Simulation Software: Fast and Full

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ATLAS Software Chain

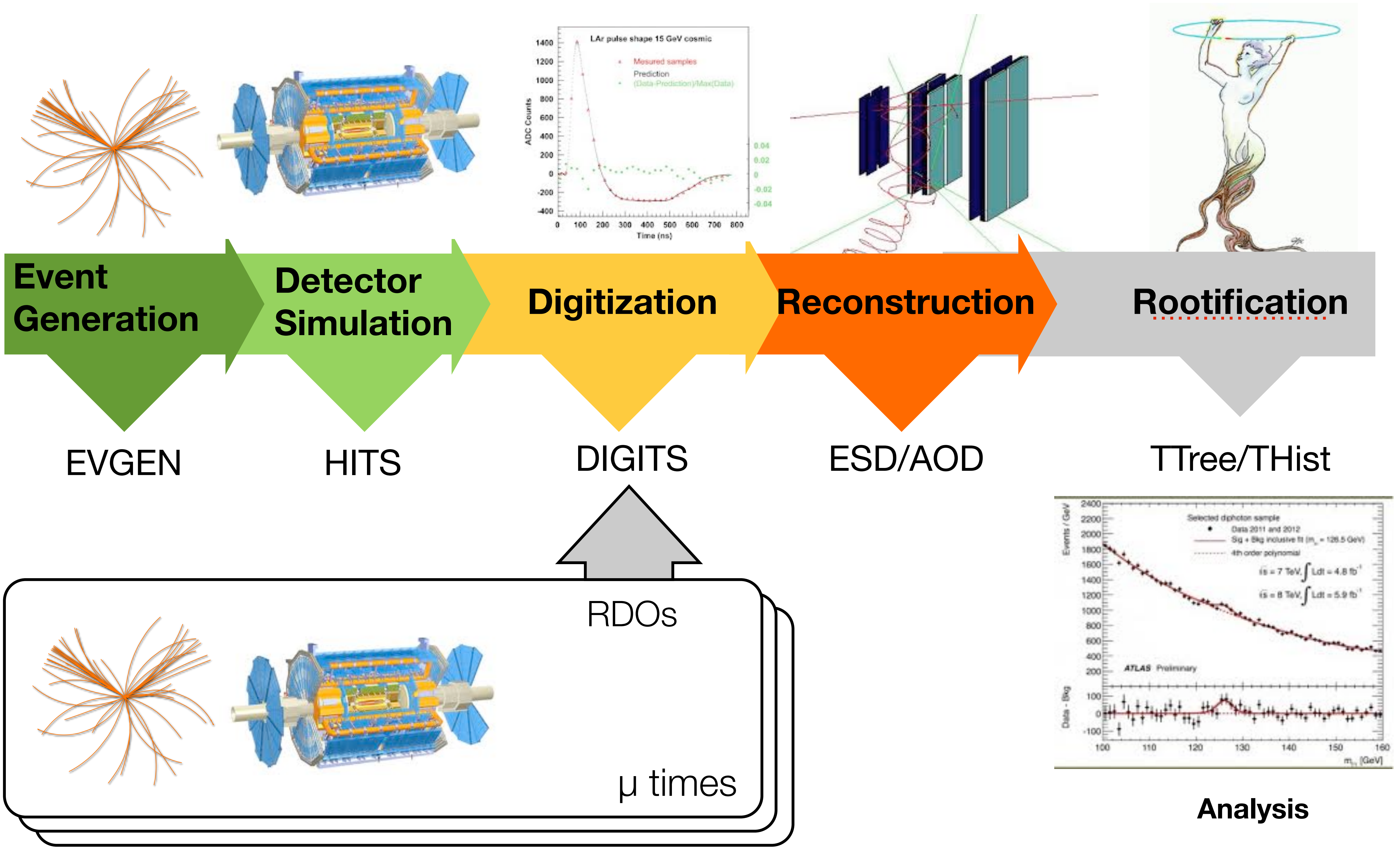
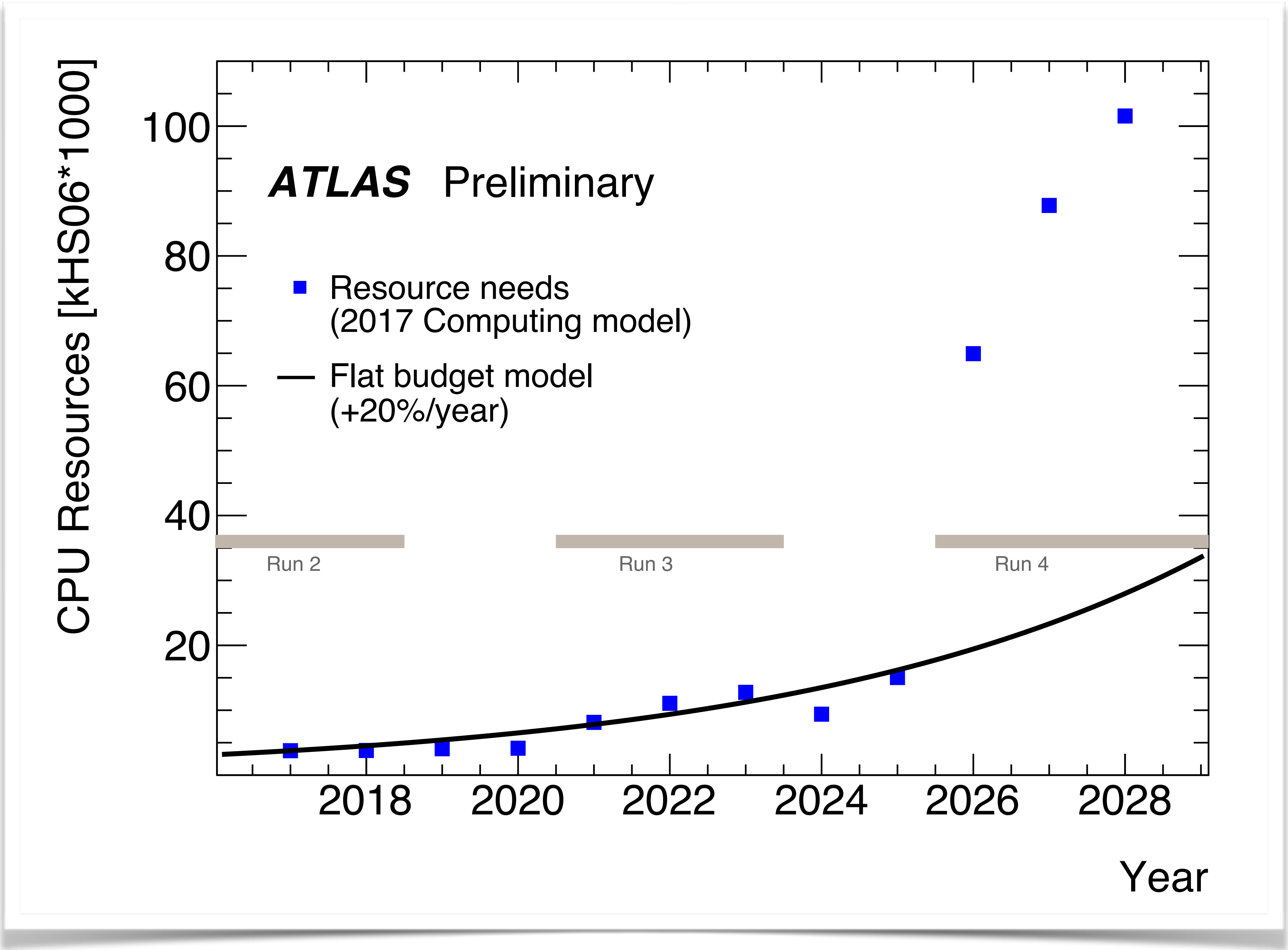


Image credit: A. Salzburger

This talk: Simulation and Digitisation

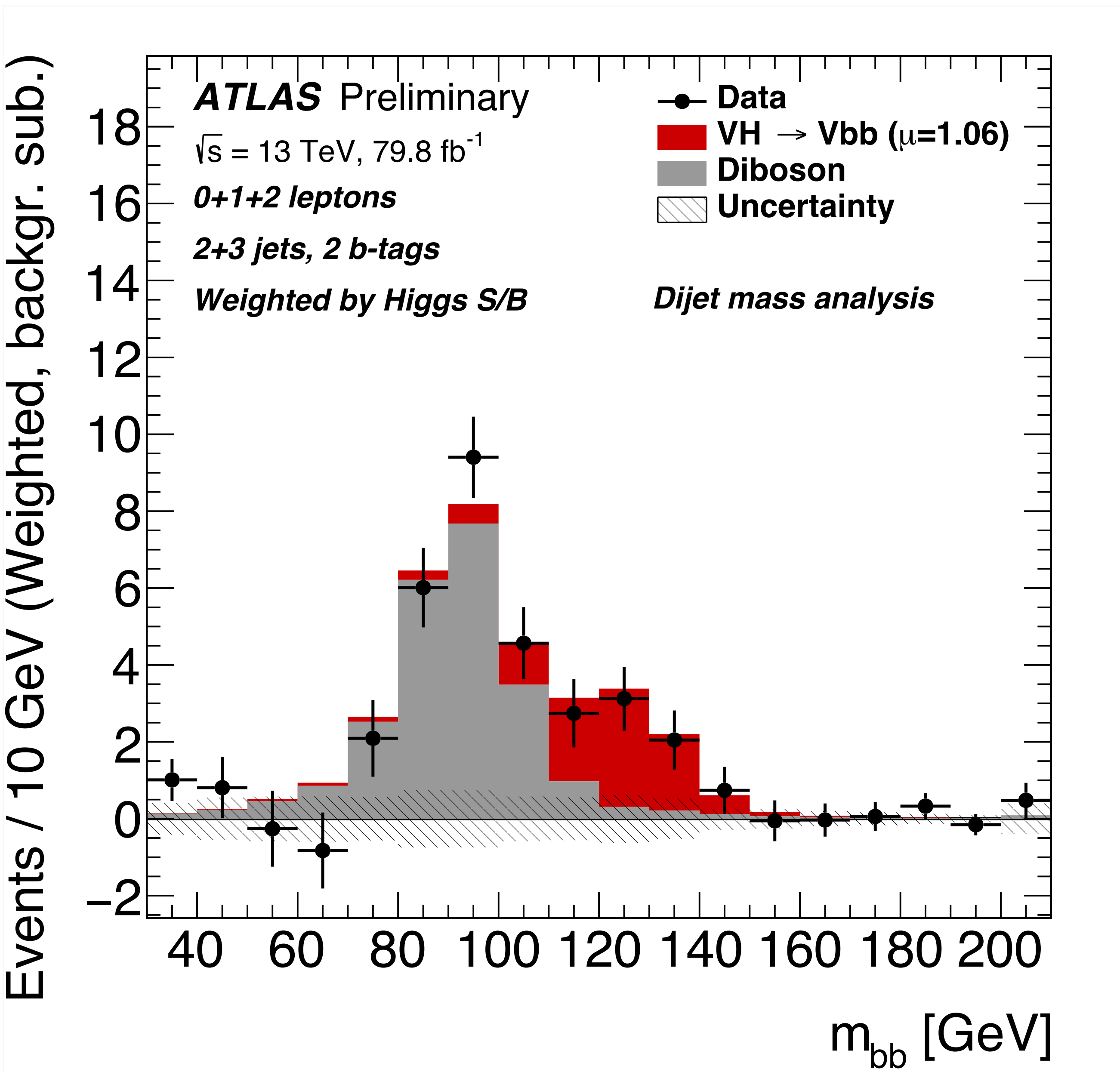
- In the **simulation** step, we simulate the interaction of the produced particles with the detector material primarily using Geant4
- In the **digitisation** step, we emulate the response of the detector electronics to the simulated particles
- These two steps are only used when producing Monte Carlo
  - With LHC data, we apply the reconstruction to the output of the detector
- This talk does not cover **event generation**: emulation of the production of particle in high-energy collisions
  - Might also be a very interesting case to consider

