Oak Ridge National Laboratory

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Full-featured Geant4 GPU acceleration using Celeritas

Seth R Johnson

Celeritas code lead

CELERITAS

Celeritas core team:

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U.S. DEPARTMENT OF ENERGY

SWIFT-HEP meeting
21 November, 2023

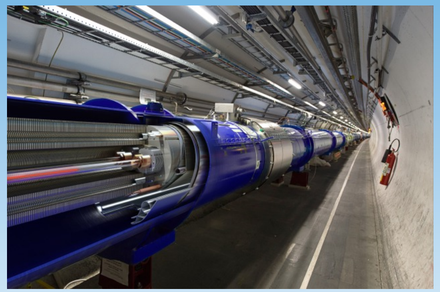
Background

Results

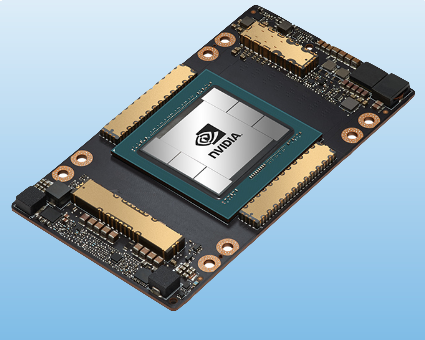
Conclusions

Project overview

- **GPU**-focused implementation of **HEP** Monte Carlo detector simulation
  - **Computing demand:** LHC-HL upgrade
  - **Computing supply:** Paradigm shift in HPC hardware
- Motivated by HL-LHC computational challenges *and* by recent success in GPU MC
  (*Exascale Computing Project [ECP] ExaSMR*)
- **Goal: accelerate production use for LHC Run 4**

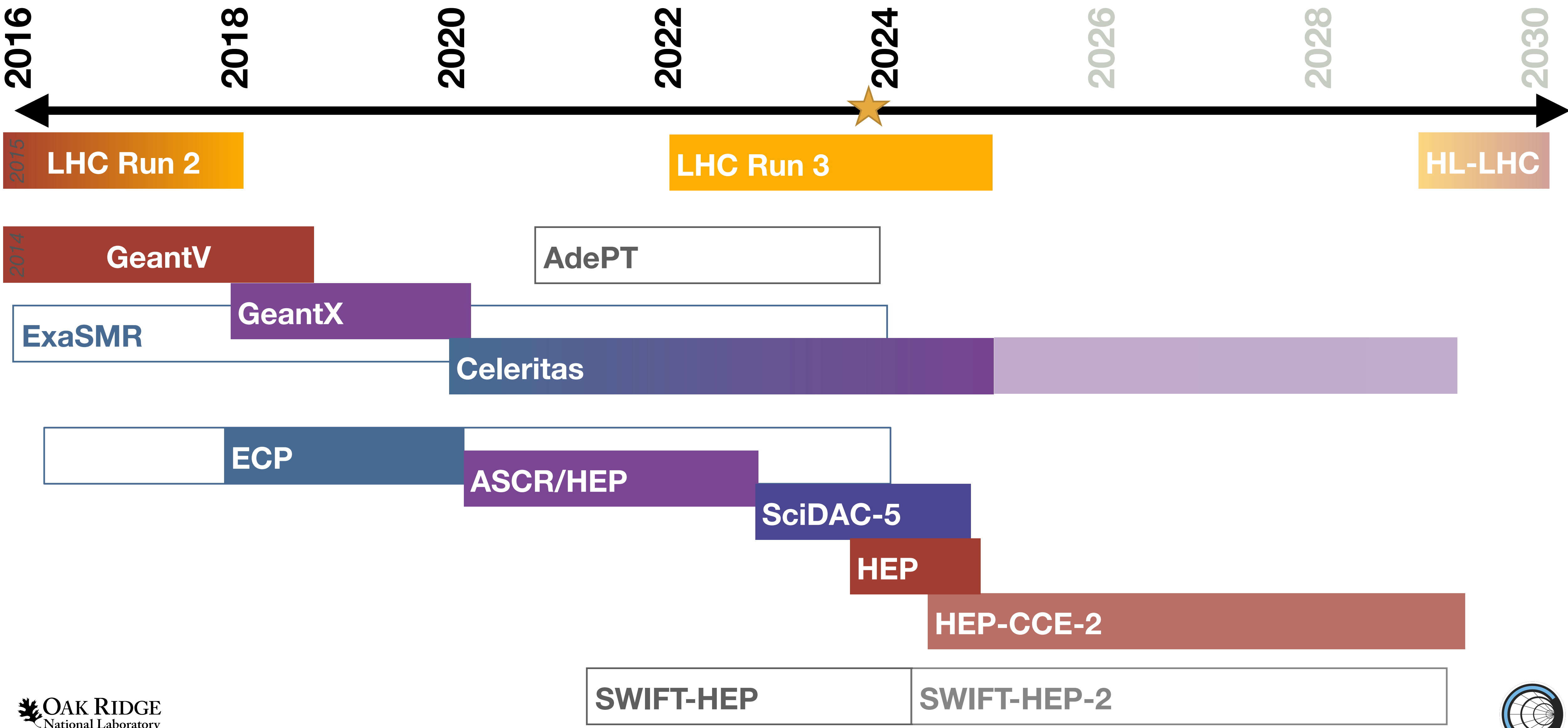


LHC beamline ©CERN



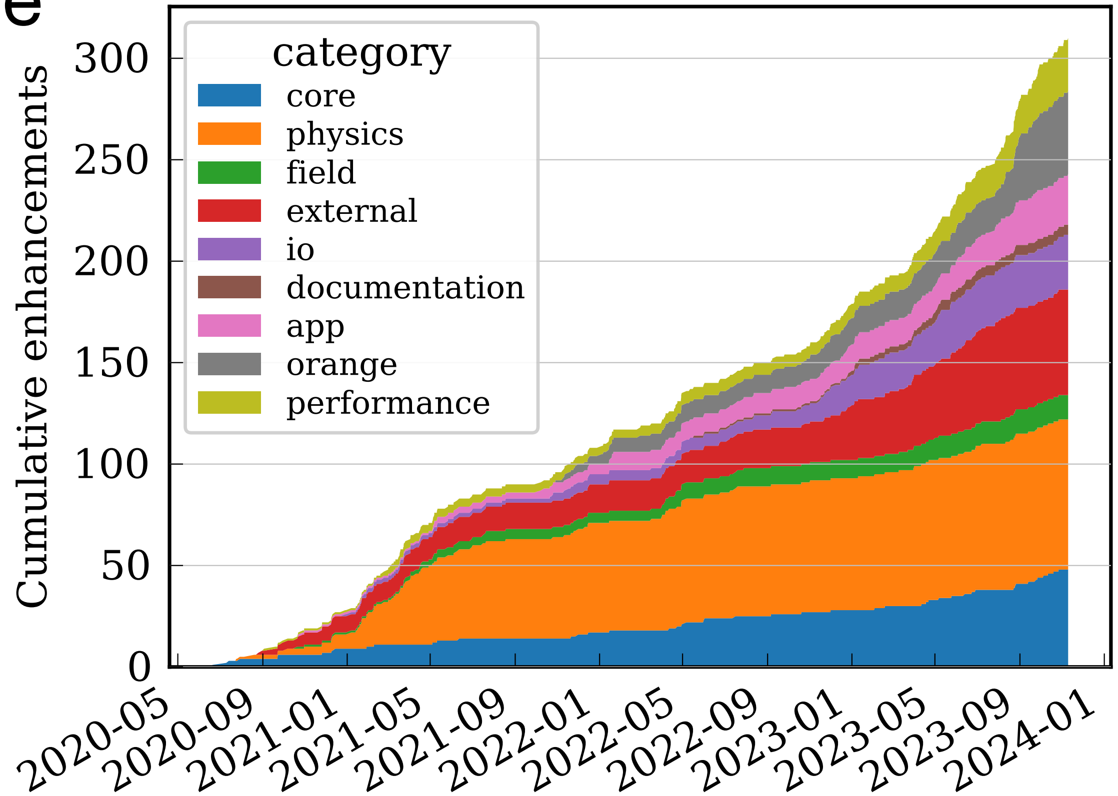
Nvidia A100 GPU (Nvidia)

Historical context



Code history and status

- 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
  - User-extensible physics, particles, detectors, …
  - Code reviews, CI, Doxygen, Sphinx, ...
- Physics is only a part of the work
- Recent focus: Geant4 integration and performance optimizaton



