Celeritas: EM physics on GPUs

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Celeritas code lead

Celeritas core team:

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Celeritas SciDAC PI:

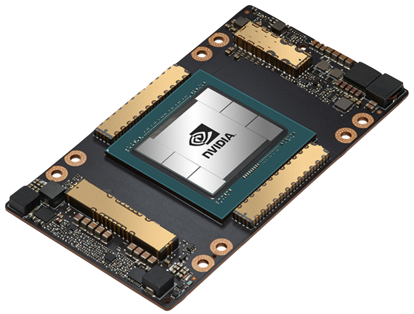
Marcel Demarteau *(ORNL)*

CalVision meeting
8 June, 2023
(derivative from CHEP 2023 presentation)

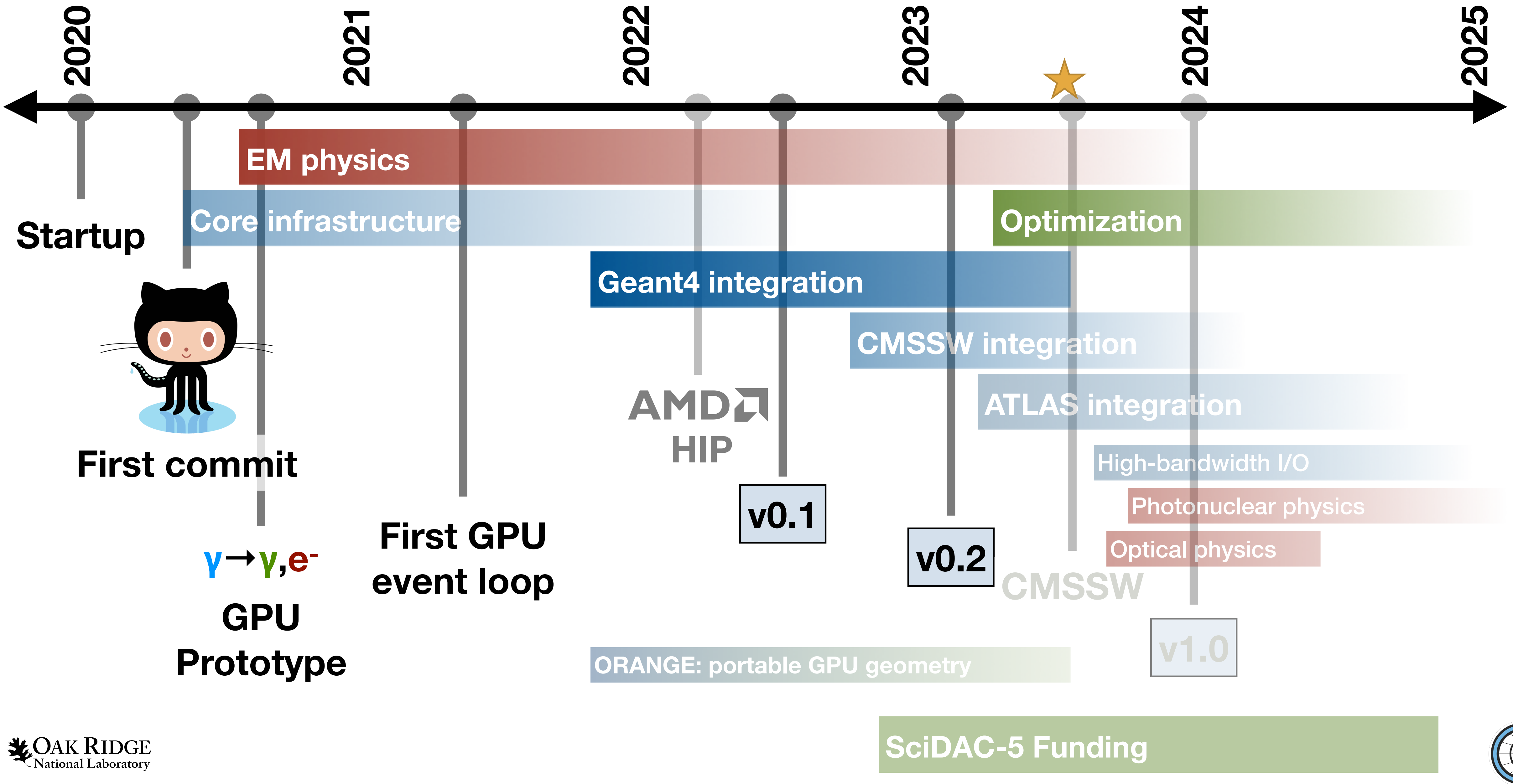
Background

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 (*ECP ExaSMR*)
- **Primary goal: accelerate production use for LHC Run 4**


Nvidia A100 GPU (Nvidia)

