High Energy Physics
Center for Computational Excellence:
ORNL: Celeritas

DOE HEP CCE All-Hands
July 22-24 2024

U.S. DEPARTMENT OF ENERGY | Office of Science
Argonne NATIONAL LABORATORY
Brookhaven National Laboratory
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BERKELEY LAB Bringing Science Solutions to the World

Phase 2 Objectives: Detector Simulation

Detector Simulation HEP-CCE Objectives

- Platform portable, accelerated optical photon transport integrated in luminescent detector frameworks
  - E.g., BACCARAT, art, CalVision, Gaudi or others
- Platform portable geometry representation and navigation
  - Monte Carlo detector simulation fully validated and accepted by experiments
  - Reconstruction e.g., integration with ACTS (ATLAS Common Tracking Software)

Completion Criterion

- Validate optical photon physics on defined benchmarks
- Improve LZ optical photon simulation throughput by 20–25× for G2; 50× for G3
- Reduce cost of geometric operations in particle event tracking loop by a factor of > 2
- Verify geometric tracking on community detector benchmark models demonstrated on DOE LCF architectures including full CMS and ATLAS/TileCal models

Cross-Cutting Activities and SIM Outreach

External Collaborations

- Participate in community meetings
  - Geant4 collaboration
  - CHEP
  - HSF Simulation Working Group
  - Experiment Software Weeks and simulation group meetings
- DOE CSGF practicums
- Current university collaborators
  - University of Virginia (CalVision)
  - University of Massachusetts - Amherst
- External Collaborators
  - SWIFT-HEP
  - AdePT (CERN SFT)
  - CMS, ATLAS, ALICE, DUNE/SBND, LHCb, LZ, CalVision simulation teams

Cross cuts across HEP-CCE

- SIM
  - Coupled event-generator/detector simulation on-device
- SOP
  - Migration to RNTuple for parallel I/O
- SMiLe
  - Training data generation

Celeritas/SIM Meetings

- **bi-weekly open slot**
  - 2/week team standups
  - update hep-sim email list
  - update indico HEP-CCE page
- **Open Issue tracking**
  - github:celeritas-project

Detector Simulation Milestones - FY24

Optical Photons

1. Implement GPU optical physics models (Nvidia/AMD)
2. Integrate GPU optical photon event loop into Celeritas with verification and baseline performance on (simplified) LZ geometry models

