# Fast simulation

HSF Parallel Session
*2019 Joint HSF/OSG/WLCG Workshop*
*Jefferson Laboratory, Newport News, VA*

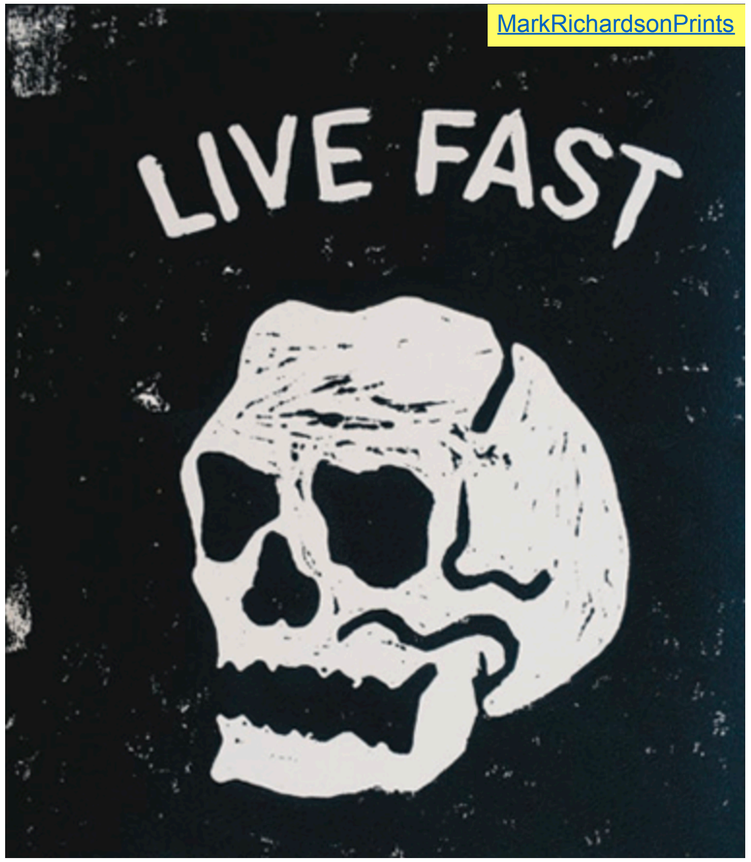
Vincent R. Pascuzzi
University of Toronto

*On behalf of the LHC experiments*

20 March 2019

# Fast agenda

- Motivation
- Current fast simulation
- Future fast simulation
- Summary



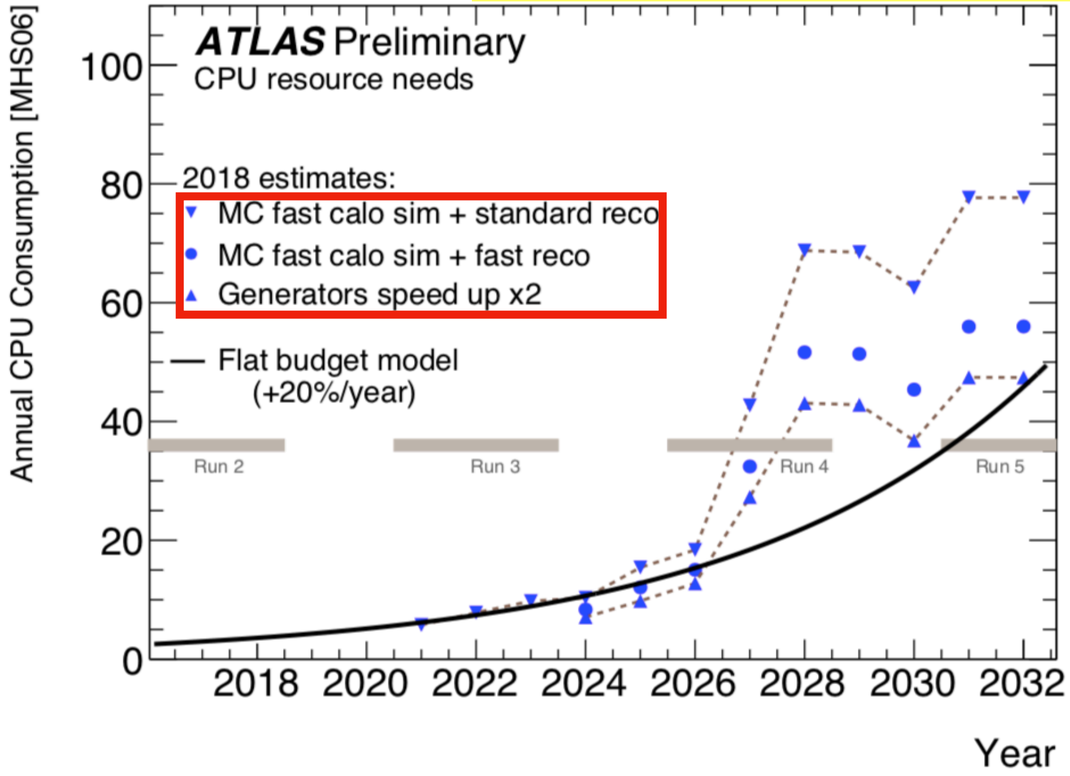
# Motivation

## *The problem*

Large MC statistics to model recorded data

- Increasing luminosity poses greater challenges

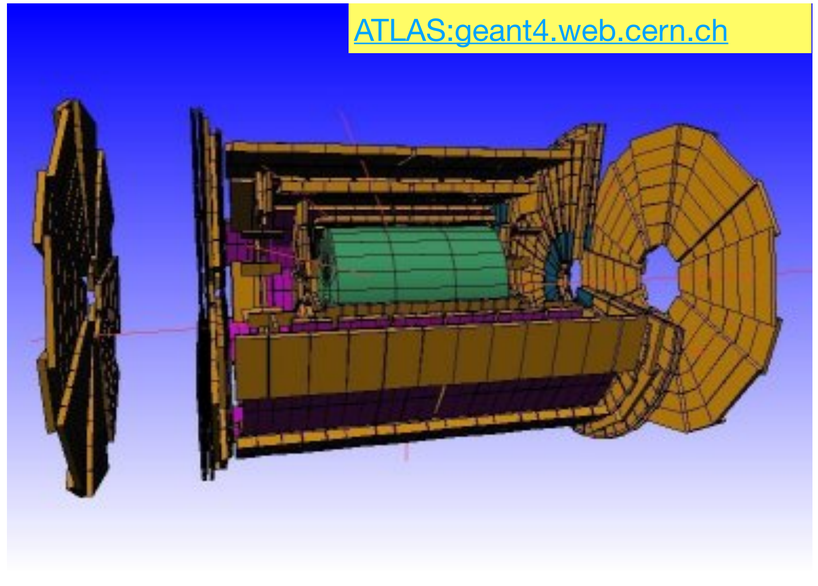
ATLAS:ComputingandSoftwarePublicPlots



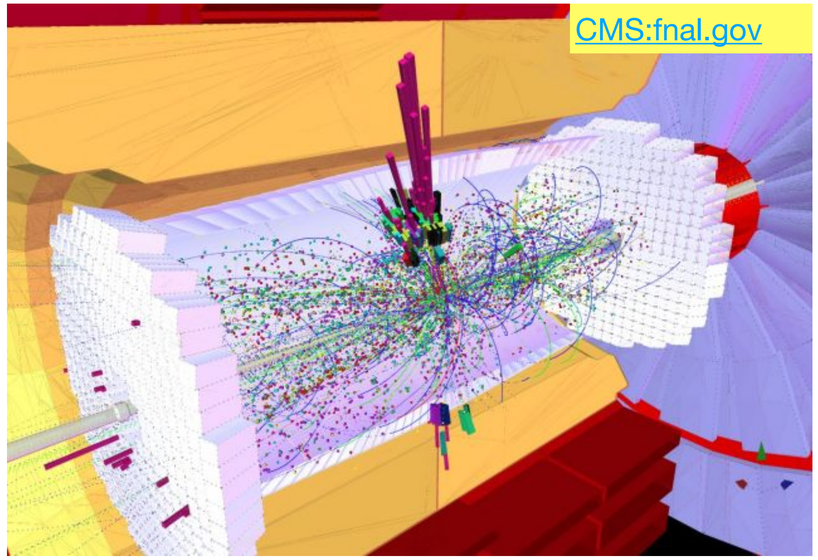

Highly-descriptive detector description not always necessary

- *e.g.* signal samples, systematics, upgrade studies

ATLAS:geant4.web.cern.ch

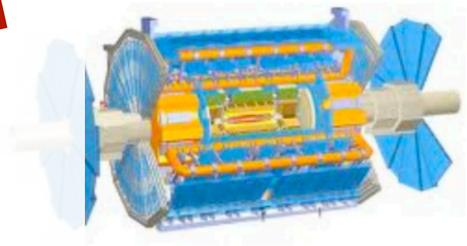


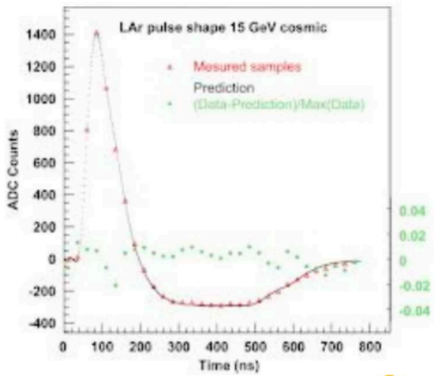
CMS:fnal.gov

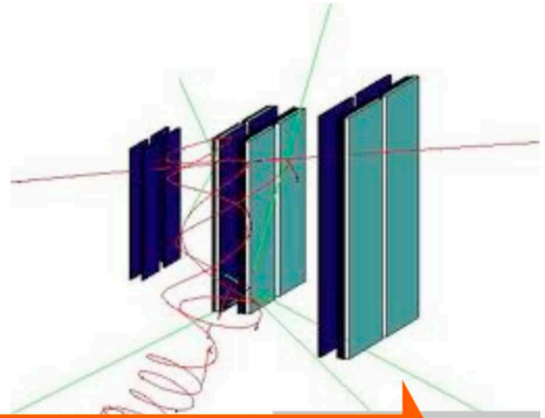


# Motivation

FAST





Event Generation → **Detector Simulation** → **Digitization** → **Reconstruction** → Rootification