Present-day timeline

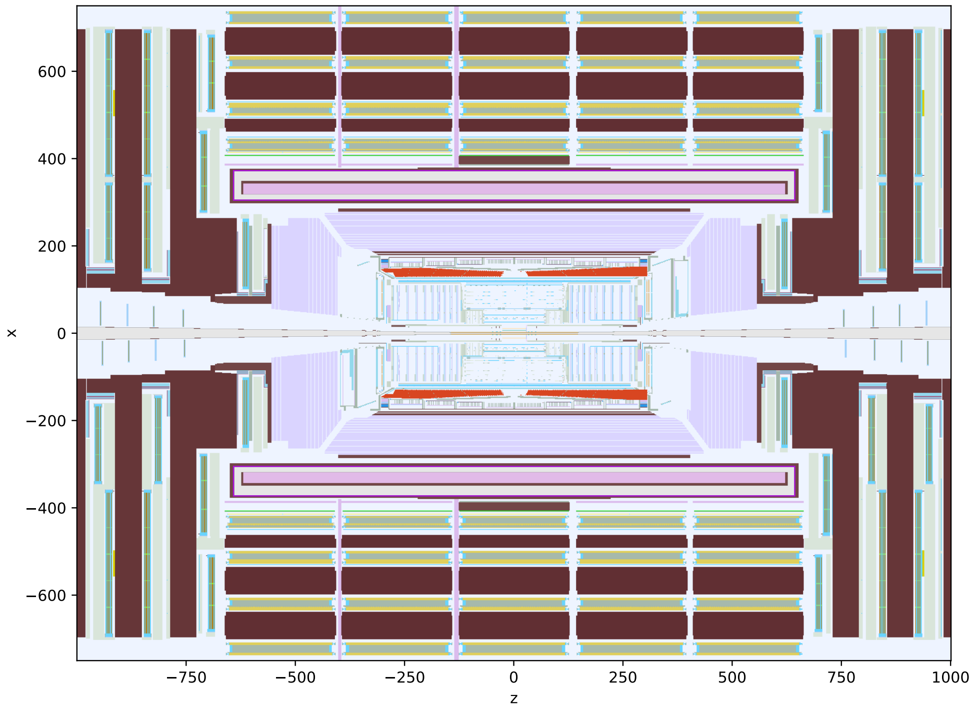


OAK RIDGE National Laboratory

Capabilities

High-level capabilities

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

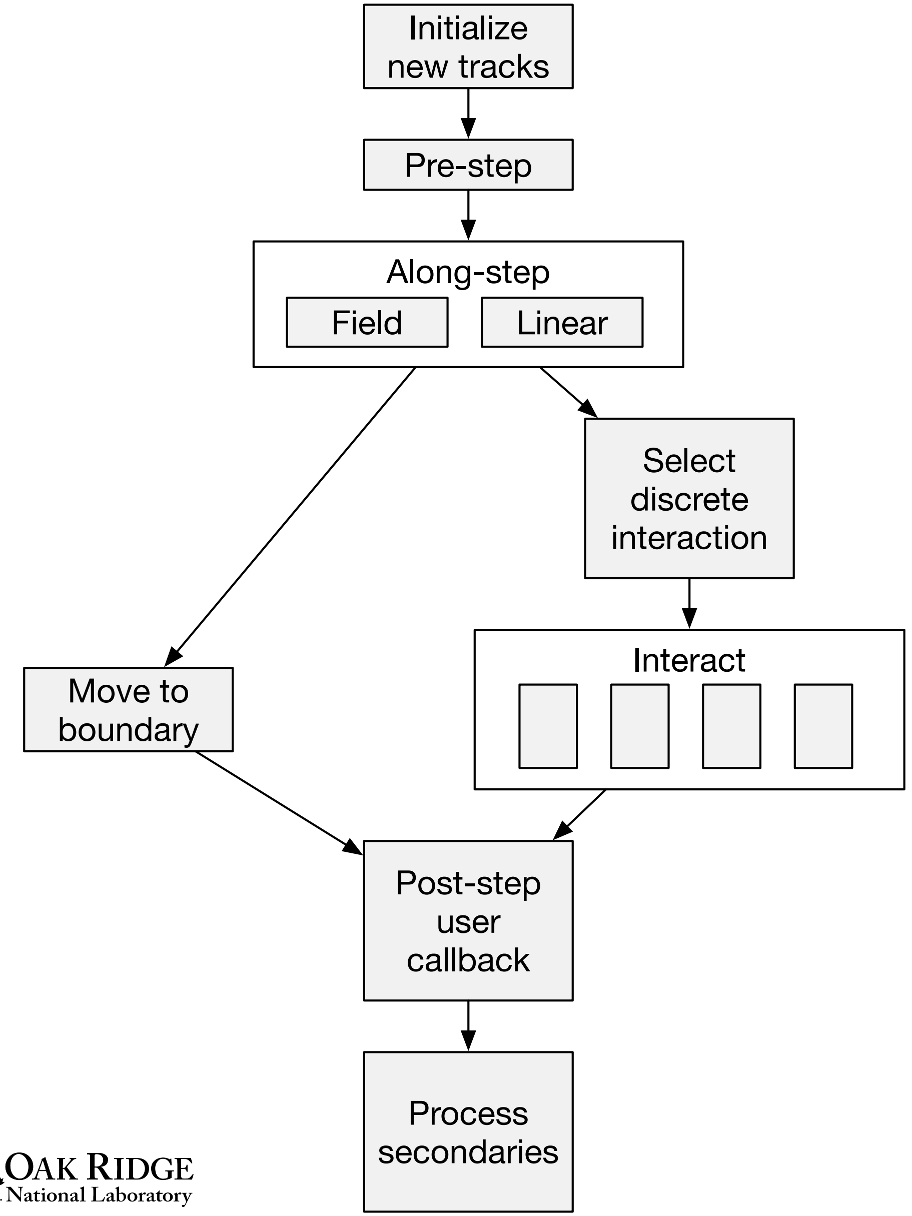


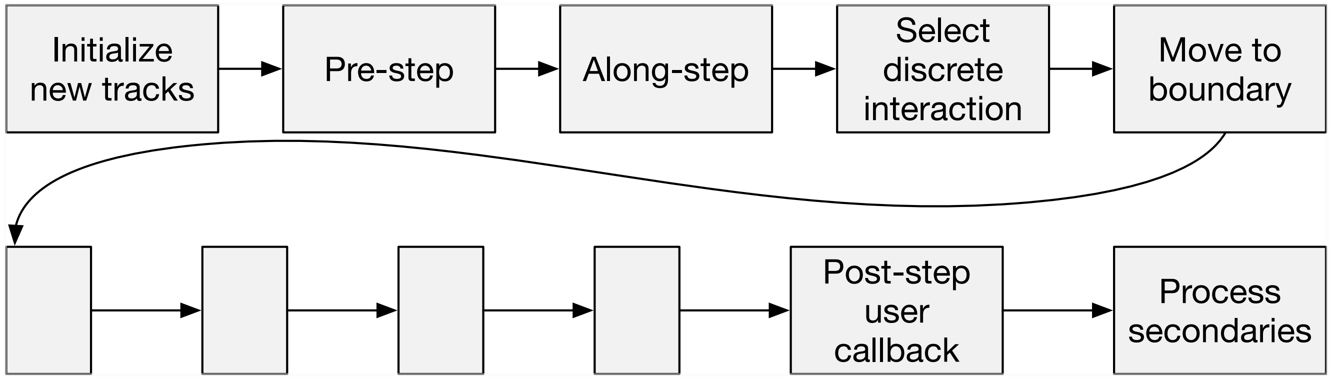
GPU-traced rasterization of CMS 2018

**VecGeom is incompatible with HIP: ORANGE GPU prototype used instead*

Verification & Validation still in progress

Stepping loop on a GPU





Topological sort: a loop over kernels

Process ~1M track batches

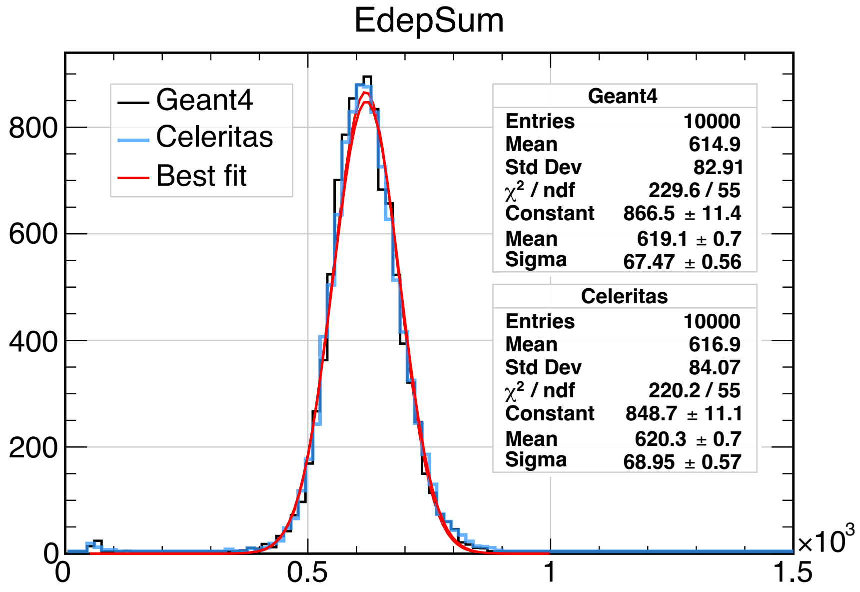
Celeritas version `0.3-dev`: Geant4 integration status

- **Imports** EM physics selection, cross sections, parameters
- **Converts** geometry to VecGeom model
- **Offloads** EM tracks from Geant4
- **Scores** hits to user “sensitive detectors”
- **Includes** GPU-optimized simple calorimeter
- **Integrates** with Geant4 10.6–11.0
- **Supports** physics/geometry/setup changes at link/run time

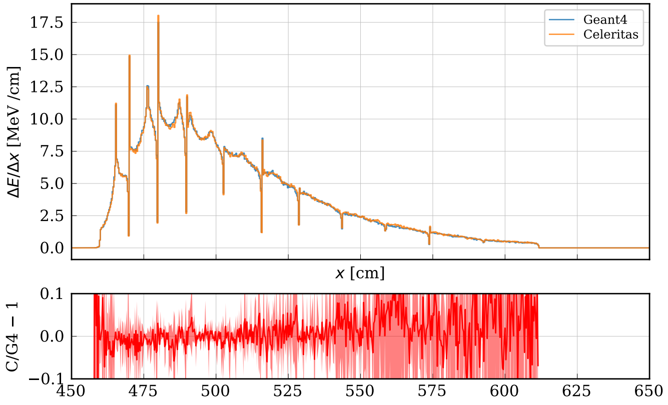
Celeritas is not designed to be a prototype code

Tilecal: ATLAS tile calorimeter test beam

- Standalone subdetector test
  - Forked from Pezzotti&Lachnit (CERN)'s work
  - 18 GeV π^+ beam, no field
  - FTFP_BERT physics
  - Primary output: energy deposition integrated over sensitive regions
- Offload e^-, e^+, γ to Celeritas
- Celeritas returns hits to user-defined `G4VSensitiveDetector`
- ~100 lines of code to integrate
- Excellent agreement



