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Celeritas v0.3: EM offloading for Geant4

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Celeritas code lead

CELERITAS

Celeritas core team:

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Celeritas core advisors:

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U.S. DEPARTMENT OF ENERGY

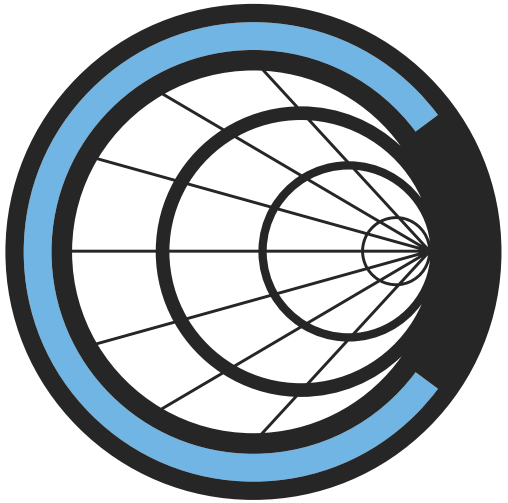
Geant4 Collaboration Meeting
28 September, 2023

Background

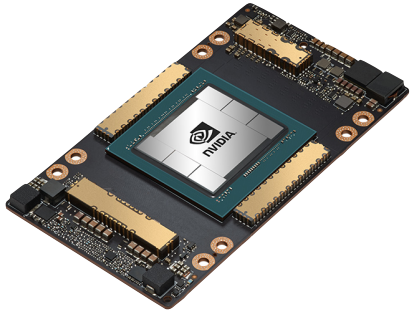
Results

Conclusions

Project overview



- **GPU**-focused implementation of experiment-agnostic **HEP** Monte Carlo detector simulation
- 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**

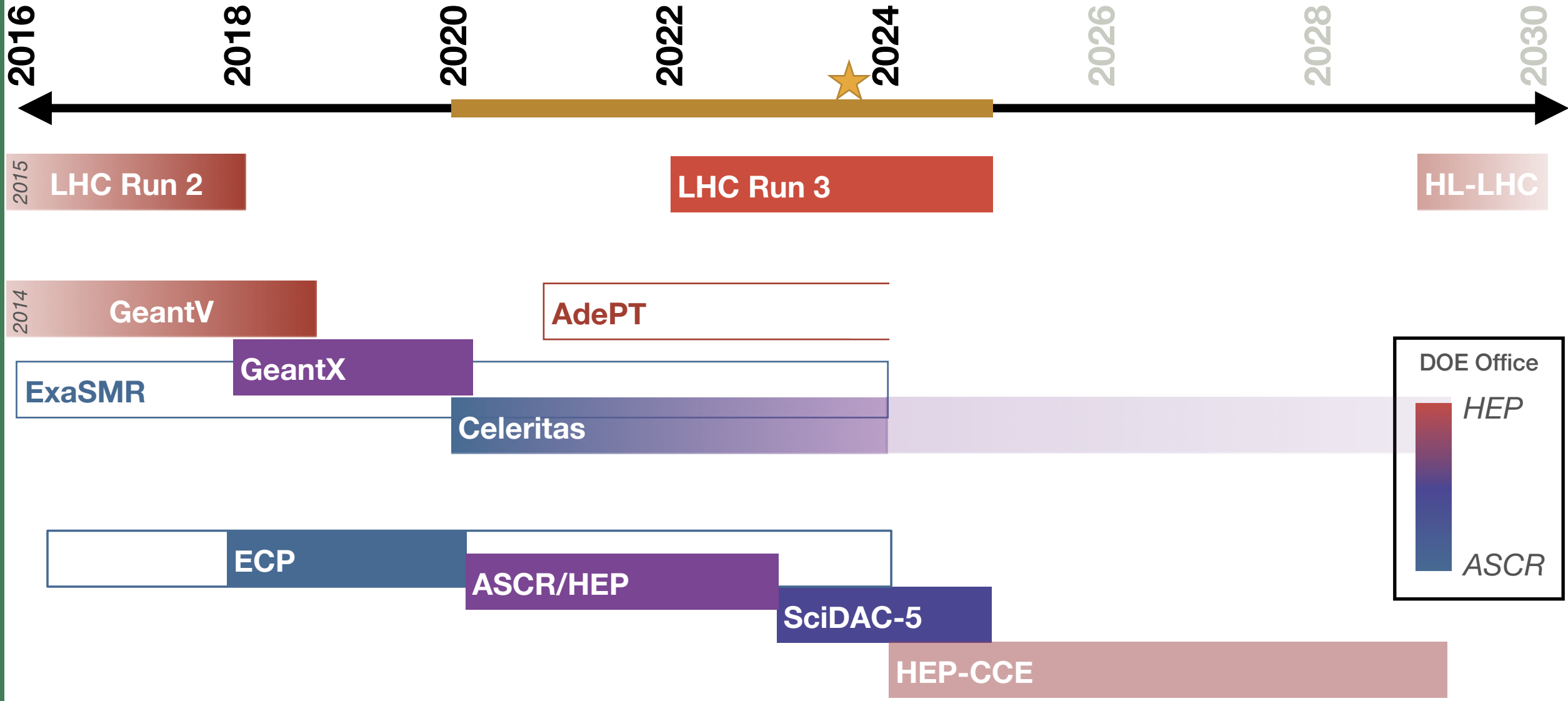


Nvidia A100 GPU (Nvidia)




Source: Johnson, S.R. CHEP 2023

Historical context



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Source: Johnson, S.R. CHEP 2023

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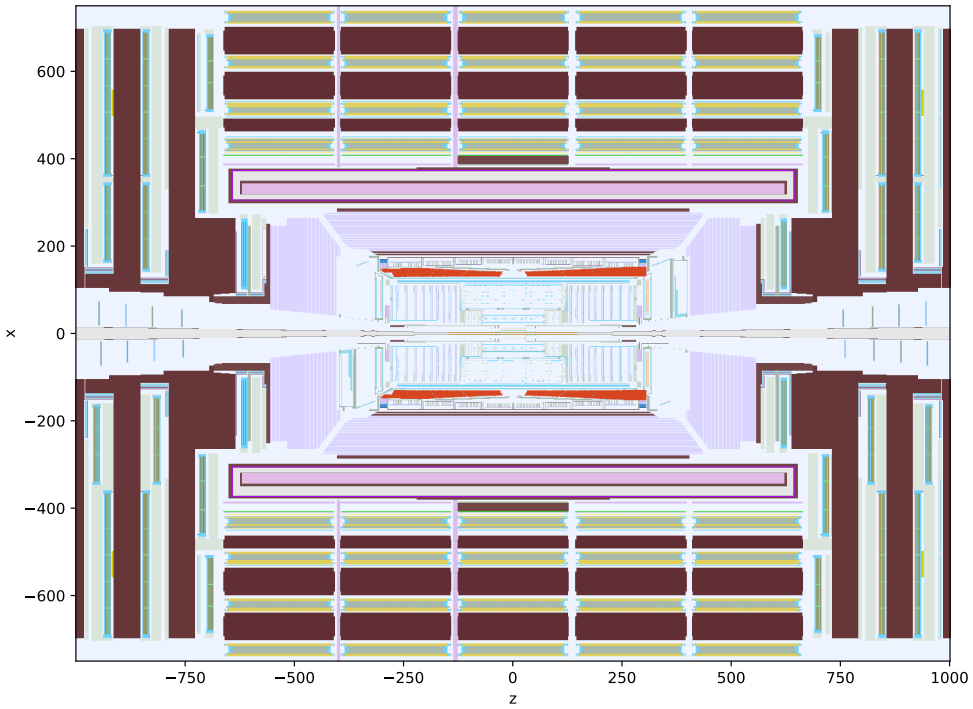
High-level capabilities