Geometry

1. Develop GPU-enabled surface-based shape models needed for ATLAS, CMS, and other experimental detector models

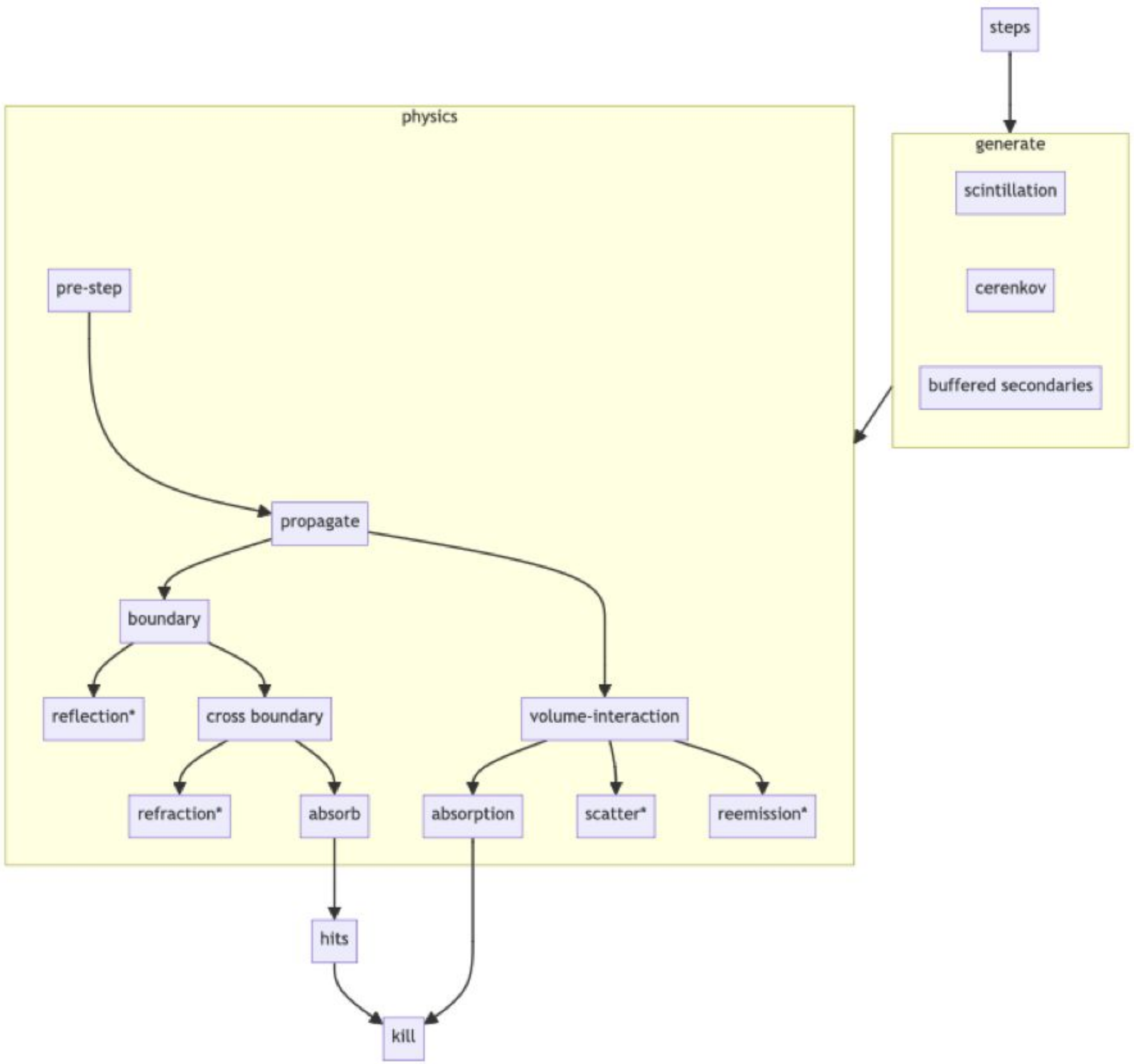
Optical Photons

Optical Photon Transport

Challenge: thousands of optical photons can be emitted per track per step, leading to long run times

Initial goal: integrated optical tracking loop with absorption by end of summer

- ✓ Geant4 optical data import
- ✓ Scintillation production
- ✓ Cerenkov production