4-vectors

Interactions of particles with matter

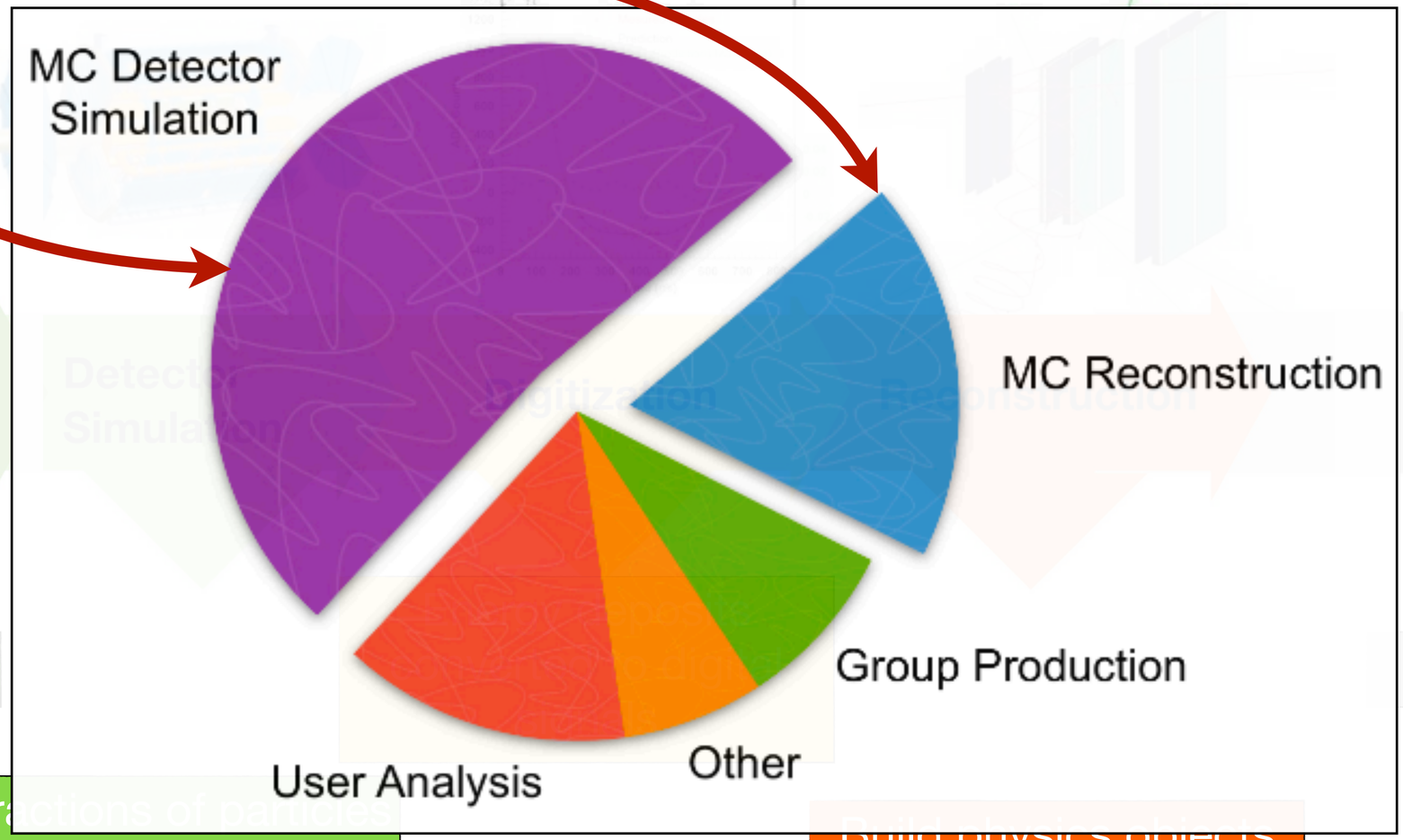
Energy deposits converted to digital signals

Build physics objects

Data for analysis

# Motivation

FAST




Event Generation

Detector Simulation

Digitization

Reconstruction

Rootification

4-vectors

Data for analysis

Interactions of particles with matter

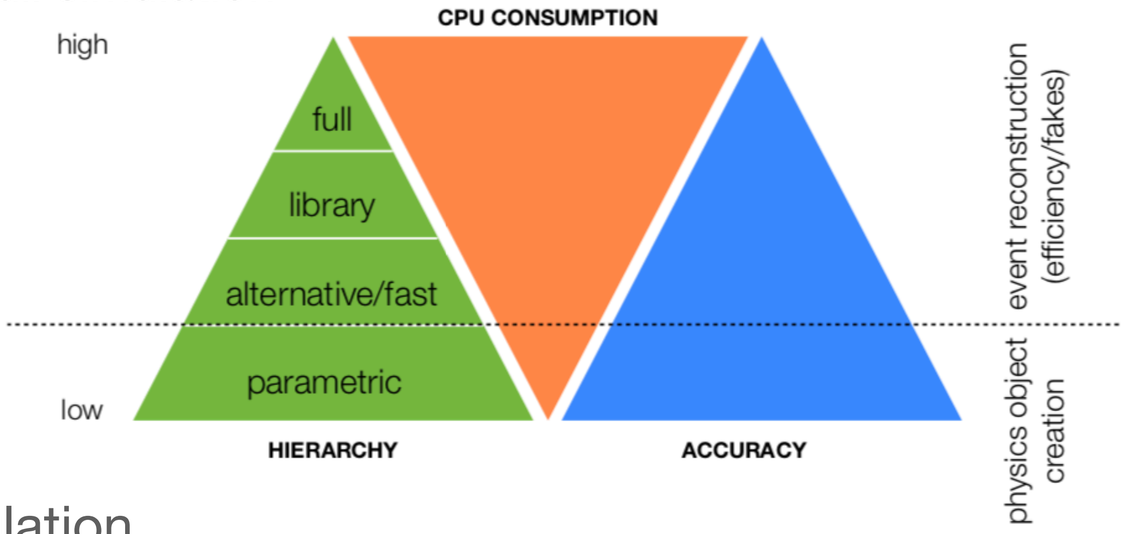
Build physics objects

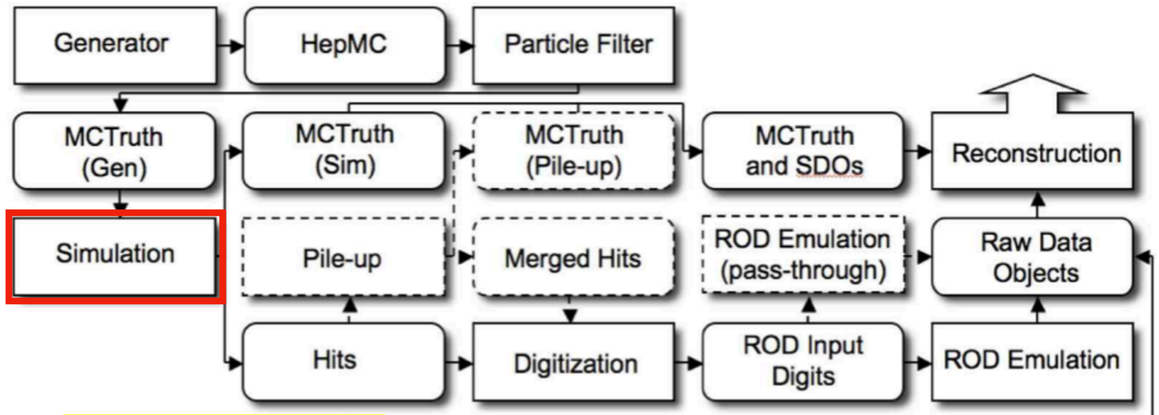
# Current fast simulation

## *Sacrifice accuracy and precision for speed*

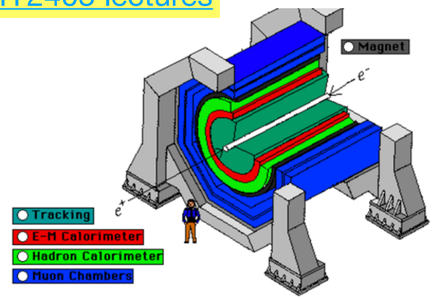
- Maintain certain level of agreement with highly-detailed full simulation
- Compatibility with offline processing chain
- Reusability and event/process recycling

J. Phys.: Conf. Ser. 664 072024




Orr: PHY2405 lectures




### Simulation

- Majority of CPU spent in calorimeters

### Digitization

- Large number of inner tracker readout channels; complex modelling of readout emulation

### Reconstruction

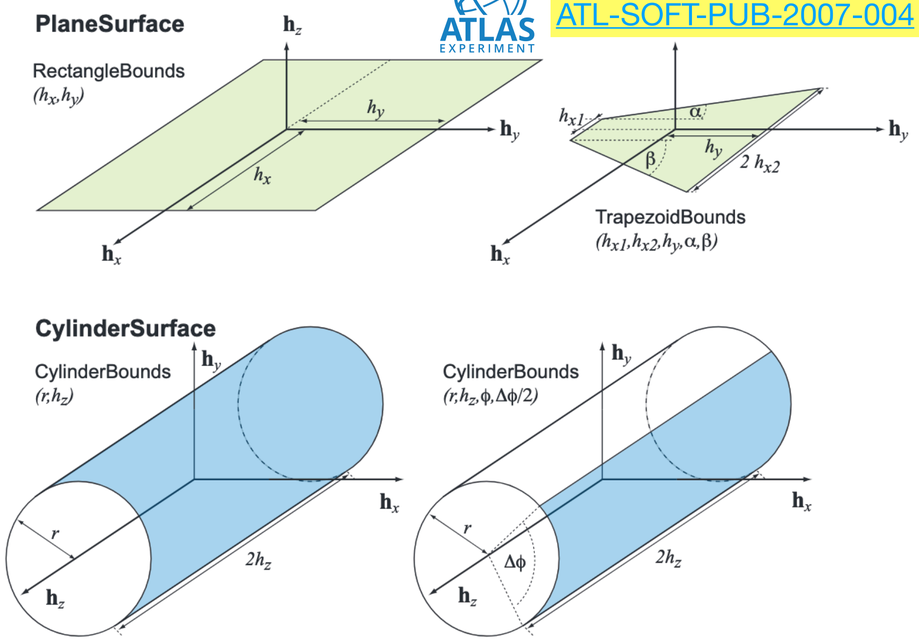
- Pattern recognition: combinatorial problem (function of $\langle\mu\rangle$)