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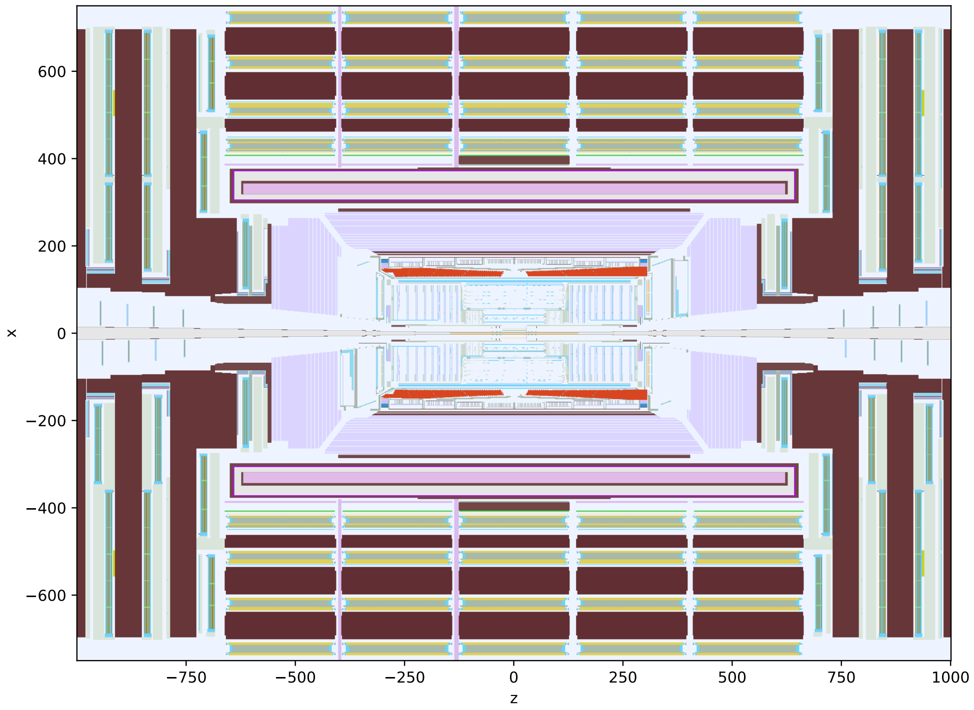
High-level capabilities

- 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

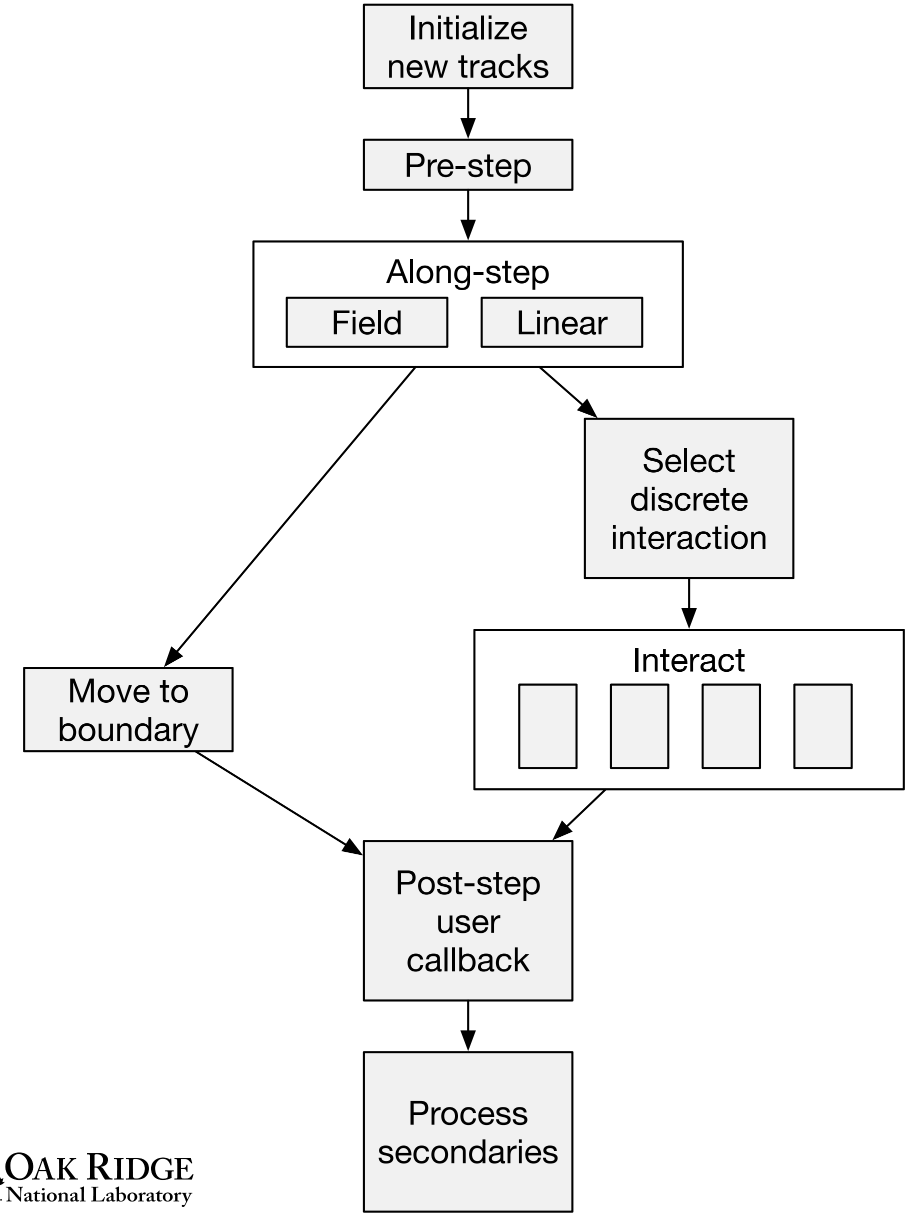


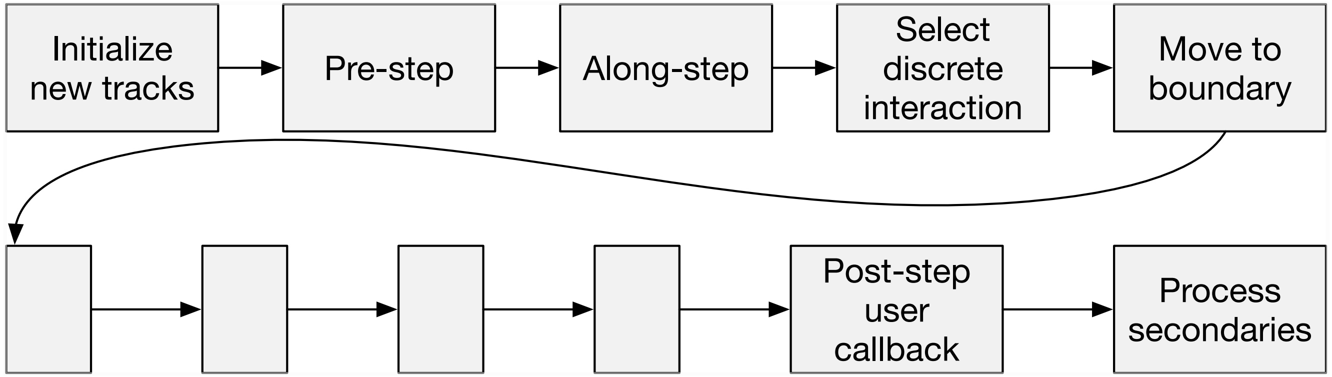
GPU-traced rasterization of CMS 2018

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

Source: Johnson, S.R. Geant4 Meeting 2023

Stepping loop on a GPU





Topological sort: a loop over kernels

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

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Source: Johnson, S.R. Geant4 Meeting 2023