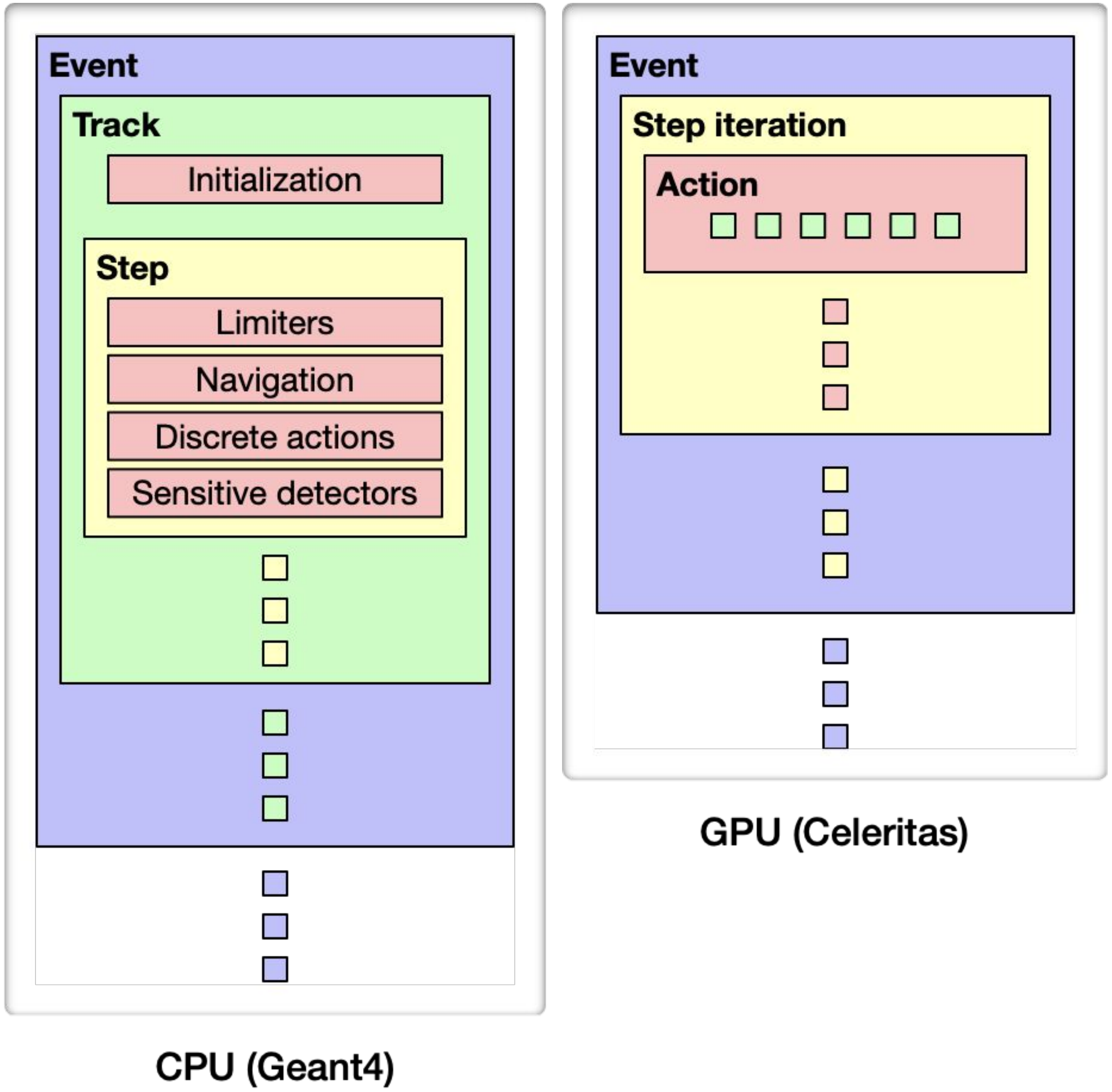


Core algorithm for simulation: stepping loop

- External synchronization point at each "event" (*p*–*p* collision)
- Dependency between steps and independence of tracks allows *loop interchange*
- Instead of polymorphic functions operating on a single track, they launch a kernel over *many* tracks

Optical photon loop has simplified physics

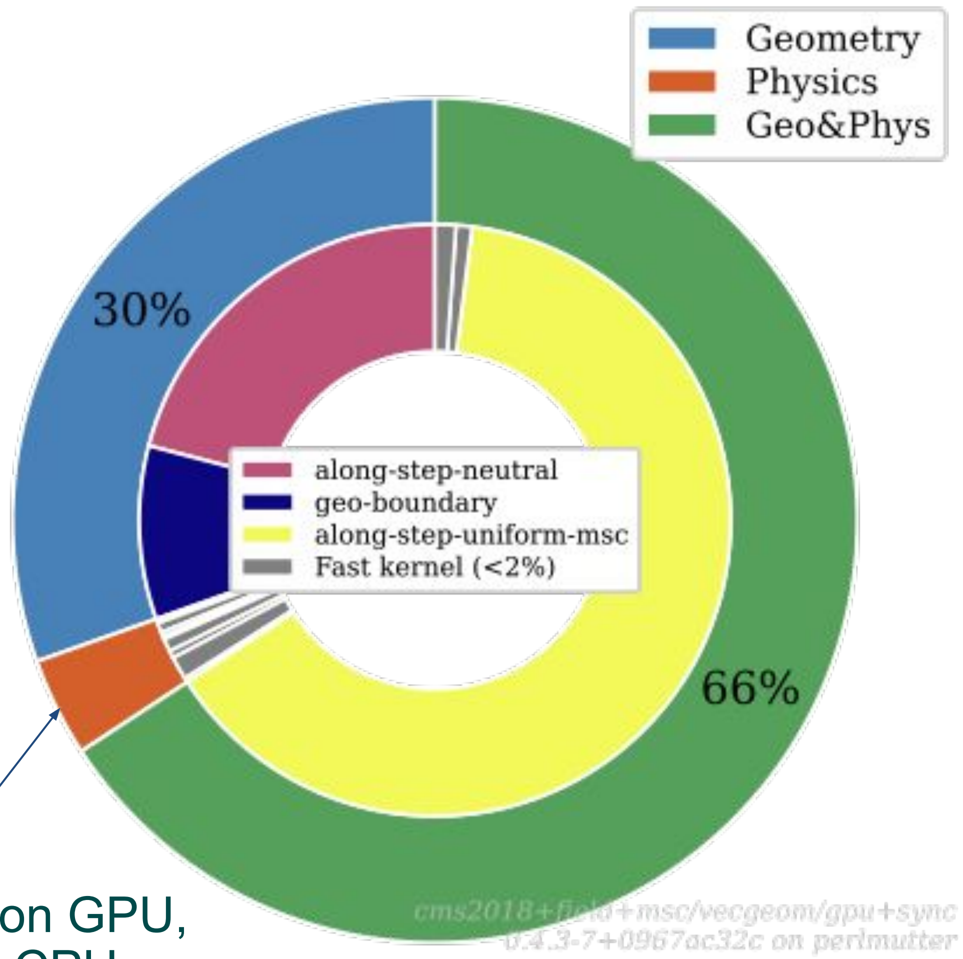
- discrete volume and surface physics only
- no safety distance
- no along-step processes
- ***specialized tracking loop to achieve desired performance***