Average energy deposition with pi+ test beam



Slab-integrated energy deposition

https://github.com/celeritas-project/atlas-tilecal-integration

Framework integration status

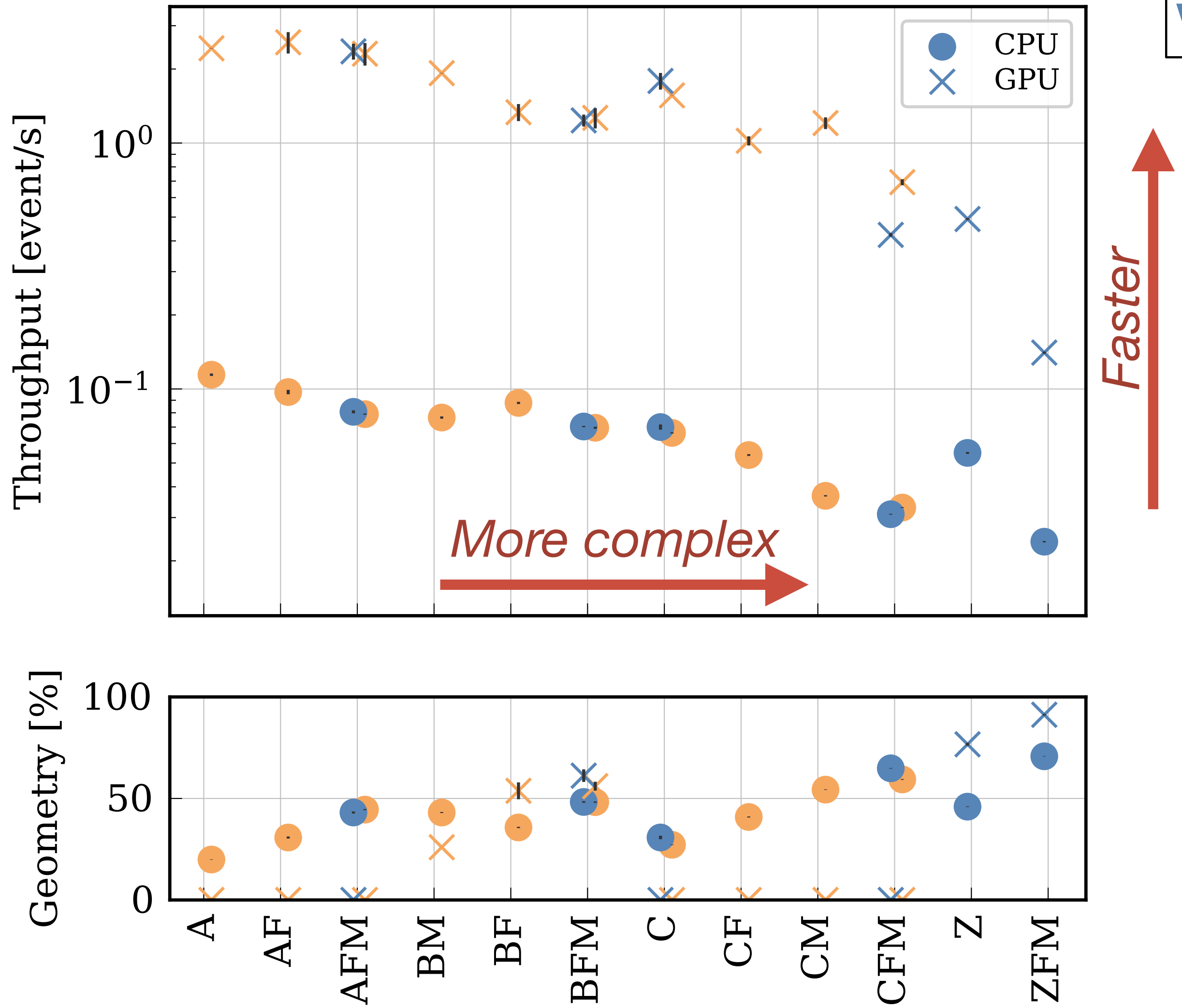
- CMS (CMSSW): offload interface implemented and running
- ATLAS (Athena): framework integration started
  - Infrastructure update for CMake compatibility: atlasexternals!1001
  - Non-custom "accordion" shape needed for VecGeom/GPU
- LHCb: seeking collaborators!
- LZ (BACCARAT): awaiting optical physics