The HL-LHC Computing Problem



Large discrepancy between budget and resource needs

Particular issue for simulation

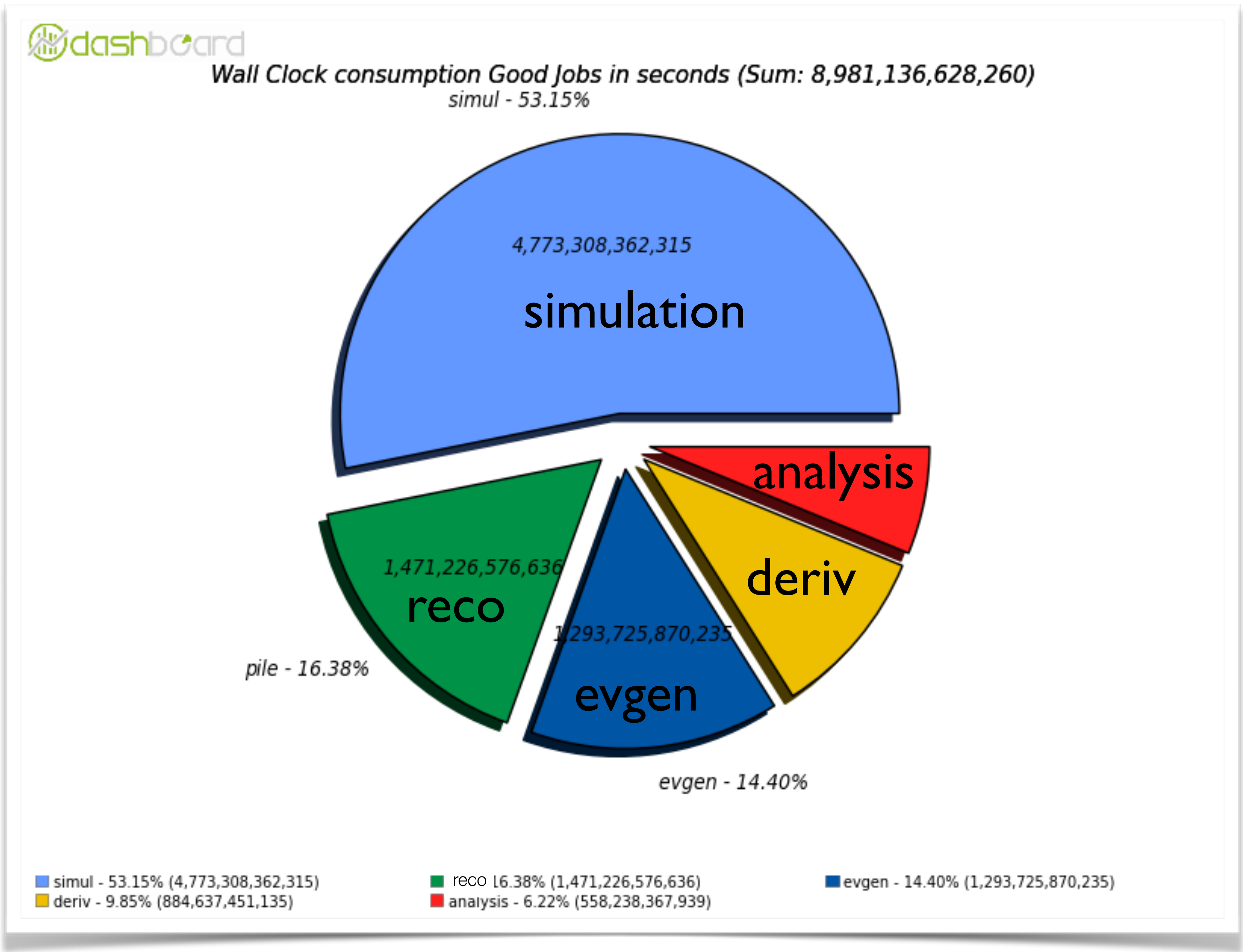


Source of uncertainty		σ_μ
Total		0.259
Statistical		0.161
Systematic		0.203
Experimental uncertainties		
Jets		0.035
E_T^{miss}		0.014
Leptons		0.009
b-tagging	b-jets	0.061
	c-jets	0.042
	light jets	0.009
	extrapolation	0.008
Pile-up		0.007
Luminosity		0.023
Theoretical and modelling uncertainties		
Signal		0.094
Floating normalisations		0.035
Z + jets		0.055
W + jets		0.060
$t\bar{t}$		0.050
Single top quark		0.028
Diboson		0.054
Multijet		0.005
MC statistical		0.070

Already now, with 80 fb-1 of data (3% of the projected total), many key analyses have MC statistics as a key systematic uncertainty

ATLAS-CONF-2018-036

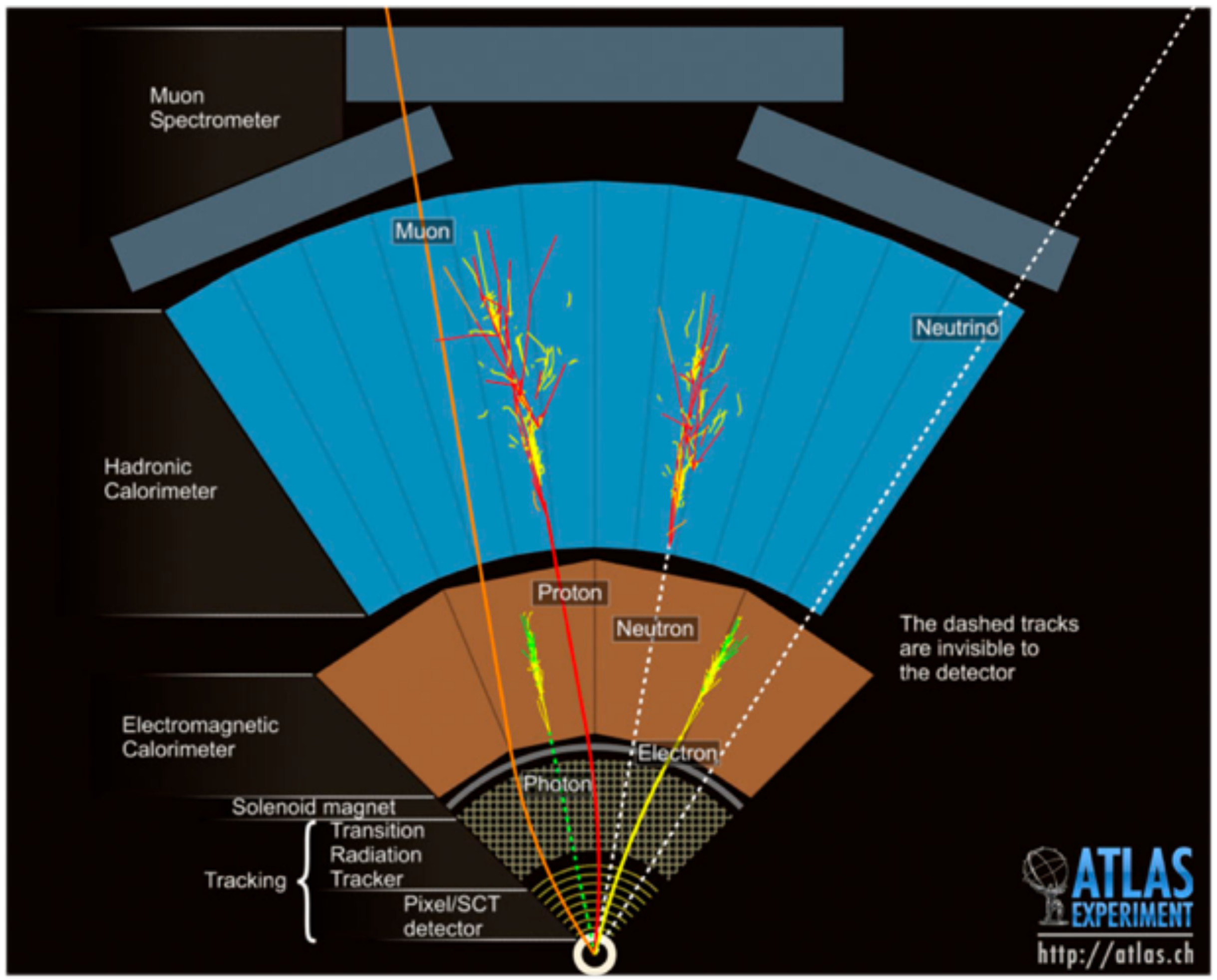
How ATLAS uses CPU

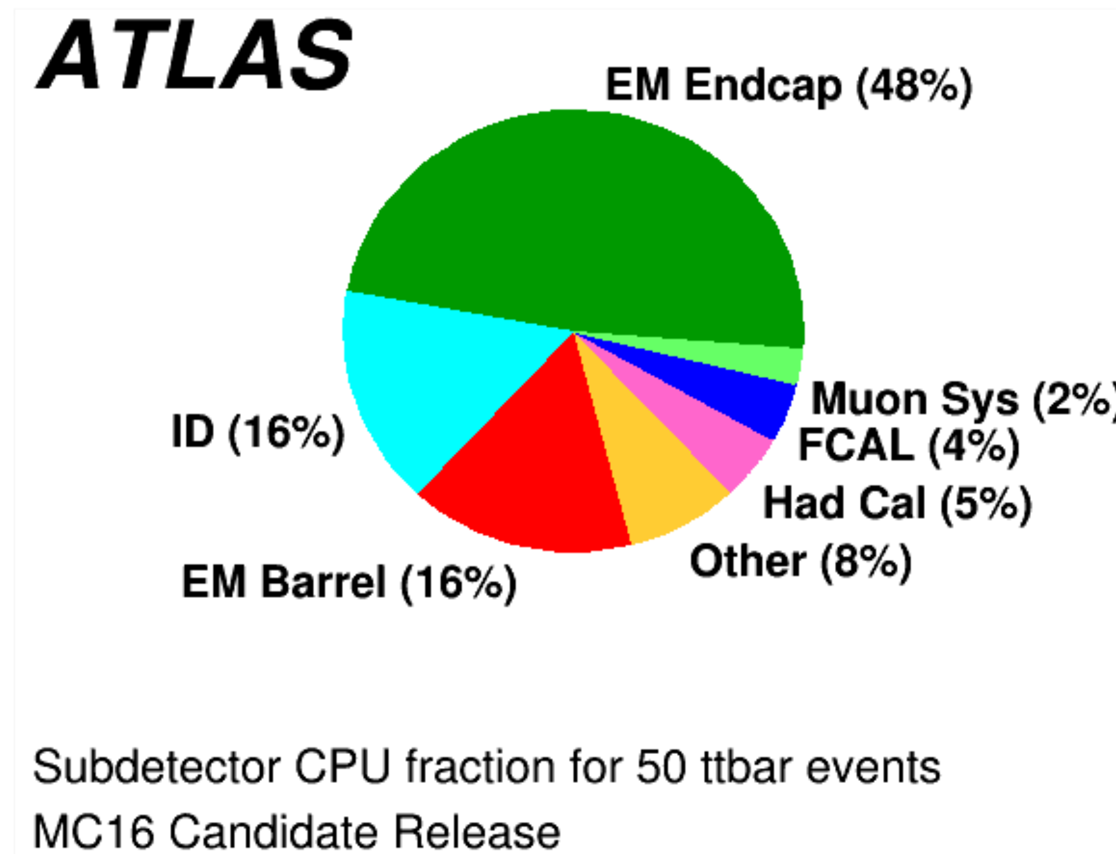


Largest fraction (53%) of CPU time is used for **simulation**

July 2017 - July 2018

Simulation by detector

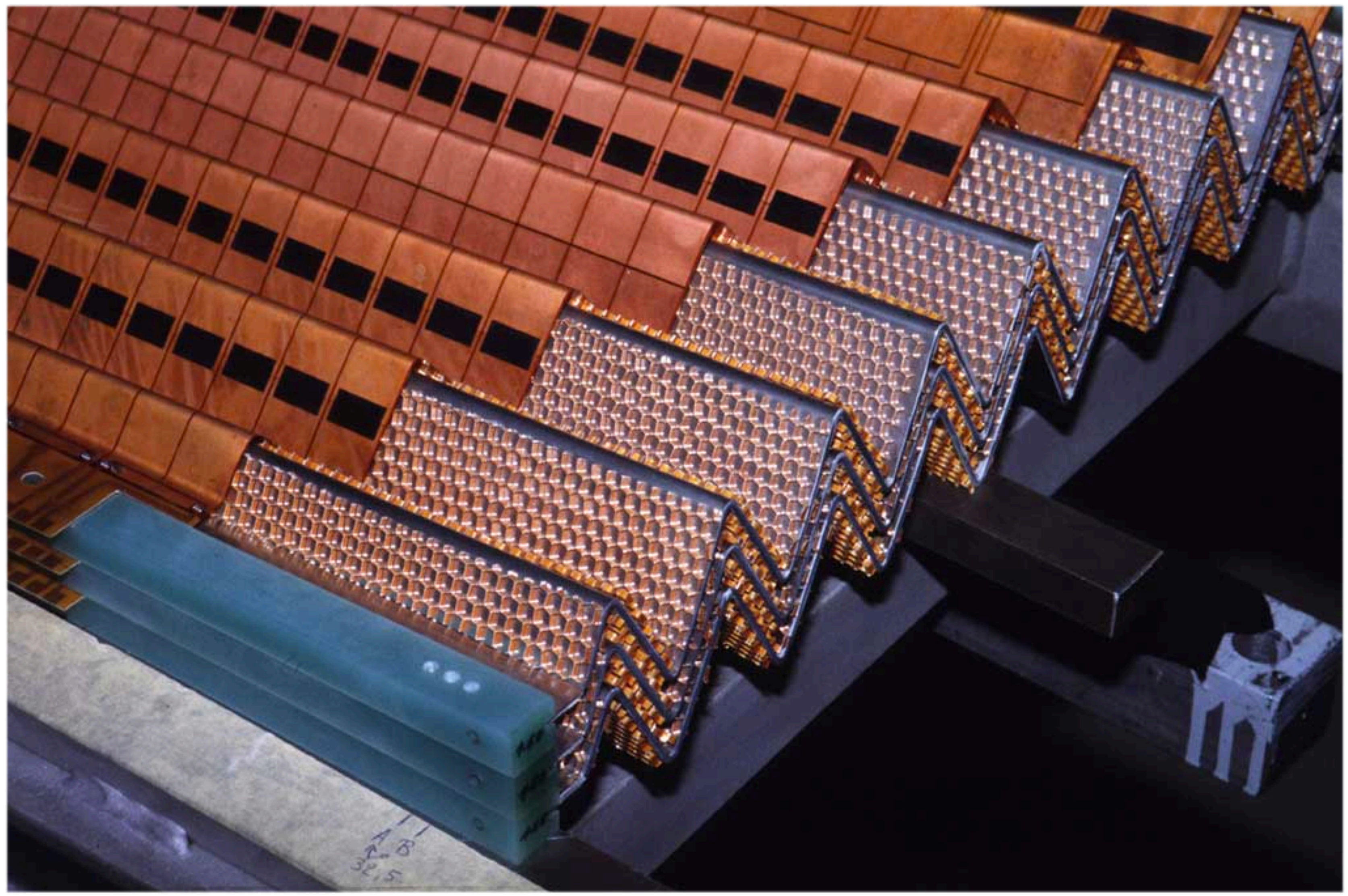




Most of the time (64%) is spent in the EM calorimeters
Followed by the Inner Detector