Celeritas version `0.4`: Geant4 integration status

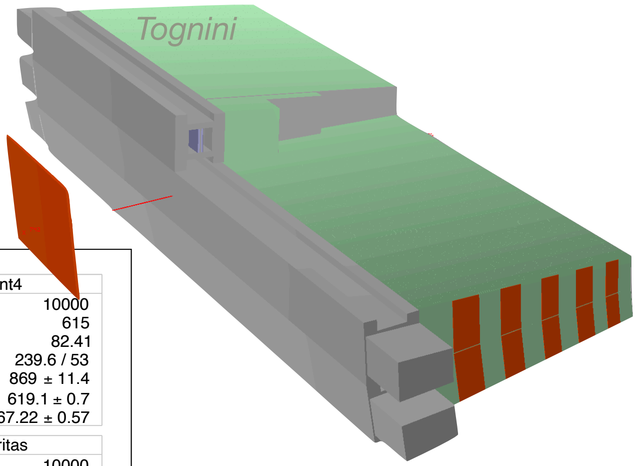
- **Imports** EM physics selection, cross sections, parameters
- **Converts** geometry to VecGeom model
- **Offloads** EM tracks from Geant4
- **Scores** hits to user "sensitive detectors"
  (Copies from GPU to CPU; reconstructs `G4Hit`, `G4Step`, `G4Track`; calls `Hit`)
- **Builds** against Geant4 10.5–11.1

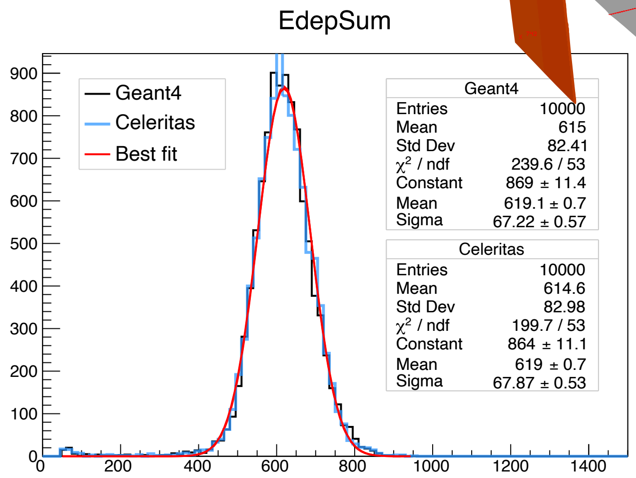
*Celeritas has **production quality** interfaces to simplify user application integration*

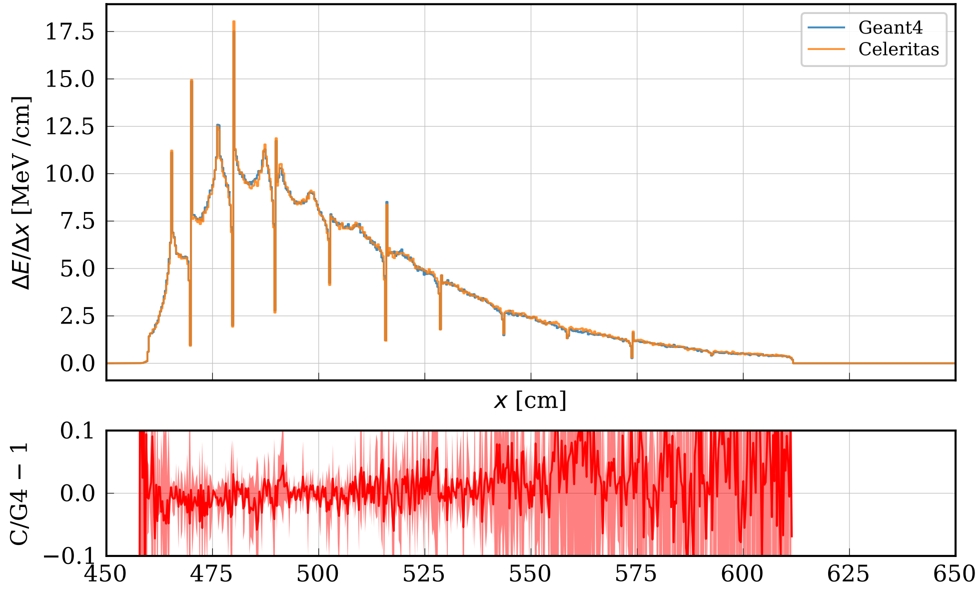
Source: Johnson, S.R. Geant4 Meeting 2023

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`
- Excellent 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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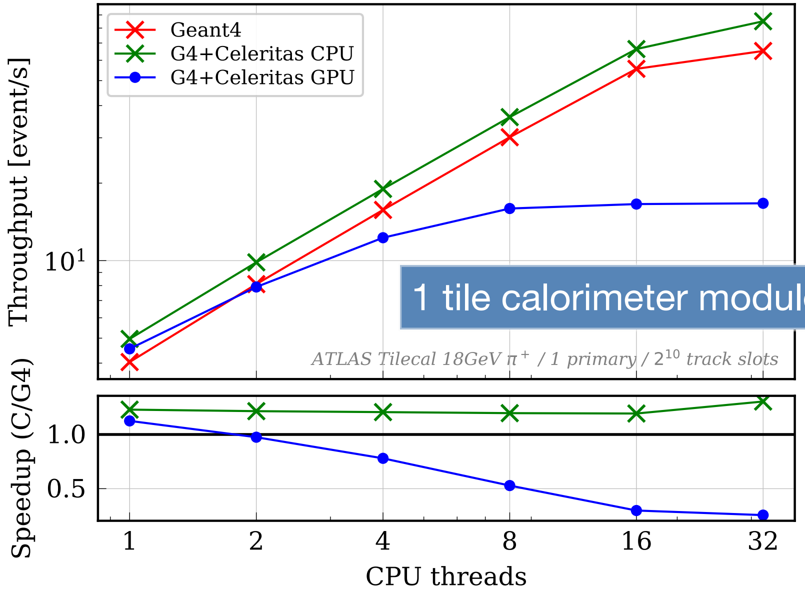
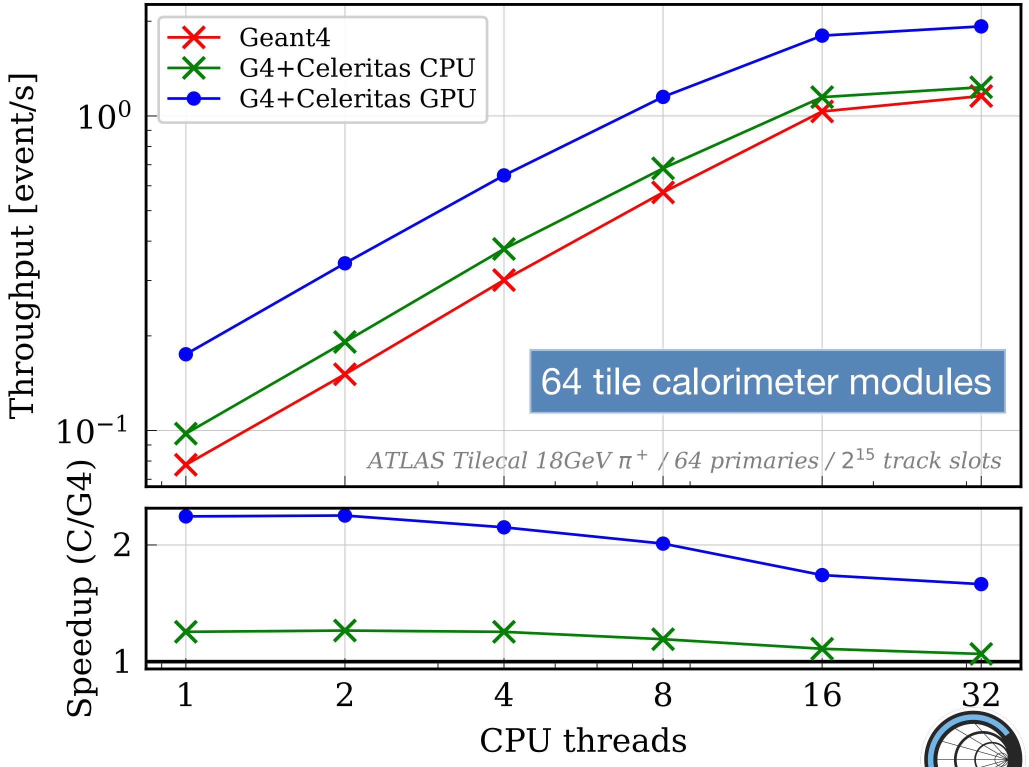
Offload performance results

- 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 *(2048 π^+ in all cases)*
- GPU speedup: **1.7–1.9×** at full occupancy
  Using all CPU cores with a single GPU
- CPU-only speedup: still **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

