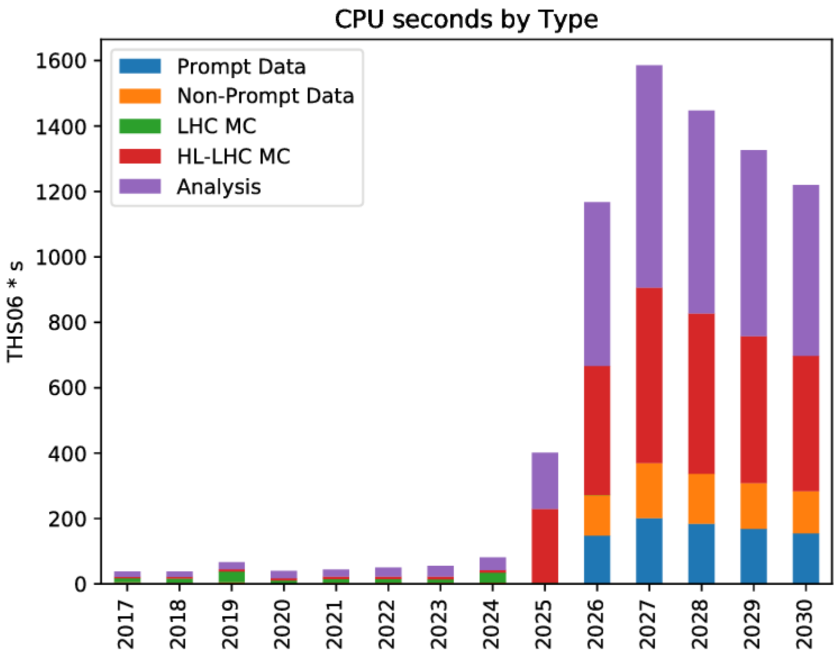
Integration of New Simulation Technologies in the Experiments

Kevin Pedro (FNAL)
on behalf of ATLAS, CMS, LHCb

Joint HSF/OSG/WLCG Workshop

March 21, 2019

Introduction



HSF Community White Paper
arXiv:1712.06982

- HL-LHC presents significant computing challenges
  - 10× data vs. Run 2/3
  - >10× increase in # channels for upgraded detectors
  - May need improved physics models to simulate complex detectors accurately
  - Reconstruction will take a larger fraction of CPU time (200PU vs. ~30PU in Run 2)

❖ Detector simulations need to produce more events with more accuracy in a more complicated geometry… w/ smaller fraction of total CPU usage

➢ Possible solutions: vectorized software and heterogeneous hardware

Vectorized Components

- **VecCore** (GitHub/root-project)
  - Libraries: Vc, UME::SIMD, CUDA
- **VecMath** (GitHub/root-project)
  - Spinoff of VecCore, dedicated to math utilities (including RNGs)
- **VecGeom** (CERN/GitLab)
  - Vectorized geometry and navigation, multi-particle interface
- **GeantV** (CERN/GitLab)
  - Vectorized transport engine for detector simulation: geometry navigation, magnetic field, EM physics
  - pre-beta tags now available, beta release coming soon

DD4hep in the Experiments

- Not a vectorized package, but a common solution for detector description
- Uses ROOT TGeo to handle geometry construction

CMS:

- Infrastructure for migration in place, tested w/ muon system (drift tubes)
- Provided significant feedback to DD4hep developers
- Contacts established to migrate other subdetectors

ATLAS:

- Testing DD4hep as a description language
- Need to use GeoModel for backend rather than TGeo (not supported)

LHCb:

- Testing w/ Gaussino, new lightweight simulation framework (CHEP2018)
- Provided feedback for TGeo (optical surfaces)
- Plan to use DDG4 simulation toolkit to convert geometry for Geant4

VecGeom in the Experiments

CMS:

- VecGeom used in scalar mode with Geant4
- 7–13% speedup with similar memory usage
  → Just from code improvements, no vectorization!