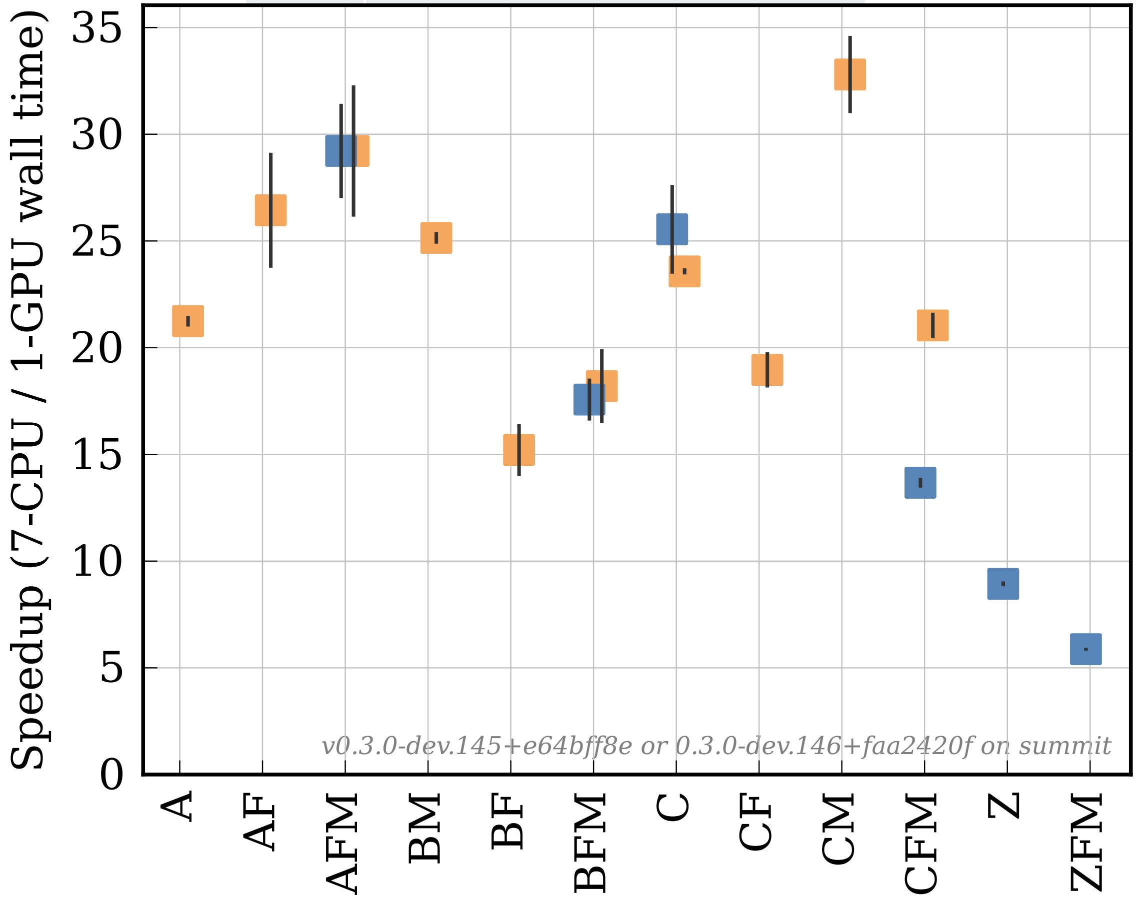
Summit GPU performance

ORANGE
VecGeom

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

	Modifier
F	+field
M	+msc



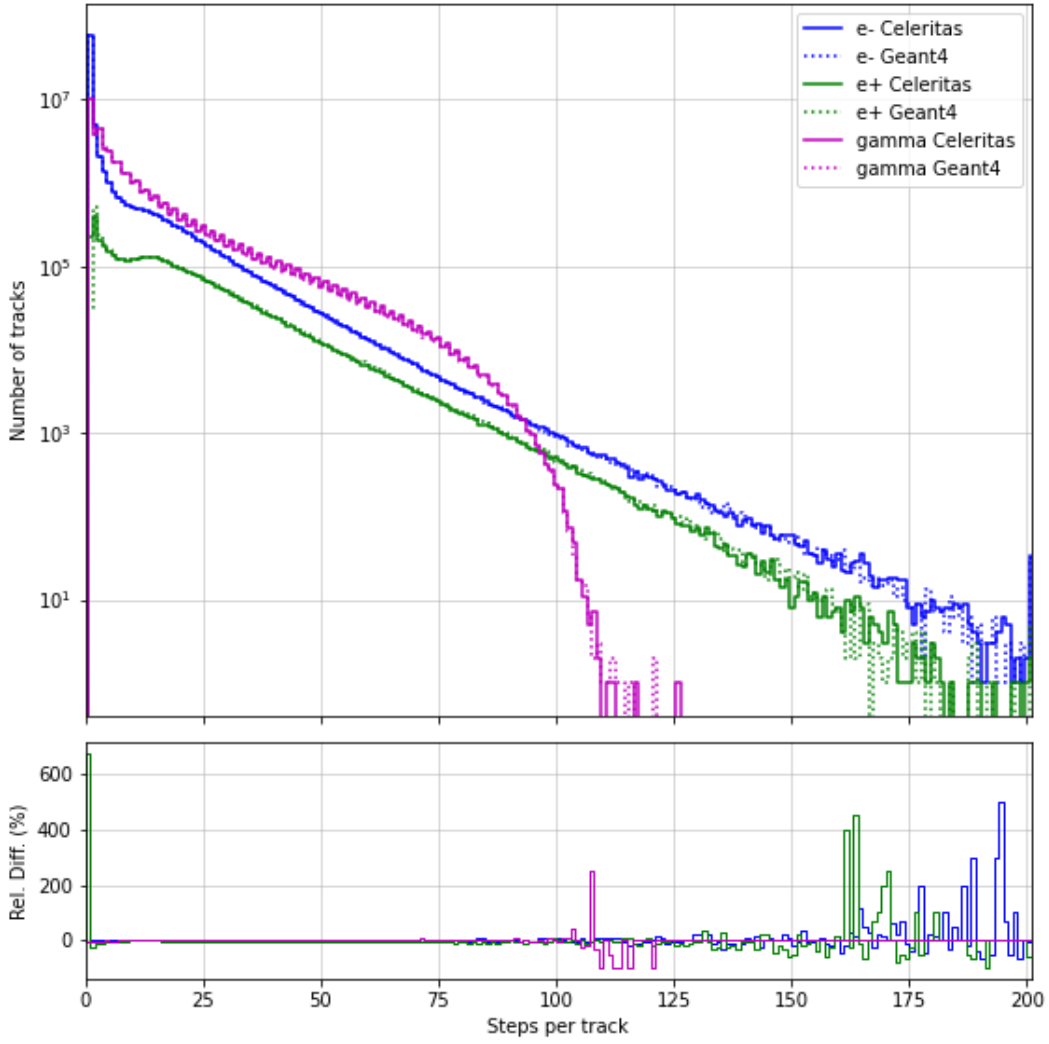


Multiply speedup by 7× for CPU:GPU equivalence

Continuing work

Validation

- Geant4 interface allows rapid comparisons
- Independent granular physics verification
- Benchmark progression problems being developed with CERN SFT (AdePT) group



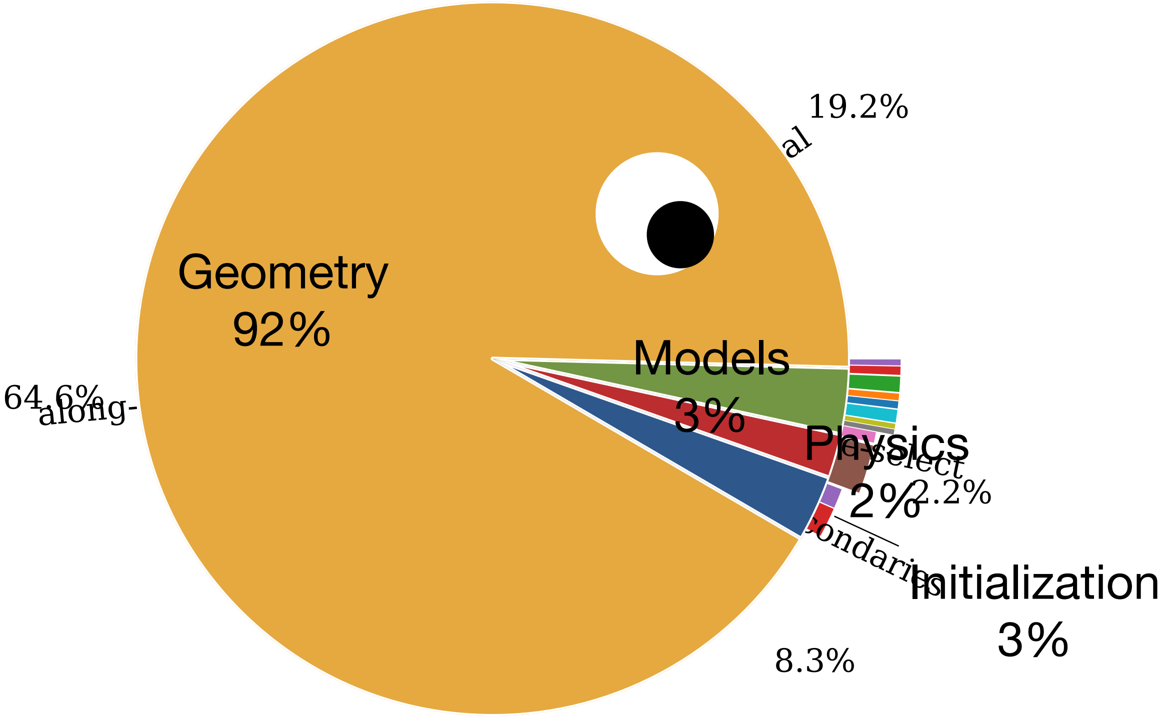
TestEM3 MSC step count verification (Amanda Lund)

Integration

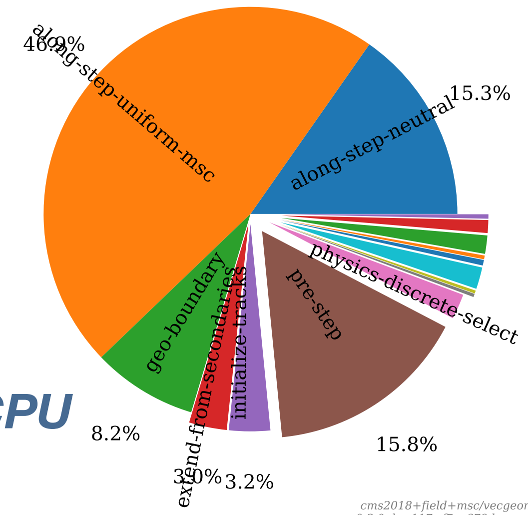
- Theoretical maximum performance gain offloading EM tracks: **~3.3×**
  (with 1000 $t\bar{t}$ events and CMS Run3 geometry)
- CMSSW offloading with RZ mapped field: **June 2023**
- ATLAS integration will require low-fidelity “accordion” for now
- Platform-agnostic optical photon acceleration in the works

Optimization

- **92%** of standalone runtime in CMS2018 is in geometry routines
- GPU native sensitive detectors
- Performance on non-HPC graphics cards still unexplored
- Goal for GPU performance for HL-LHC electron shower:
  - **2×** per watt vs CPU *(efficiency)*
  - **160×** CPU:GPU *(capacity)*