Computational Tracking Geometry

Primary LHC Bottleneck: Geometry

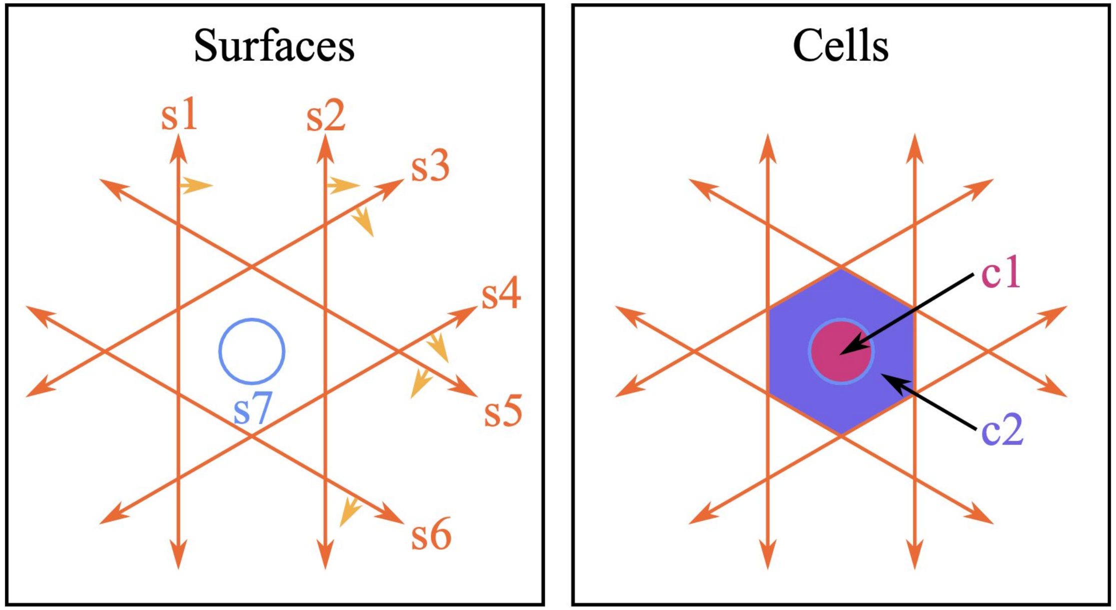
- Each step* may require 100 “distance to boundary” evaluation
  ** ~1B steps per simulation!*
- Up to ~10^5 distinct geometric elements per detector model
- CERN (VecGeom) and ORNL (ORANGE via HEP-CCE2) both implementing potential solutions