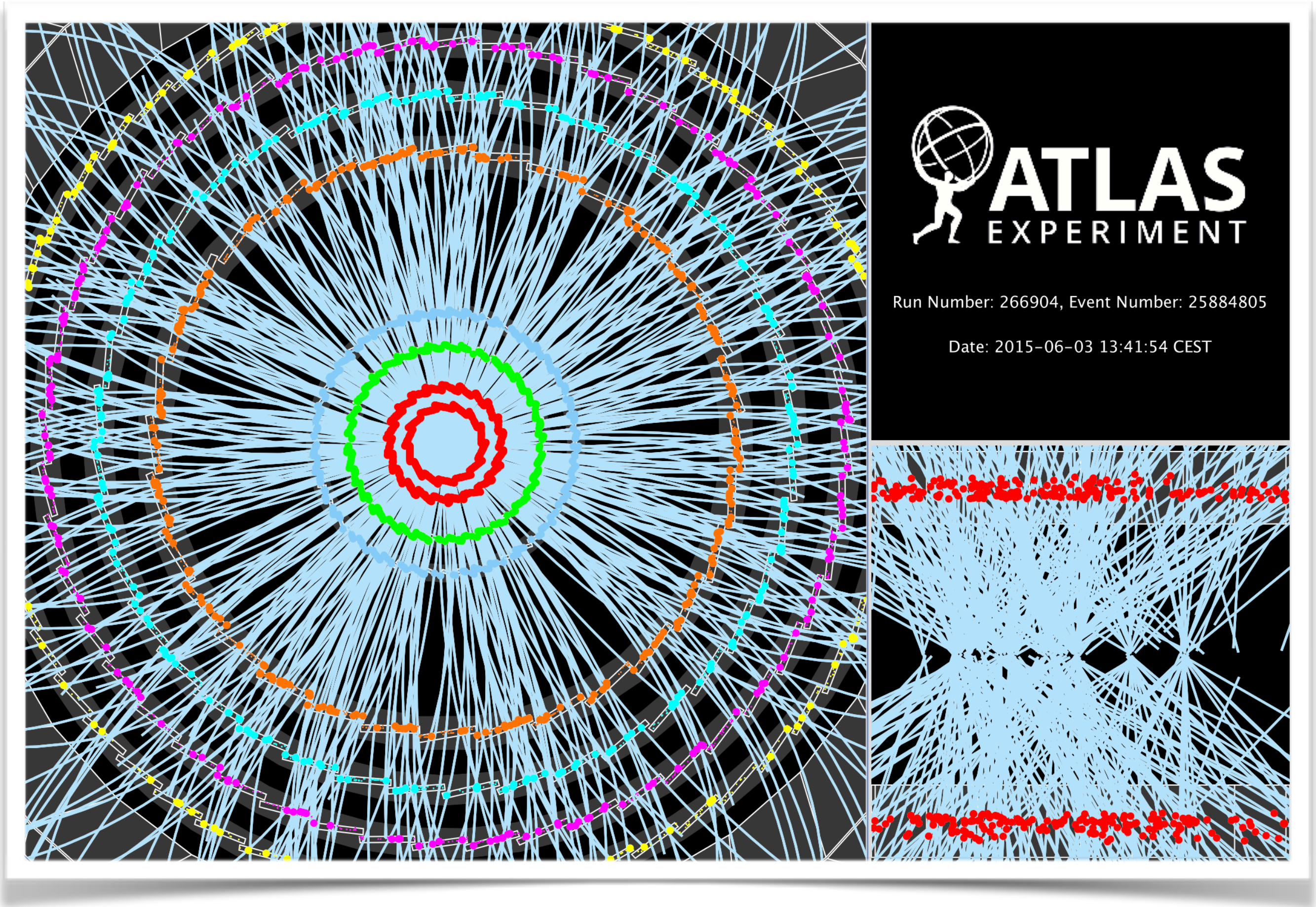
ATLAS Calorimeters

See talk by W. Lampl for more details



Main reason is the complex accordion structure of the calorimeters

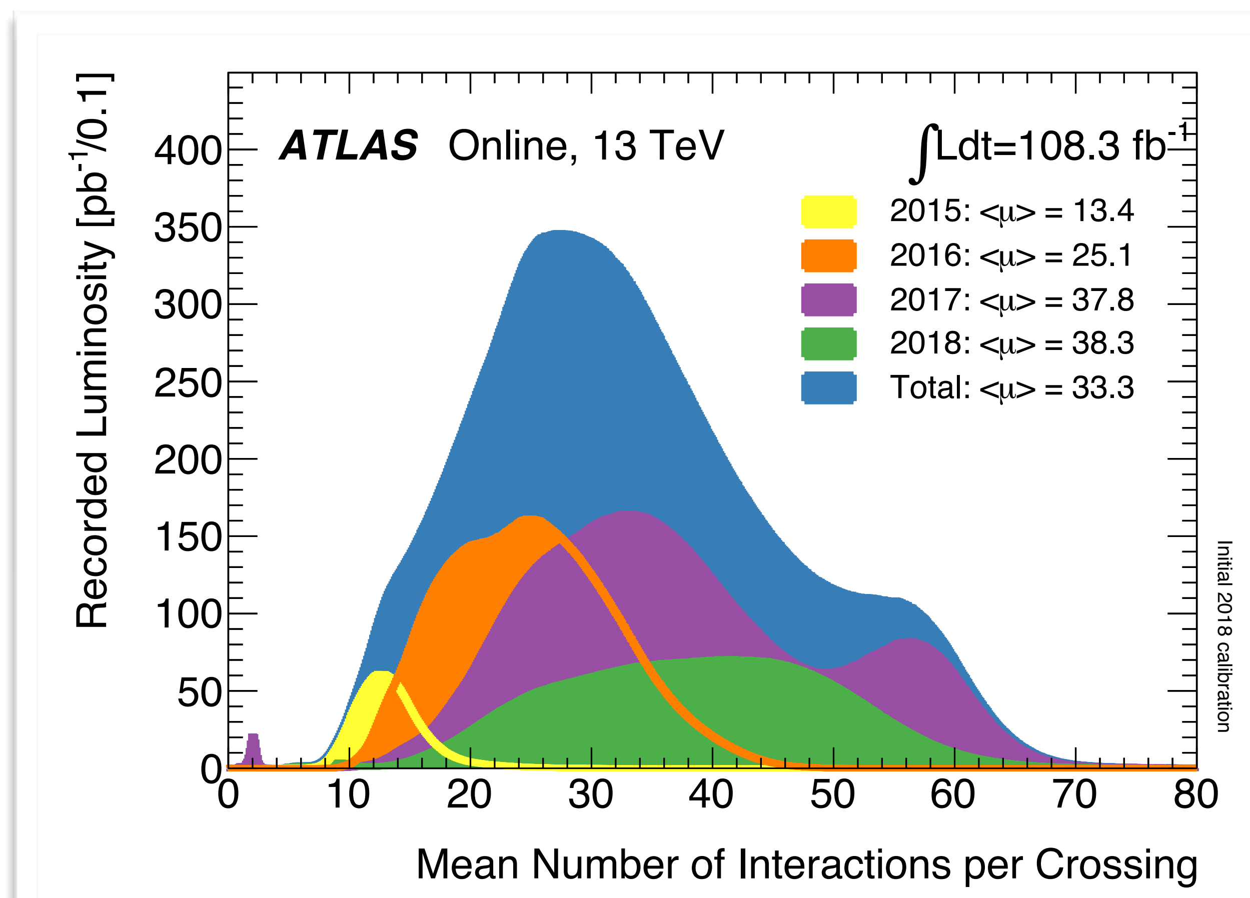
Additional Challenge: Pile up



Event display of a typical LHC event

Typically need to simulate ~40 additional proton-proton interactions per collision

Want to save time by reusing pile up events, but this introduces significant complications to the chain