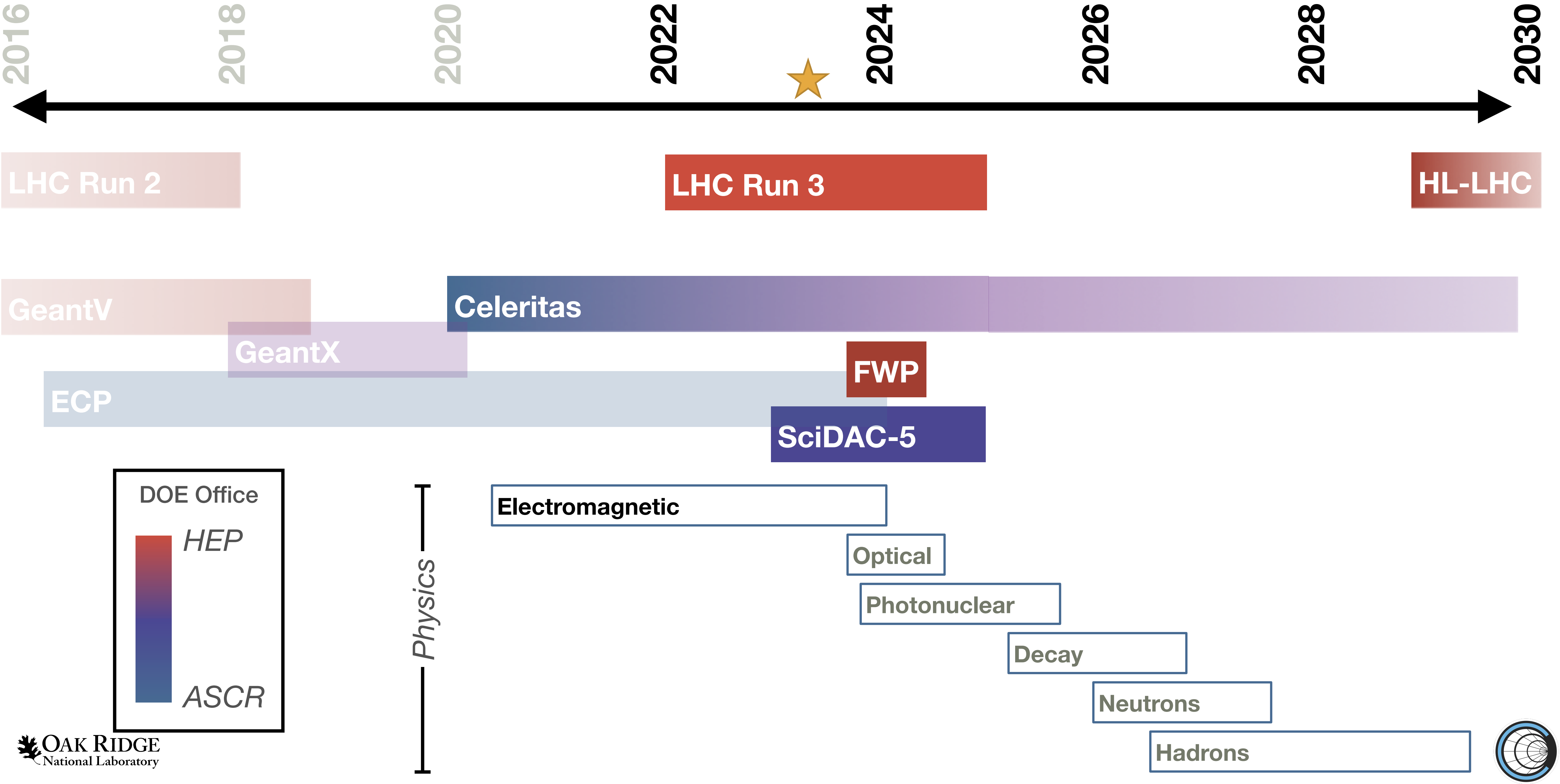
CMS2018 GPU



CMS2018 CPU

cms2018+field+msc/vecgeom/cpu v0.3.0-dev.117+f5cc679d on summit

Celeritas future timeline



Summary

- Many steps toward polished GPU detector simulation framework
- Current test problems show **~6–30× performance boost** for Celeritas detector simulation using GPUs on Summit
  (42–210× GPU/CPU core equivalence)
- Upcoming capabilities will extend our problem domain beyond LHC

Acknowledgments

Celeritas v0.2 code contributors:

- Elliott Biondo (@elliottbiondo)
- Philippe Canal (@pcanal)
- Seth R Johnson (@sethrj)
- Soon Yung Jun (@whokion)
- Guilherme Lima (@mrguilima)
- Amanda Lund (@amandalund)
- Ben Morgan (@drbenmorgan)
- Paul Romano (@paulromano)
- Stefano C Tognini (@stognini)

Past code contributors:

- Doaa Deeb (@DoaaDeeb)
- Tom Evans (@tmdelellis)
- Vincent R Pascuzzi (@vrpascuzzi)

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

Backup slides

Execution plan: EM physics and integration

1: Implement minimal feature set to offload EM particles

(importing Geant4 physics data, recreating G4Hit structure, implementing EM models)

2: Establish baseline performance with minimum, verified features

Standalone CMS2018 with magnetic field and full EM physics is our key problem

3: Optimize performance

- Standalone GPU performance
- Multitask/thread+GPU performance
- GPU-based sensitive detectors (calorimeters, etc)

Modular software design and robust testing is key

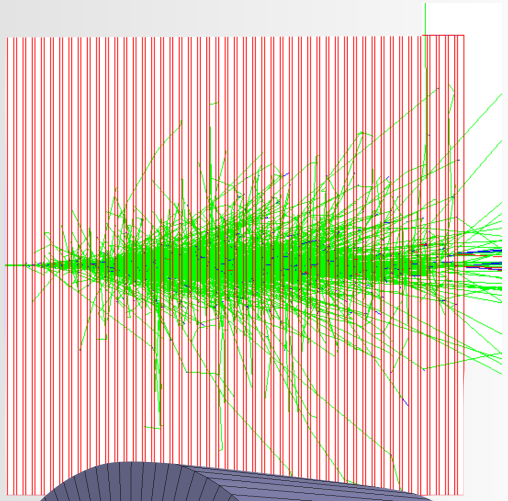
Extensibility

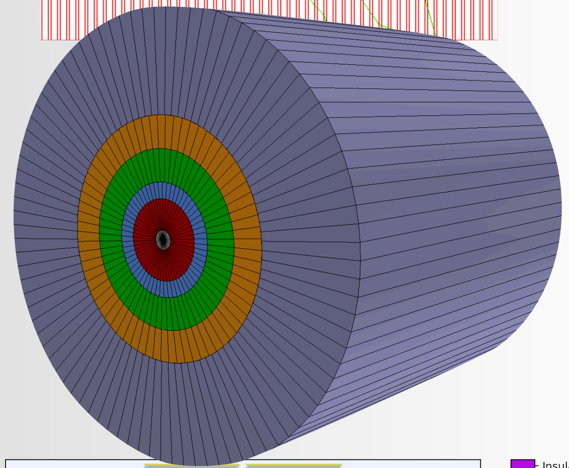
- New models and detector integrations can be added **at link time**
  (maybe even `dlopen` in the future)
- Robust integration pathways for frameworks and applications
- Code is amenable to major refactoring with minor changes
  - Modular structure
  - Composition-based classes
  - Data-oriented design

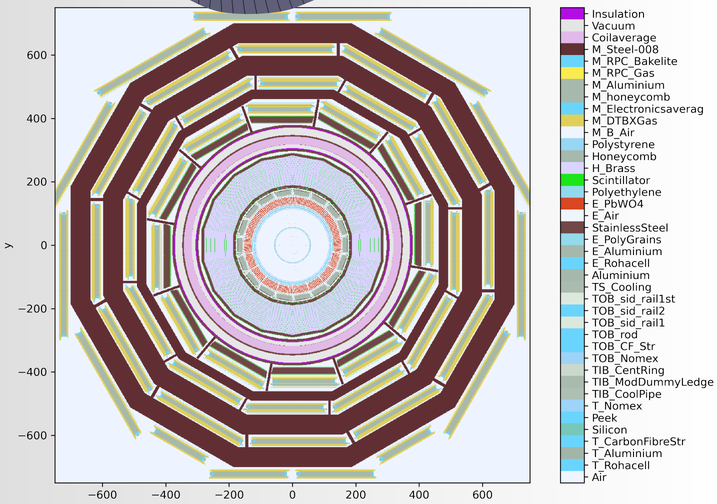
Celeritas is not designed to be a prototype code