Physics is 4% on GPU,
but 19% on CPU

Geometry background and goals

- Universal volume-based detector geometry description
  - Multiple front ends: DD4HEP, GDML
  - Multiple back ends: Geant4, ROOT, VecGeom
- Volume-based tracking is not performan on GPU
- ORANGE: GPU-optimized geometry representation using surfaces
  - New: Geant4 volume conversion
  - In progress: safety distance



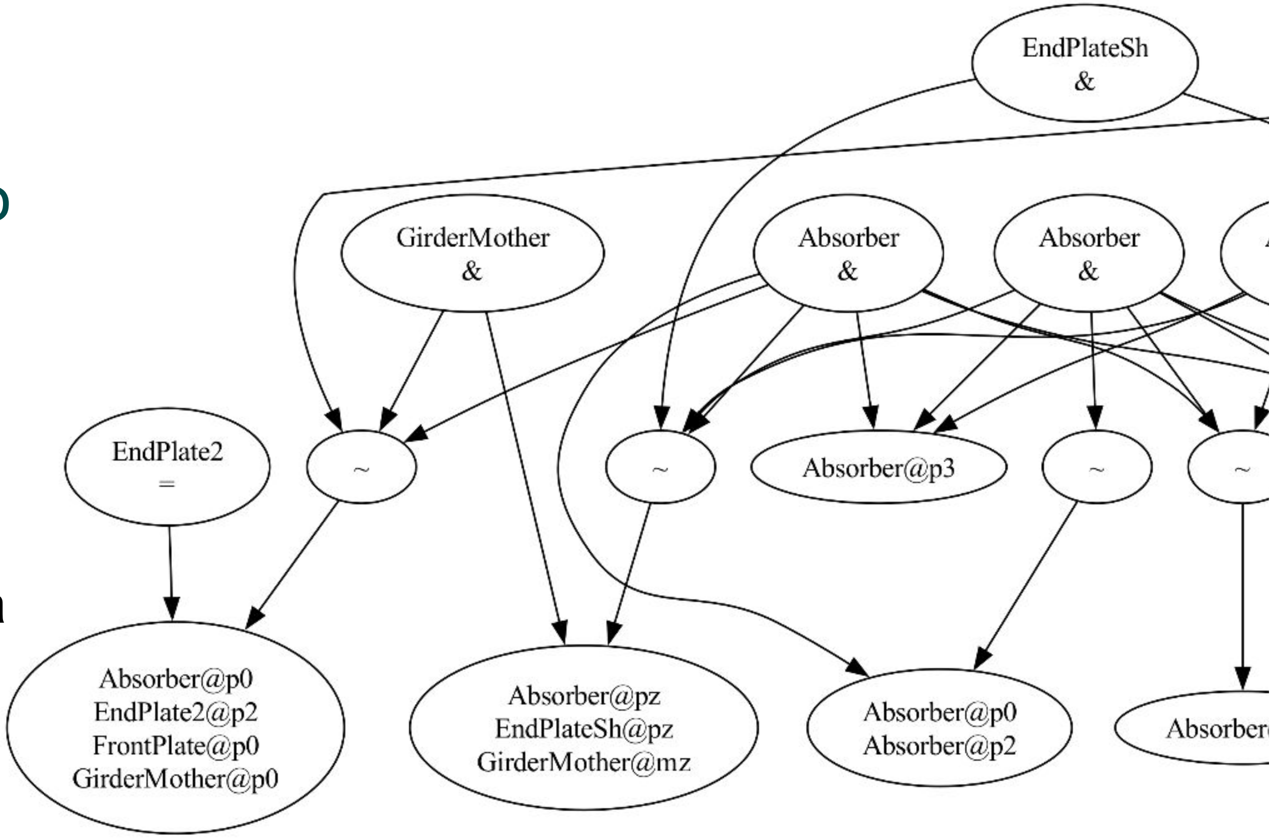
Logic used to form cells

c1: -s7

c2: +s1 -s2 +s3 -s4 +s5 -s6 +s7

Volume-to-surface conversion

- Constructed in-memory using Geant4
- Combine multiple related volumes into a repeatable “unit”
  - Single-use volumes
  - Leaf nodes (no embedded volumes)
- For each unit:
  - Construct surfaces from each volume in a local reference frame
  - Apply transformations
  - Merge nearly-coincident surfaces