# Current fast simulation

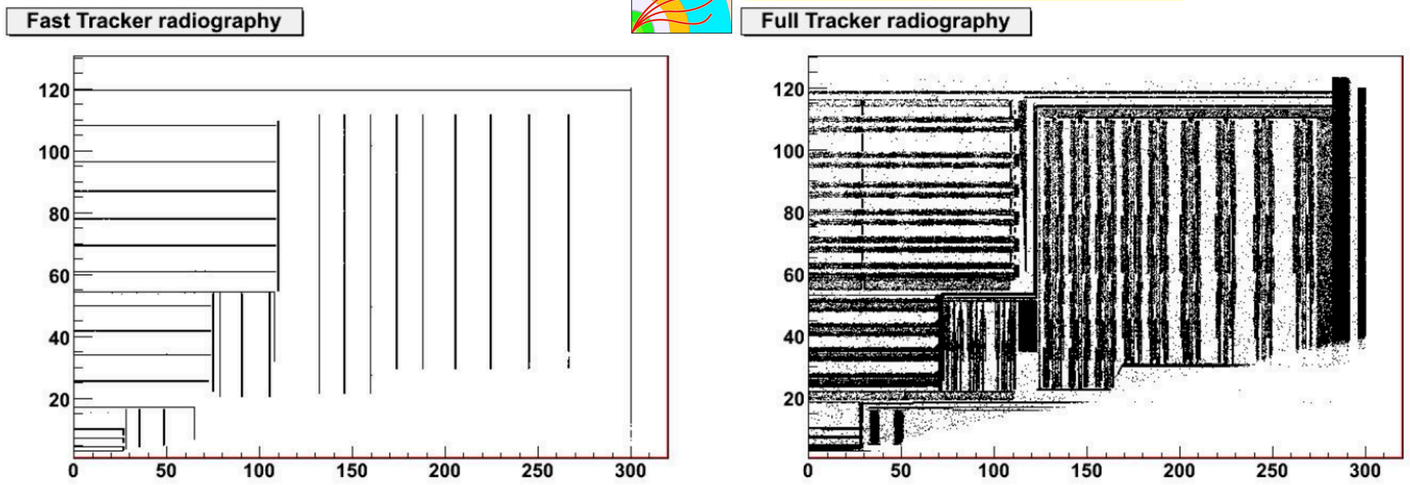
## *Simplified geometries*

- Approximations of full Geant4-based geometry for tracking and calorimetry
- Physical volumes -- e.g. cuboids, cylinders -- built from primitive surfaces rather than complex `G4VSolids`
- Detailed volume materials projected onto 2D surfaces

ATL-SOFT-PUB-2007-004




J. Phys.: Conf. Ser.513 022012




- Particle-material interactions on surfaces determined by surface 'thickness' measured in radiation/interaction lengths
- Database-lookup for detector properties, e.g. alignment, element extents

# Current fast simulation

## Calorimetry

### Geant4 EM and hadronic templates

- Simulate *e*, *γ*, *π*± shower shapes/energy profiles
  - *π* used for all (charged+neutral hadrons)

### Longitudinal and lateral profiles

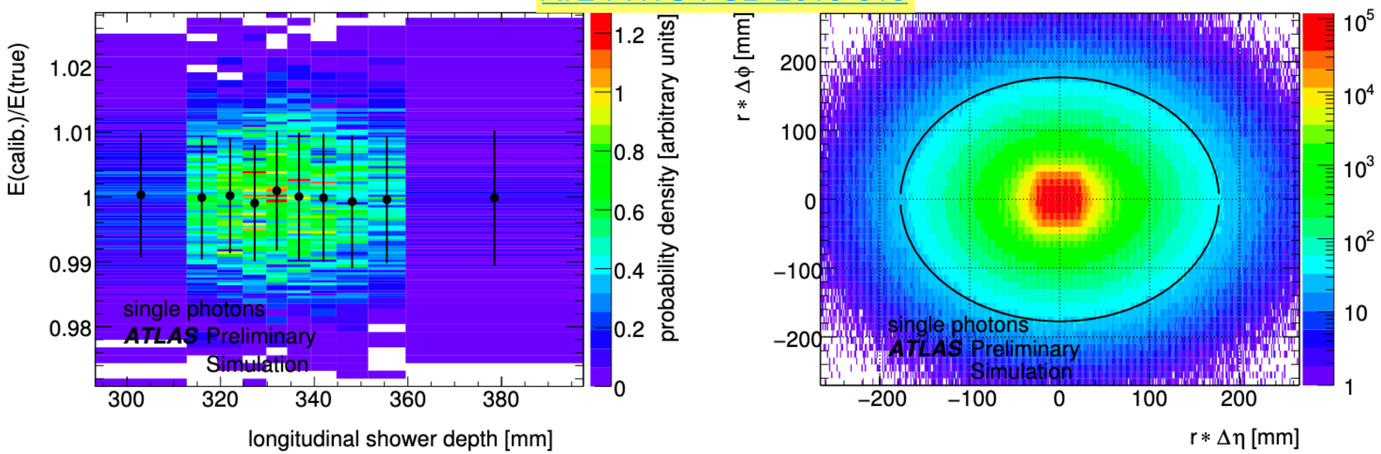
- Determine *E*-/*η*-dependent parameterization of shower properties: start and shape
- Fit parameterization to template and extract best parameters
- Sample energy deposits to create 'hits'

$$L(x) = \frac{x^{\alpha-1}e^{-x}}{\Gamma(\alpha)}$$

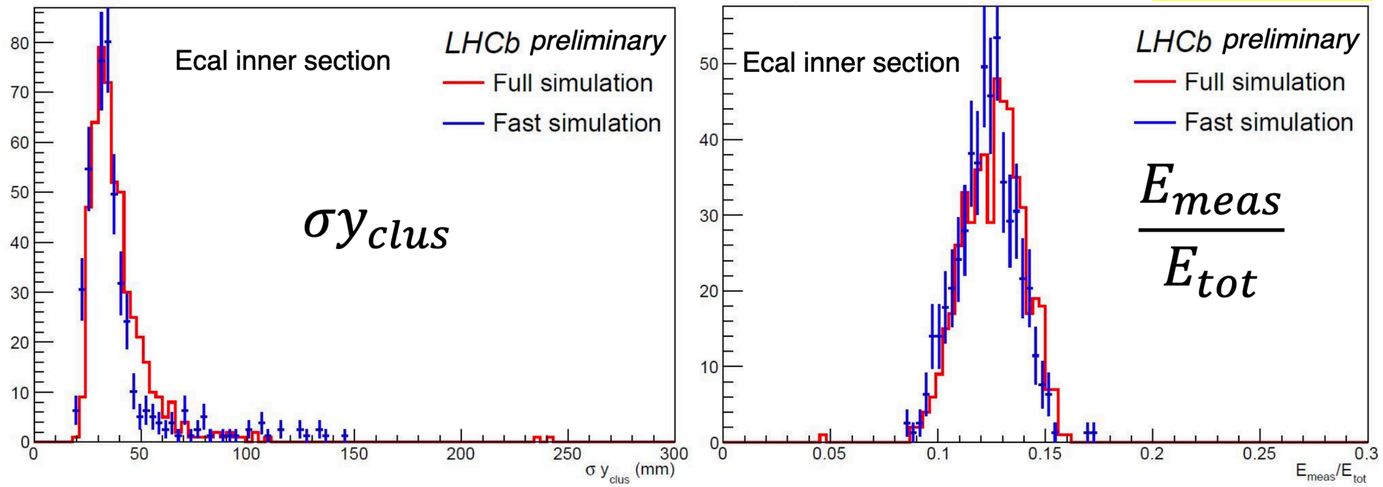
J. Phys.: Conf. Ser.293 012023

$$R(r) = \frac{2rR_0^2}{(r^2+R_0^2)^2}$$

ATL-PHYS-PUB-2010-013




Rama:CHEP18




### Shower libraries

- Homogeneous assumption does not hold
- Thresholds/cutoffs for low-*E* particles
- Geant4-based 'libraries' of showers
  - Compression achieved through, *e.g.* clustering and truncation cutoffs => rescaling

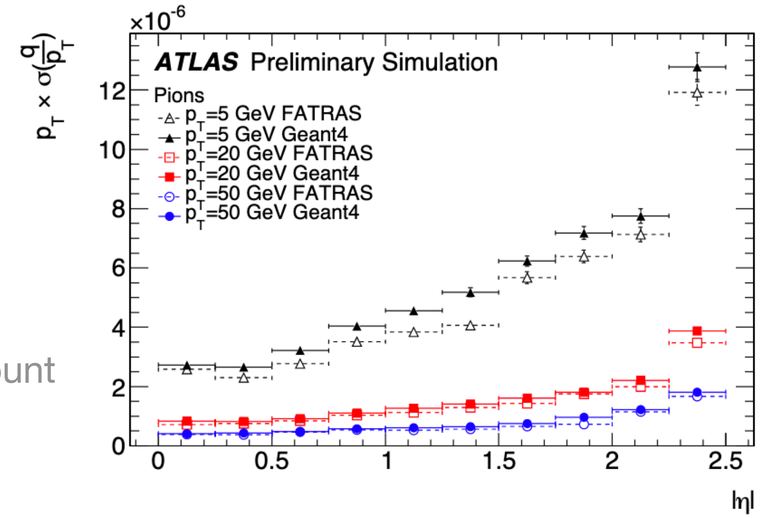
# Current fast simulation

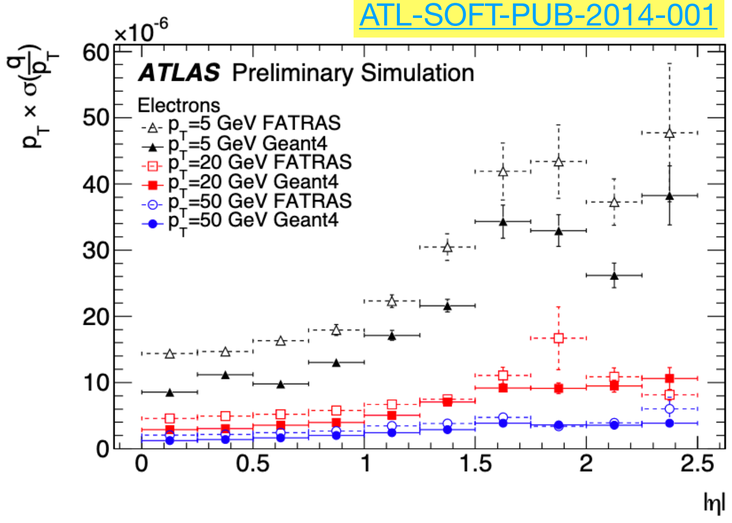
## *Tracking*

### Simulation

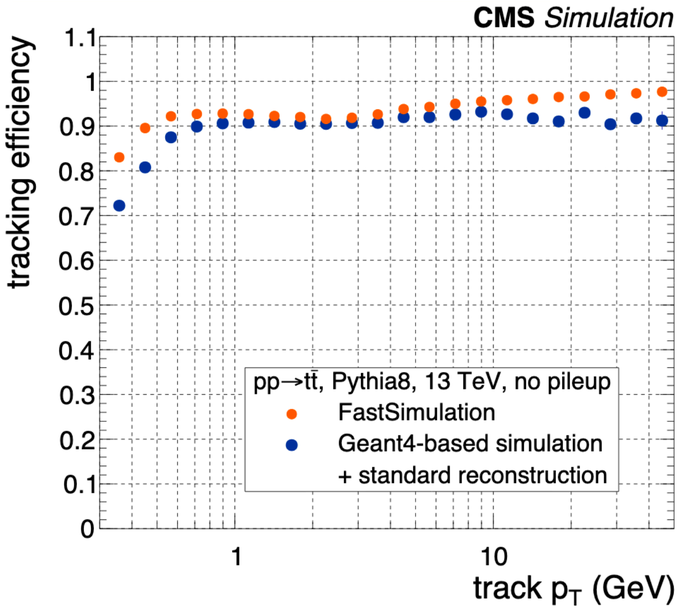
- Parameterizations models for particle-material interactions
- Material effects for, *e.g.* bremsstrahlung and photon conversions, multiple-scattering; dependent on amount of material traversed