Simulation Flavours

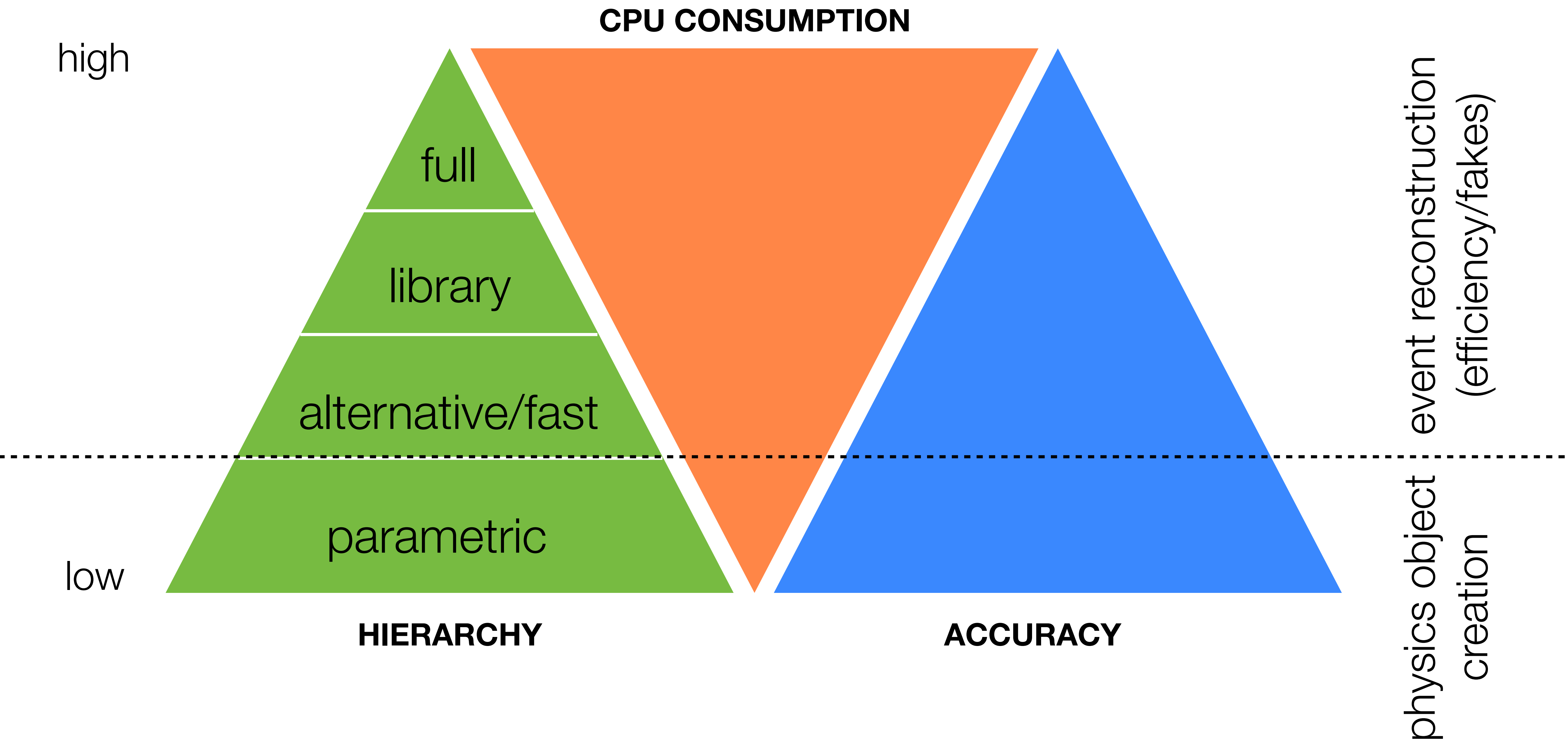


Image credit: A. Salzburger

ATLAS Simulation Tools

FastCaloSim

Parametrised calorimeter response

Fatras

Fast inner detector simulation

FastDigi

Fast inner detector digitisation

Pseudotracking

Truth information to skip pattern recognition

The Idea: Integrated Simulation Framework

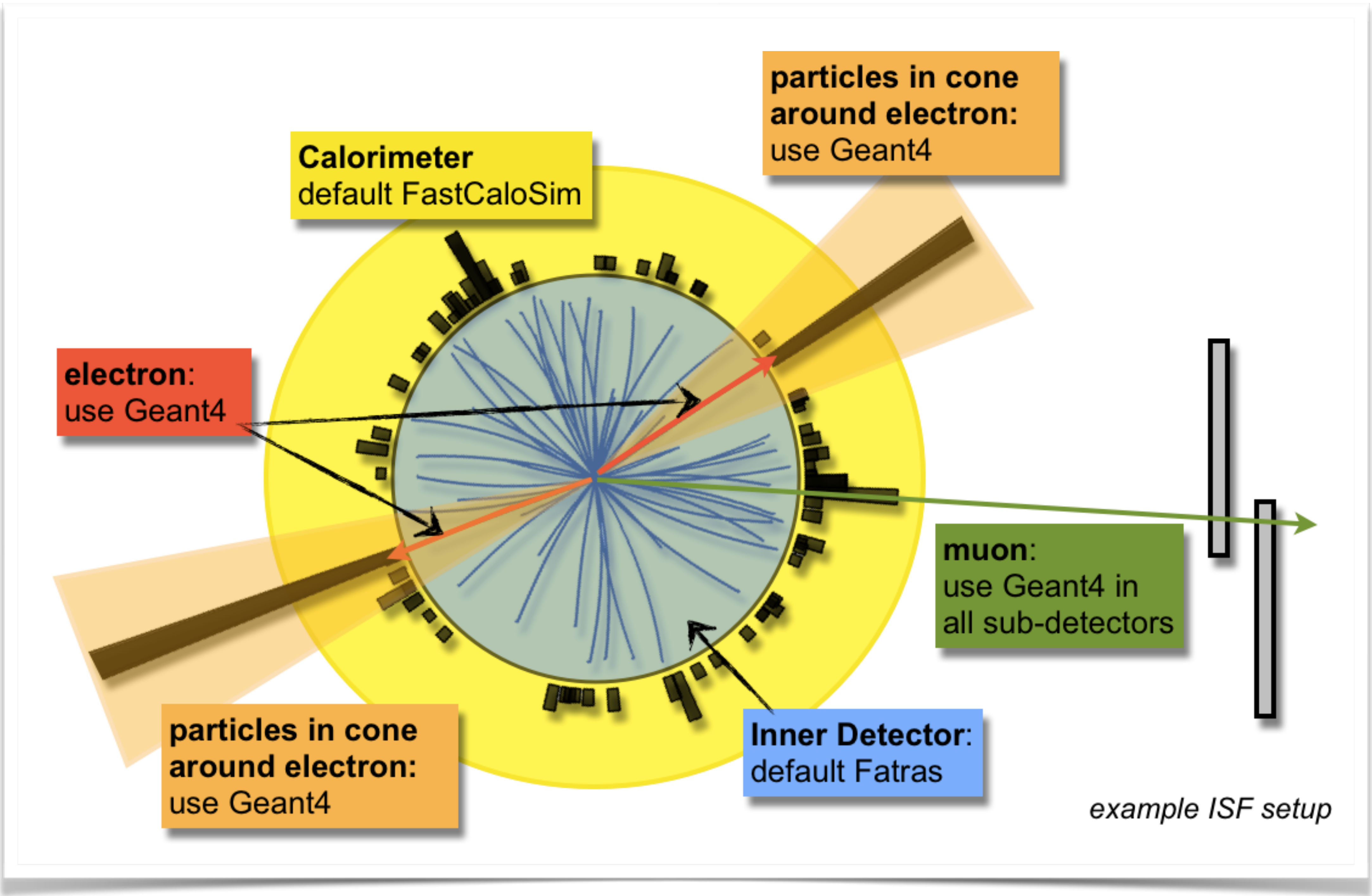
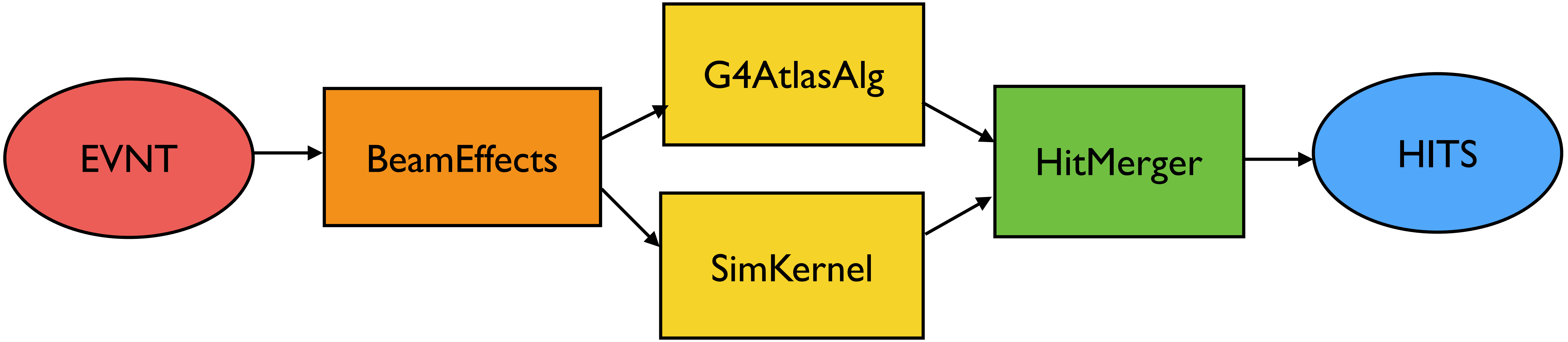


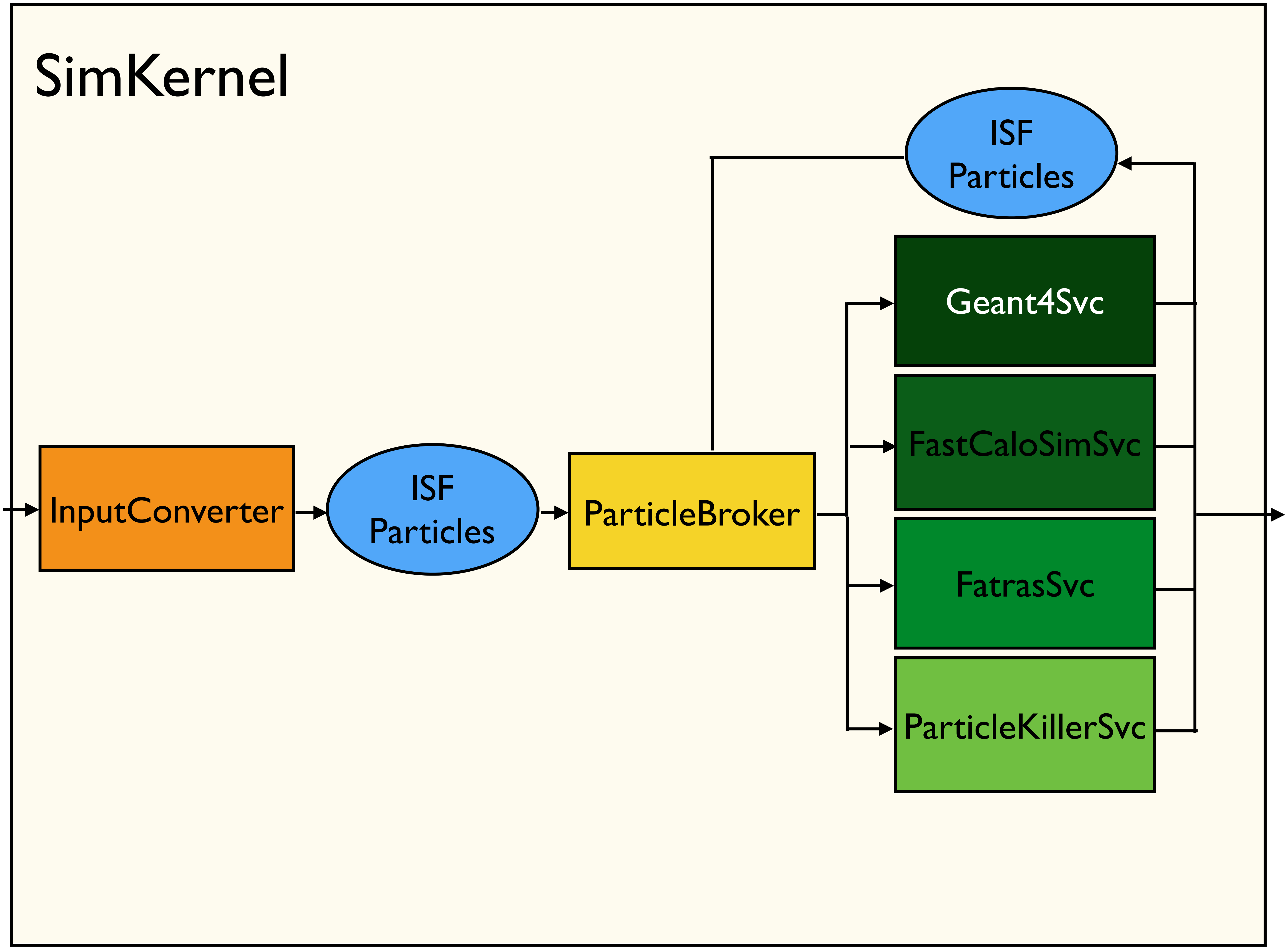
Image credit: A. Salzburger

We have the capabilities to produce events like this, but in reality we use the ISF to use different simulation flavours in different detectors

Simulation Overview



Simulation: SimKernel



Geant4Svc

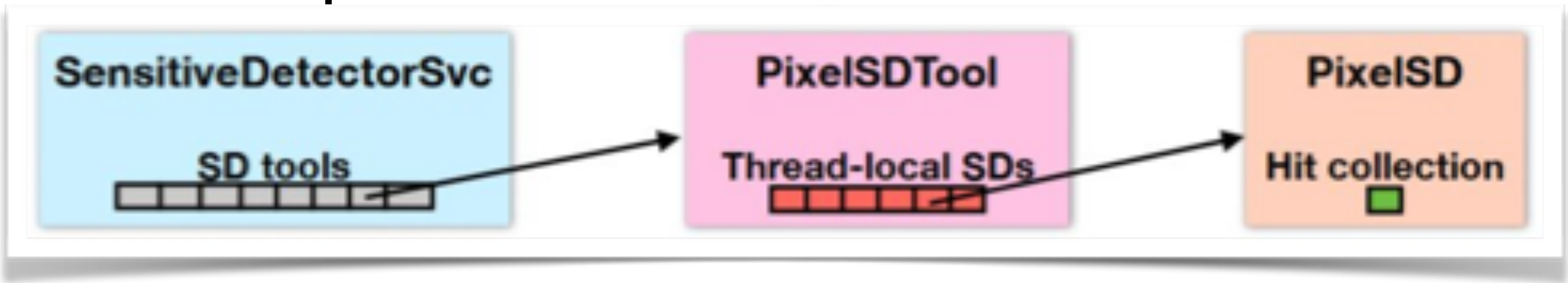
- The simulation is done in the external Geant4 package, but we have an interface to configure the following
  - Geometry
  - Sensitive detectors
  - Magnetic field
  - Physics list
  - Additional processes
  - User actions
  - Fast simulation models (e.g. frozen showers)

http://geant4.cern.ch/

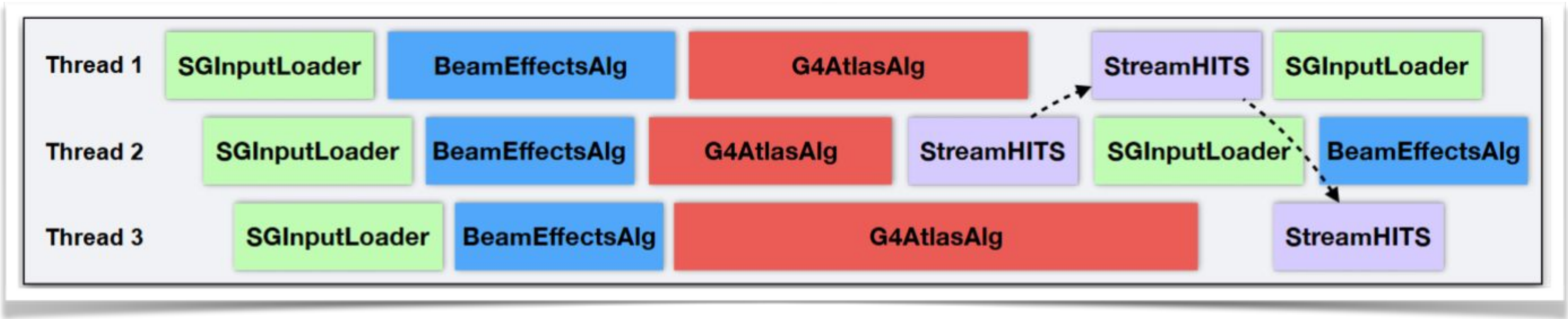
- Comments
  - G4 can already run multithreaded (but only in our upcoming release)
  - ISF needs to be migrated to MT
    - In the longer term, should think about how much we want to maintain ISF vs rely on G4 to handle fast simulation models

Geant4MT in AthenaMT

- Composite model of Gaudi/Athena components that create + manage thread-local G4 components



- Thread-local workspaces setup via new thread initialisation tool framework mechanism
- Processing algorithms are clone to execute on different events concurrently
- One instance of the output stream algorithms (StreamHITS) services all worker threads: Being replaced by SharedWriter to handle multiple parallel threads



Slide from J. Chapman

Speeding up the Full Simulation

Improvements already in place

Configuration	MinBias	ttbar
Nominal production configuration: shower libraries in the forward calorimeter, nominal range cuts, NystromRK4 stepper, FTFP_BERT_ATL physics list, 250ns neutron time cut, simulation of primary particles with pseudo-rapidity below 6.0	1.0	1.0
No shower libraries	1.5	1.3
ClassicalRK4 stepper instead of NystromRK4	1.09	1.07
No neutron time cut	1.02	1.01

Detector simulation white paper: arxiv:1803.04165

G4 10.2p03.