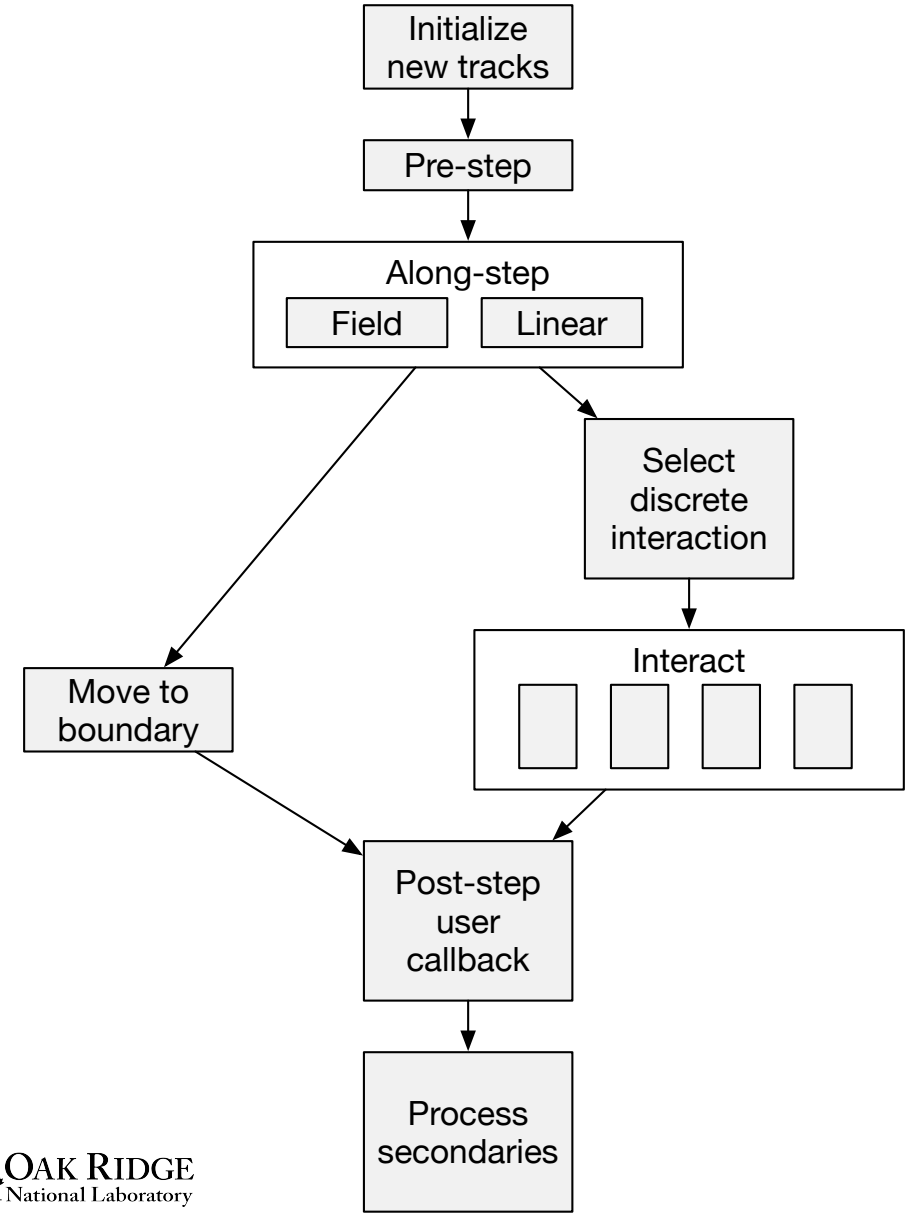
- Equivalent to `G4EmStandardPhysics`
  …using Urban MSC for high-E MSC; only γ, e±
- Full-featured Geant4 detector geometries using VecGeom 1.x
- Runtime selectable processes, physics options, field definition
- Execution on CUDA (Nvidia), HIP* (AMD), ***and CPU*** devices

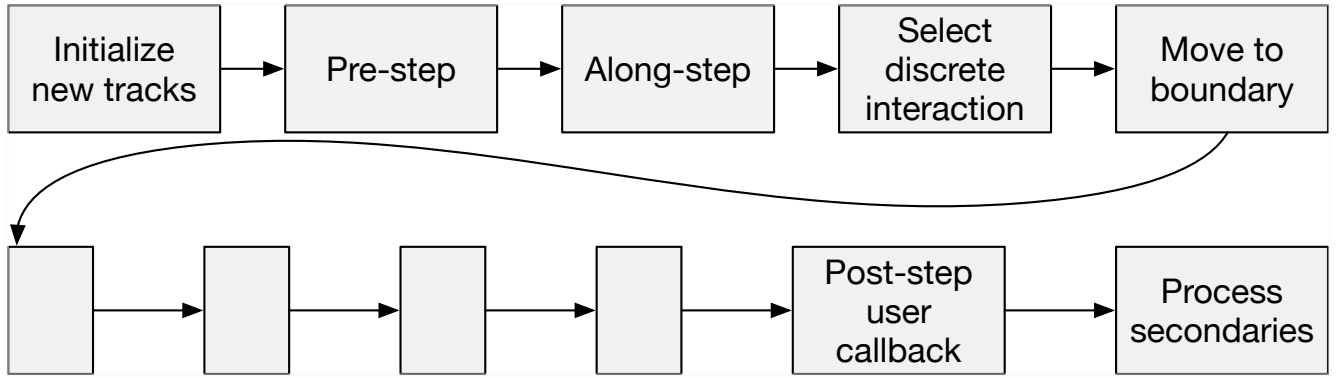


GPU-traced rasterization of CMS 2018

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

Stepping loop on a GPU





Topological sort: a loop over kernels

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

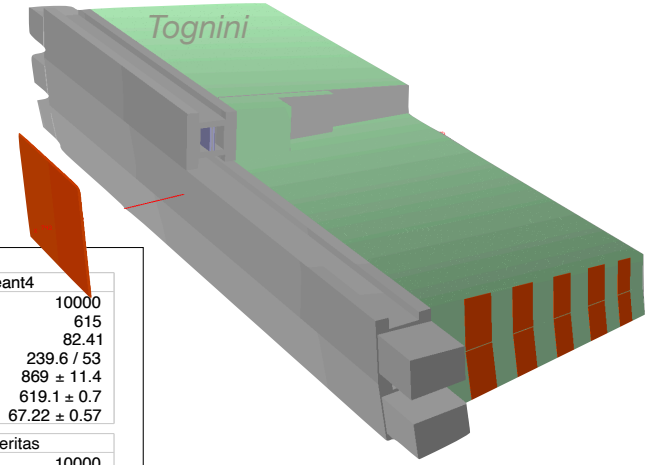
Celeritas version `0.3`: Geant4 integration status