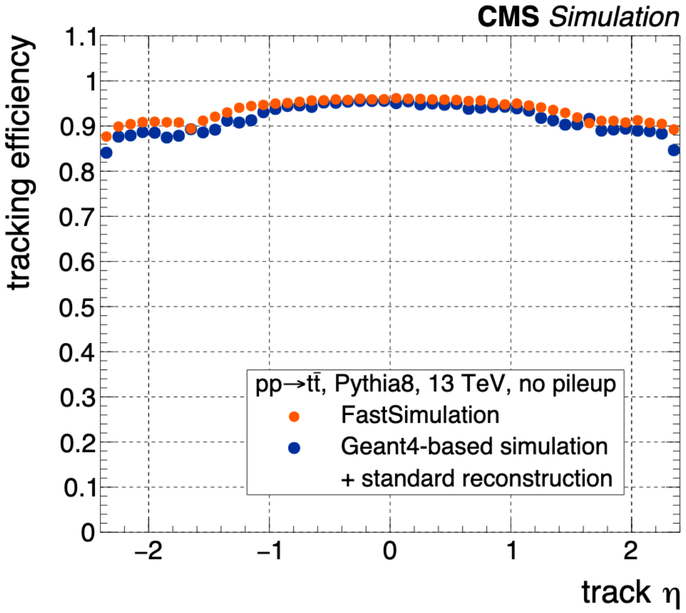
ATL-SOFT-PUB-2014-001




J. Phys.: Conf. Ser. 898 (2017) 042034



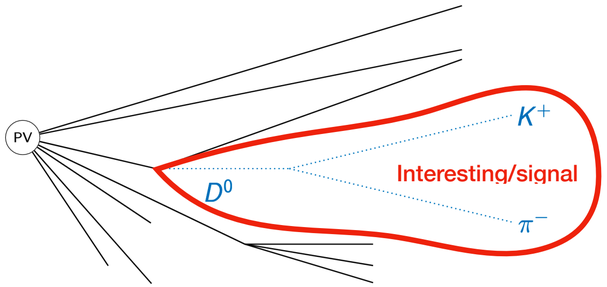

### Reconstruction

- Exploit MC generator, *i.e.* truth, information (ideal detector)
  - Skip pattern recognition, seeding and ambiguity treatment
- Manipulate true hits to remove bias in track fitting
  - Hit content and efficiencies
  - Merging of near-by hits, track-sharing, 'fake' tracks

# Current fast simulation

## *ReDecay*

Eur. Phys. J. C (2018) 78: 1009

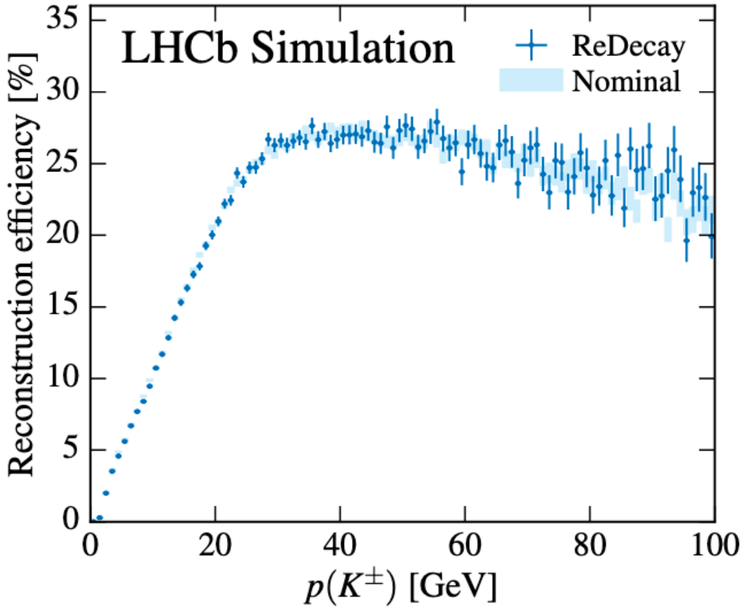



### Philosophy

- Should spend majority of time simulating interesting processes, not rest of event (ROE)

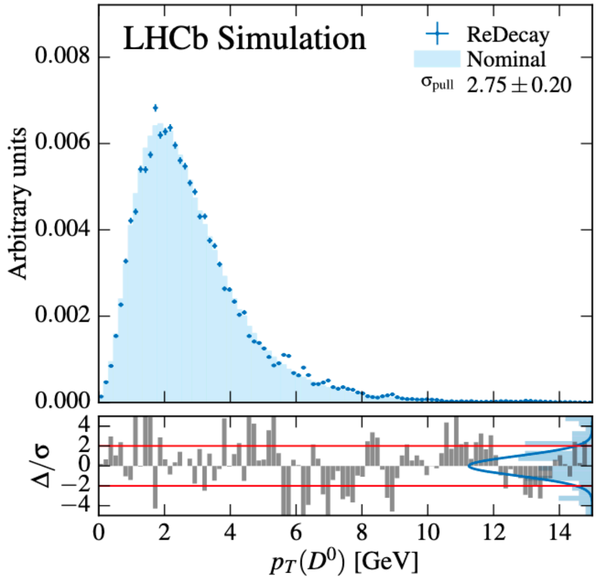
### Generate ROE once, signal $N_{\text{ReDecay}}$ times

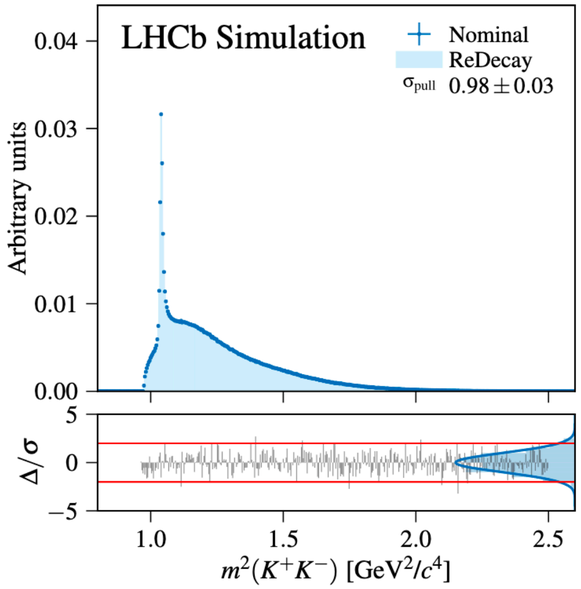
- New $D^0$ decay vertex along fixed momentum vector
  - New decay product kinematics
- Same efficiencies and resolution (by construction)




### All shapes in agreement but correlations exist

- Effect of statistical uncertainties depend on studied observable
  - Sample original events and take all *ReDecay*'d replicas
- Most observables are unaffected



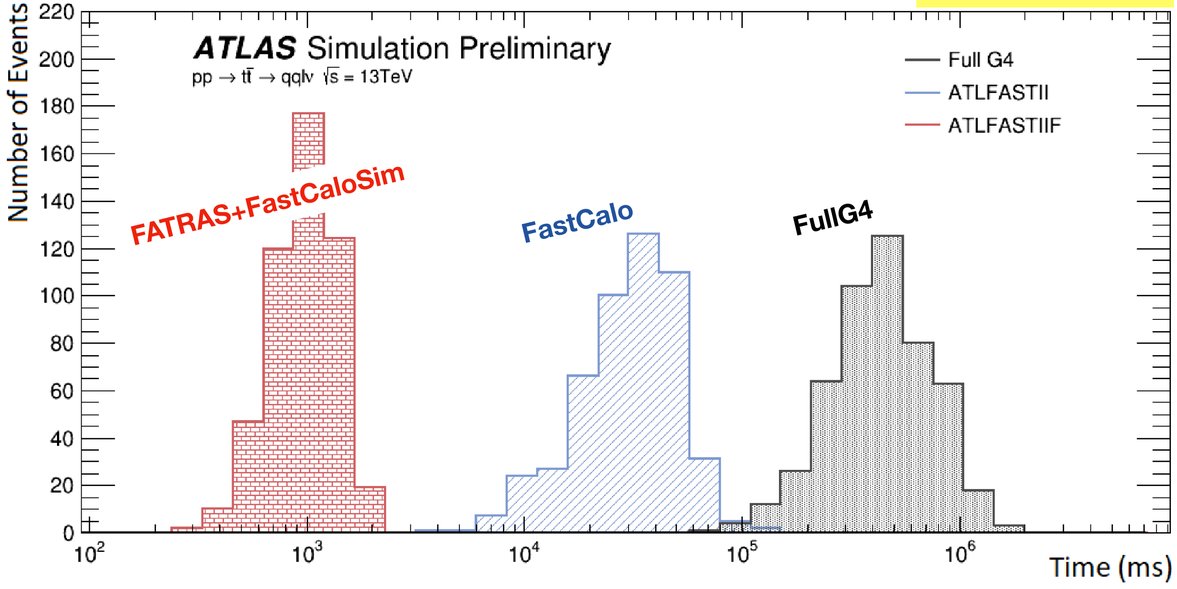

**CMS simulates all pile-up using FastSim that is mixed with hard-scatter events in SimHits or RecHits. ATLAS is working on MC+MC overlay (see talk from T. Novak).*