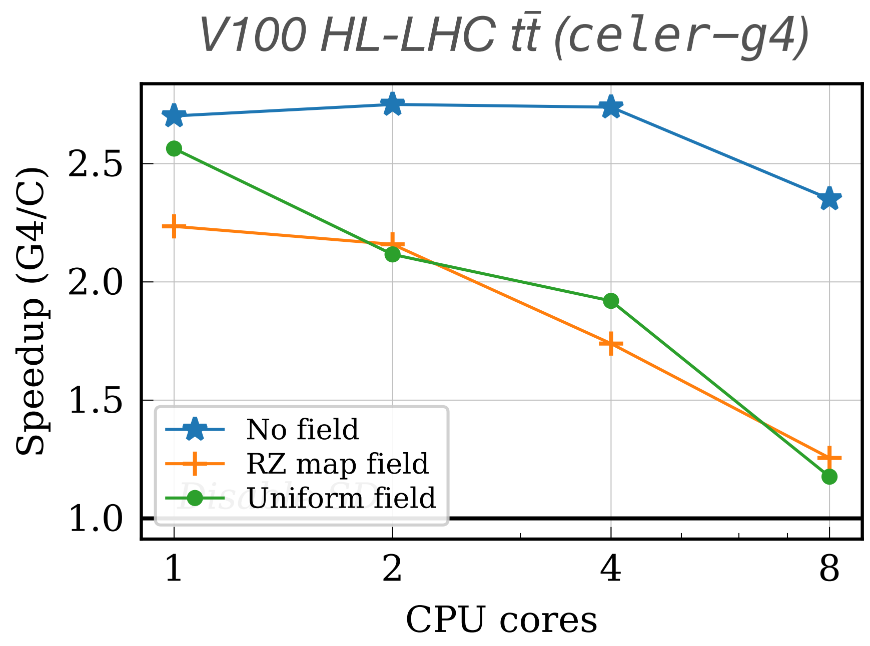


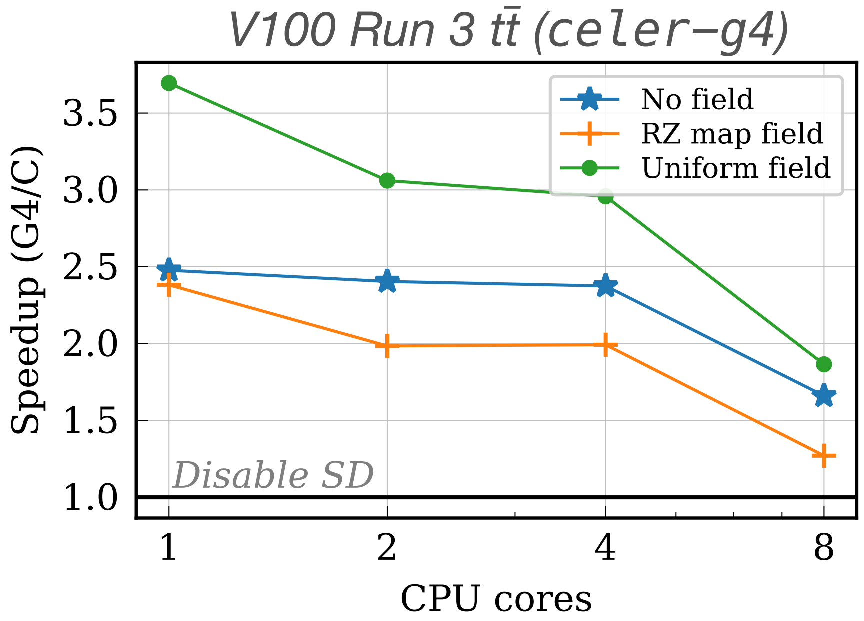


Source: Johnson, S.R. Geant4 Meeting 2023

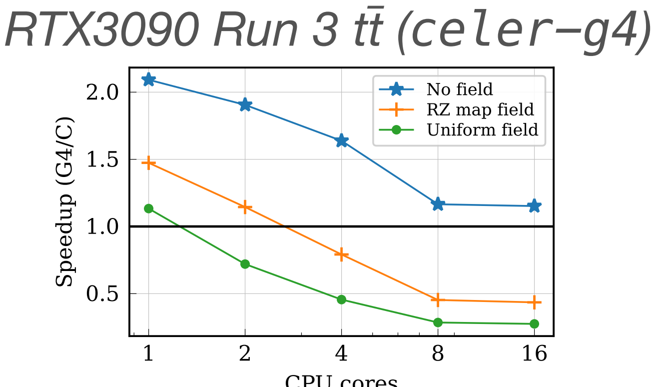
CMS performance results

- Initial CMSSW integration “works”
  - ~500 lines to integrate
  - Performance isn’t comparable due to different physics
- Standalone Geant4 app
  - FTFP_BERT, discretized+interpolated RZ magnetic field
  - Without Celeritas, 8× slower than CMSSW
- Promising results
  - SD reconstruction is <15% of runtime
  - Initial comparison of hits shows good agreement
  - Possibly over factor of 2 speedup in production
- Plenty to investigate
  - Magnetic field driver
  - Single-precision





Hardware: Intel Xeon Gold 6152 CPU 22c 2.10GHz
+ NVIDIA Tesla V100 SXM2 w/32GB HBM2
Input: 8 tt̄ events @ 14 TeV from LHC pp collision



Hardware: Intel Xeon i9-10900K CPU 20c 3.70GHz
+ NVIDIA Tesla RTX3090 w/32GB HBM2
Input: 8 tt̄ events @ 14 TeV from LHC pp collision

Standalone EM performance

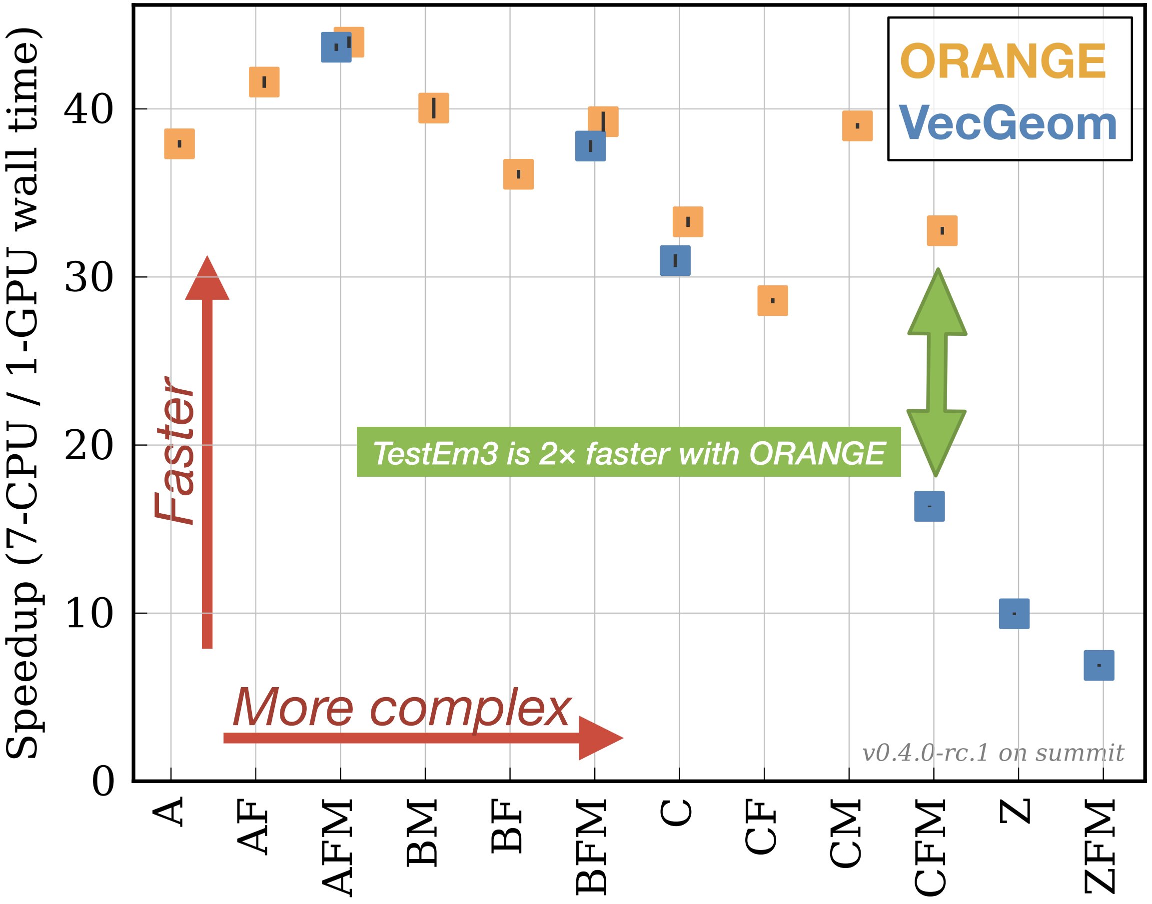
	Problem definition
A	testem15
B	simple-cms
C	testem3
Z	cms2018