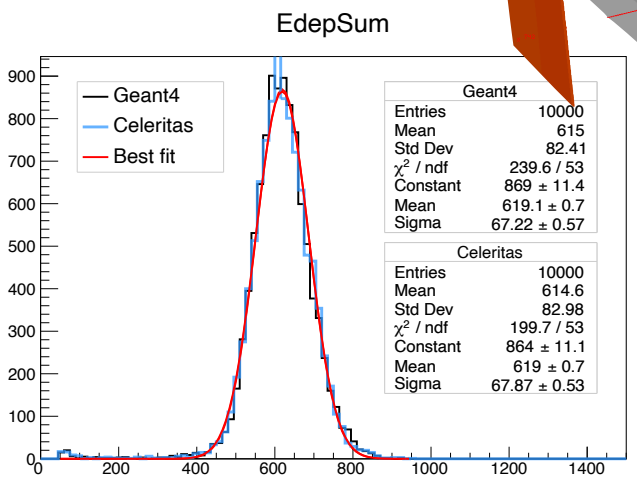
- **Imports** EM physics selection, cross sections, parameters
- **Converts** geometry to VecGeom model
- **Offloads** EM tracks from Geant4
- **Scores** hits to user "sensitive detectors"
  (Copies from GPU to CPU; reconstructs `G4Hit`, `G4Step`, `G4Track`; calls `Hit`)
- **Builds** against Geant4 10.5–11.1

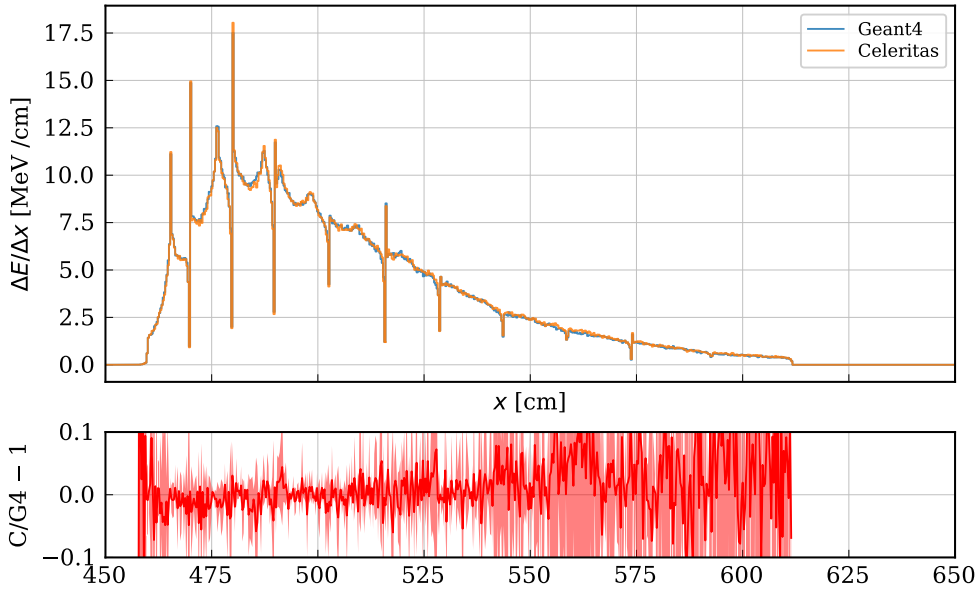
*Celeritas has **production quality** interfaces to simplify user application integration*

EM offloading with FullSimLight

- ATLAS FullSimLight: hadronic tile calorimeter module segment
  - 64 segments in full ATLAS, 1 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

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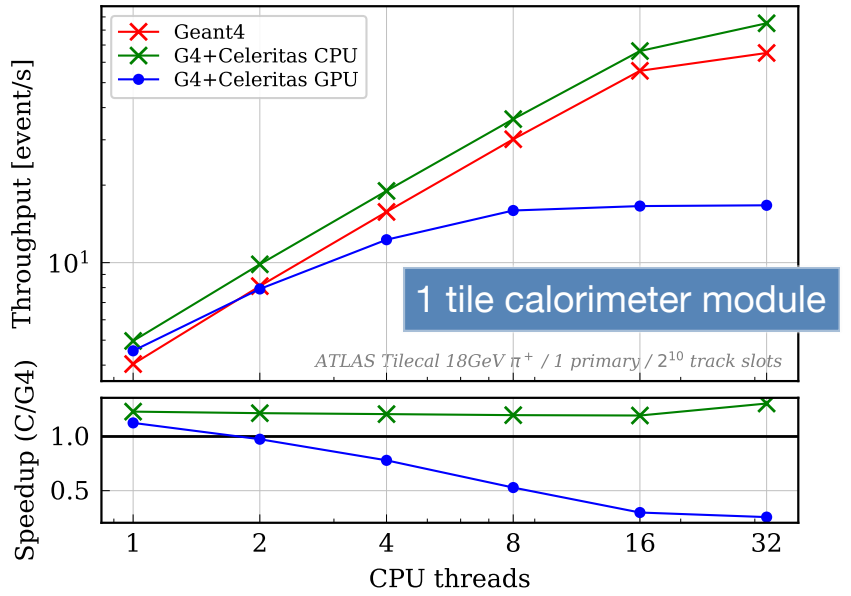
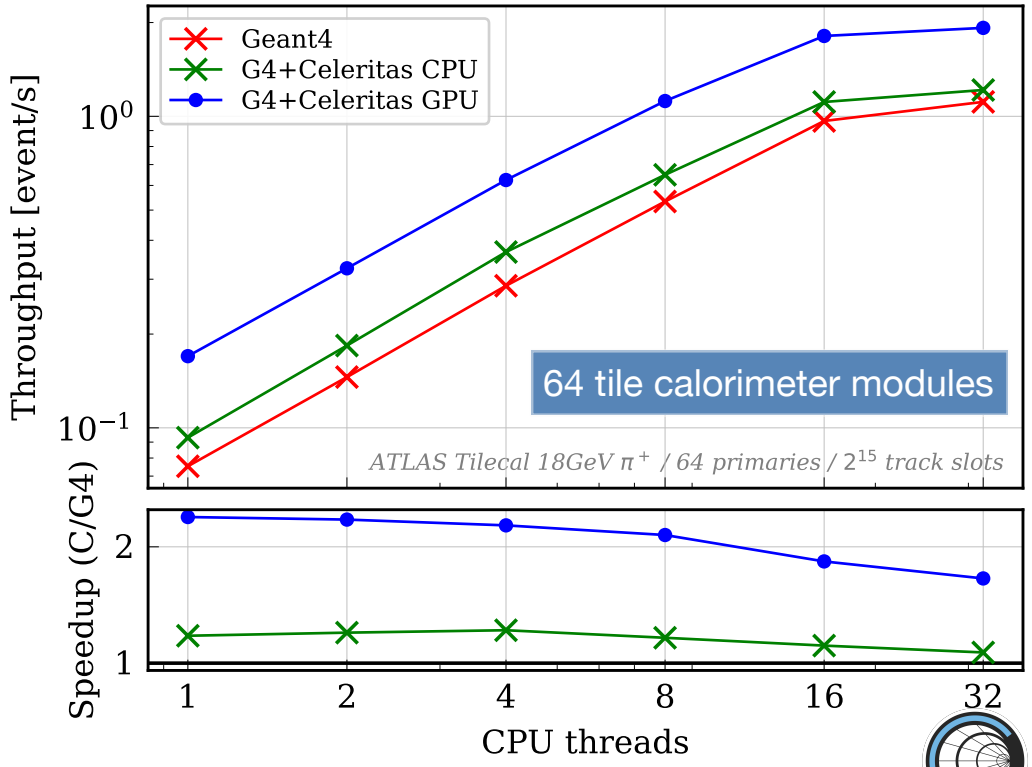
Test problem: Lachnit, Pezzotti; FSL integration: Morgan