# Current fast simulation

## *Mini-summary I*

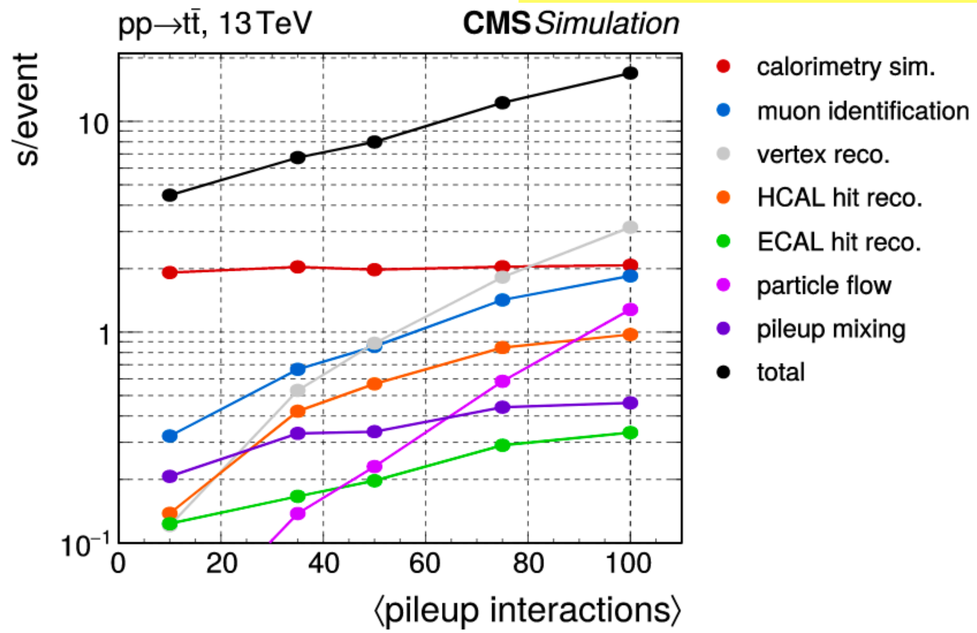
- Parameterized calorimeter simulations used for large fraction of Run-2 MC production
- Combine configurable **Fast** (simulation + digitization + reconstruction) **Chain**

SIM-2019-002




- Fast tracking, calorimeter and fast emulation of track reconstruction for significant fraction of Run-2 MC production; 20~100x speed-ups
- Ongoing accuracy/precision improvements, support for Phase-2

J. Phys.: Conf. Ser. 898 (2017) 042034

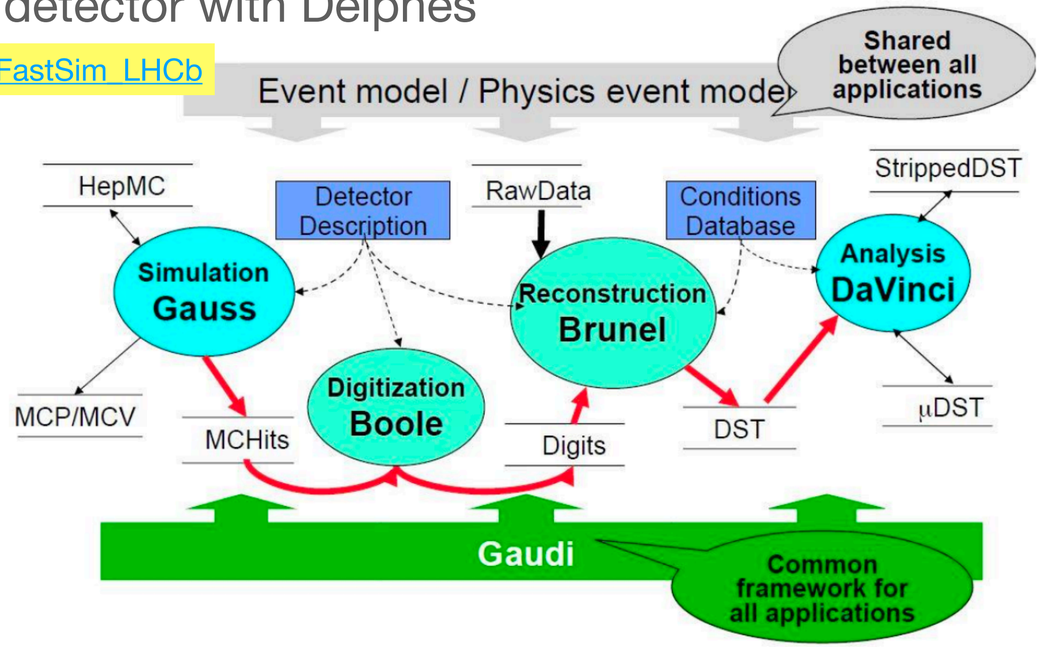


# Current fast simulation

## *Mini-summary II*

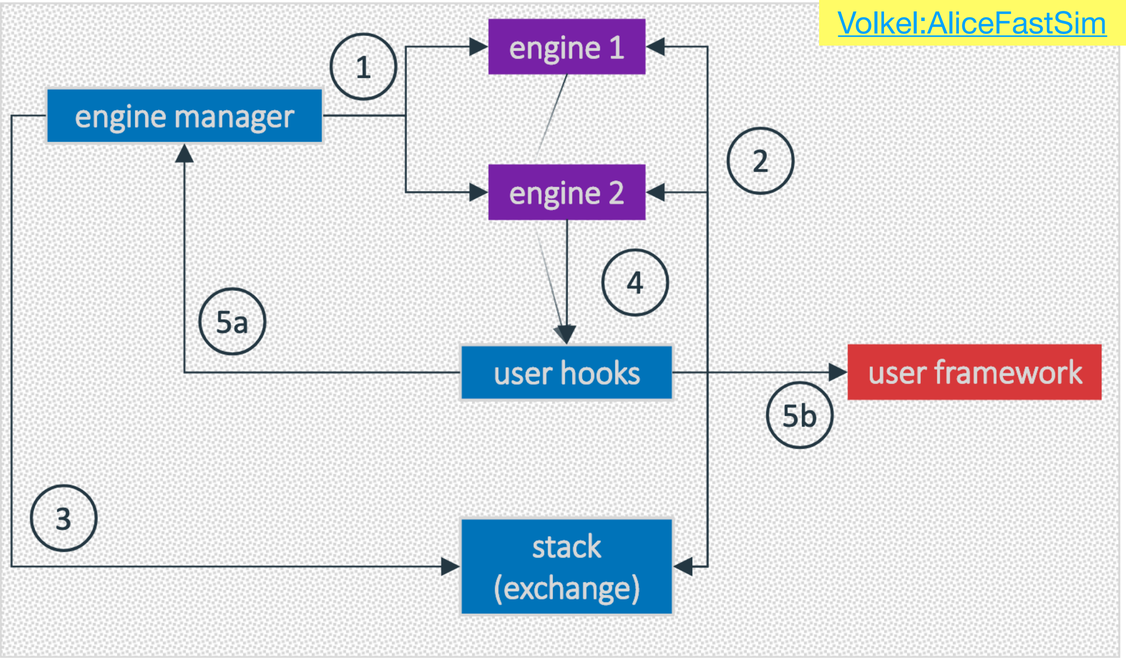
- ReDecay used for O(100M) events already, up to 50x speed-ups; additional 30-50x from frozen showers
- Other ideas: disable subdetectors, fully parameterized detector with Delphes

Müller:FastSim_LHCb




- Detector simulation based on ROOT VMC
- Intending to have ability to mix multiple full simulation engines with fast simulation kernels
  - Extension to VMC

Volkel:AliceFastSim



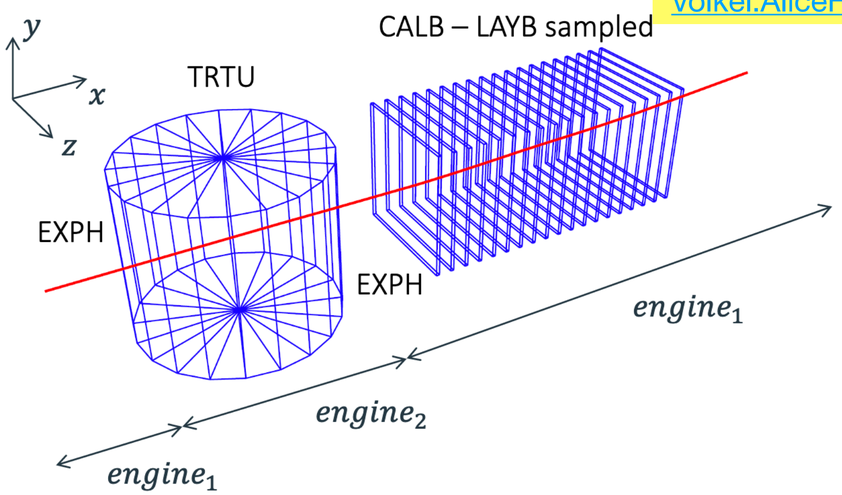
# Future fast simulation

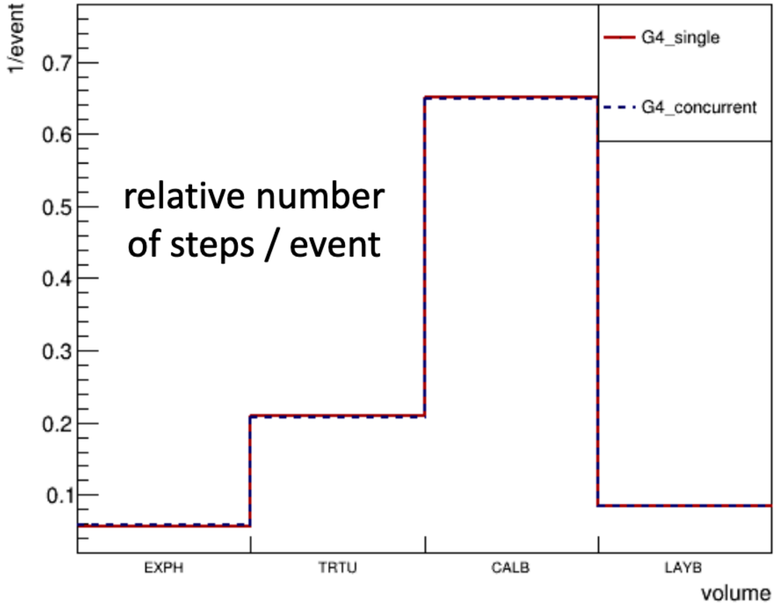
## *Harmonizing full + fast simulation techniques*

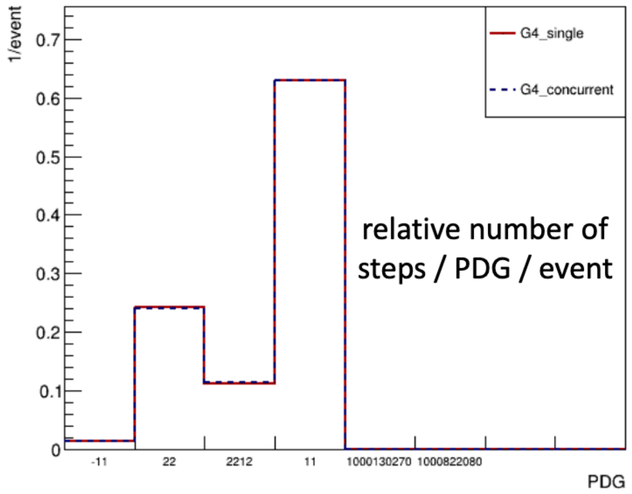
### Philosophy

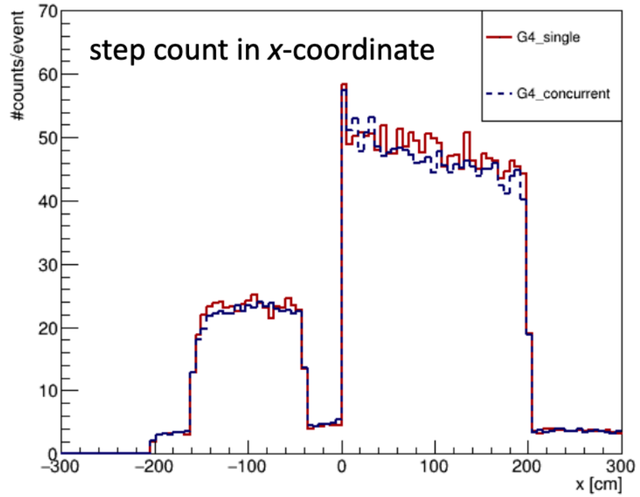
- Fully simulate only signal objects or specific subdetector, fast everything else
  - Streamline full+fast simulation techniques

Volkel:AliceFastSim




### Proof-of-concept

- Mixing of two simulation "engines" with toy model
- Check between single and concurrent Geant4 instances

*ATLAS developed the Integrated Simulation Framework (ISF) but a number of difficulties -- e.g. defining scale factors, many types of MC -- are encountered.