➢ Included in production for >1 year

ATLAS:

- VecGeom tested in scalar mode with Geant4: just Cones and PolyCones used
- 1–3% speedup observed
- Testing with all shapes from VecGeom in progress
  - Also testing w/ different Geant4 versions (10.4.2, 10.5)

LHCb:

- VecGeom tested in scalar mode with Geant4
- No speedup observed: likely due to simple shapes in detector geometry

GeantV in the Experiments

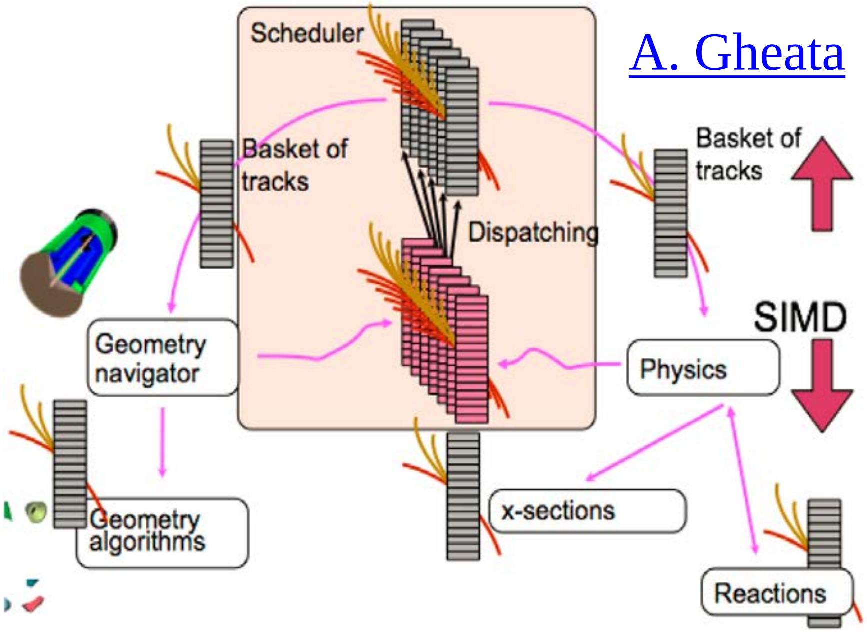
CMS:

➢ Significant effort in testing

- First stage: cmsToyGV (in GeantV alpha)
  - o Integrate w/ simplified toy-mt-framework
  - o Demonstrate compatible threading model
  - o Example of ExternalLoop mode
- Second stage: integration in CMSSW
  - o See SimGVCore
  - o In progress, details to follow
- Third stage: performance testing
  - o Use beta release when available

LHCb:

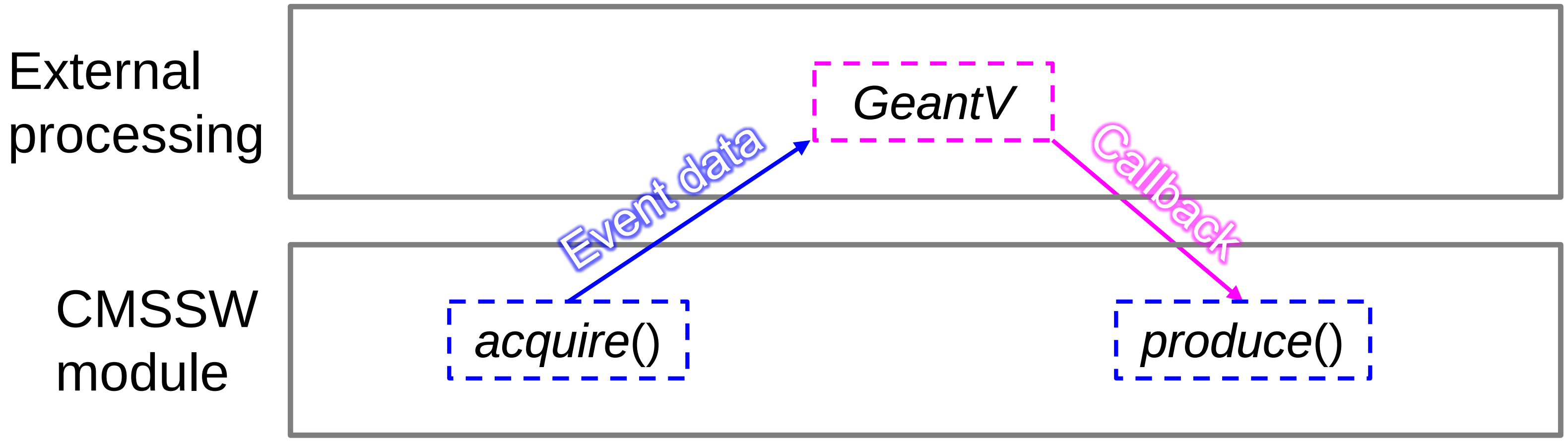
- Plan to integrate w/ Gaussino



A. Gheata

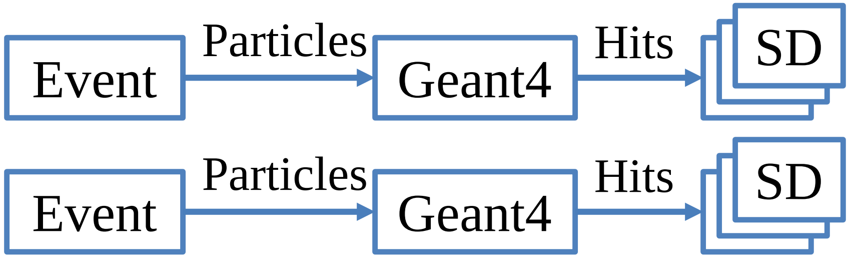
Elements of GeantV Integration in CMSSW

- ✓ Generate events in CMSSW framework, convert HepMC to GeantV format
- ✓ Build CMSSW geometry natively and pass to GeantV engine (using TGeo)
- Using constant magnetic field, limited EM-only physics list
- Adaptation of sensitive detectors and scoring in progress
- Up to date with latest tag pre-beta-4
- Run GeantV in "external loop" mode using CMSSW ExternalWork feature:
  - Asynchronous task-based processing

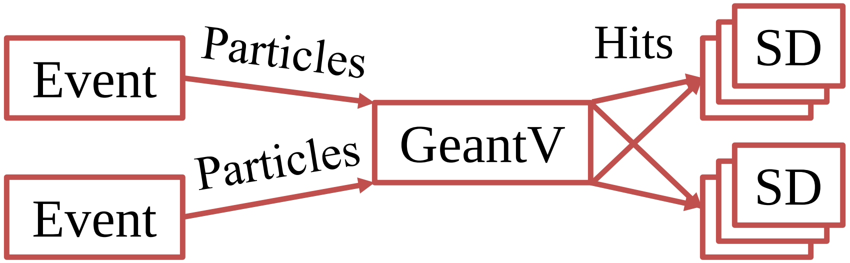


Geant4 vs. GeantV Scoring

- Sensitive detectors (SD) and scoring trickiest to adapt
  - Necessary to test "full chain" (simulation → digitization → reconstruction)
  - Significantly more complicated than Geant4 MT



Geant4 shares memory, but each event processed in separate thread



Each event processed in multiple threads, mixed in with other events

- Duplicate SD objects per event per thread, then aggregate → 4 streams = 16 SD objects
  - GeantV TaskData supports this approach

Technical Details of Scoring

- SD code uses Geant4 objects heavily: G4Step, G4LogicalVolume, etc.
- GeantV instead has Geant::Track, vecgeom::LogicalVolume, etc.
- ➢ Need “Rosetta stone” to translate various operations
  - Geometry volumes and replica numbers, material properties, etc.
  - Thanks to GeantV developers for sending this information
- How to avoid upsetting delicate and complicated SD code?
- ➢ Template wrappers to unify interfaces and operations
  - Store pointers or references to original objects – minimize memory overhead
  - No extra cost from virtual table (vs. using inheritance)
- Implementation in progress using simplified SD class
  - Future: connect to TaskData, then migrate real SD classes

ATLAS FastCaloSim on GPU

- Self-contained simulation → feasible target to profile and explore GPU port
- Standalone version runs in ROOT interpreter
  - ➢ Working on compiled version (easier profiling and porting/parallelization)
- Identified possible parallelization for `TFCSLateralShapeParametrizationHitChain::simulate()`
  - o Implementing CUDA kernel & device functions
  - o Try to minimize data transfer between CPU and GPU
- Next steps:
  - o Optimize CUDA functions
  - o Apply CUDA stream
  - o Use many GPU devices in same node (e.g. Summit) or distributed nodes
- Funded by HEP-CCE
- Collaboration between ATLAS and BNL Computational Science Initiative