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



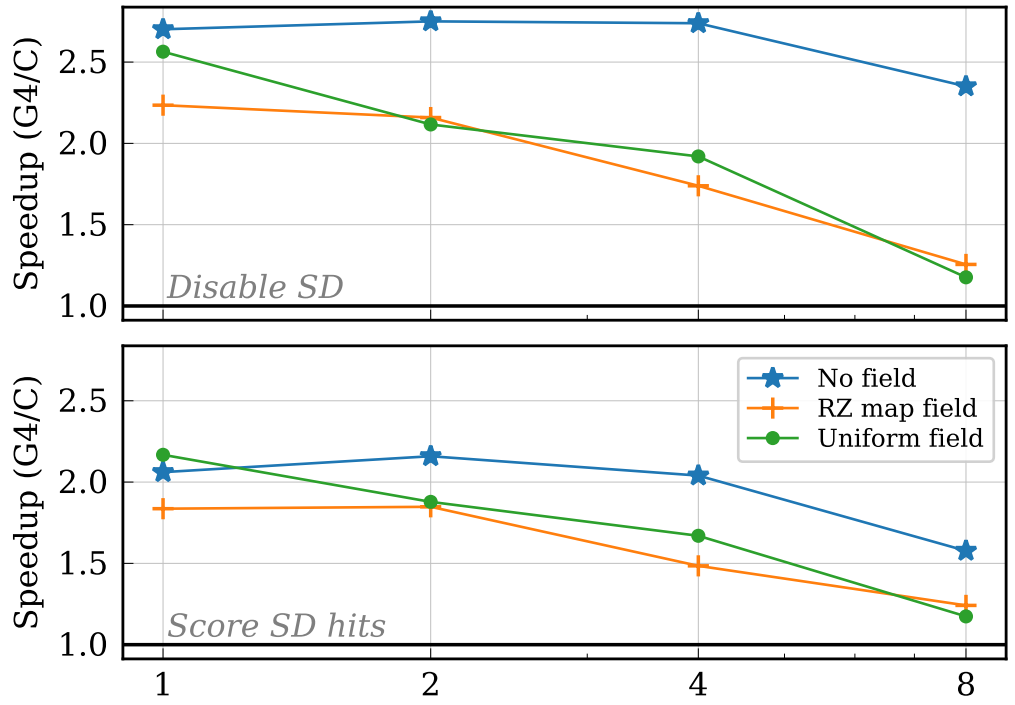


Initial CMSSW integration

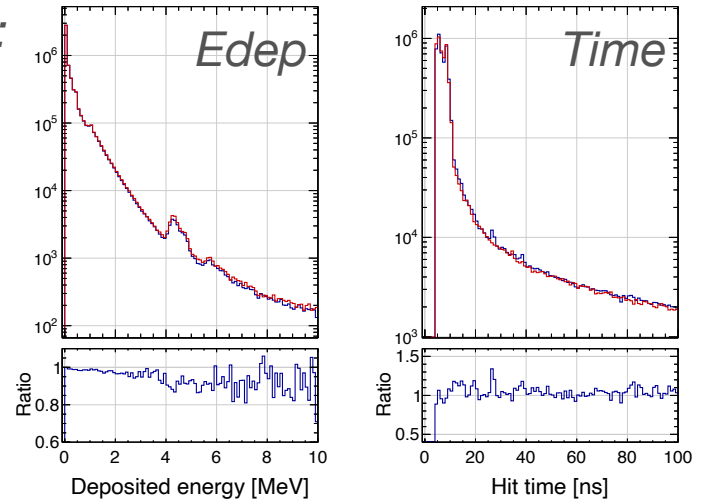
- ~500 lines of code to integrate
  - Offload e^-, e^+, γ to Celeritas
  - R–Z field map preprocessed for Celeritas
  - Celeritas reconstructs hits and sends to CMSSW SDs
  - No support for MC truth or track-level granularity
  - CMSSW has numerous fine-grained tweaks to physics/propagation compared 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)

Standalone app results (Run 3)



EcalHitsEB_HC: promising preliminary comparison!



Hardware: Intel Xeon Gold 6152 CPU 22c 2.10GHz + NVIDIA Tesla V100 SXM2
Geometry: CMS detector (Run 3 configuration)
Input: 8 $t\bar{t}$ events @ 14 TeV from LHC pp collision

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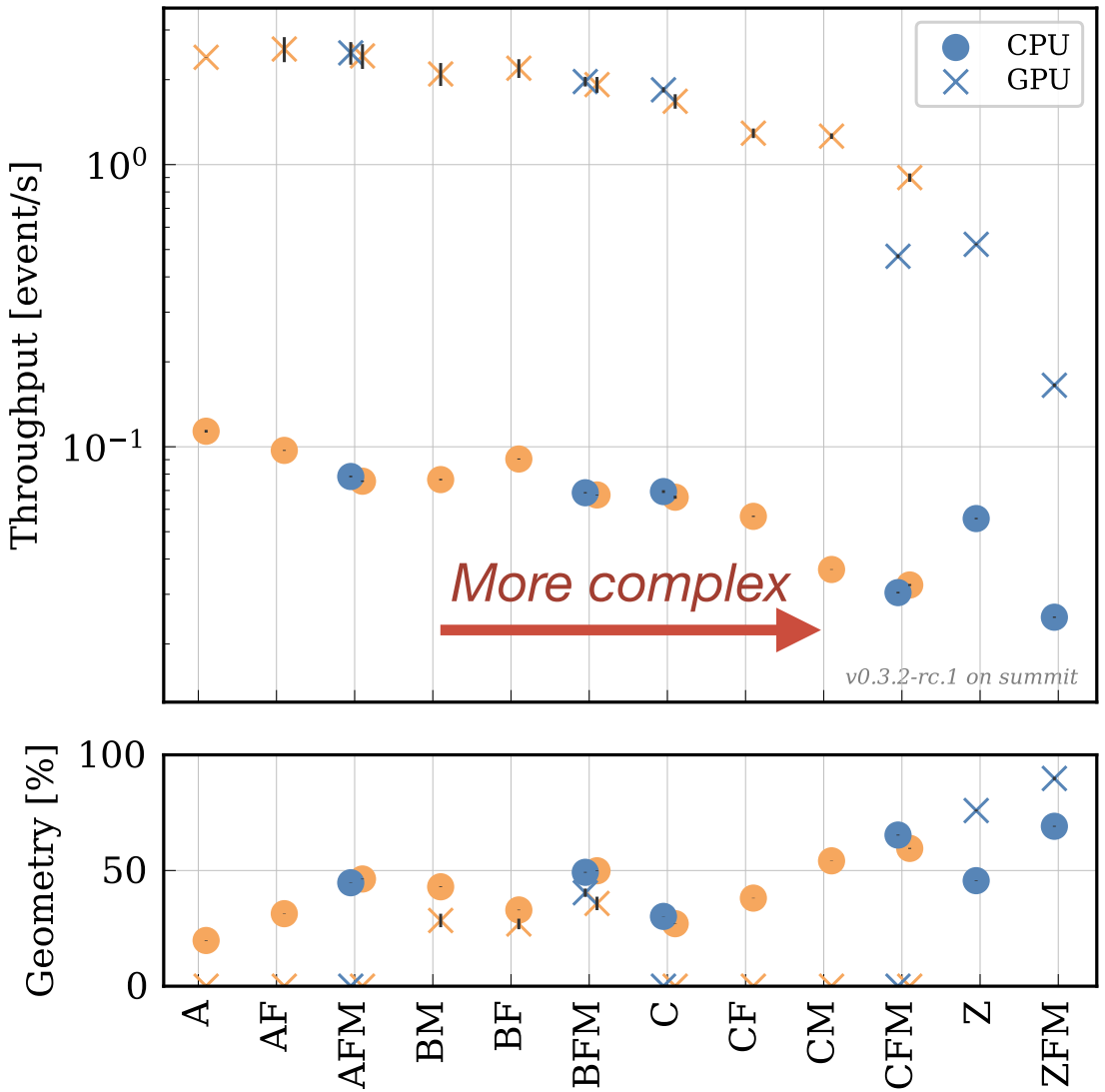
EM-only GPU performance