Further Improvements

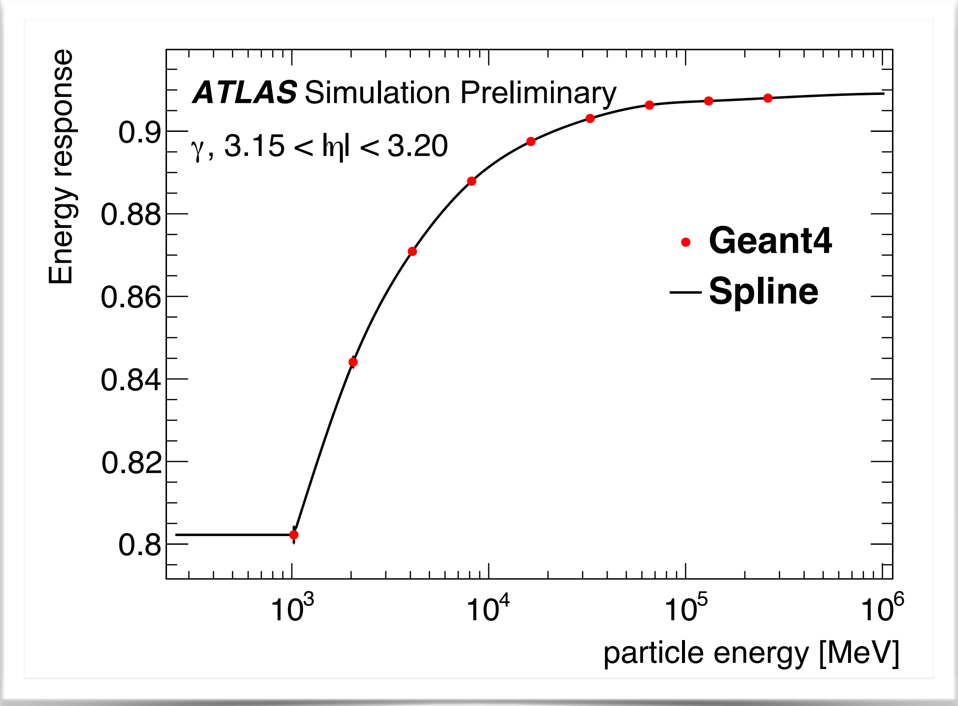
- Optimizations
  - Improved G4Solid implementations. (4%)
  - Optimize choice of G4Solids used to create given volumes.
  - Big Library (static-linking) (10%)
  - Profile-guided optimization (5%?)
- Simplifications
  - Geometry simplification
  - Hadronic cross-section tables
  - More aggressive G4 cuts
  - Russian roulette for neutrons

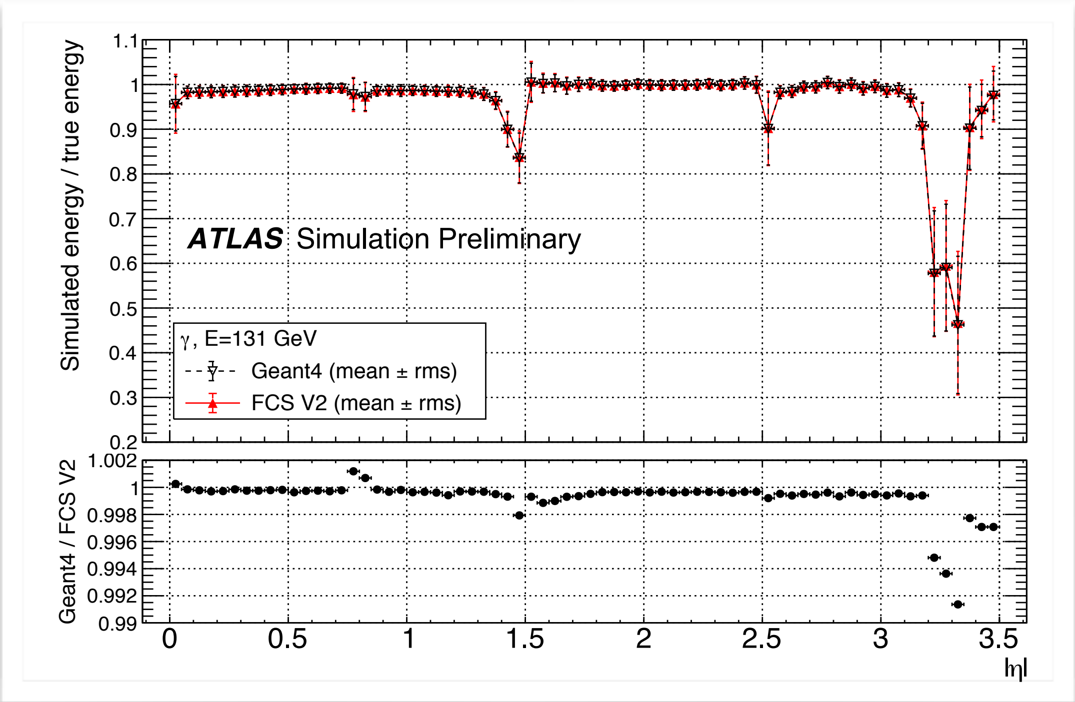
Fast Simulation

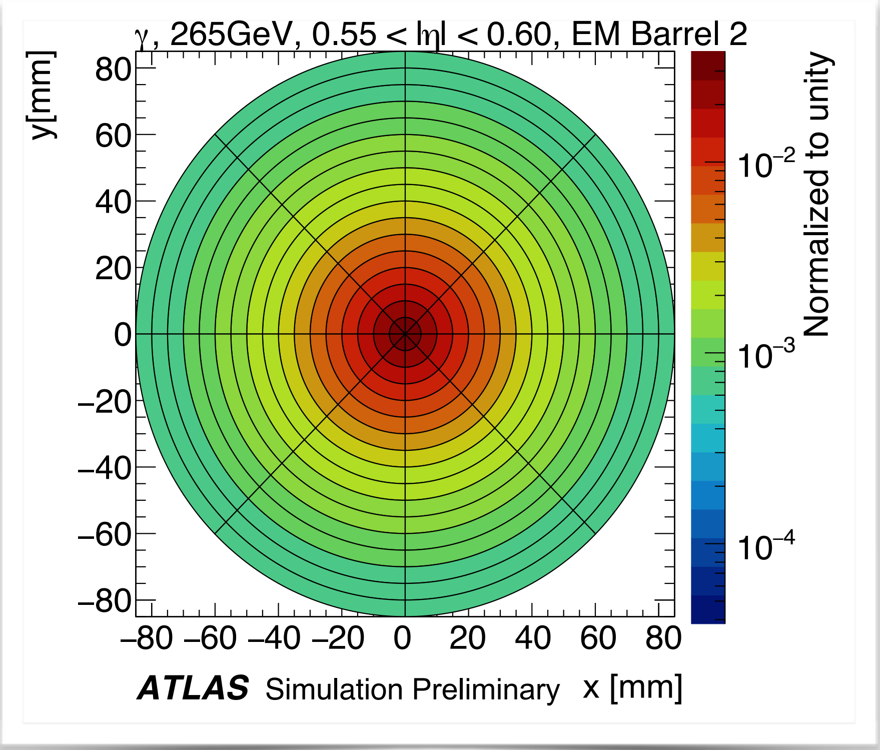
- **FastCaloSim**
  - Updated version is under development to provide improved physics performance (similar speed is expected)
  - Framework updates required so that it is not thread hostile
  - Quite a bit of work will be required to make it thread-safe
- **Fatras**
  - Little manpower for maintenance
  - Significant work required to make it thread-safe
  - G4 used for hadronic interactions
    - Could consider making the interaction with G4 closer for the future?

FastCaloSim

- Parametrise the energy and shower shape for single particles in the calorimeters as a function of energy and direction (η)