Regression/timing suite

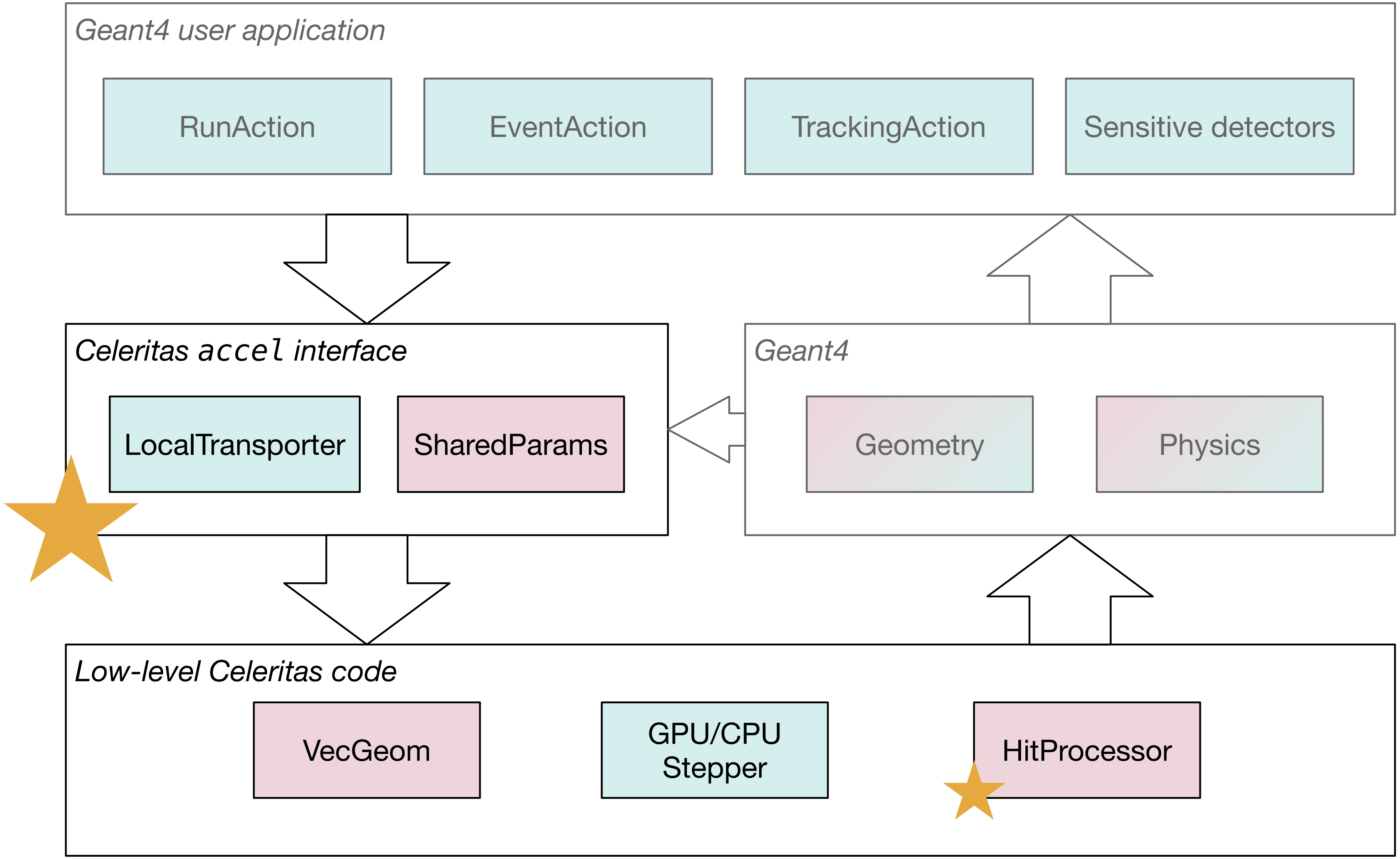
- Run on single node of Summit at full capacity
  - 6 separate runs simultaneously (different seed for each)
  - Each run: 7 CPU (OpenMP) vs. 1 GPU (+1 CPU)
  - Demonstrate performance “loss” by neglecting GPU resources
- 1300 10 GeV e^- per event, 7 events per run
- Preliminary set of problem definitions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