	Modifier
F	+field
M	+msc

- 1300 × 10 GeV e-, 7 events
- ⅙ Summit node

  1 × Nvidia V100 GPU, 7 × IBM Power9 CPUs
- Celeritas GPU vs CPU

  CUDA (1 CPU thread) vs OpenMP (7 CPU threads)
- "Speed of light": **7–44×**



Multiply speedup by 7× for CPU:GPU equivalence

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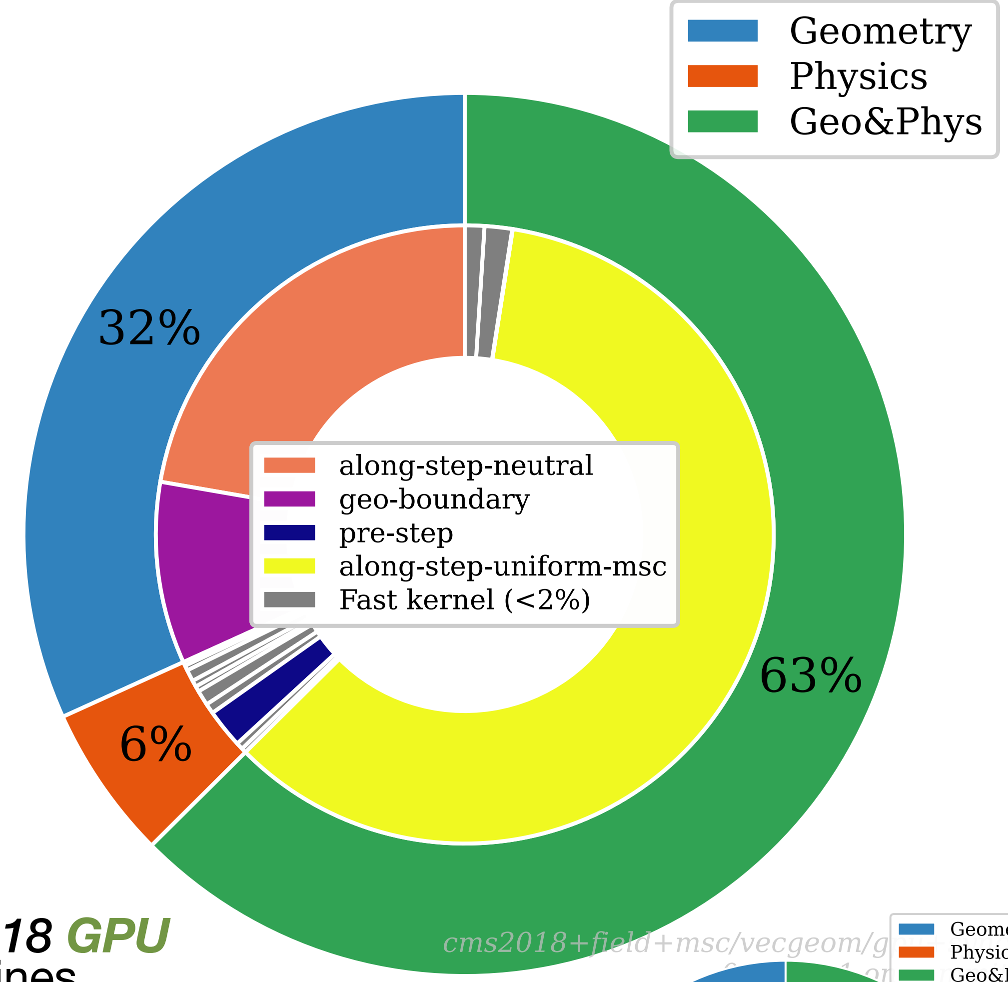
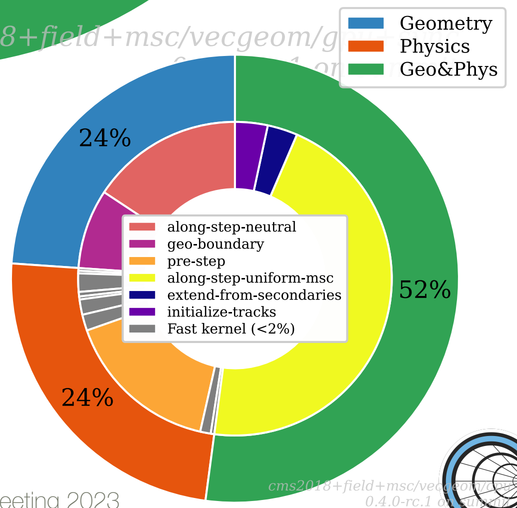
Ongoing work

- Integration
  - CMSSW
  - Athena (ATLAS) framework
- Verification & validation
  - EM test problems
  - CMSSW workflow
  - Benchmark problems with AdePT team
- Optimization and geometry
  - **95%** of standalone runtime in CMS2018 is in geometry routines
  - Performance tuning “knobs” have vast and mostly unexplored parameter space
  - GPU native sensitive detectors
  - ORANGE navigation



CMS2018 GPU



CMS2018 CPU

Source: Johnson, S.R. Geant4 Meeting 2023

Future work

- Optimize magnetic field propagation and geometry
- Validate for use in frameworks (CPU or GPU)
- Evaluate performance on commodity graphics cards
- Implement optical physics for other HEP experiments

Goals for Celeritas GPU EM-only performance
2× per watt vs CPU *(efficiency)*
160× CPU:GPU *(capacity)*

Summary

- Proven real-world performance for GPU EM physics **and** ease of integration for client codes
  - Comparisons with 1 GPU, multicore CPU, against pure Geant4
  - Calorimeter test beam net improvement: **10–30% faster** on CPU, **1.8–2.2×** on GPU (Nvidia A100)
  - CMS Run 3 configuration standalone simulation speedup: **12–87% faster** on GPU (Nvidia V100)
- Anticipated performance even higher
  - Standalone EM problems: **~7–34× faster** (Celeritas CPU vs GPU) on Summit (Nvidia V100) (49–238× GPU/CPU core equivalence)
  - ORANGE vs current VecGeom for TestEM3: **85% faster**

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

Acknowledgments

Celeritas v0.4 code contributors:

- Elliott Biondo (@elliottbiondo)
- Philippe Canal (@pcanal)
- Julien Esseiva (@esseivaju)
- Tom Evans (@tmdelellis)
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- Seth R Johnson (@sethrj)
- Soon Yung Jun (@whokion)
- Guilherme Lima (@mrguilima)
- Amanda Lund (@amandalund)
- Ben Morgan (@drbenmorgan)
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- Paul Romano (@paulromano)