Conclusions

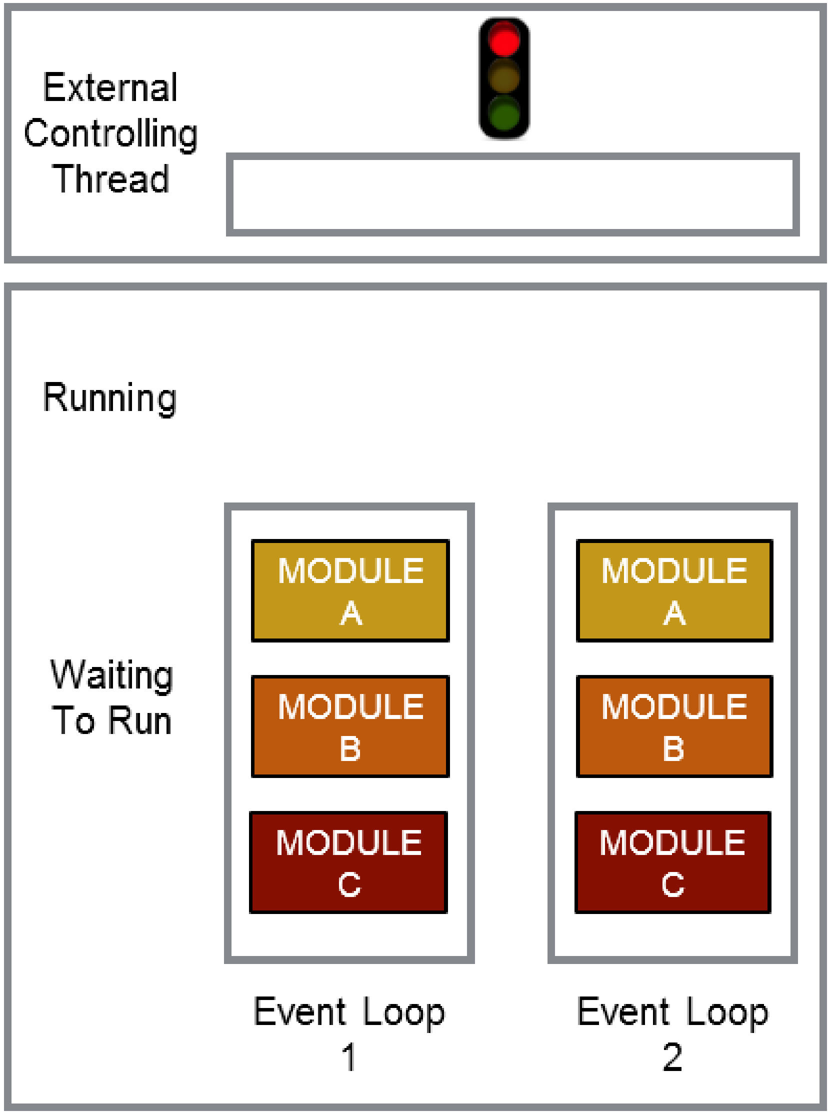
- New packages relevant to simulation are available:
  - Common solutions (DD4hep)
  - Vectorized components (VecGeom, GeantV, etc.)
- Experiments are making progress testing and integrating these packages
  - Providing frequent feedback to developers
  - Continued communication is essential to the success of these projects
  - Observed speedups vary; many factors at play, and still early
- In particular, CMS integration testing of GeantV is maturing
  - Next step: performance testing w/ beta release
    - Check if speedup translates to experimental software framework
    - Check if existing CMS speedups are compatible w/ GeantV
    - Understand full cost of migration to new interfaces
  - Provide a path for other experiments to follow

Backup

External Work in CMSSW (1)

Setup:

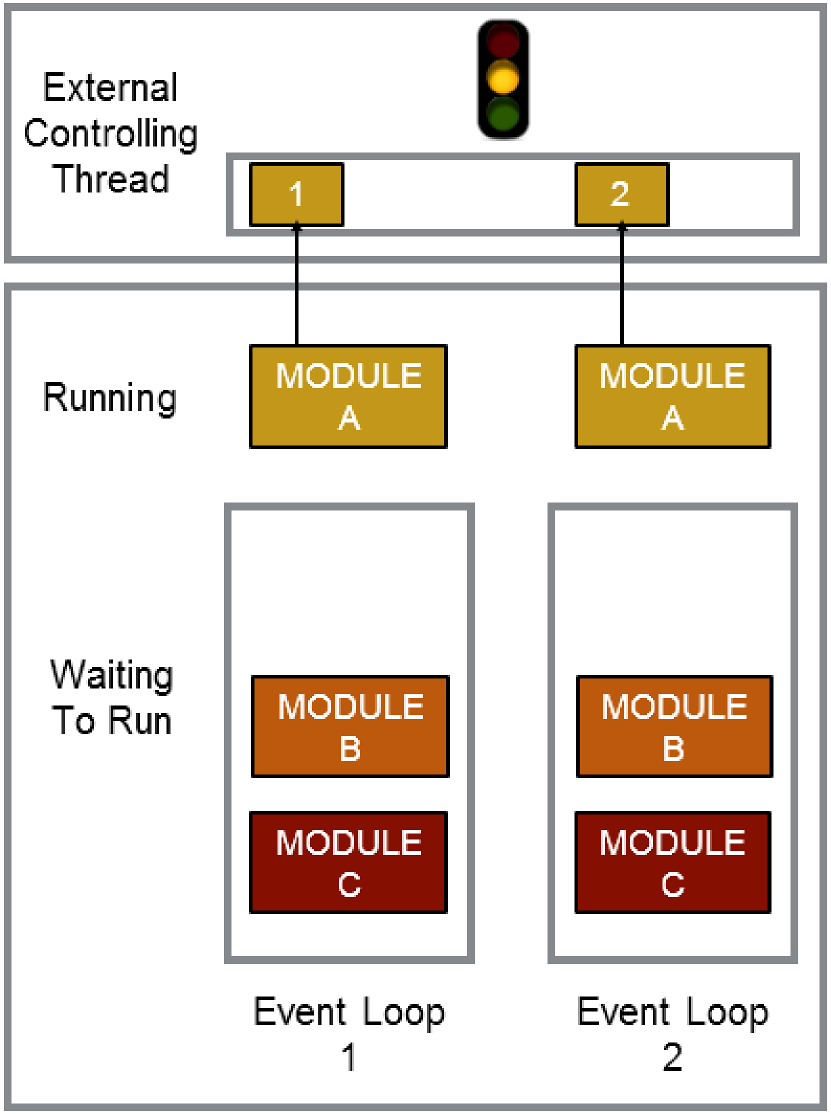
- TBB controls running modules
- Concurrent processing of multiple events
- Separate helper thread to control external
- Can wait until enough work is buffered before running external process



External Work in CMSSW (2)

Acquire:

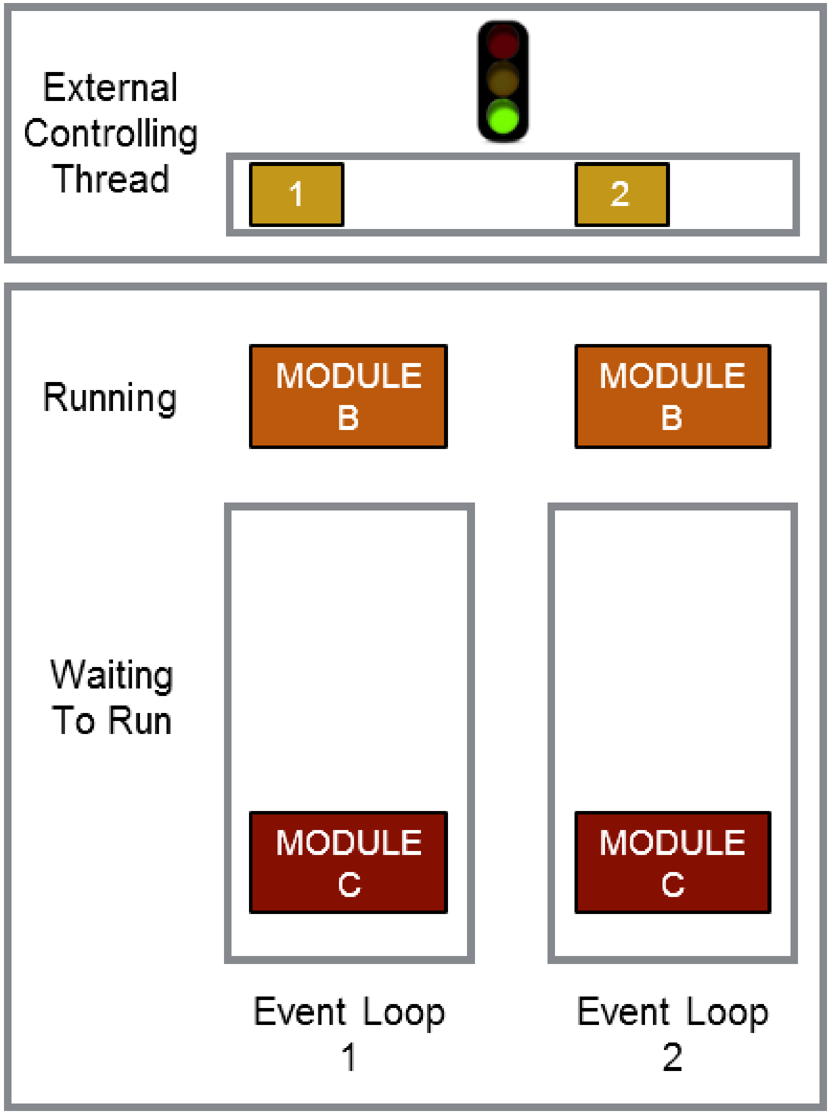
- Module *acquire*() method called
- Pulls data from event
- Copies data to buffer
- Buffer includes callback to start next phase of module running



External Work in CMSSW (3)

Work starts:

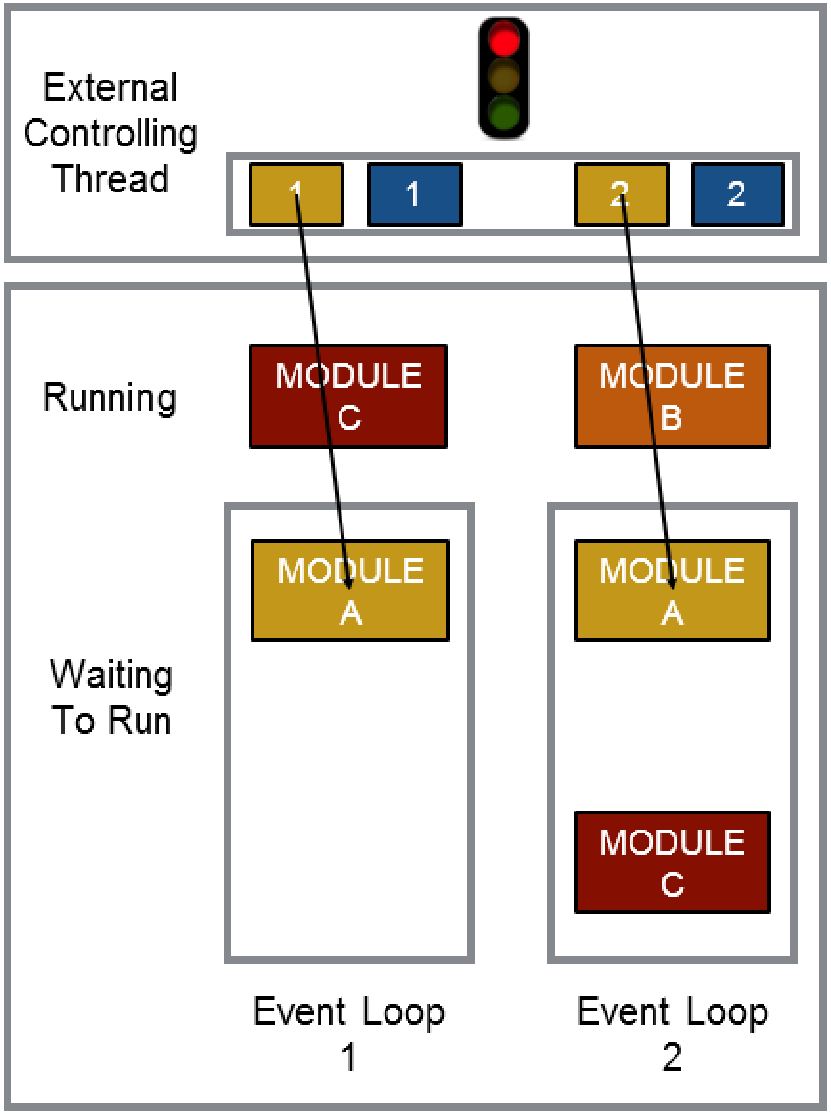
- External process runs
- Data pulled from buffer
- Next waiting modules can run (concurrently)