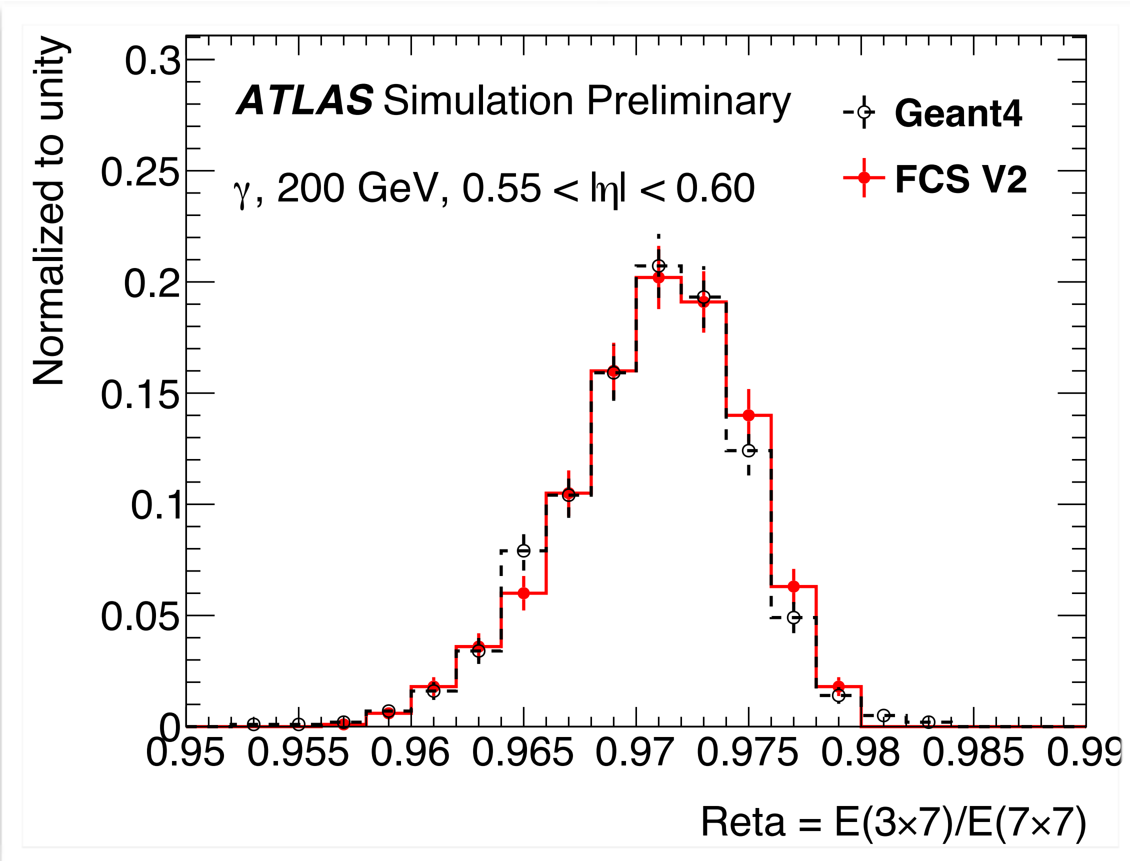


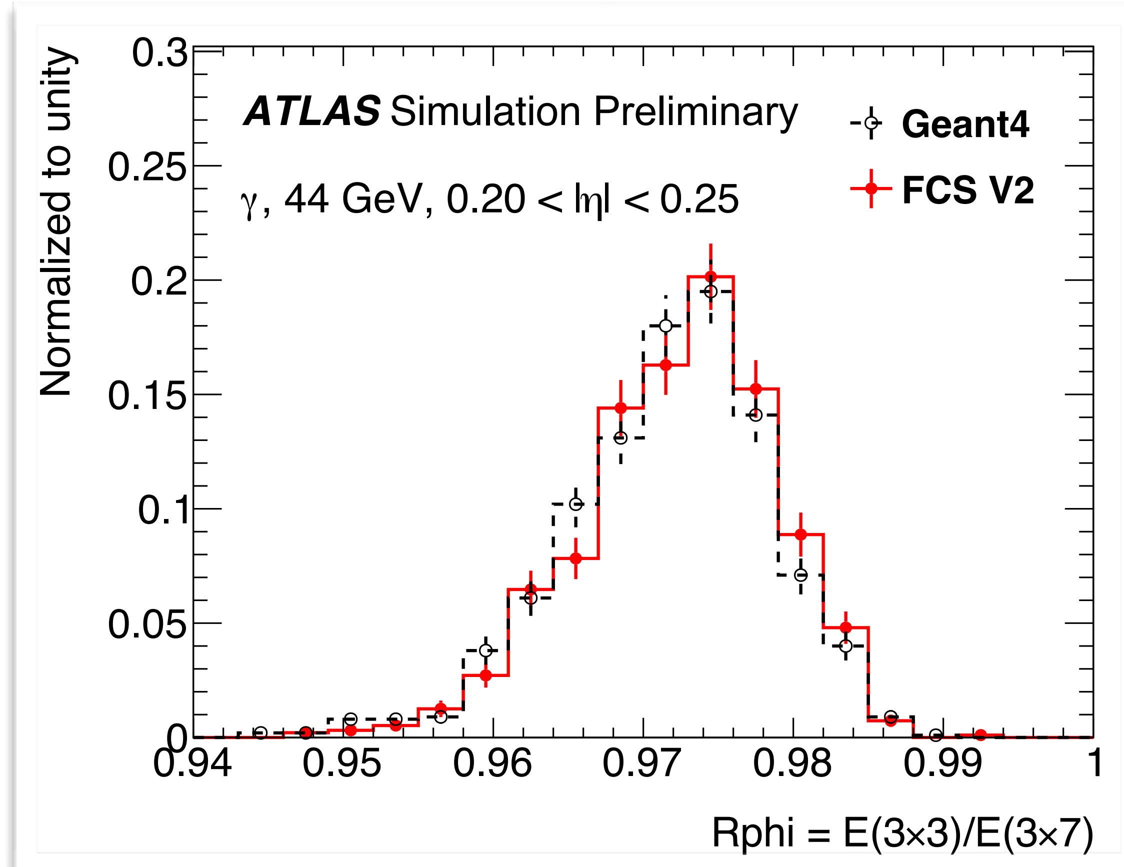


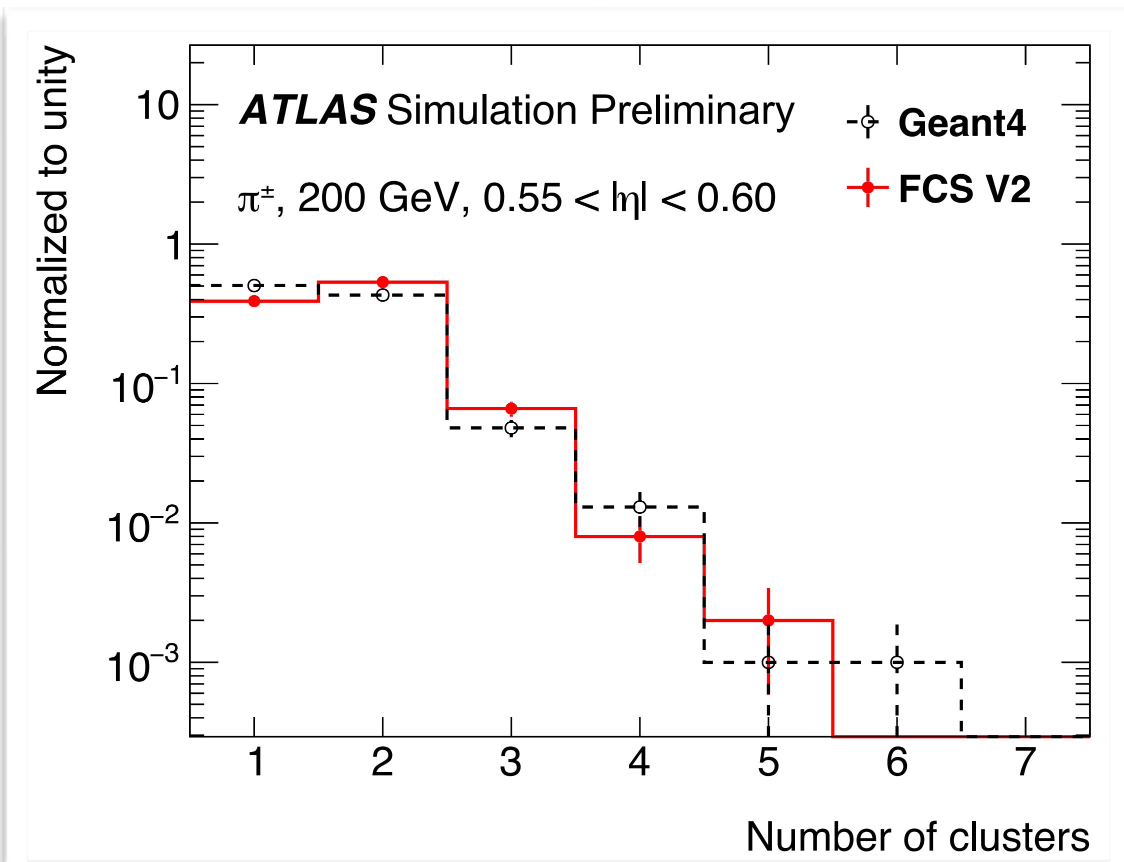


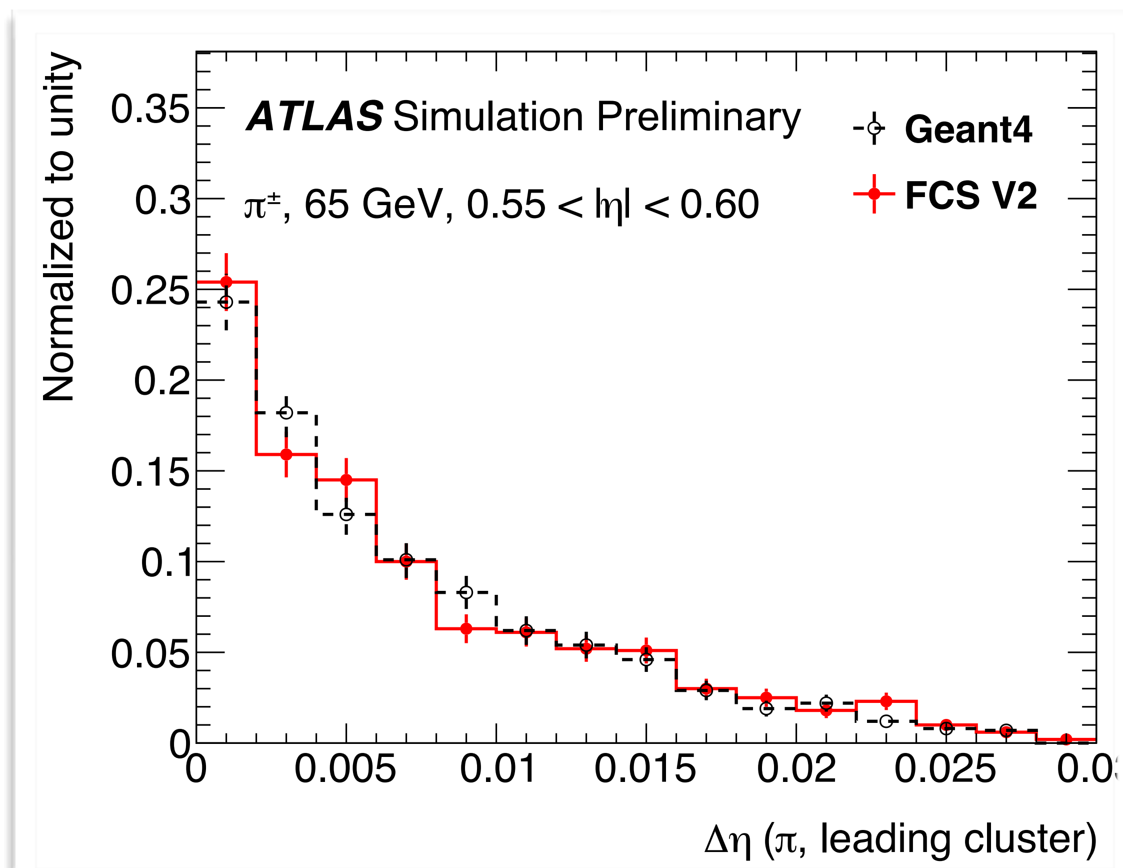
More details

Performance of FastCaloSim

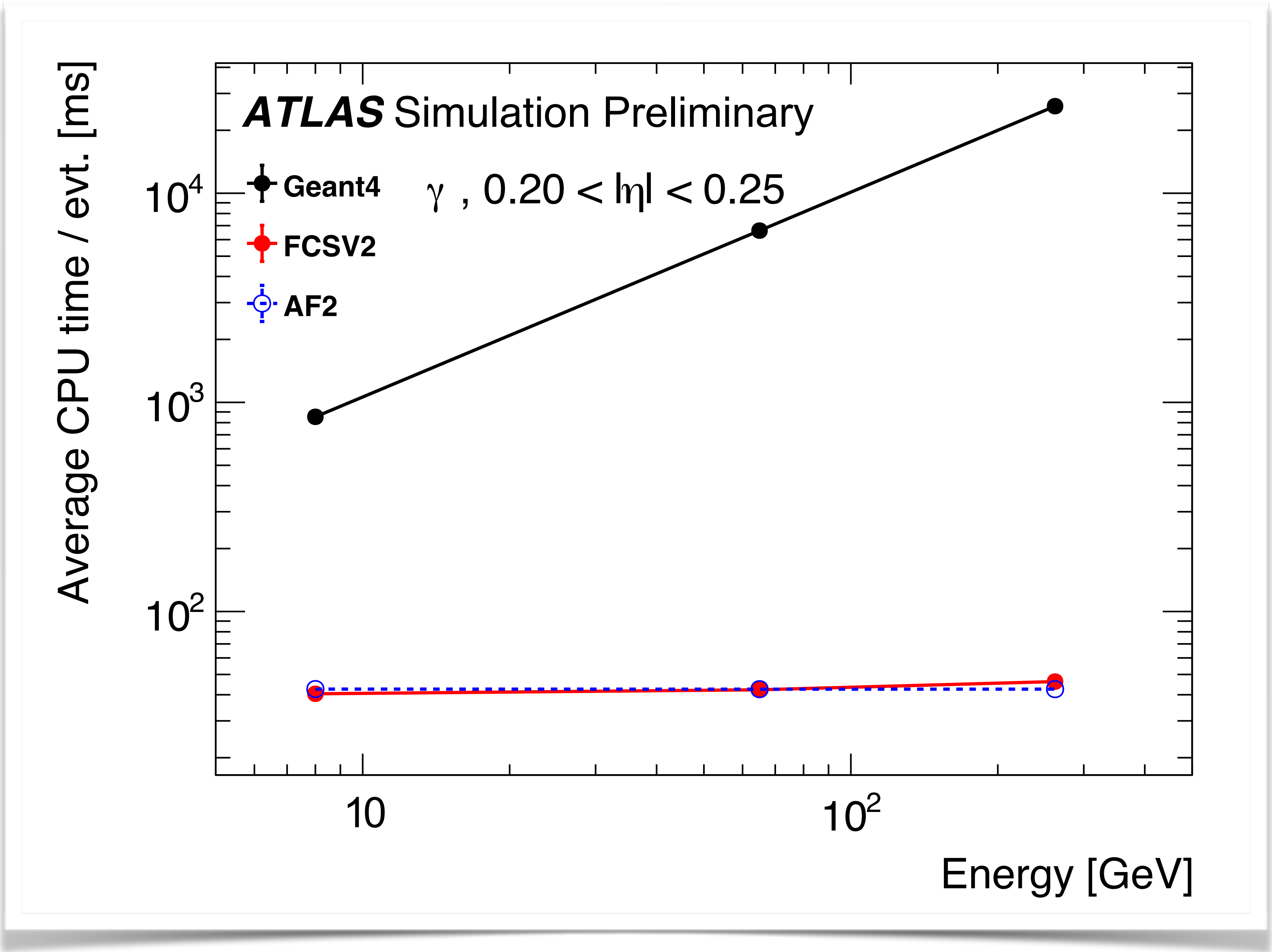








Dramatic CPU savings



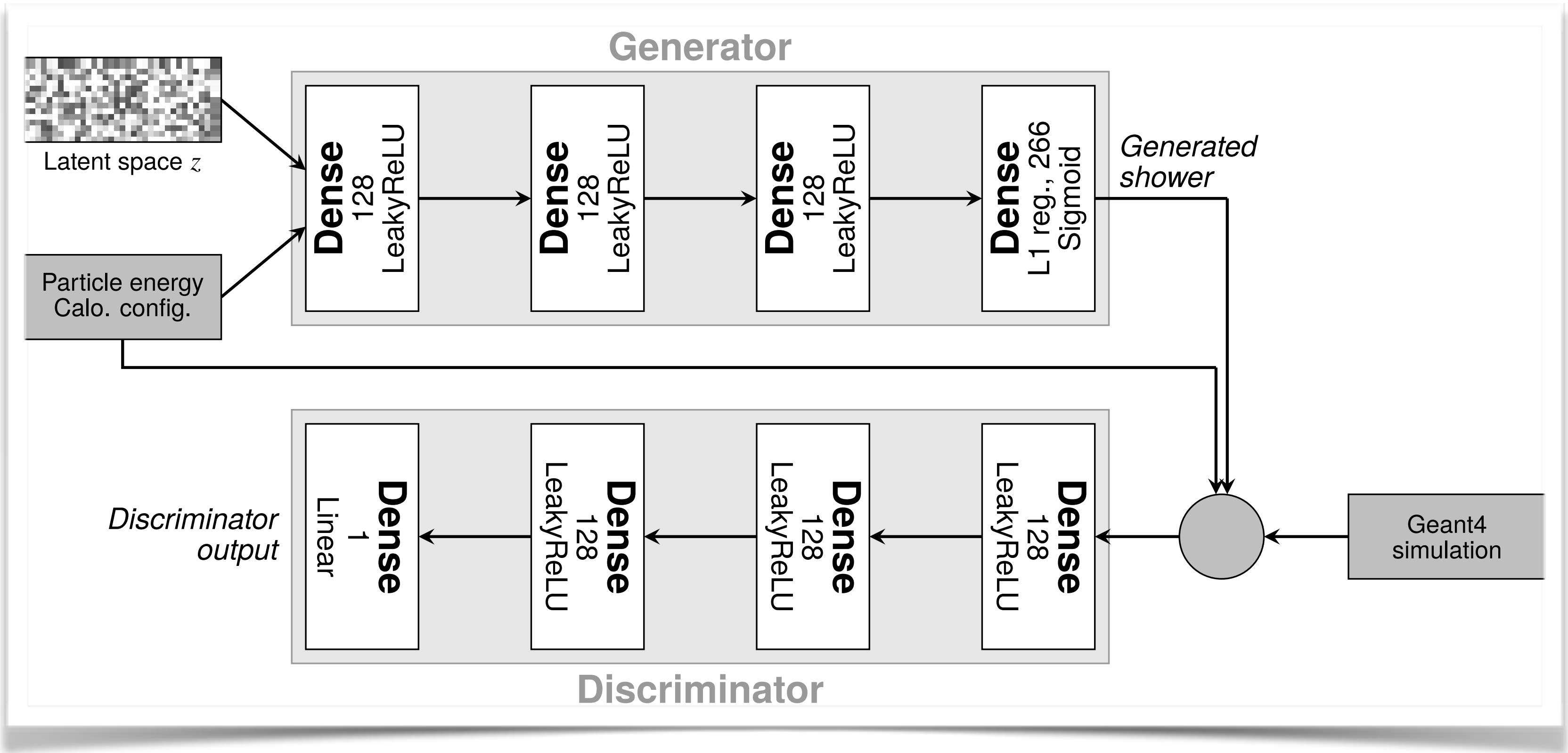
Simulation from the inner calorimeter surface only