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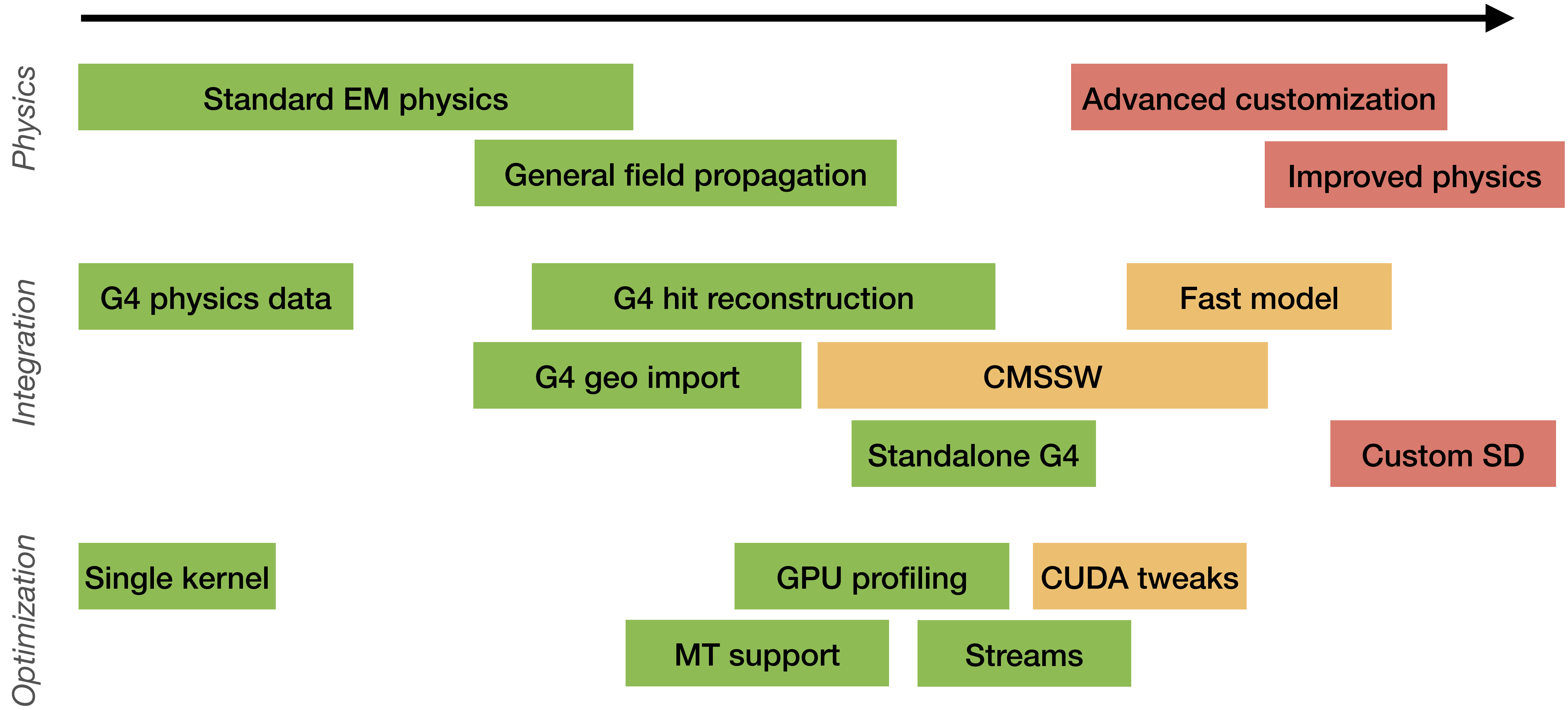
Backup slides

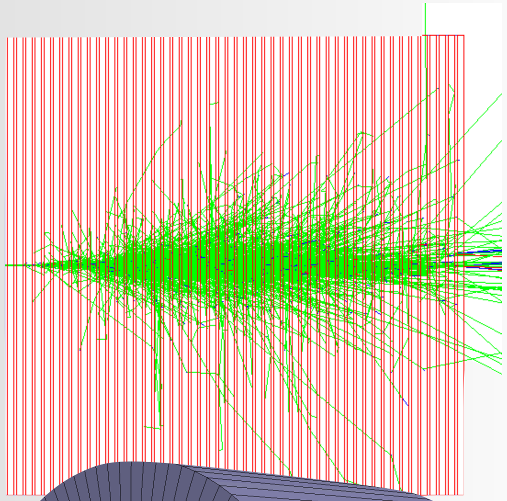
Qualitative timeline

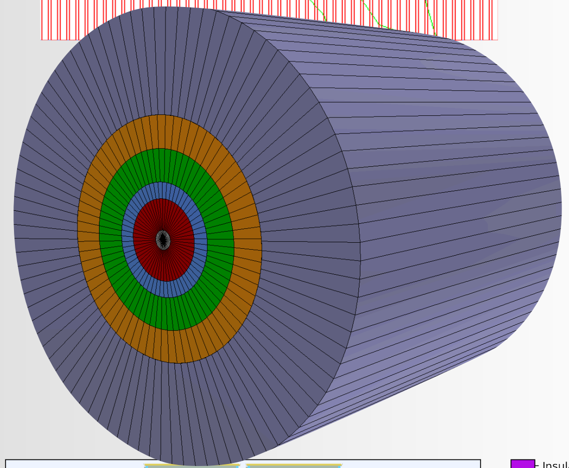


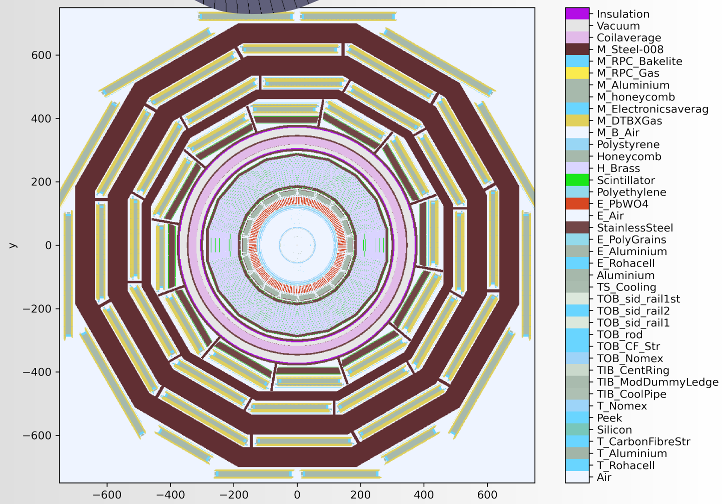
Regression/timing suite

- Run on single node of Summit at full capacity
  - 6 separate runs simultaneously (different seed for each)
  - Each run: 7 CPU (OpenMP) vs. 1 GPU (+1 CPU)
  - Demonstrate performance “loss” by neglecting GPU resources
- 1300 × 10 GeV e^- per event, 7 events per run
- Preliminary set of problem definitions

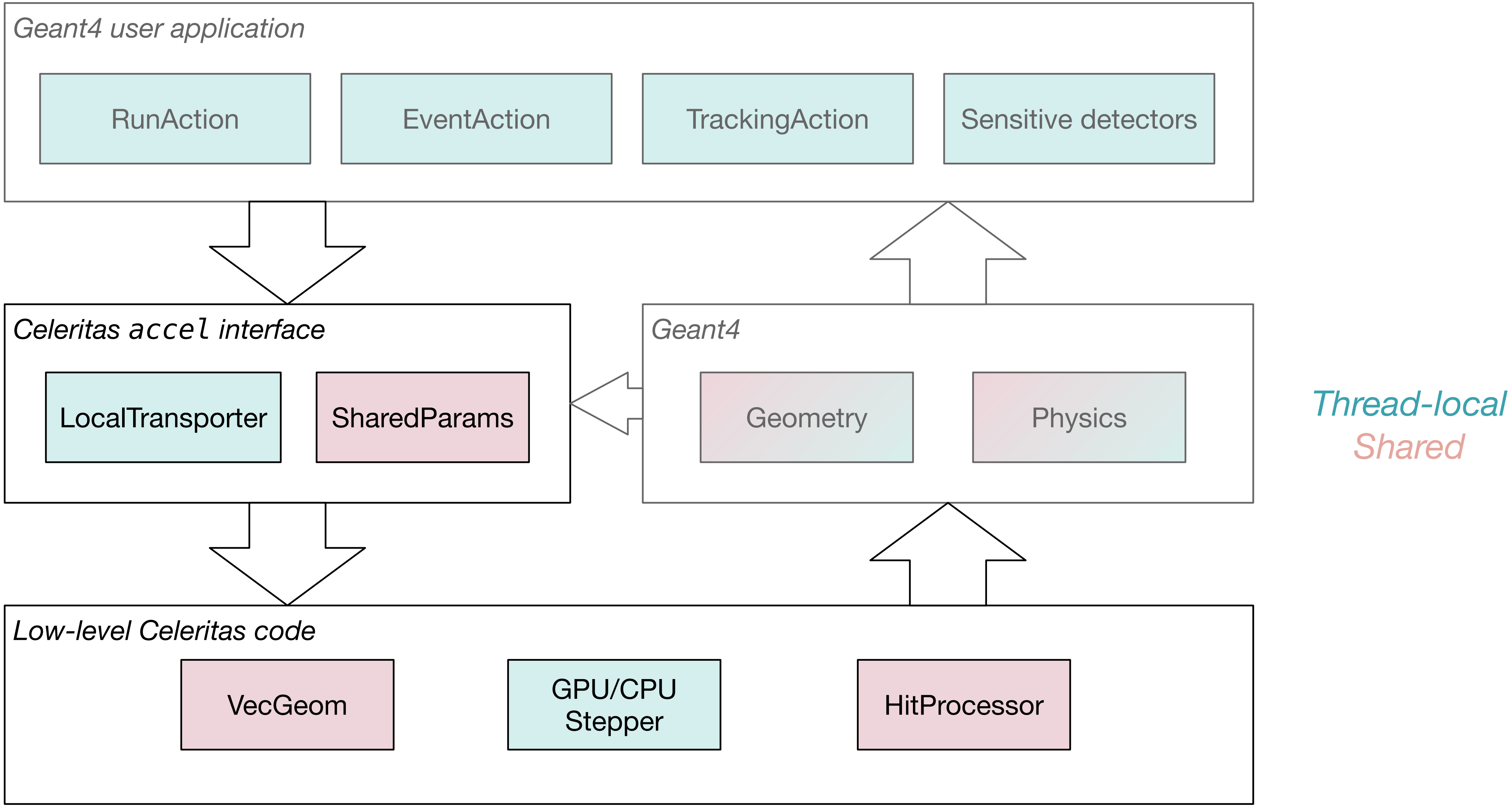
  (working with AdePT team to develop)
- Initial optimizations
- Initial results are apples-to-apples