External Work in CMSSW (4)

Work finishes:

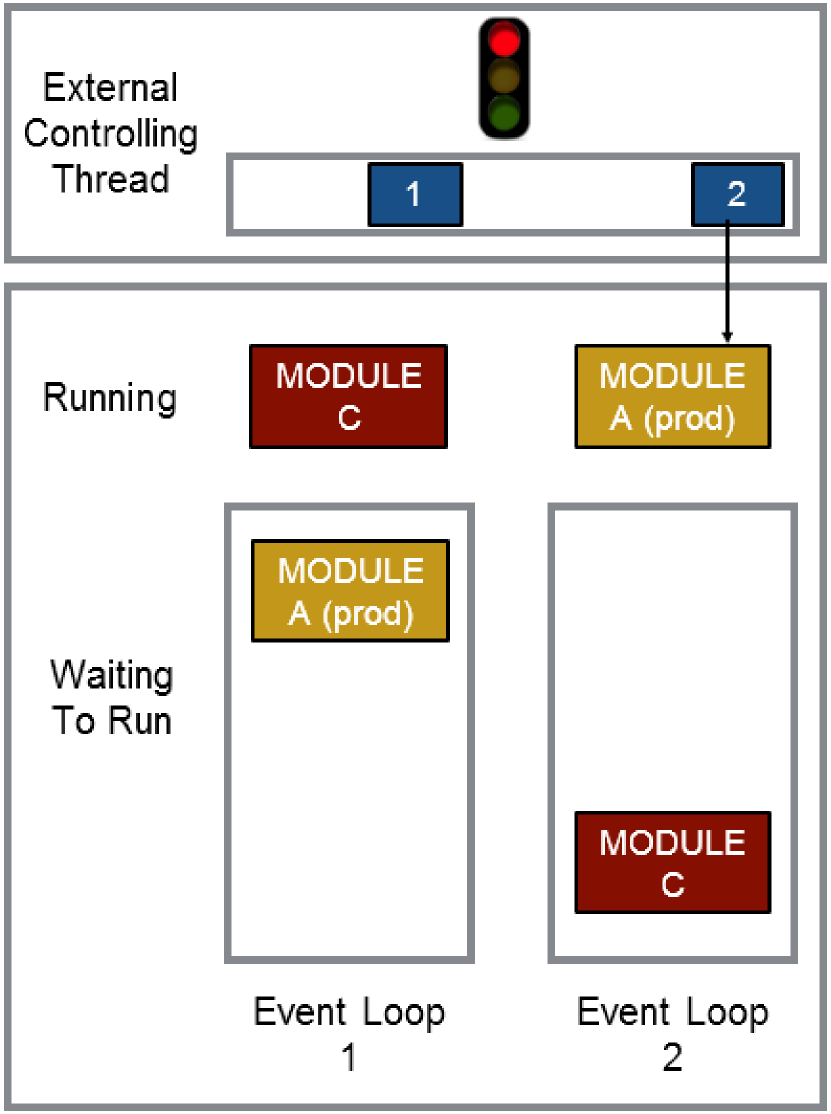
- Results copied to buffer
- Callback puts module back into queue



External Work in CMSSW (5)

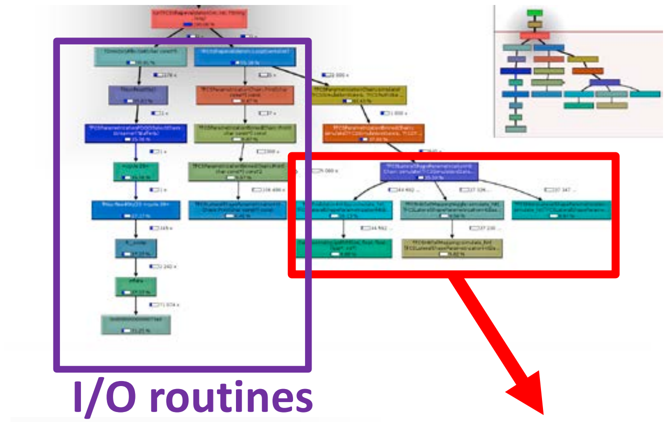
Produce:

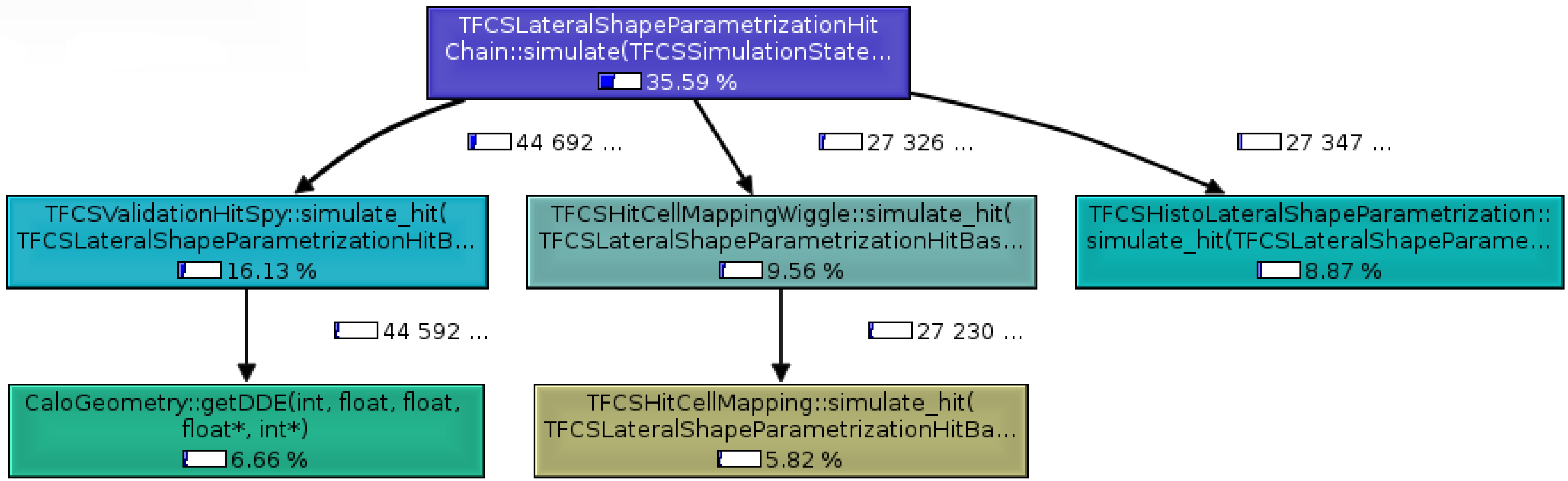
- Module *produce*() method is called
- Pulls results from buffer
- Data used to create objects to put into event



FastCaloSim Profile

- **TFCSLateralShapeParametrizationHitChain::simulate()** is the most significant routine except I/O parts.
- The running time of **TFCSLateralShapeParametrizationHitChain::simulate()** will increase as the number of hits increases.
- **TFCSLateralShapeParametrizationHitChain::simulate()** is a possible candidate to parallelize.





FastCaloSim Analysis

TFCSLateralShapeParametrizationHitChain::simulate() Structure

TFCSLateralShapeParametrizationHitChain::simulate() {

…

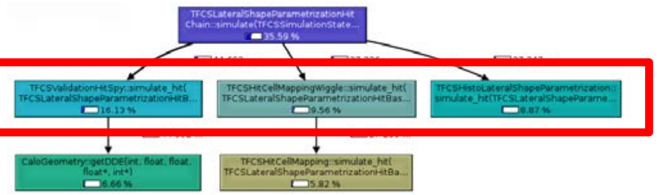
…

Loop on **nhit** → **Possible** Parallelization

…

Loop on hit_simulation_chain

Call →



→ **Impossible** Parallelization because of data dependency

End Loop

…

End Loop

…

}