# Future fast simulation

## *Ex machina: learned machines*

### Existing methods effective, however...

- Average lateral shower properties, uncorrelated energy fluctuations
- Sub-clusters not well modelled
- Pre-simulated showers => finite library size

### Unsupervised learning

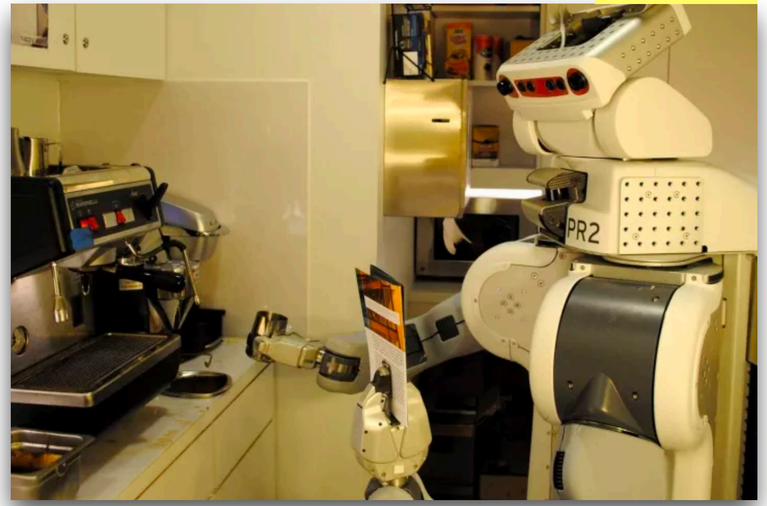
- Learn relationships between dataset properties and classify without being told the 'answer'
  - Principle Component Analysis **(PCA)**
  - Generative Adversarial Networks **(GANs)**
  - Variational Auto-Encoders **(VAEs)**

### Exploit accelerators

- Ideal use-case for GPUs and FPGAs
  - *e.g.* hyperparameter scans

coursera.org

Roborista




wikipedia.org/CDC 6600


theverge.com/circuitbreaker

# Future fast simulation

## *FastCaloSimV2*

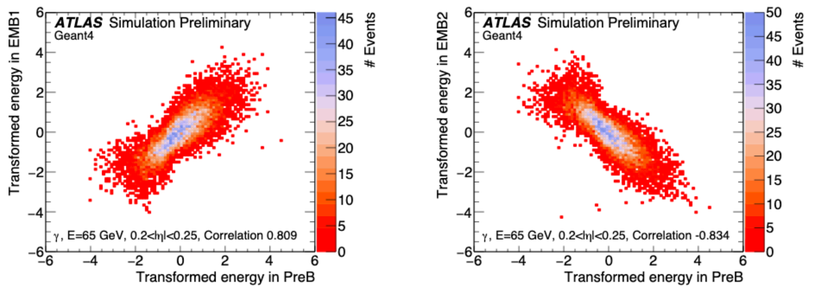
ATL-SOFT-PUB-2018-002

Improved energy and shape parameterizations

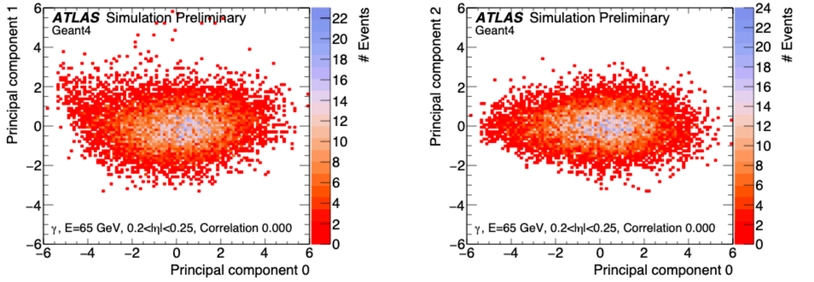
- Decorrelate using PCA
- Speed comparable to legacy FastCaloSim
  - Add forward calorimeters, improved lateral shower profiles

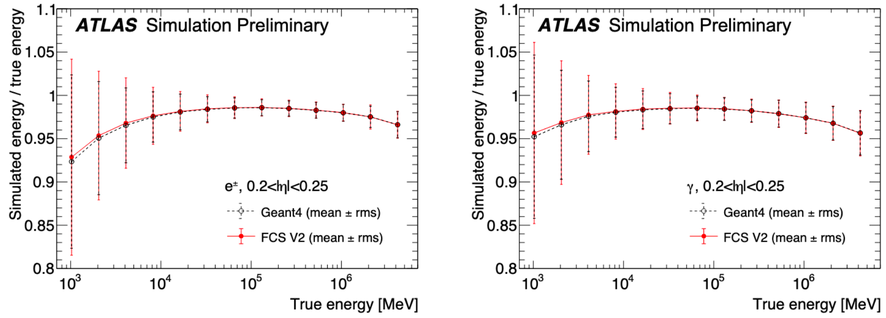
| Step | Description |
|---|---|
| **Input** | $E_{tot}$ and $E_{frac}$ from Geant4 samples |
| **Transform** | Construct cumulative distributions (integrating over all events) from inputs, transformed into Gaussians |
| **PCA** | Construct PCA matrices; first principal component (PC) is rotated in direction of maximum variance |
| **Bin** | Divide input shower samples into 'PCA bins' consisting of equal number of events (*i.e* probabilities) |
| **Reiterate** | Assign each sample a PCA bin and perform PCA chain again |

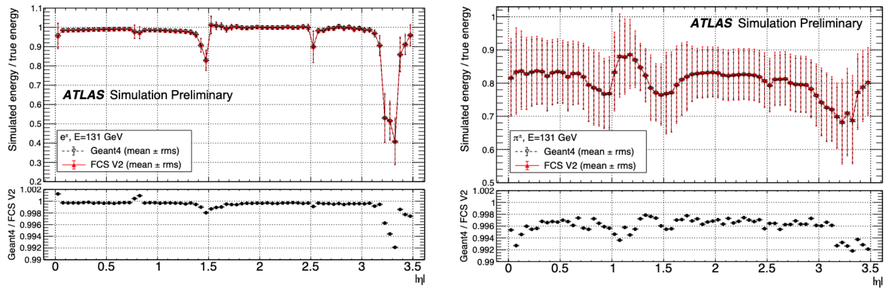
**Before rotation**




**After rotation**



# Future fast simulation

## *Deep generative models* HSF Simulation Working Group

Generate new samples following probabilistic distribution as training set

- Try to learn true data distribution -> reproduce it
- Learn 'approximation function' of true distribution

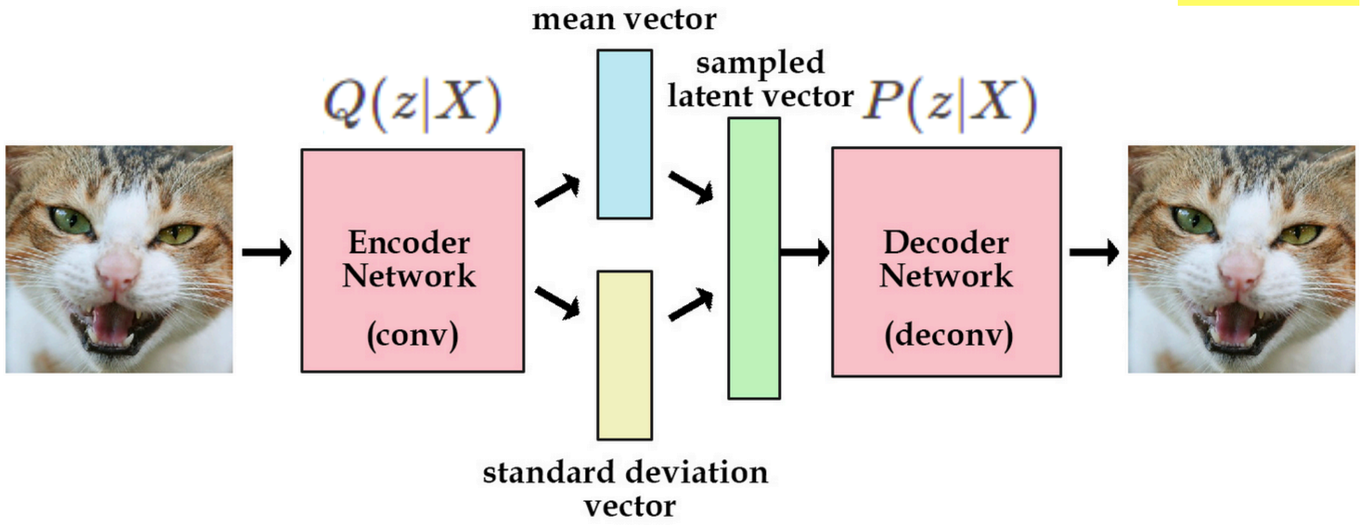
VAEs

- Maximize lower bound of data log-likelihood
  - Generate samples with variations
- Depend on learning probability density
  - Low-dimensional latent space => blurry images output