Some surfaces and volumes constructed from ATLAS TileCal

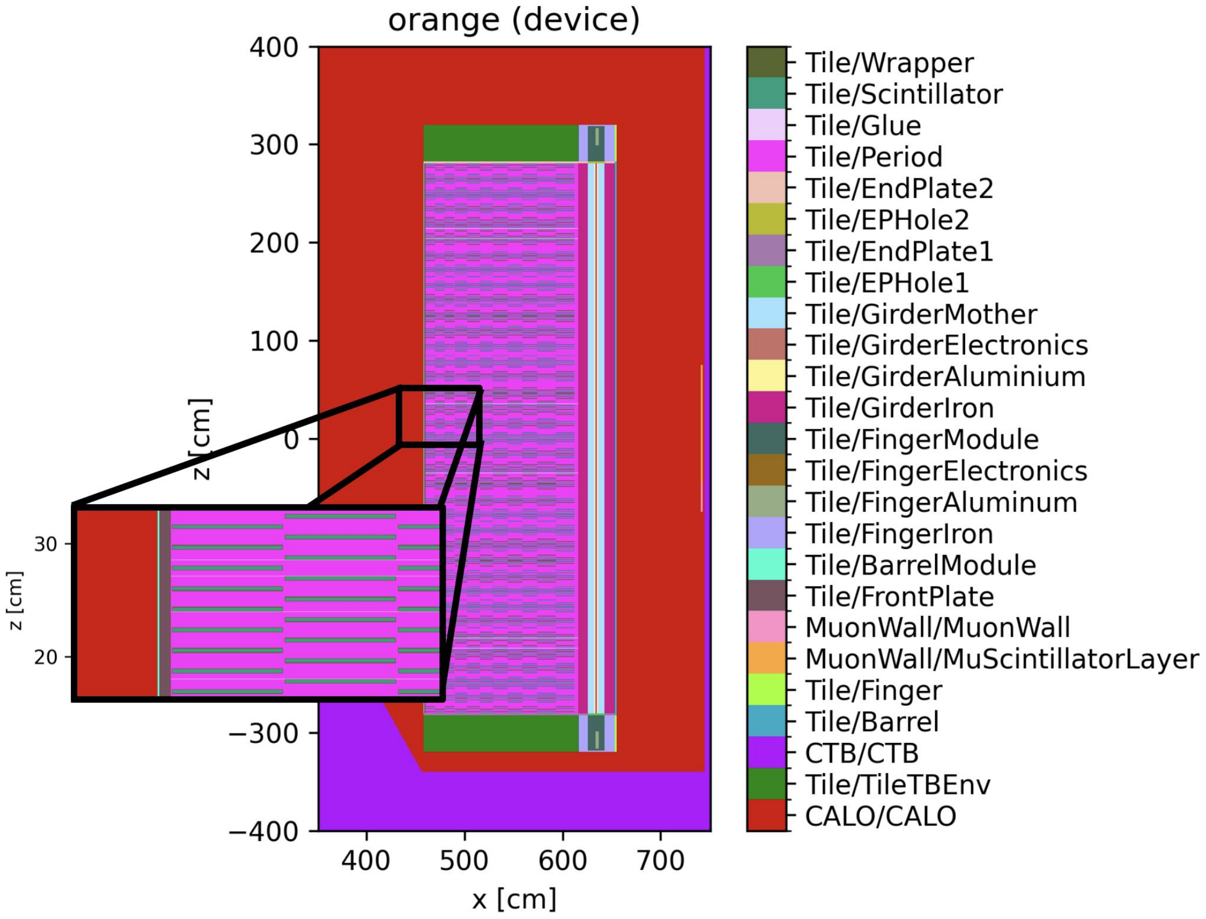
Task list

Challenge: most compute-intensive aspect of EM simulation on the GPU

- ✓ Model conversion
- ✓ Robust surface construction
- ➢ Model verification
- ➢ Performance optimization
- ✖ Safety calculation

Initial targeted geometry

- ATLAS TileCal
- CMS HGCal
- ATLAS EMEC



GPU ORANGE ray trace of ATLAS tile calorimeter

Full physics performance coupling to Geant4 (VecGeom)