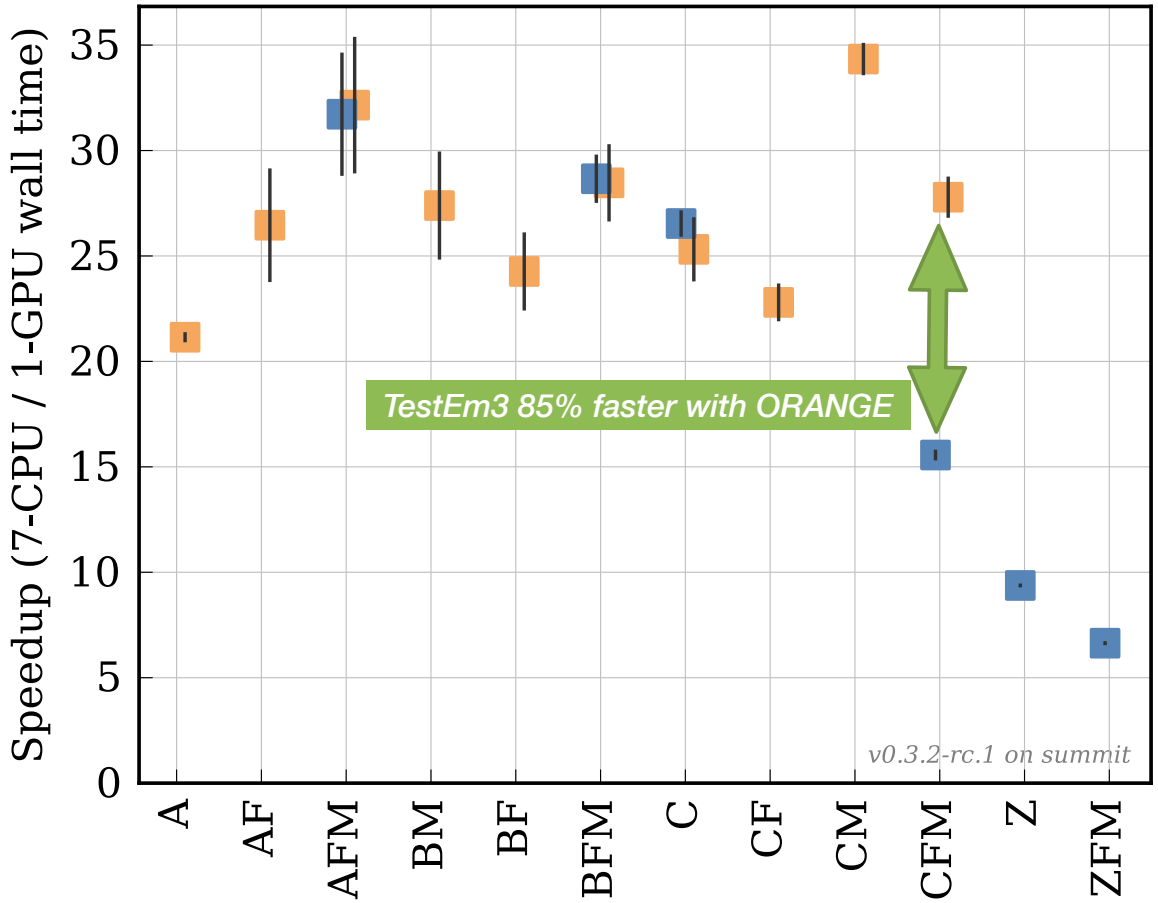


Faster

ORANGE
VecGeom

Problem definition	
A	TestEm15
B	Simple CMS
C	TestEm3
Z	CMS 2018

Modifier	
F	+field (1T)
M	+msc (Urban)



Multiply speedup by 7× for CPU:GPU equivalence

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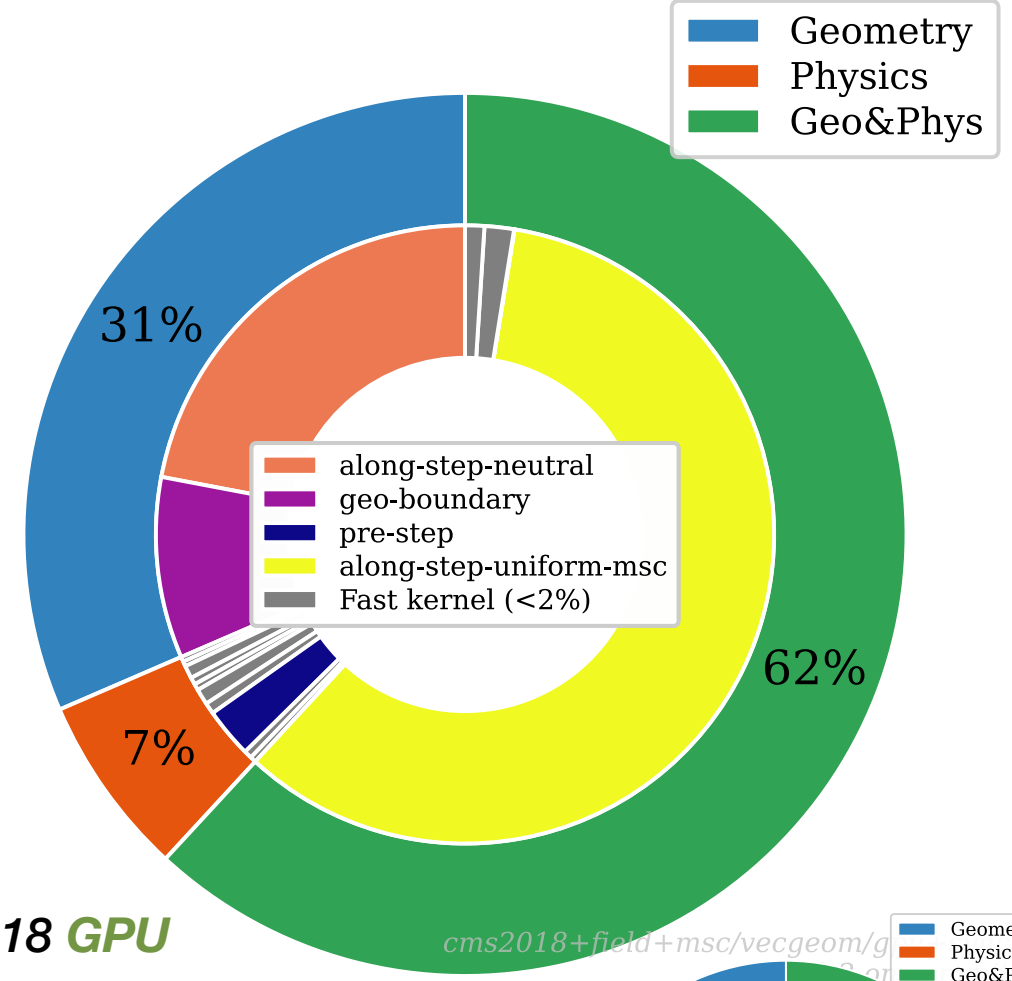
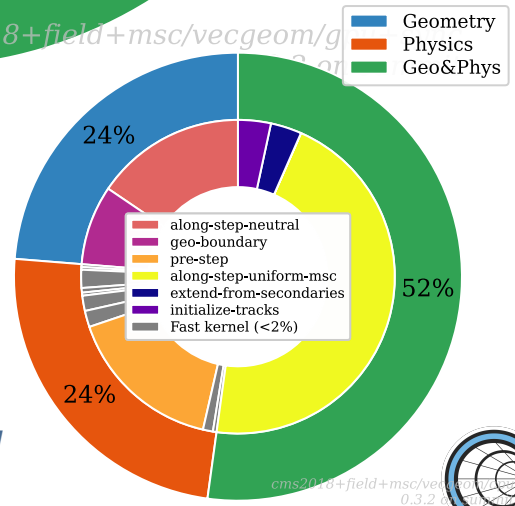
Ongoing work