Geant4 interface library



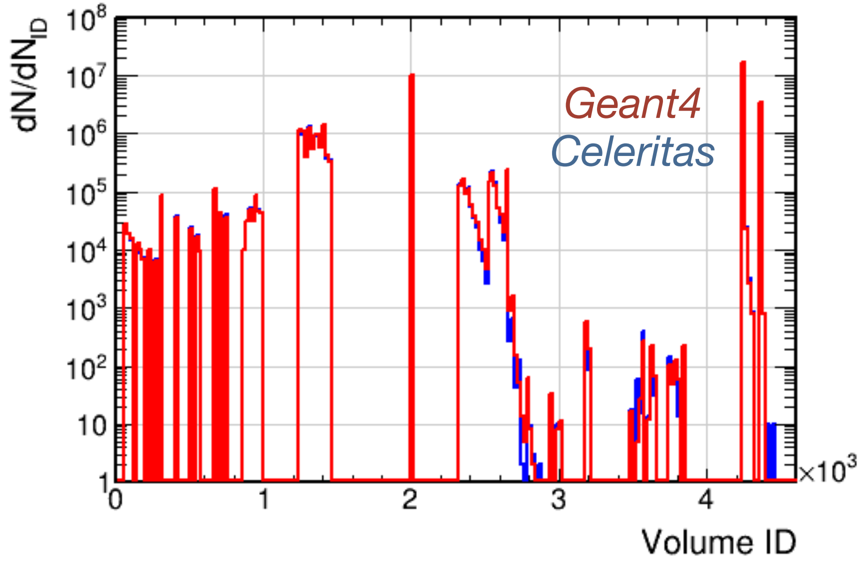
https://celeritas-project.github.io/celeritas/user/index.html

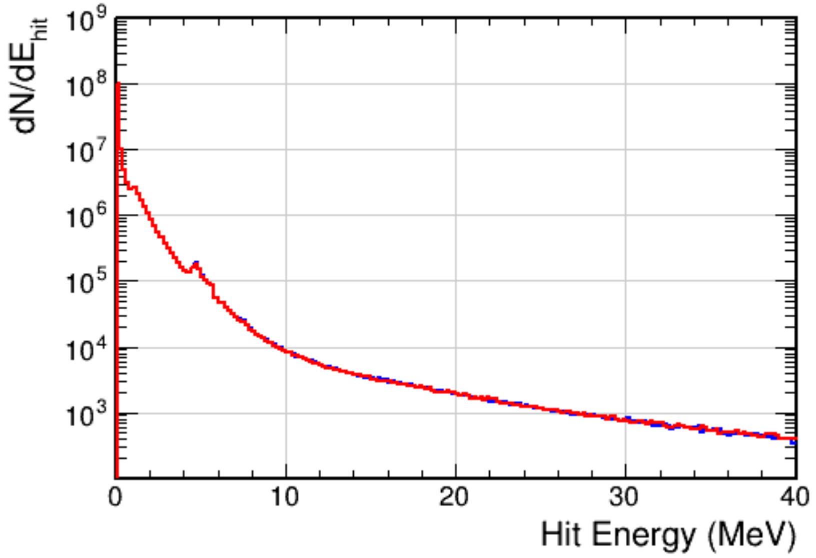
Johnson, Seth R. "Celeritas v0.2: Offloading EM tracks to GPU from Geant4," 21 Feb 2023.

Initial CMSSW integration

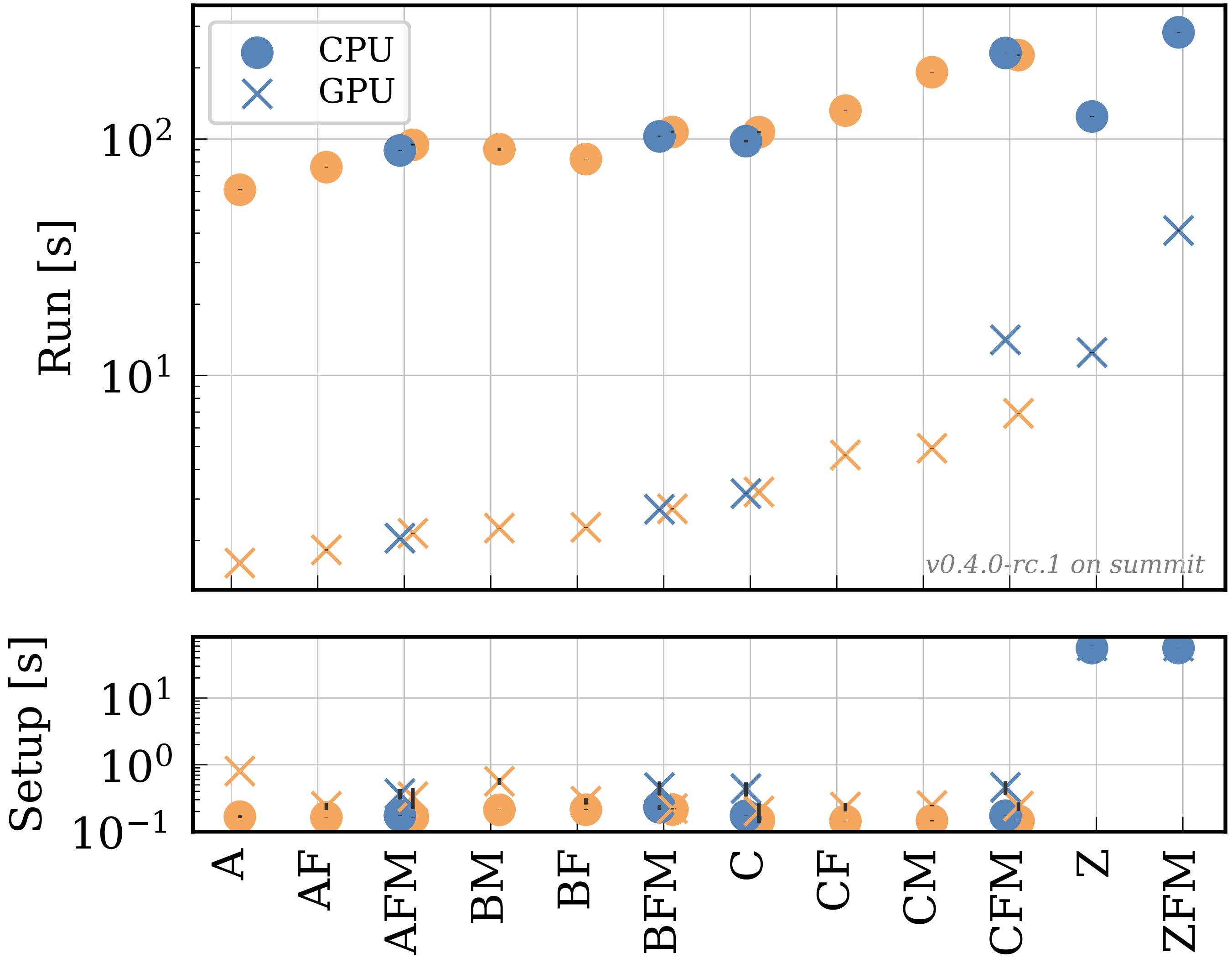
- ~500 lines of code to integrate
  - Offload e^-, e^+, γ to Celeritas
  - R–Z field map preprocessed for Celeritas
  - Celeritas reconstructs hits and sends to CMSSW SDs
  - No support for MC truth or track-level granularity
  - CMSSW has numerous fine-grained tweaks to physics/ propagation compared to default EM
- Initial “fair” performance comparison
  - Current approach: export CMS geometry and detectors to GDML, run through standalone Geant4+Celeritas app
  - 8 CPU+1 GPU standalone simulation: **17–87% faster**
  - **Theoretical** max speedup in framework: 230%