Challenges for FastCaloSim

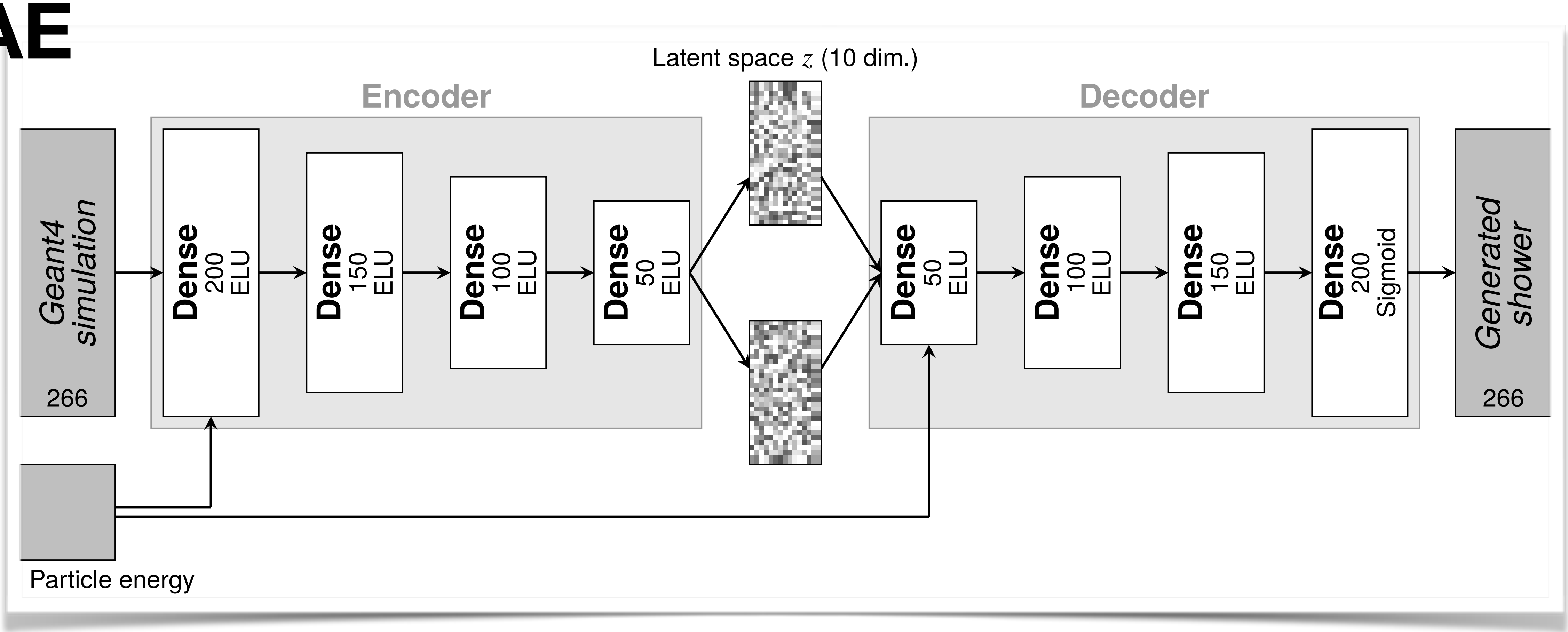
- Producing and managing the large number of events required to derive the parametrisation
  - O(150M)
- Accurately modelling the correlations in the energy between the different layers
  - Use a PCA approach to decorrelate
- Modelling the shower fluctuations
  - Exploring approaches based on ML
- Parametrising the calorimeter response accurately and efficiently
  - A simple histogram-based solution would require 8 GB of memory …