- Integration
  - CMSSW
  - Athena (ATLAS) framework
- Verification & validation
  - EM test problems
  - CMSSW workflow
  - Benchmark problems with AdePT team
- Optimization and geometry
  - **~90%** 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

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Future work

- Optimize magnetic field propagation
- 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

- Straightforward integration into existing Geant4 apps
- Demonstrated performance gains by offloading EM to Celeritas
  - 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 v0.3 code contributors:

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

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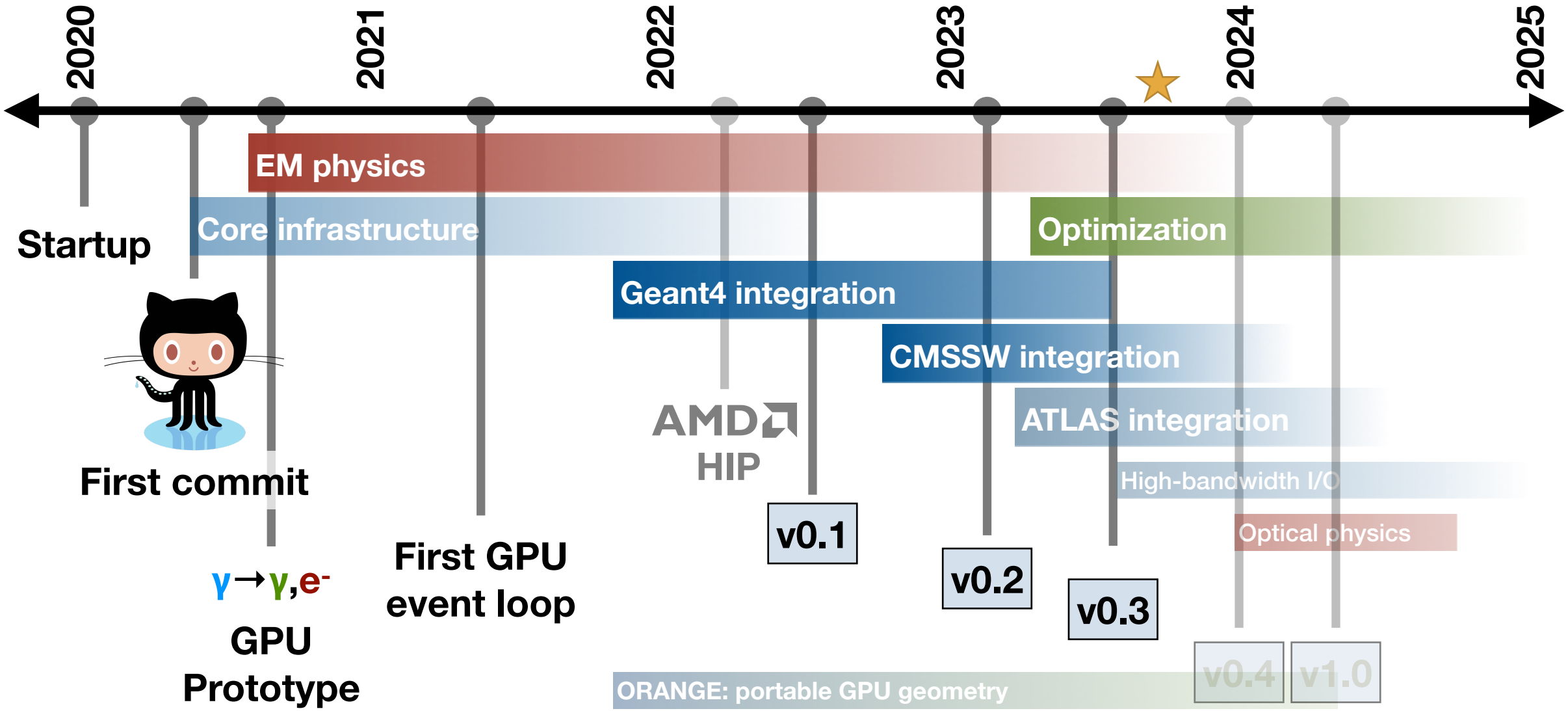
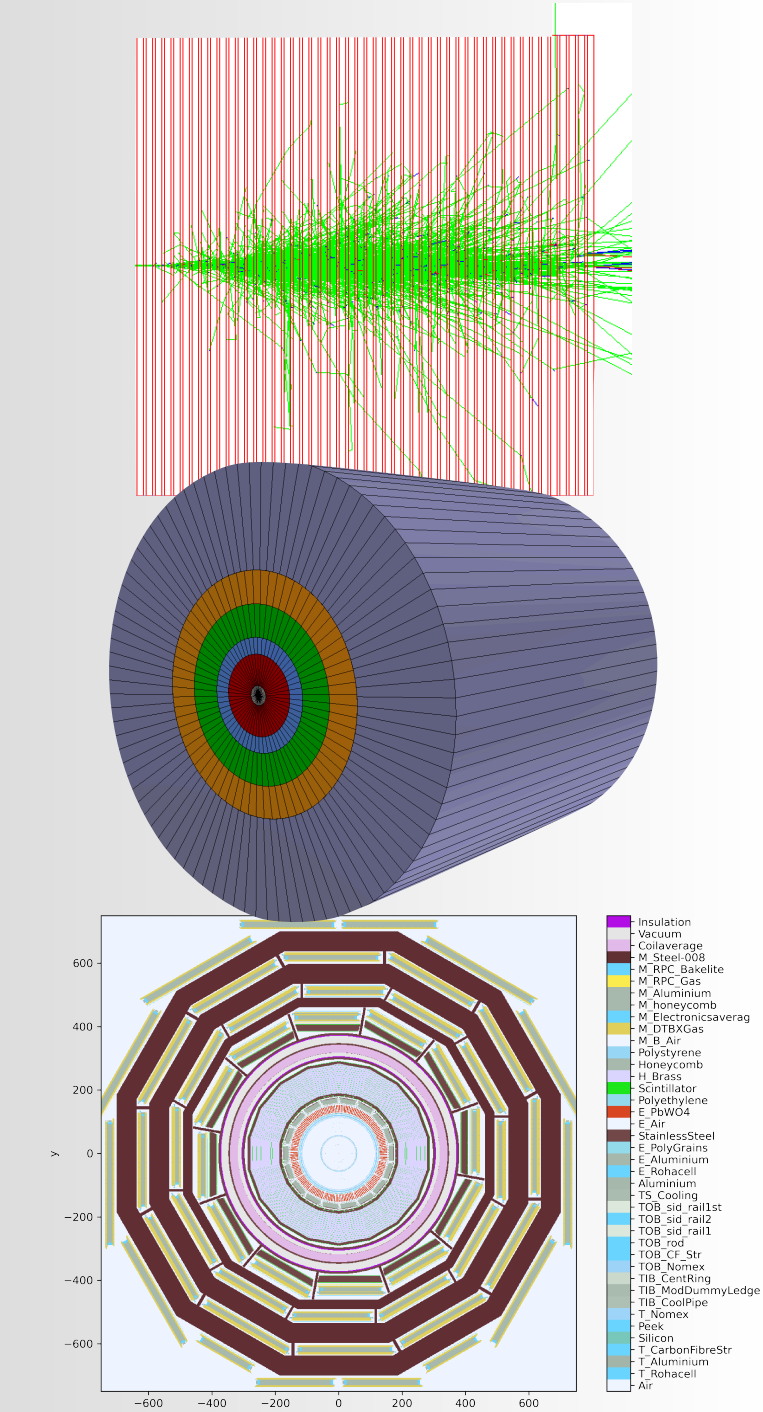
Backup slides