($t\bar{t}$ events, CMS Run3 geometry, tuned physics, full fidelity magnetic field)





Regression problem run time



ORANGE
VecGeom

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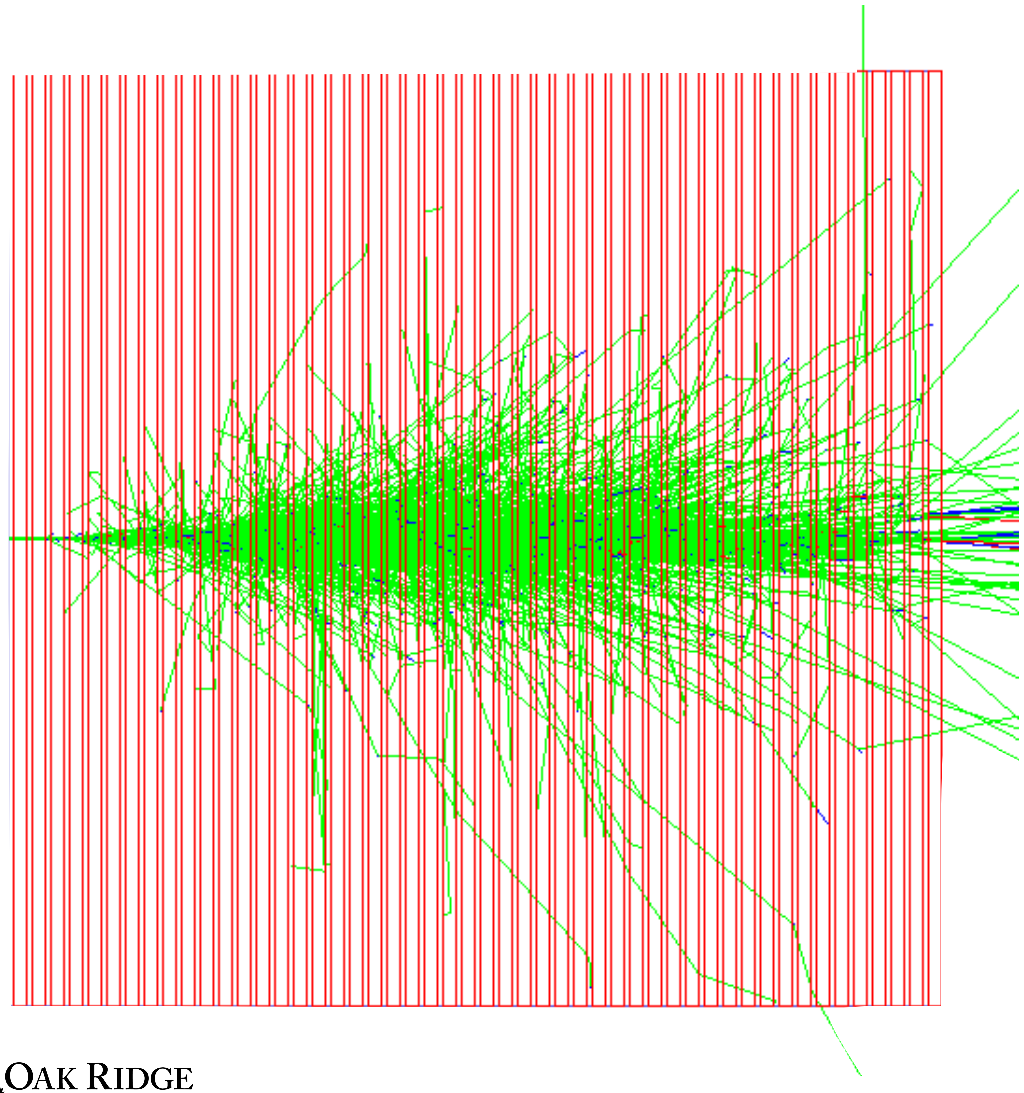
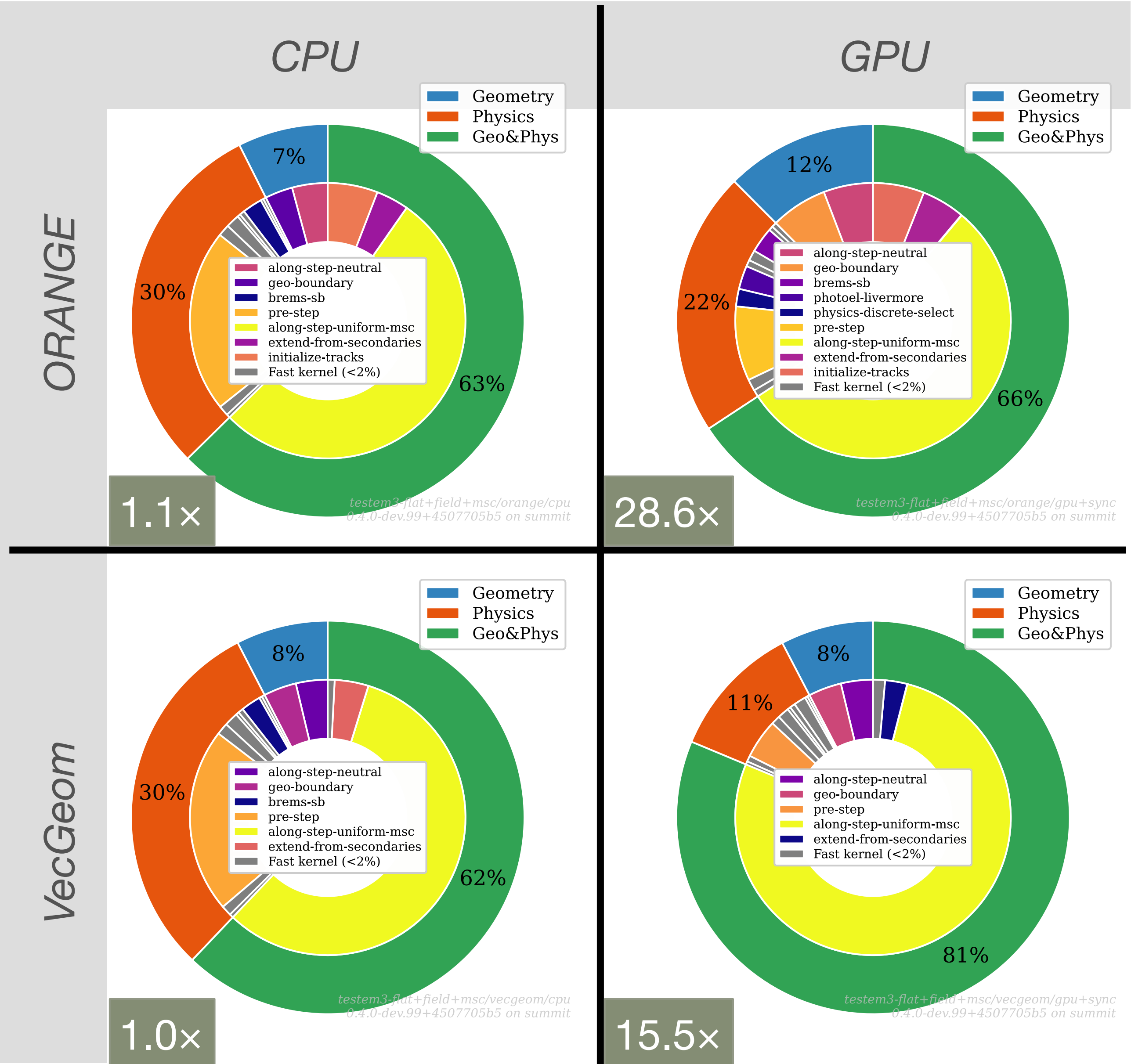
TestEM3 performance





Stargazing

- Interest in GPU HEP is growing!