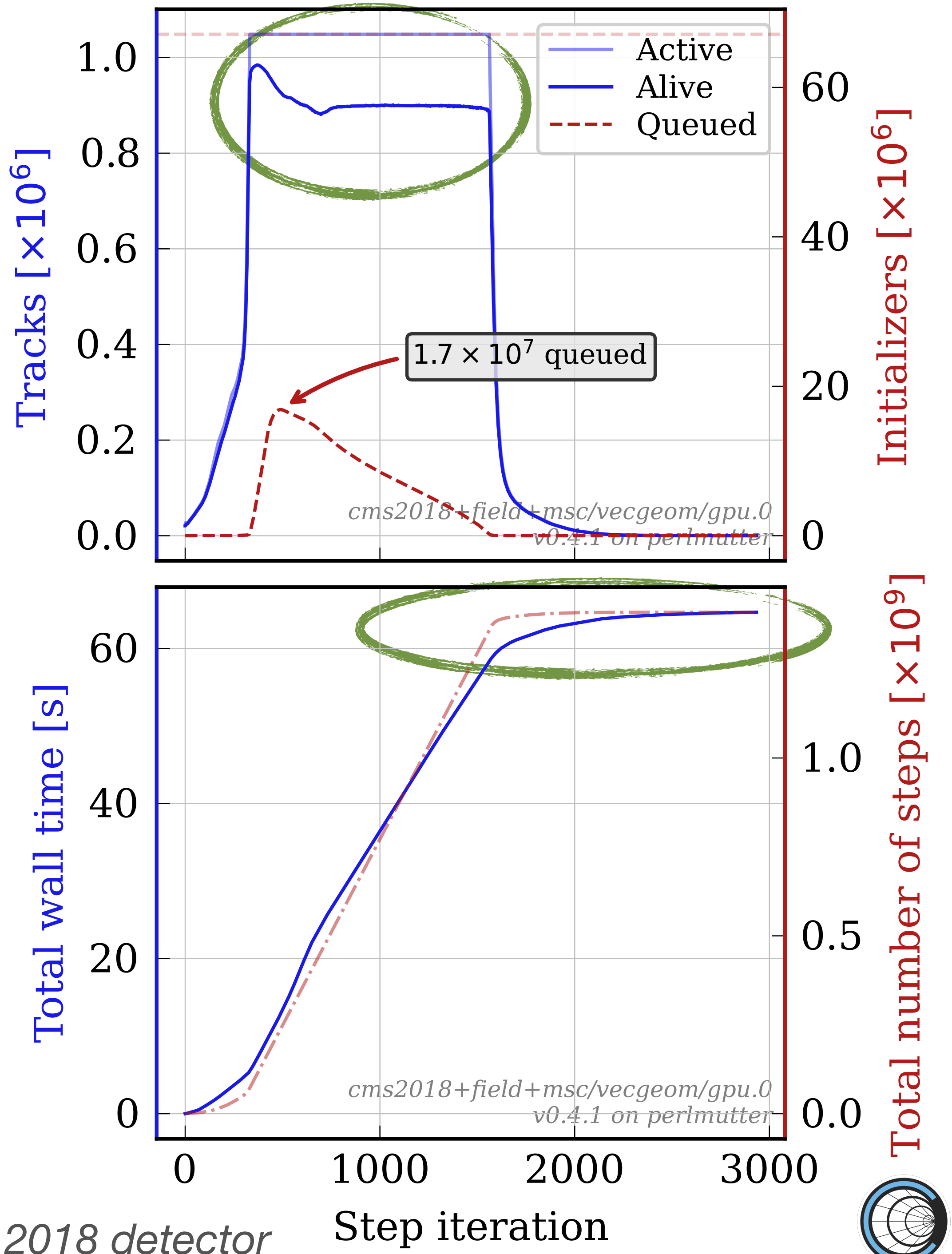


Thread-local
Shared

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

Step-dependent behavior

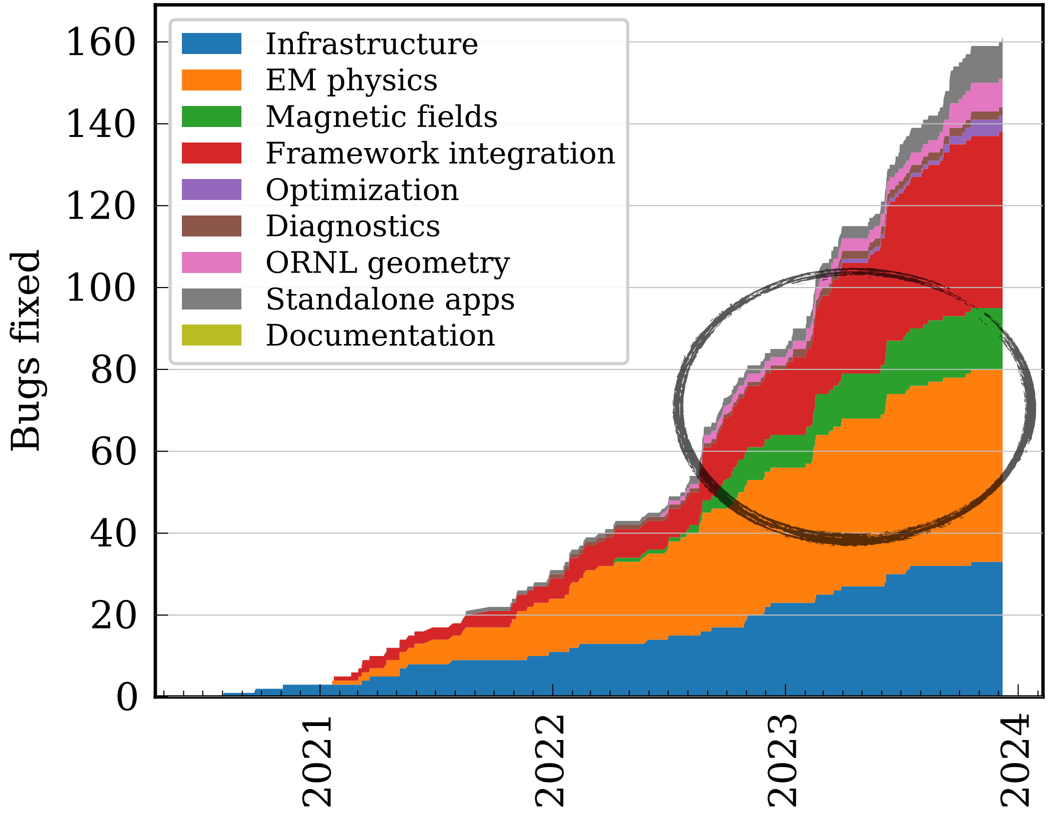
- Number of active particle tracks changes drastically due to EM shower
- Saturated GPU takes the most time but <50% of step iterations
  Despite using masking instead of sorting!
- Converting the tail of long-lived tracks does *not* kill us



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

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*