Present-day timeline

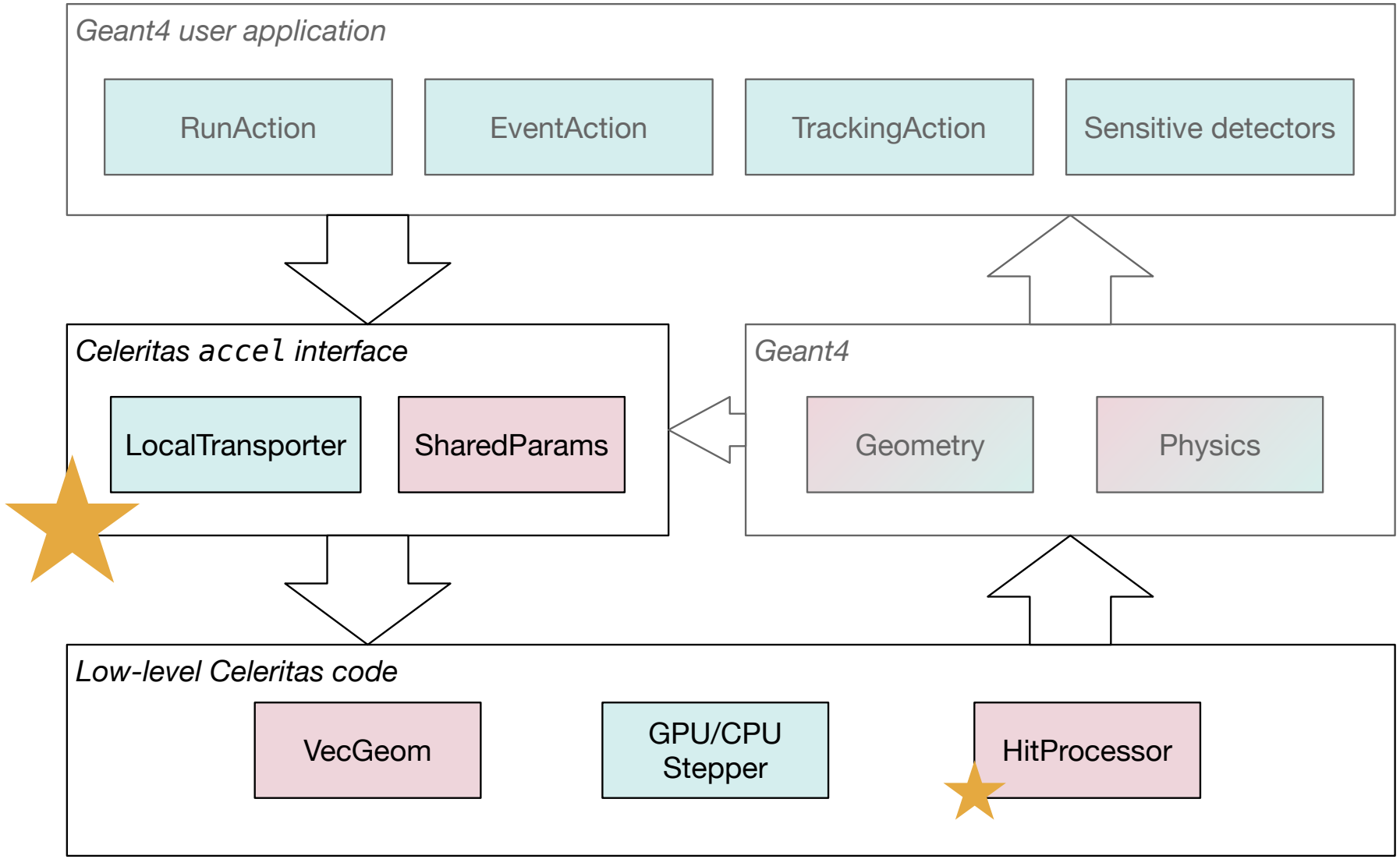


Regression/timing suite

- 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



Thread-local
Shared

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

**New code for v0.2*

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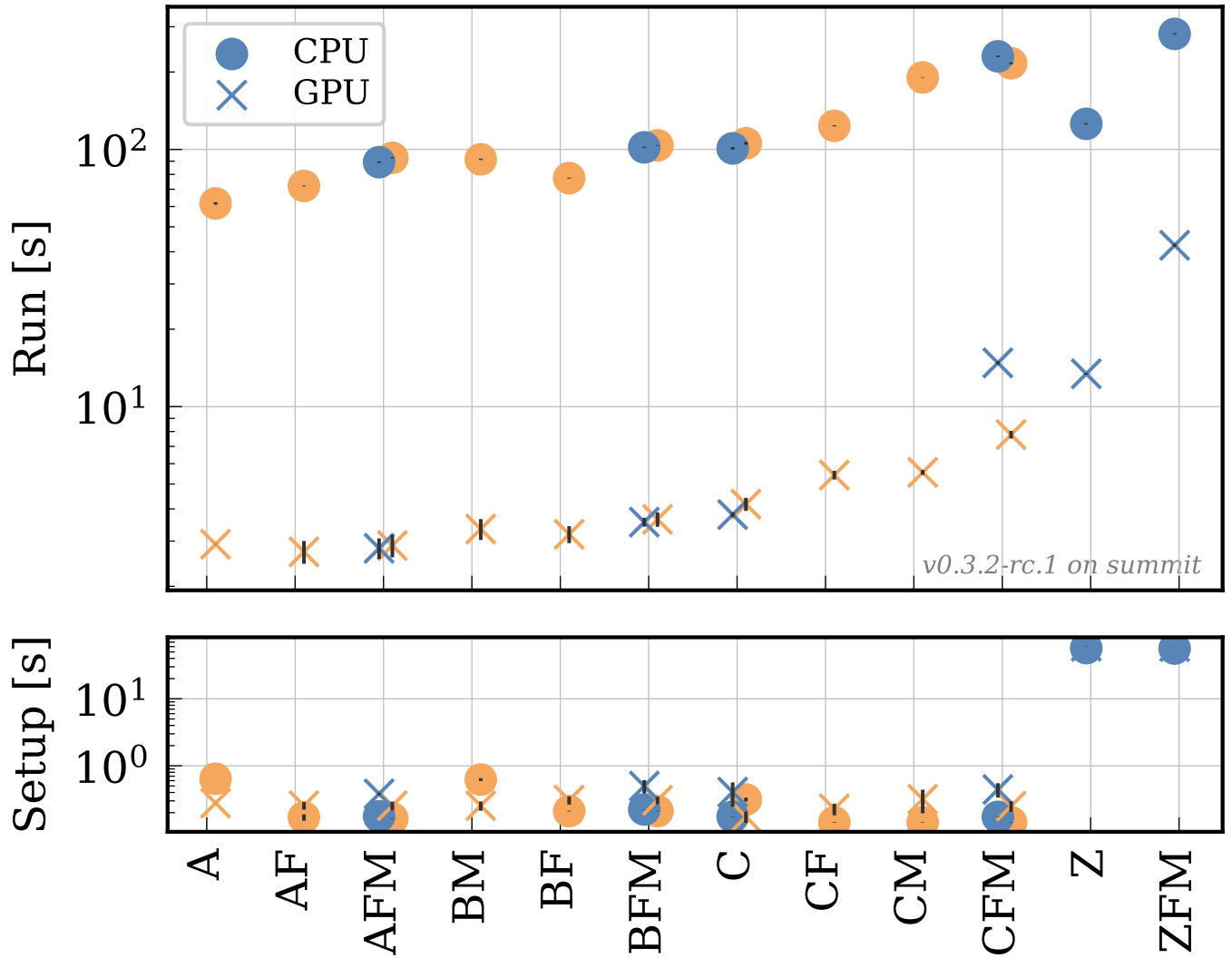
Regression problem run time