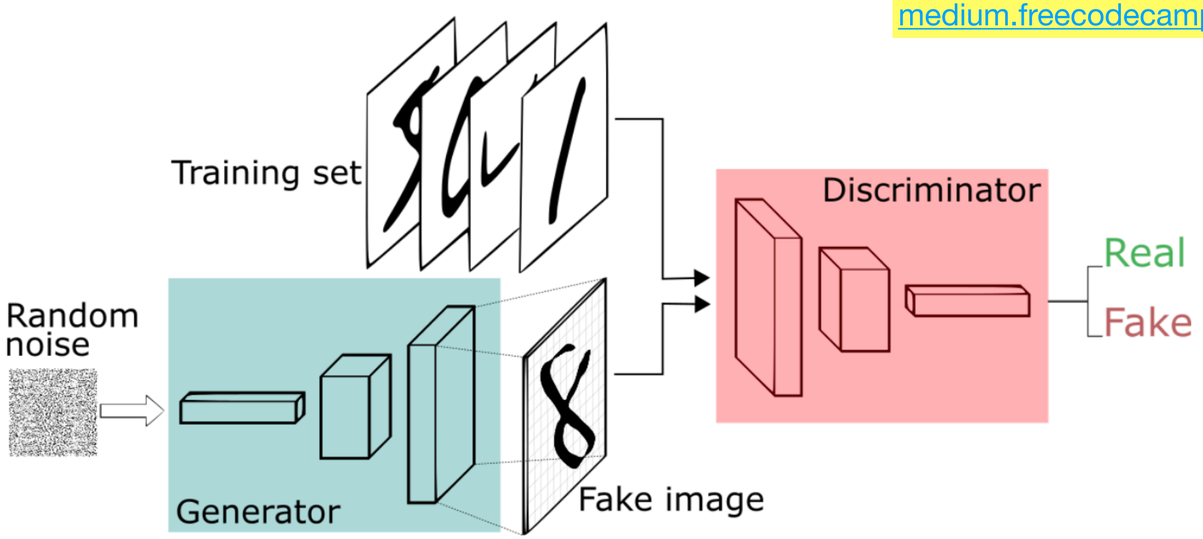
GANs

- Equilibrium between generator and discriminator
- High-quality images output but complicated to work with

kvfrans.com



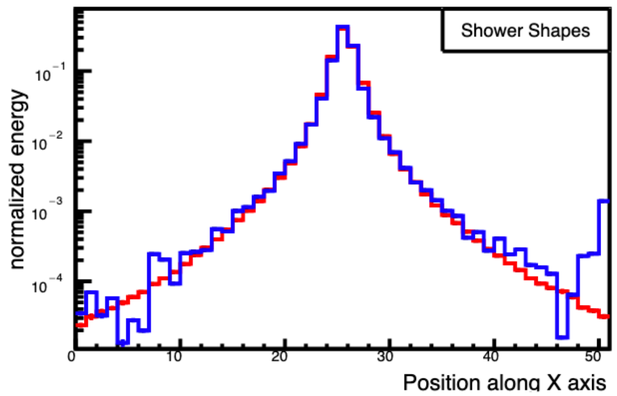

medium.freecodecamp.org

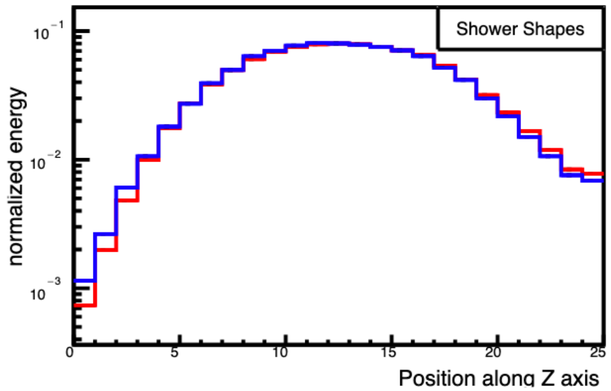


# Future fast simulation

## *DL efforts at the LHC* HSF Simulation Working Group

CERN openlab 3D convolutional GANs

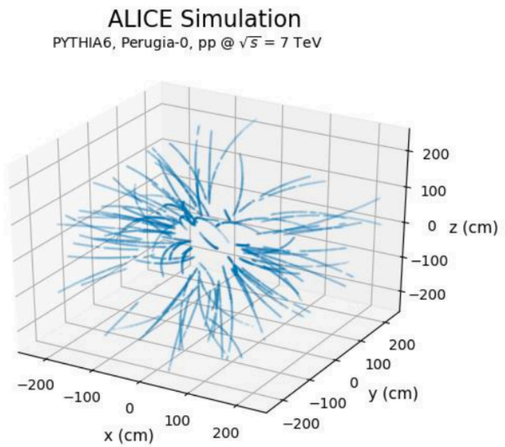


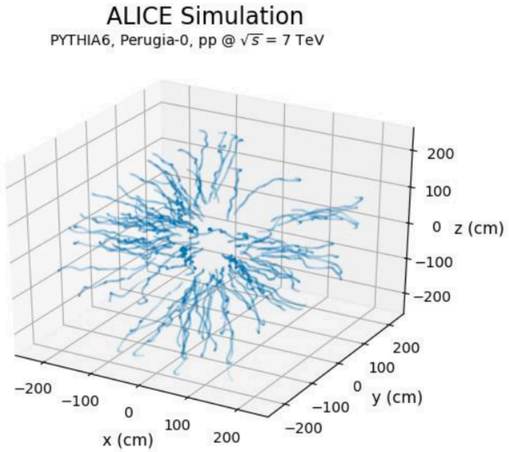




- Inference testing on GPUs, FPGAs
- TensorFlow+MKL-DNN
  - Speedups ~ 10000
  - 1ms/shower

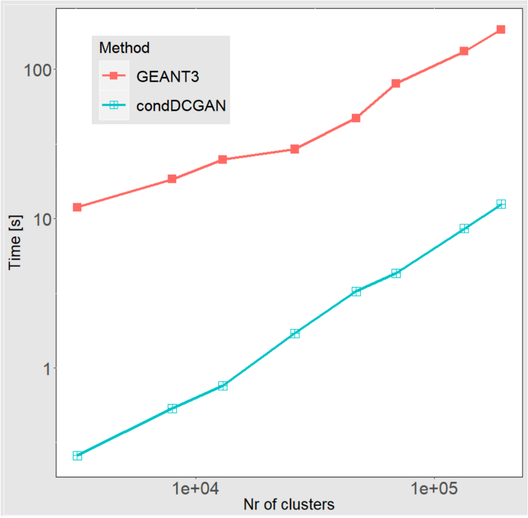
| Time to create an electron shower | | |
|---|---|---|
| Method | Machine | Time/Shower (msec) |
| **Full Simulation (geant4)** | Intel Xeon Platinum 8180 | 17000 |
| **3d GAN (batch size 128)** | **Intel Xeon Platinum 8180 (TF 1.4)** | **7** |

ALICE condDCGAN



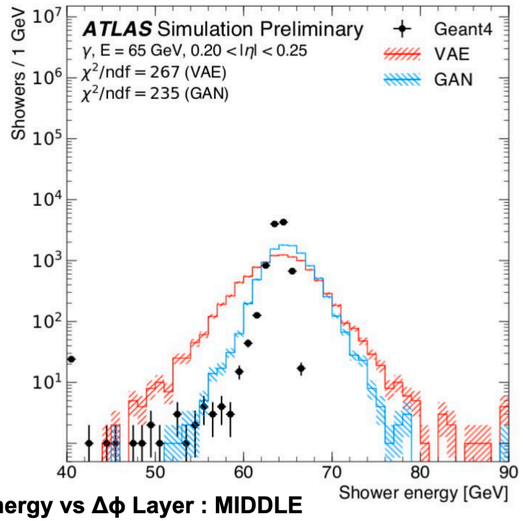

- Performance measured i7-6850K (single core)
- Anticipate additional order of magnitude with Titan XP



# Future fast simulation

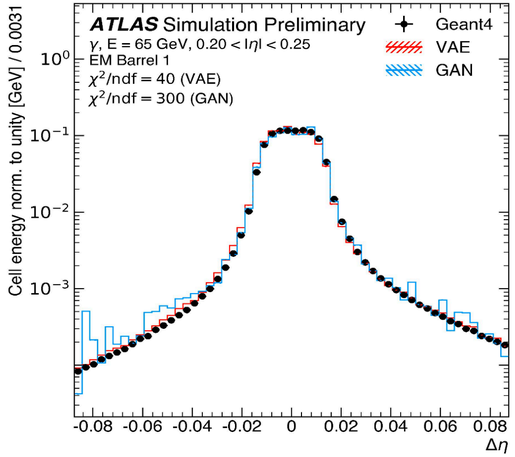
## *DL efforts at the LHC* HSF Simulation Working Group

### VAEs and GANs

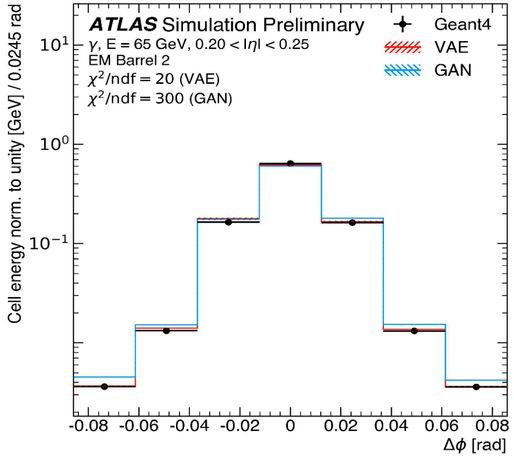



- Single $\gamma$, $E$ = 65 GeV, $0.2 < |\eta| < 0.25$
- Challenges posed by layers with small (and sparse) energy deposits

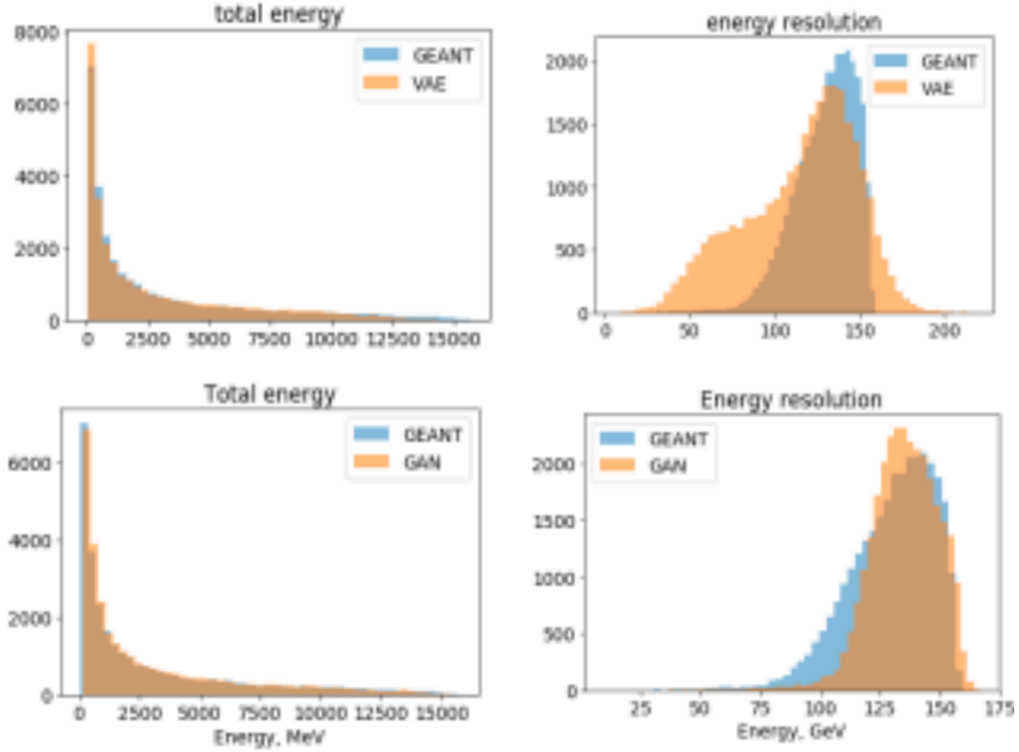
**Average energy vs Δη Layer : STRIP**




**Average energy vs Δϕ Layer : MIDDLE**




### VAEs and GANs




*"For image generation we are usually happy if the result looks like it is desired...In science we need the result to reasonably well match the given set of requirements."*