R&D: Ideas from Machine Learning

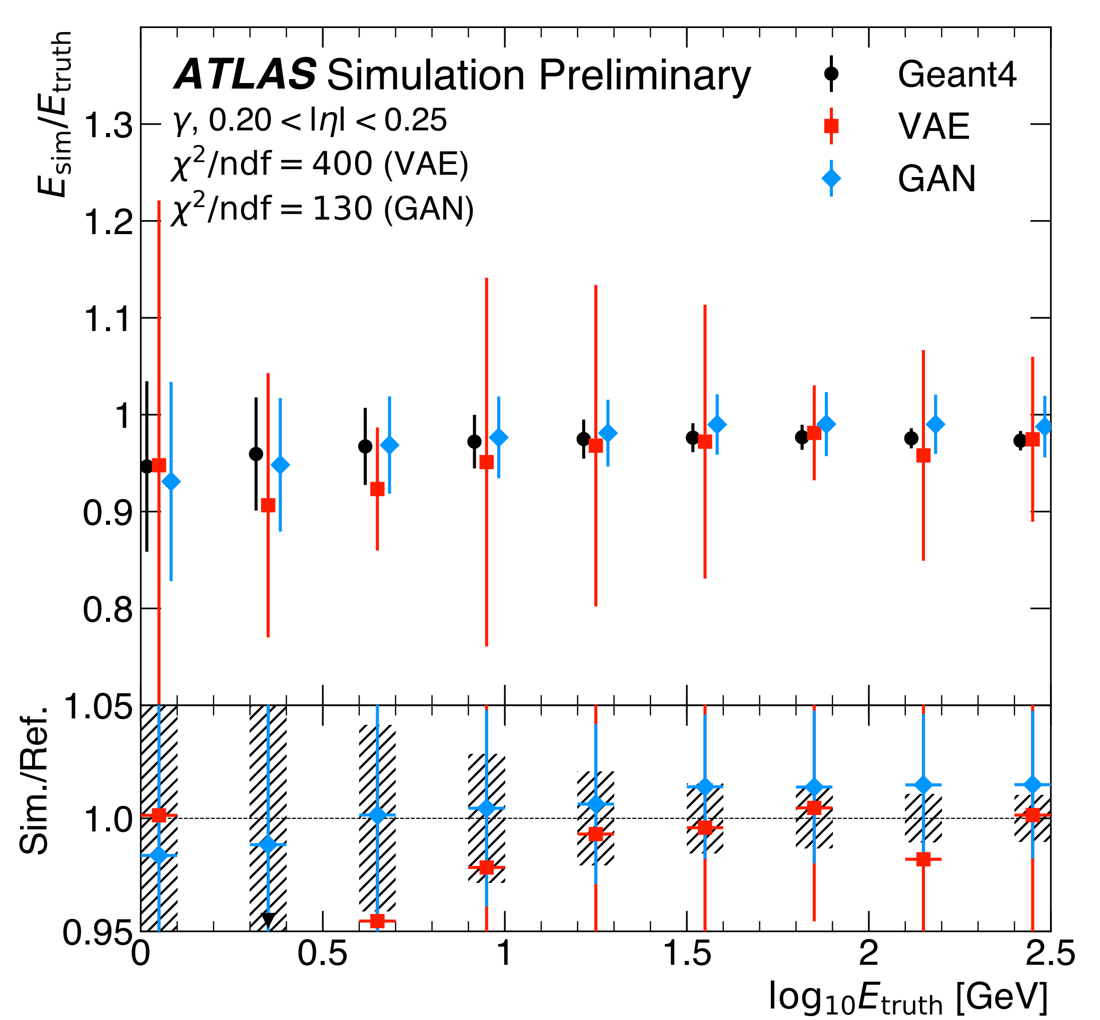
GAN

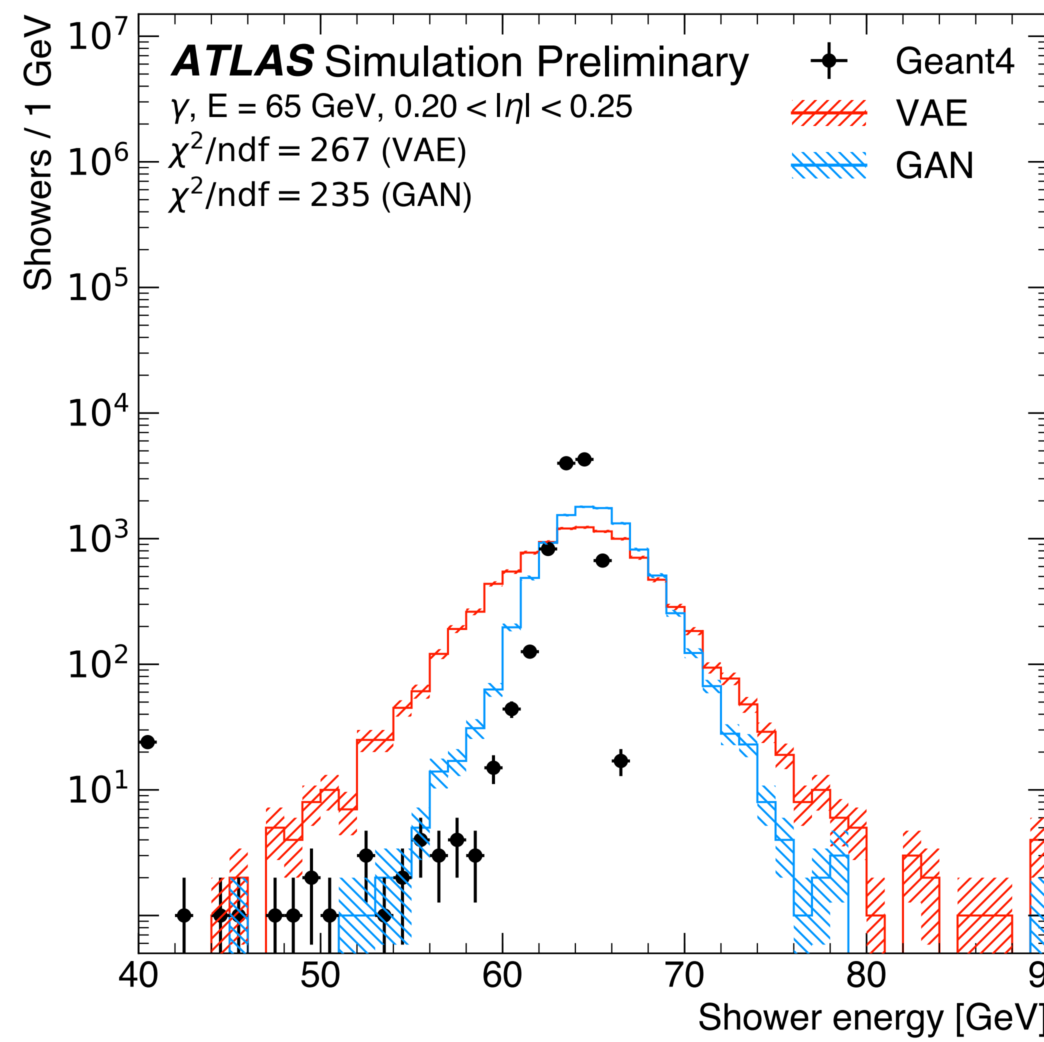


VAE



Early Results

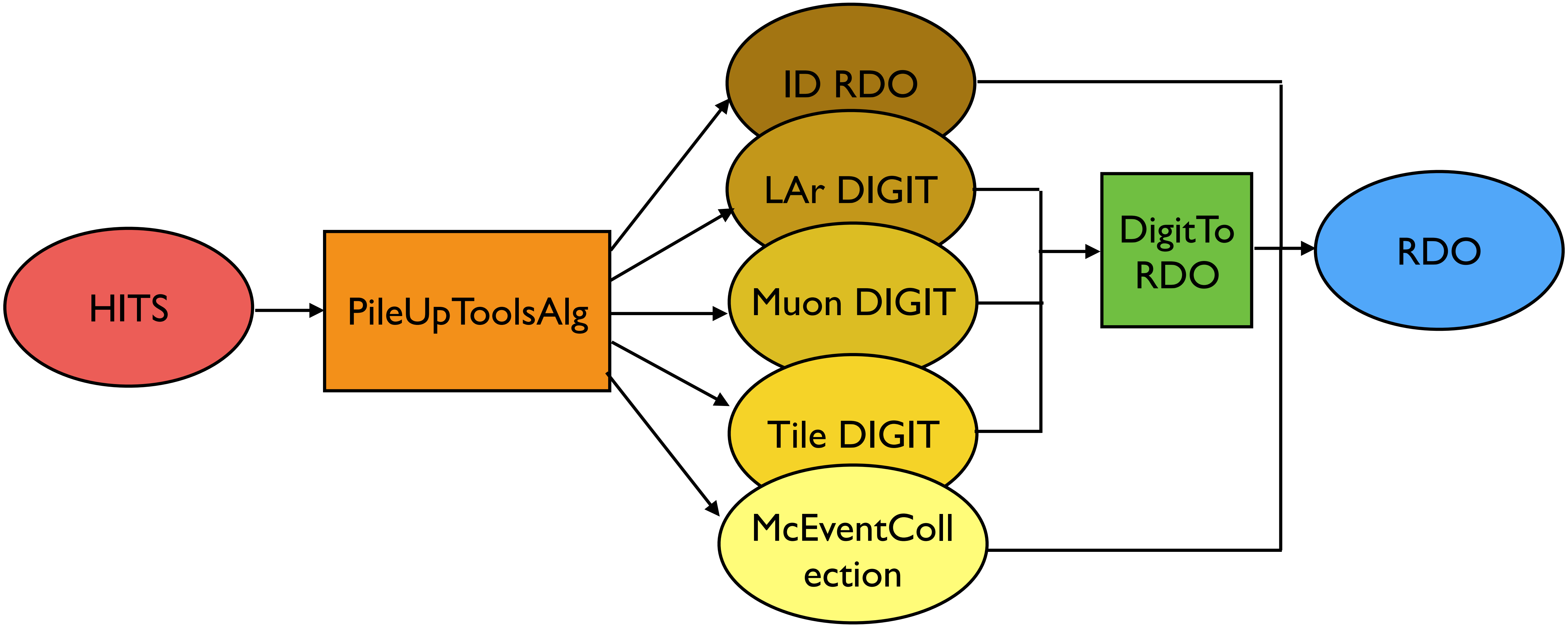




More results

Digitisation Overview

Hard scatter only



DIGITs also contain additional trigger information

Producing events with pile up

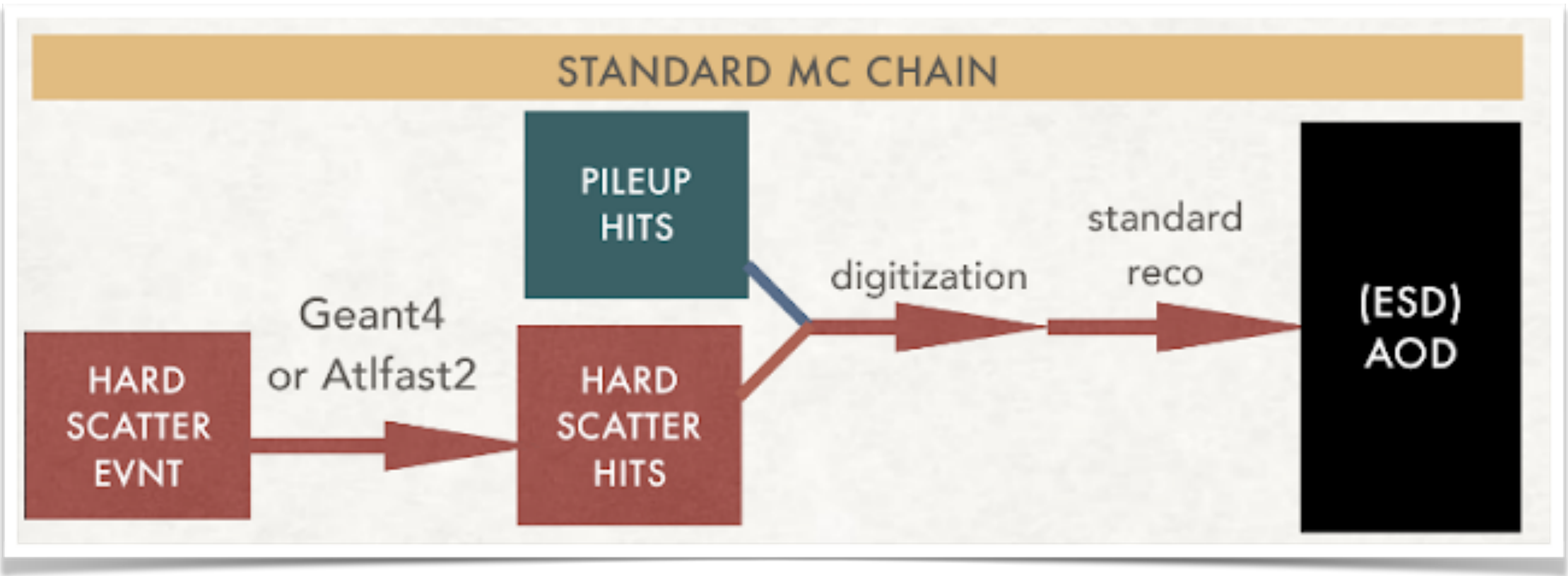


Image credit: T. Lari

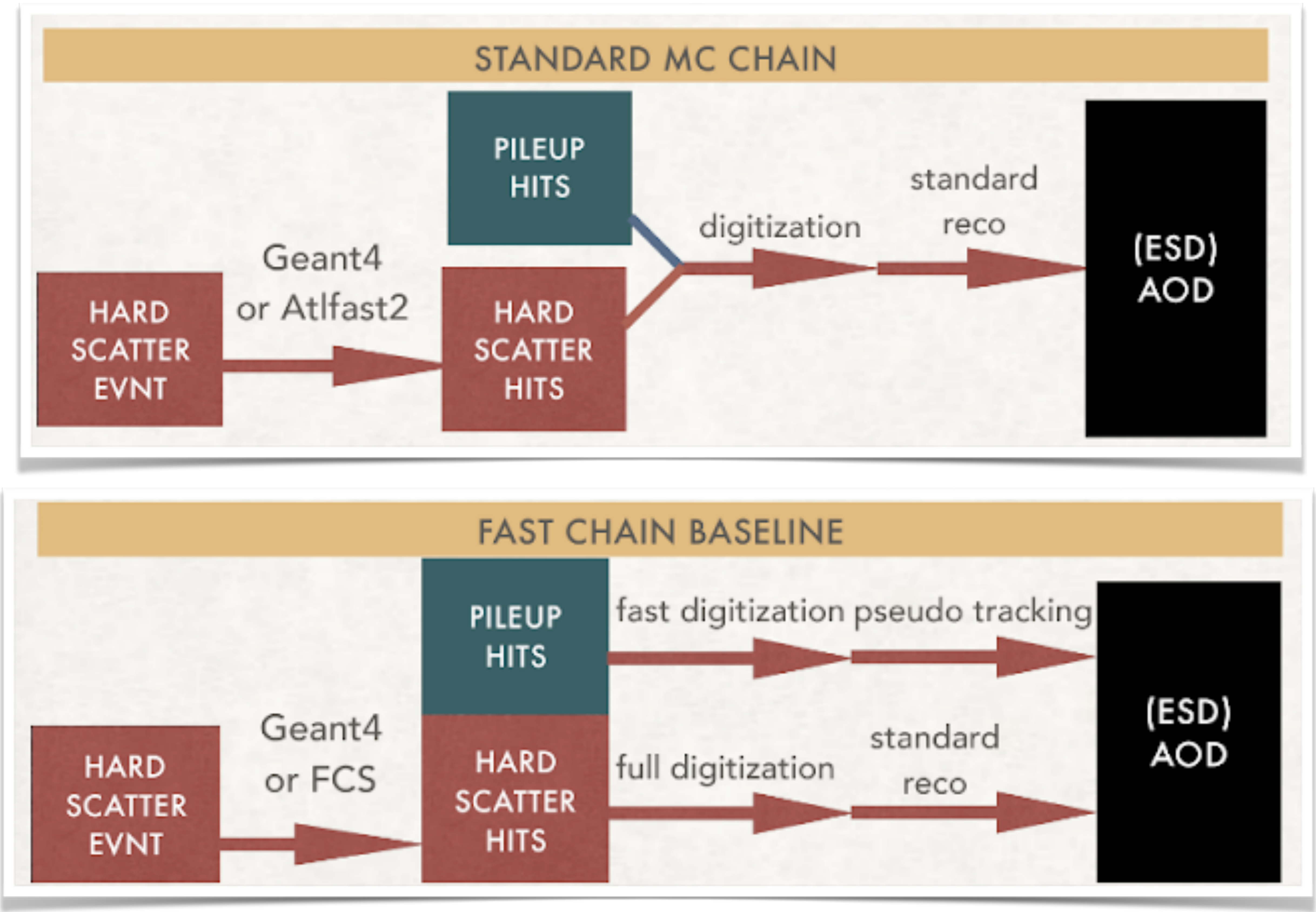
Digitisation (with pile up)

- PileUpEventLoopMgr replaces the AthenaEventLoopMgr
- BkgStreamsCache (1 per pile up type: low pT minbias, high pT minbias, etc)
  - Array of EventSelectors (O(4000))
  - For each bunch-crossing (39 in total):
    - Get <μ>by sampling from a Poisson random distribution to obtain the actual μ = N
    - Pick N background events from the caches
  - Create a new xAOD::EventInfo object with references to all required StoreGates with a record of which BCID each is used for
- PileUpToolsAlg
  - For each bunch crossing
    - Queries each PileUpTools: are you interested ?
    - If yes, pass list of StoreGates to look at and process
    - Clear used events after all PileUpTools have been queried (memory)

Comments on MT Digitisation

- Can already run single hard scatter events with MT
- Challenge is in the treatment of the pile up
  - Need to minimise memory
  - Also ensure that events aren't used too many times
- Potential Strategy
  - Share pool of background events between threads
  - Events need some sort of state
    - Have they been used?
    - Are they currently in use?
    - Discard once used sufficient times
- This would require significant core athena development as these concepts don't exist in Gaudi

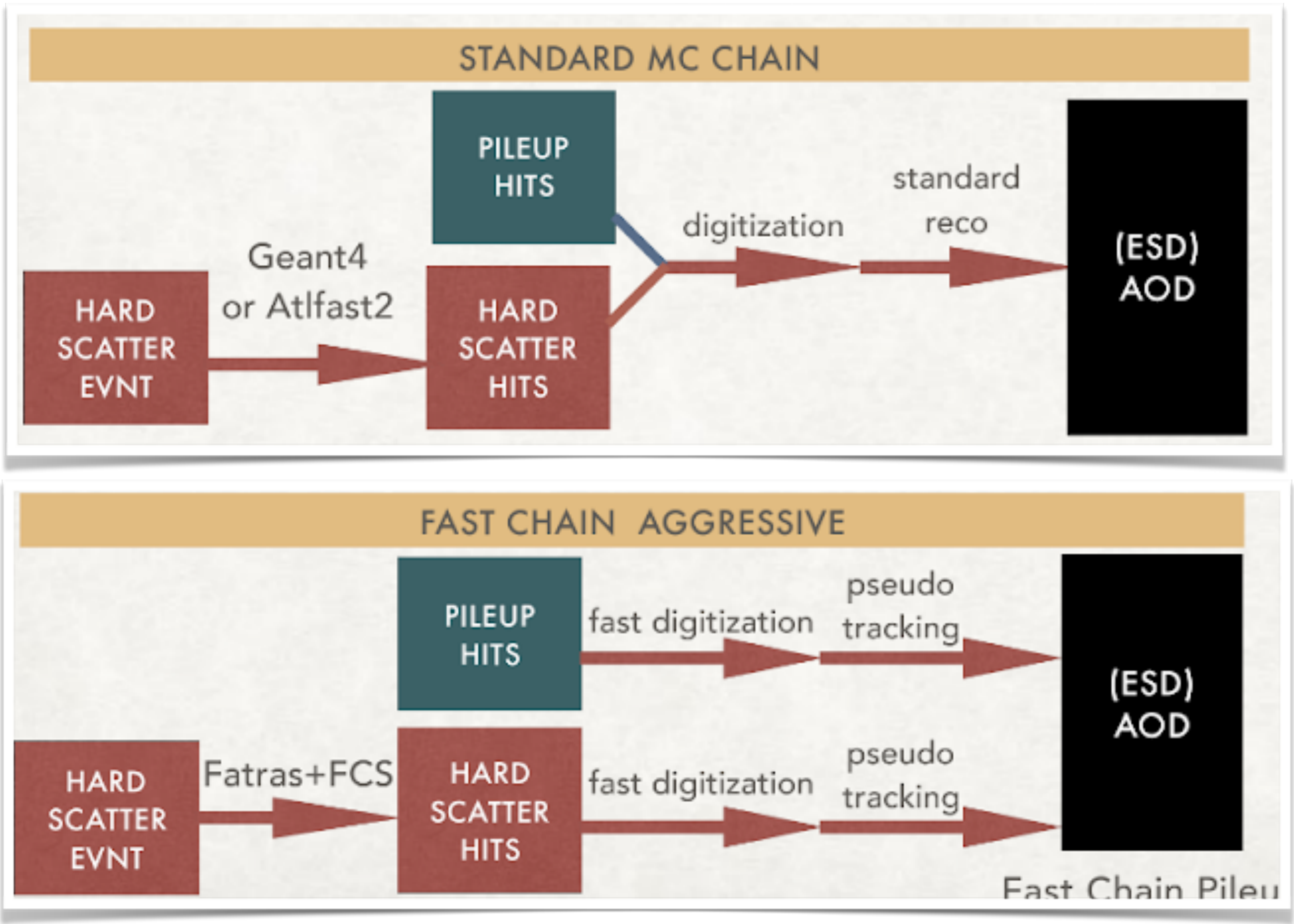
FastChain: Baseline



O(300)x faster

Image credit: T. Lari

FastChain: Aggressive



O(300)x faster

Image credit: T. Lari

Conclusion

- Detector simulation is the main driver of CPU in the production of simulated datasets for the ATLAS experiment
  - In the future, with larger datasets and more pile-up the problem will become even more challenging
- Presented a brief overview of simulation (both full and fast) and digitisation in the context of the ATLAS experiment
- Highlighted aspects of our current practises, work in progress and ideas for future directions
- Comments and feedback are very welcome !