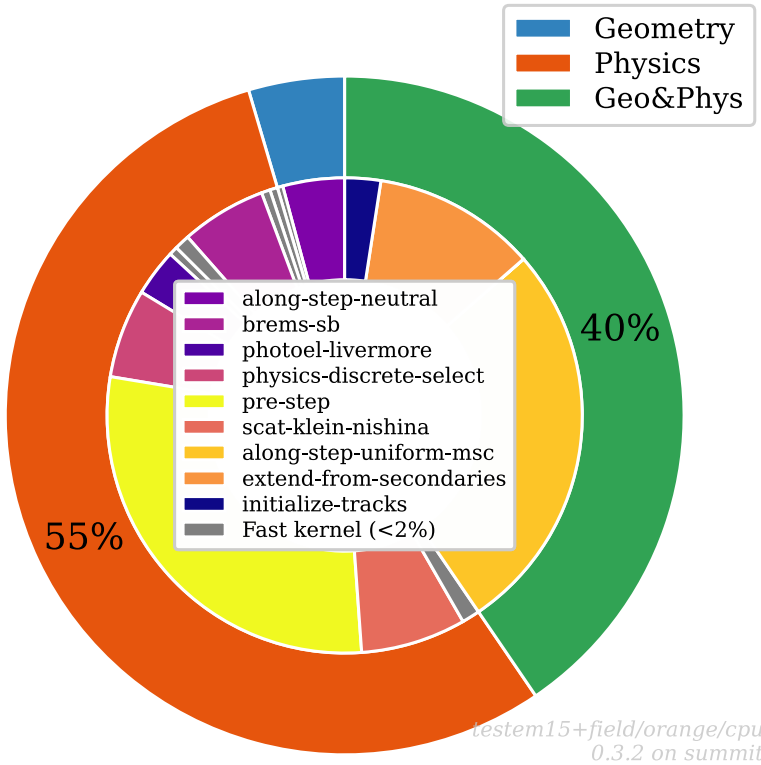


ORANGE
VecGeom

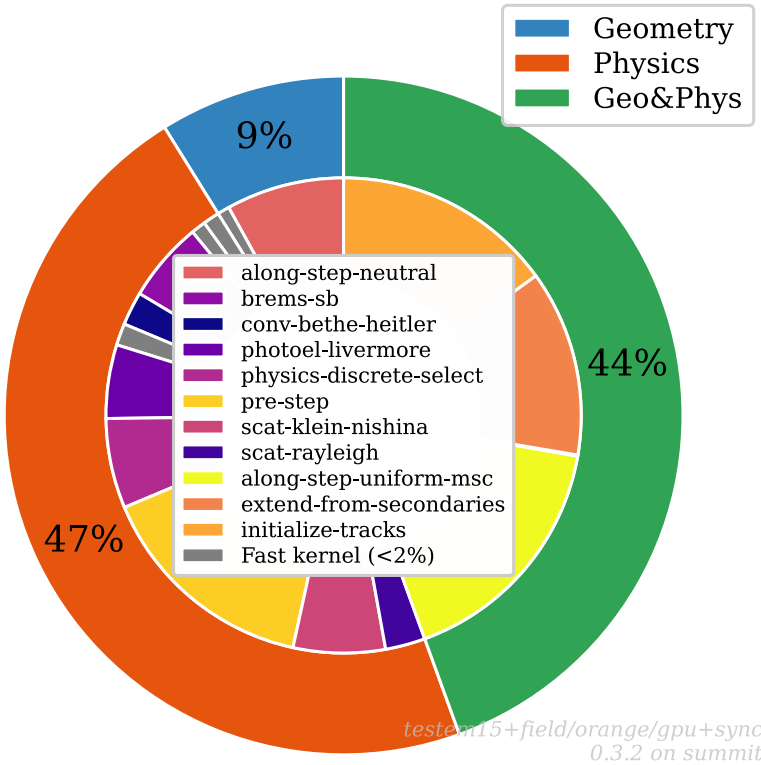
	Problem definition
A	testem15
B	simple-cms
C	testem3
Z	cms2018

Modifier	
F	+field
M	+msc

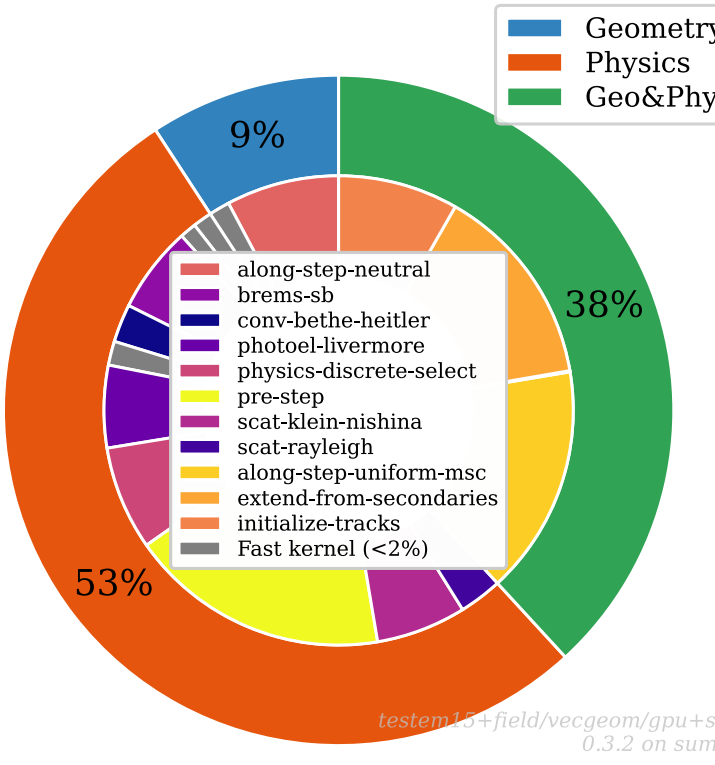
Infinite medium hotspots



ORANGE CPU



ORANGE GPU



VecGeom GPU

*GPU cross section calculation is comparatively **faster** than CPU*

TestEM3 fractional performance