Geant4 interface library

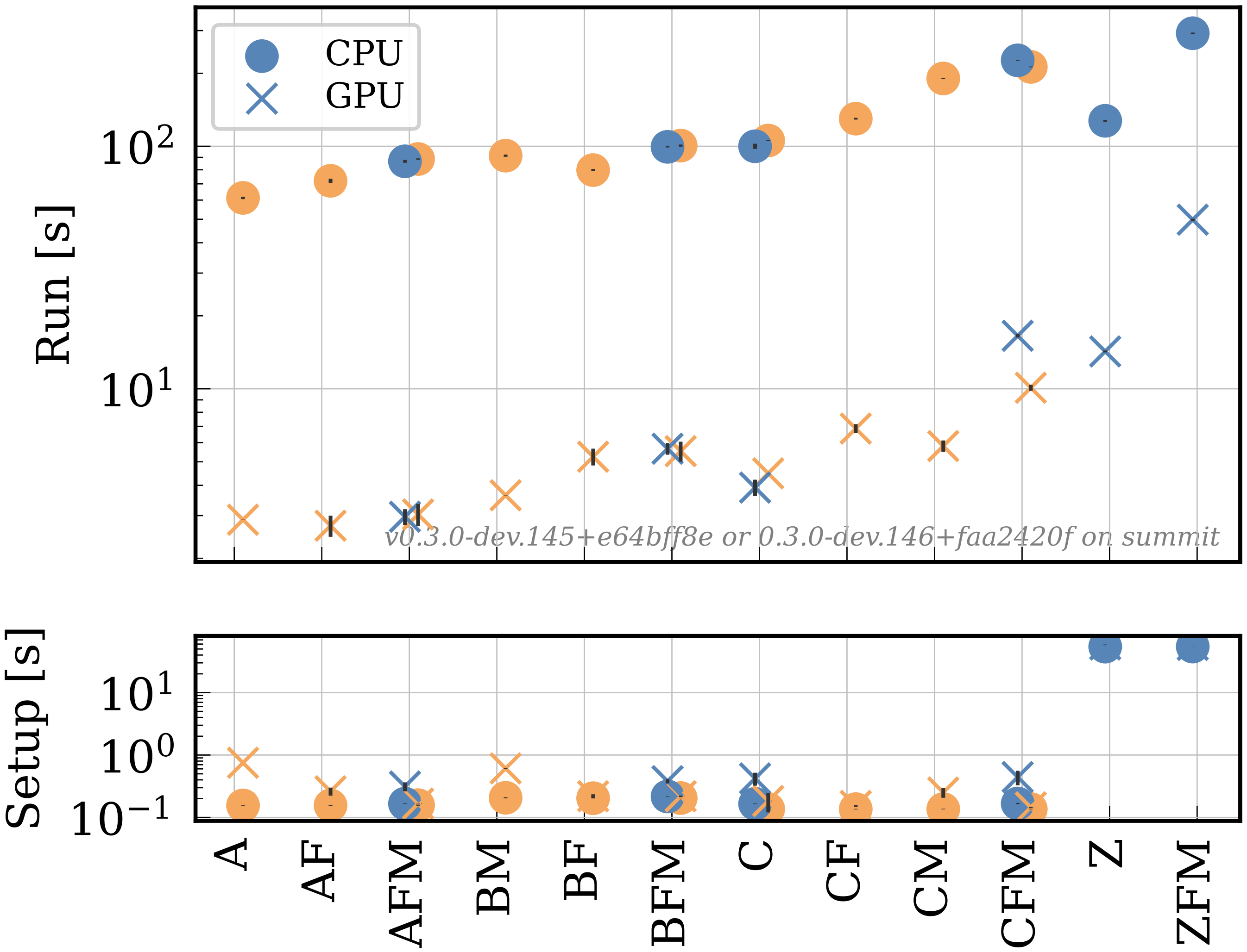


Thread-local
Shared

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

**New code for v0.2*

Regression problem run time



ORANGE
VecGeom

Problem definition

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Modifier

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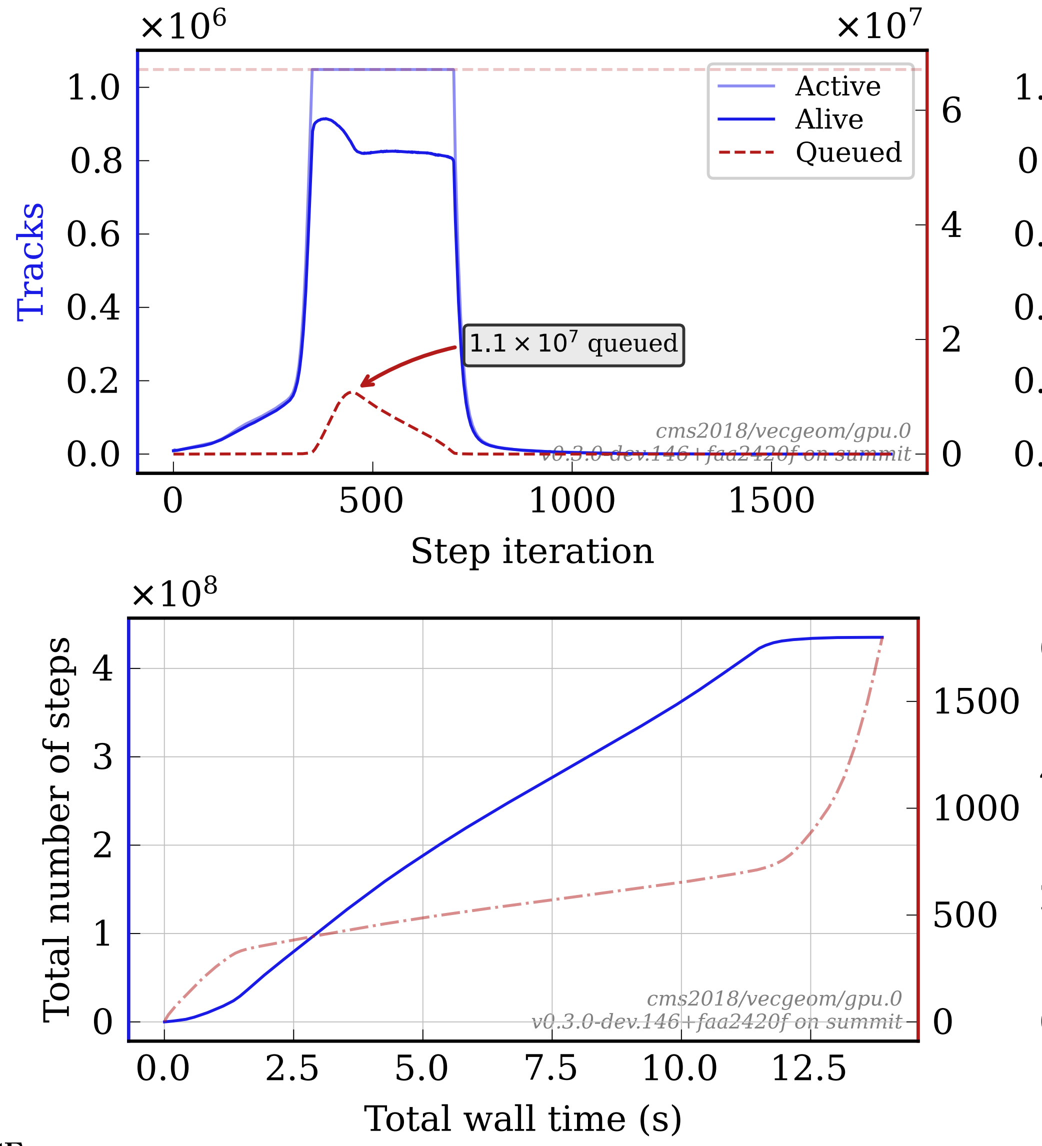
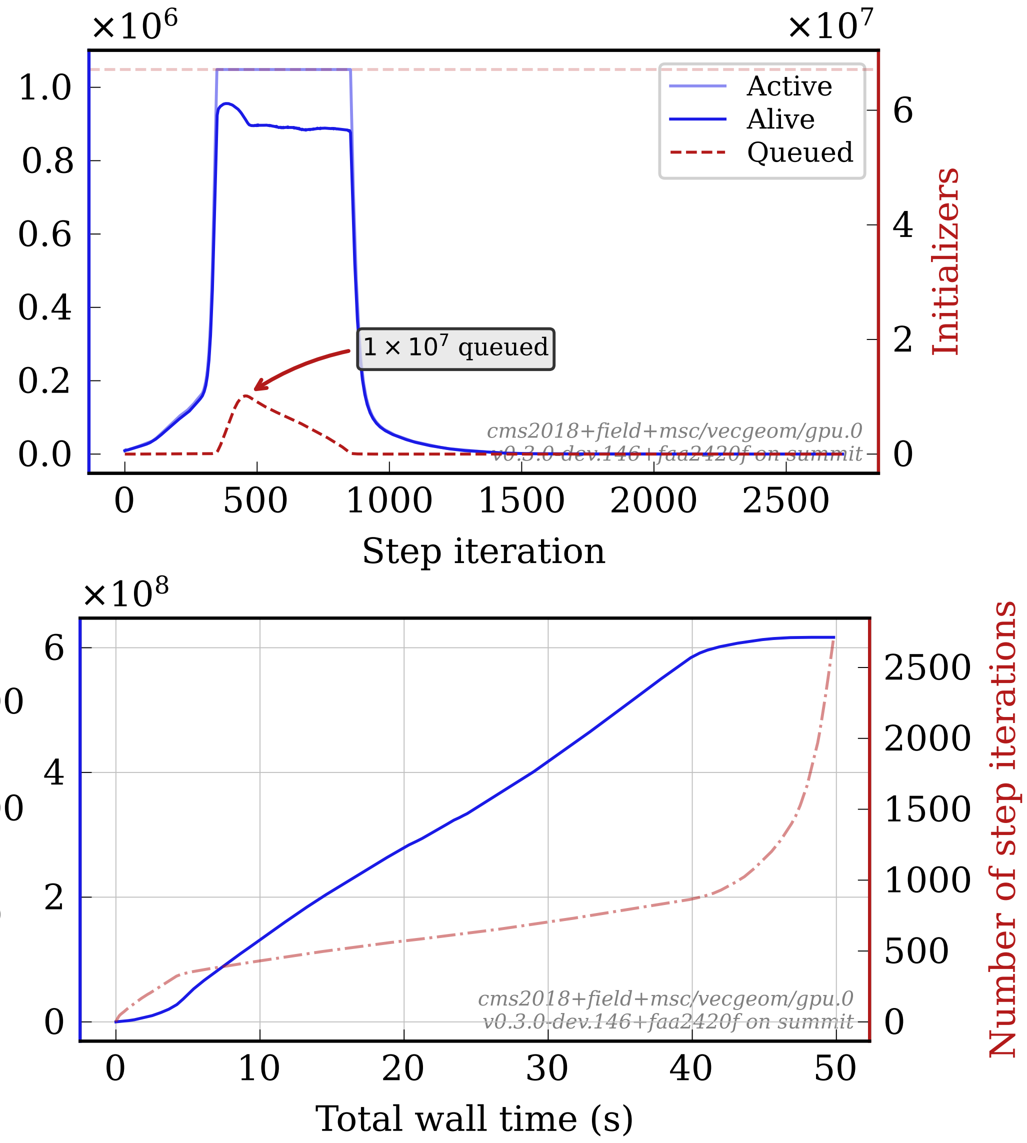
CMS2018 performance



CMS2018 ***GPU*** *without field or MSC*



CMS2018 ***GPU*** *with field and MSC*

ORANGE *Oak Ridge Advanced Nested Geometry Engine*

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

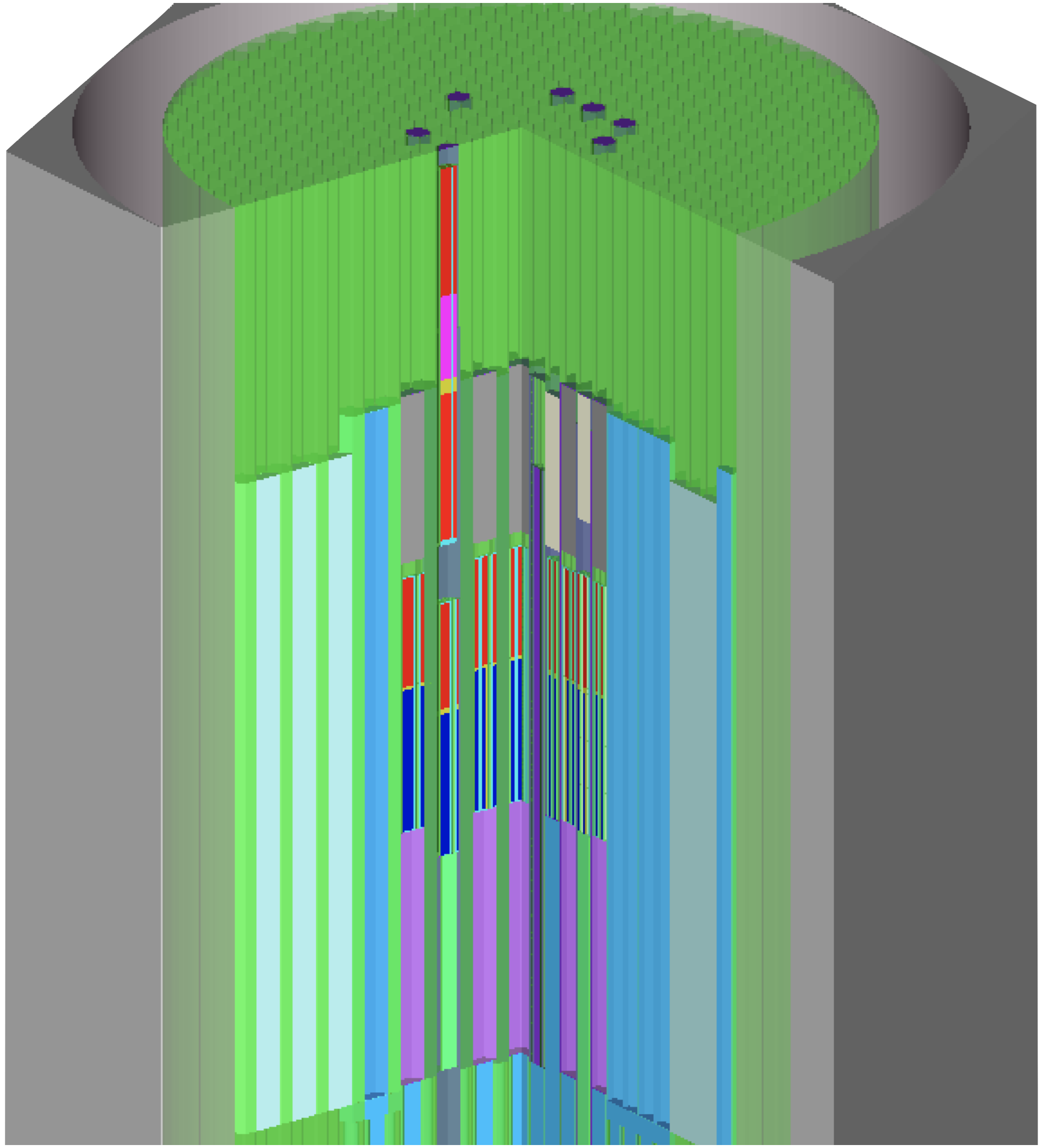
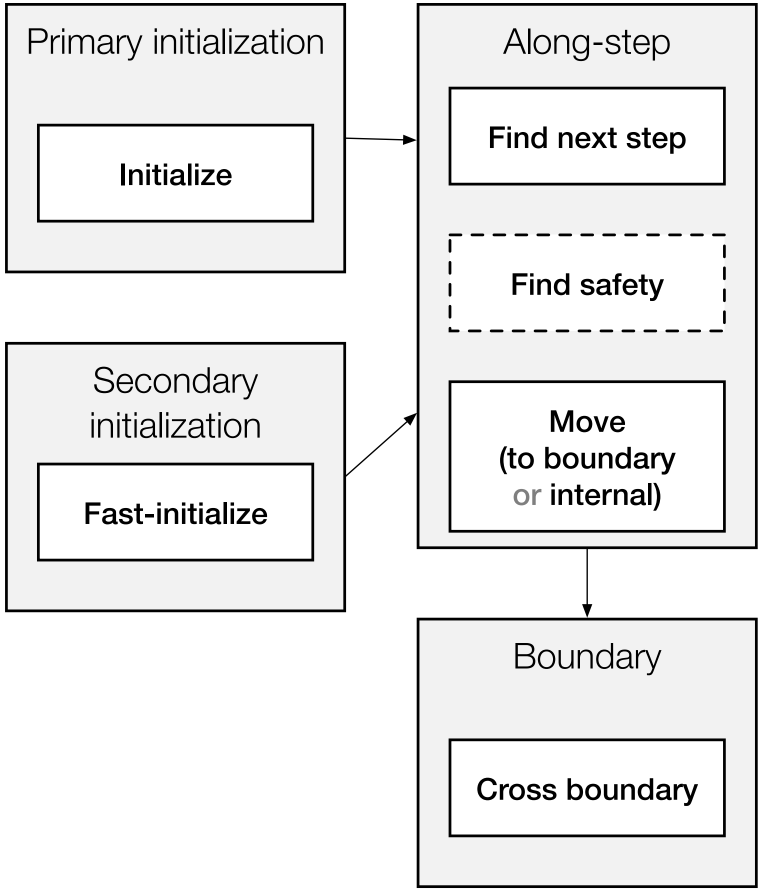


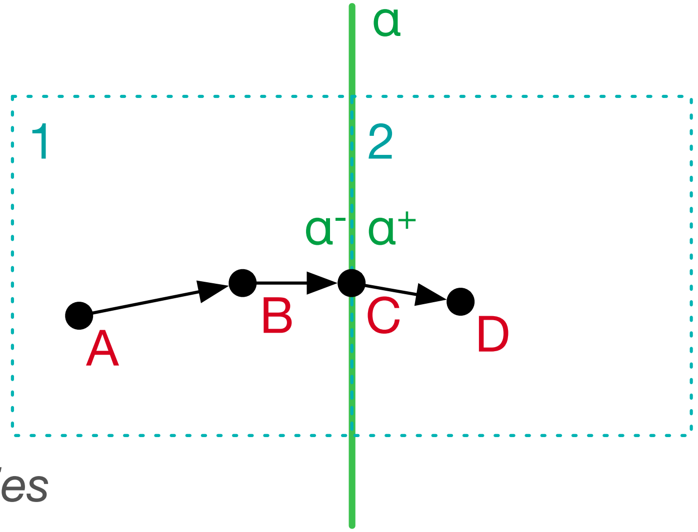
Image credit: Steve Skutnik (ORNL)

ORANGE surface-based tracking methodology

Celeritas geometry interface

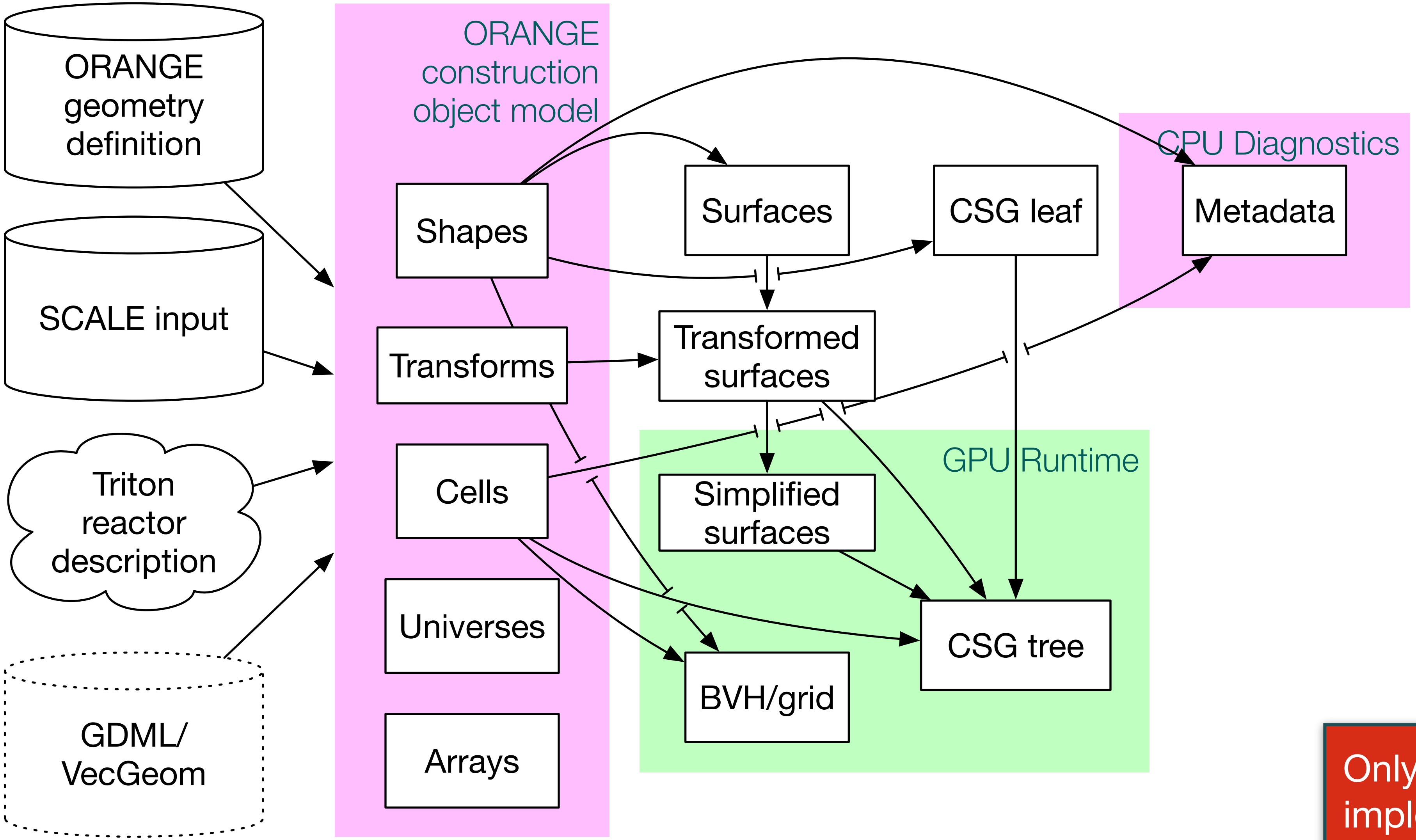


	Position	Volume	Surface+Sense
(input)	A	—	
Initialize	A	1	—
Find step	A	1	—
Move internal	B	1	—
Move to bdy	C	1	α inside
Cross bdy	C	2	α outside
Move internal	D	2	—



**exact handling of direction changes on boundaries*

ORANGE surface/volume construction



Only **partially** implemented in Celeritas ORANGE