# Summary

With an increasing (HL-)LHC luminosity, we need to look towards fast simulations

- Some techniques employed for nearly a decade, worked well
  - Parameterizations, reduced geometries, other simplifications
- We already know these won't suffice in the future
  - Some cases accuracy is also a problem

Next generation of fast simulation requires new strategies

- Integration of full+fast techniques into harmonized framework
- Much effort ongoing to exploit advanced statistical techniques and fast hardware
  - Machine learning
  - Accelerators and HPC

Deep learning shows promise

- LHC experiments devoting human-power into generative algorithms
  - Detector-agnostic implementation, use of GPUs, FPGAs, HPC
- Still some R&D before hitting mainstream/production
  - Scientific requirements and considerations are crucial

# Backup

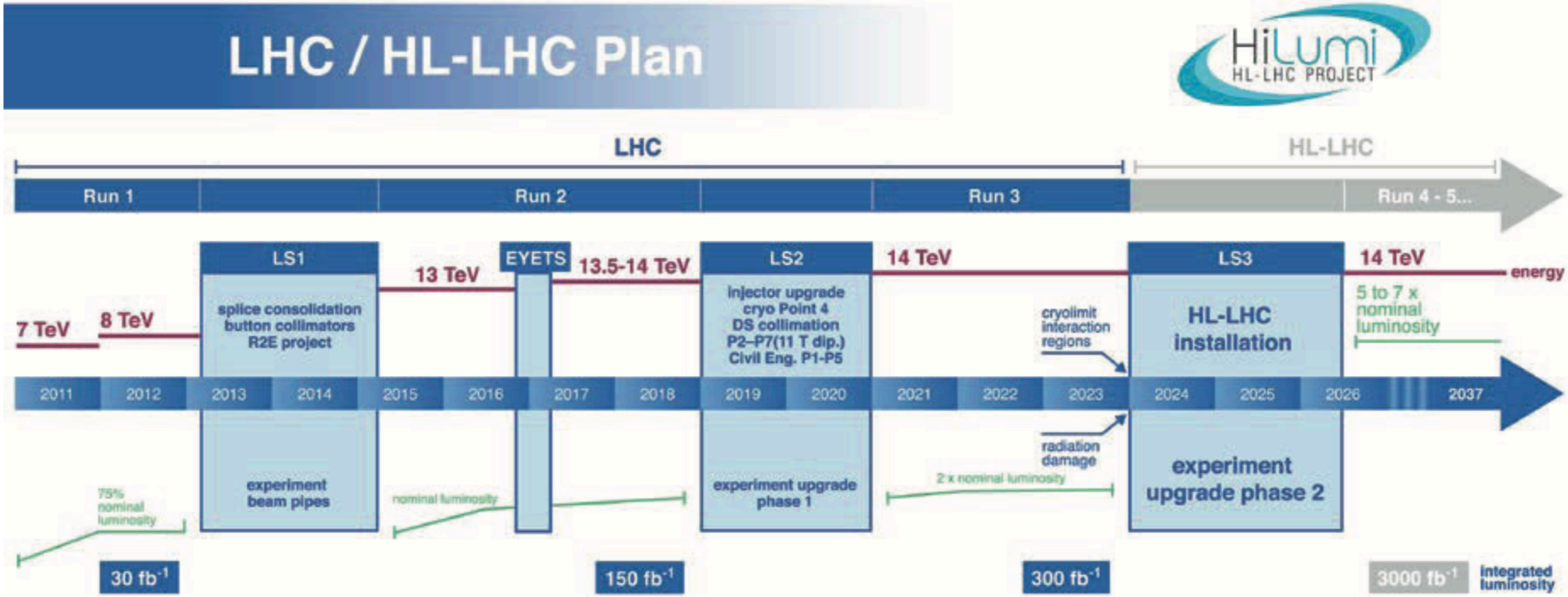

cbc.ca/sports/hockey

(The joke: Calvin Pickard is/was a backup goalie.)

# Projected LHC programme

LHC has been increasing luminosity since its inception

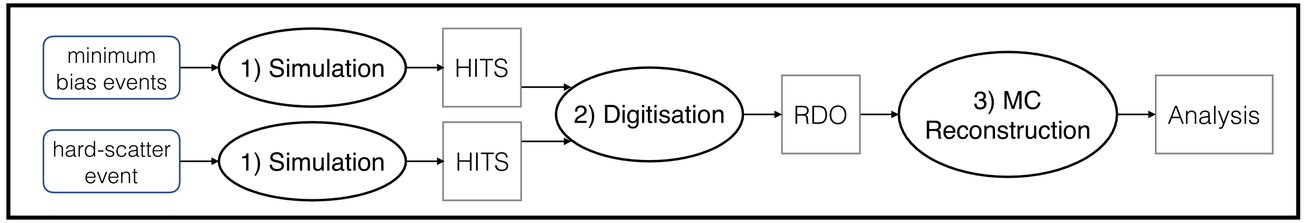
CERN-2017-007-M

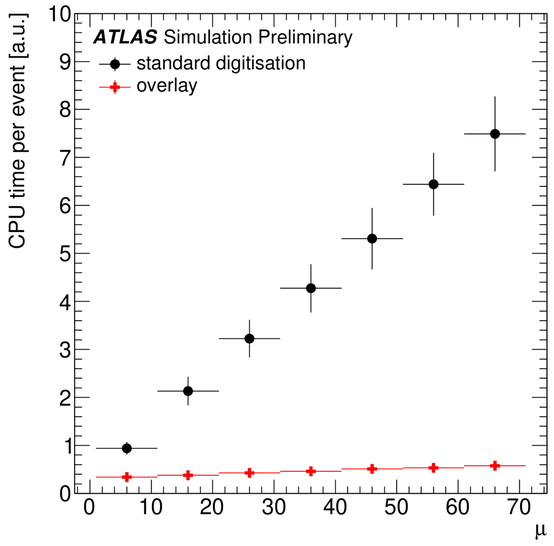


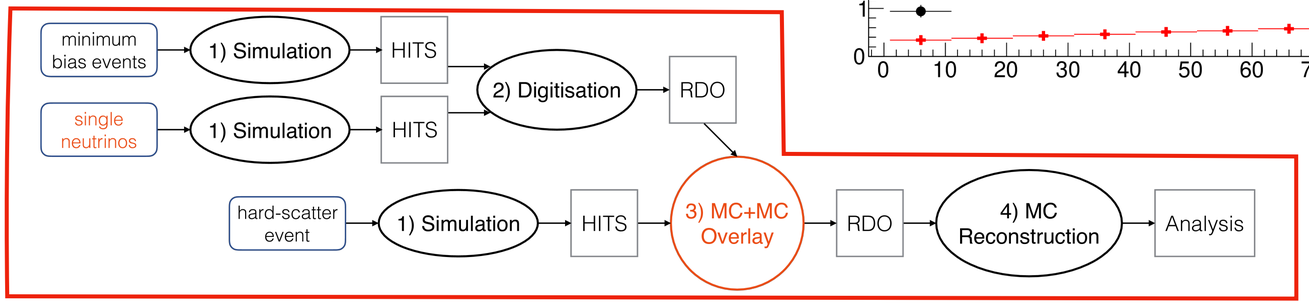
# Current fast simulation

## *Ongoing work*

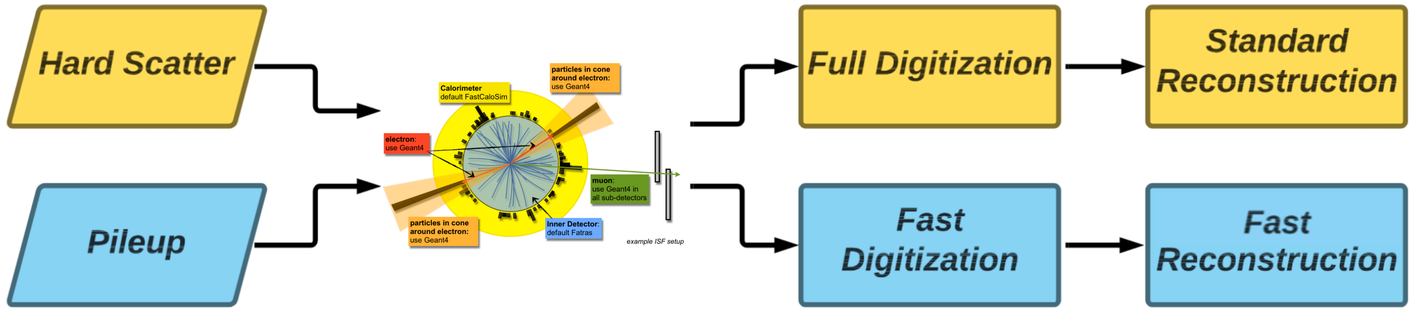
### Recycling: MC+MC overlay

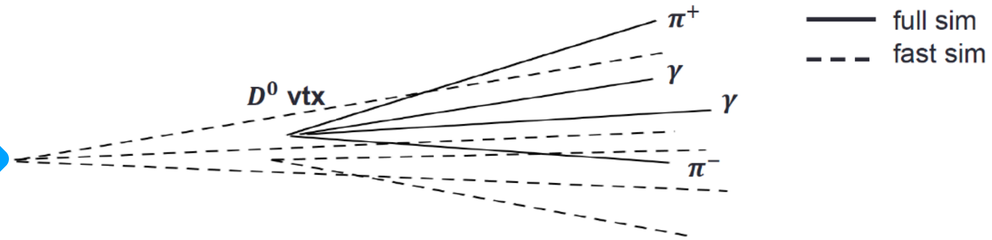


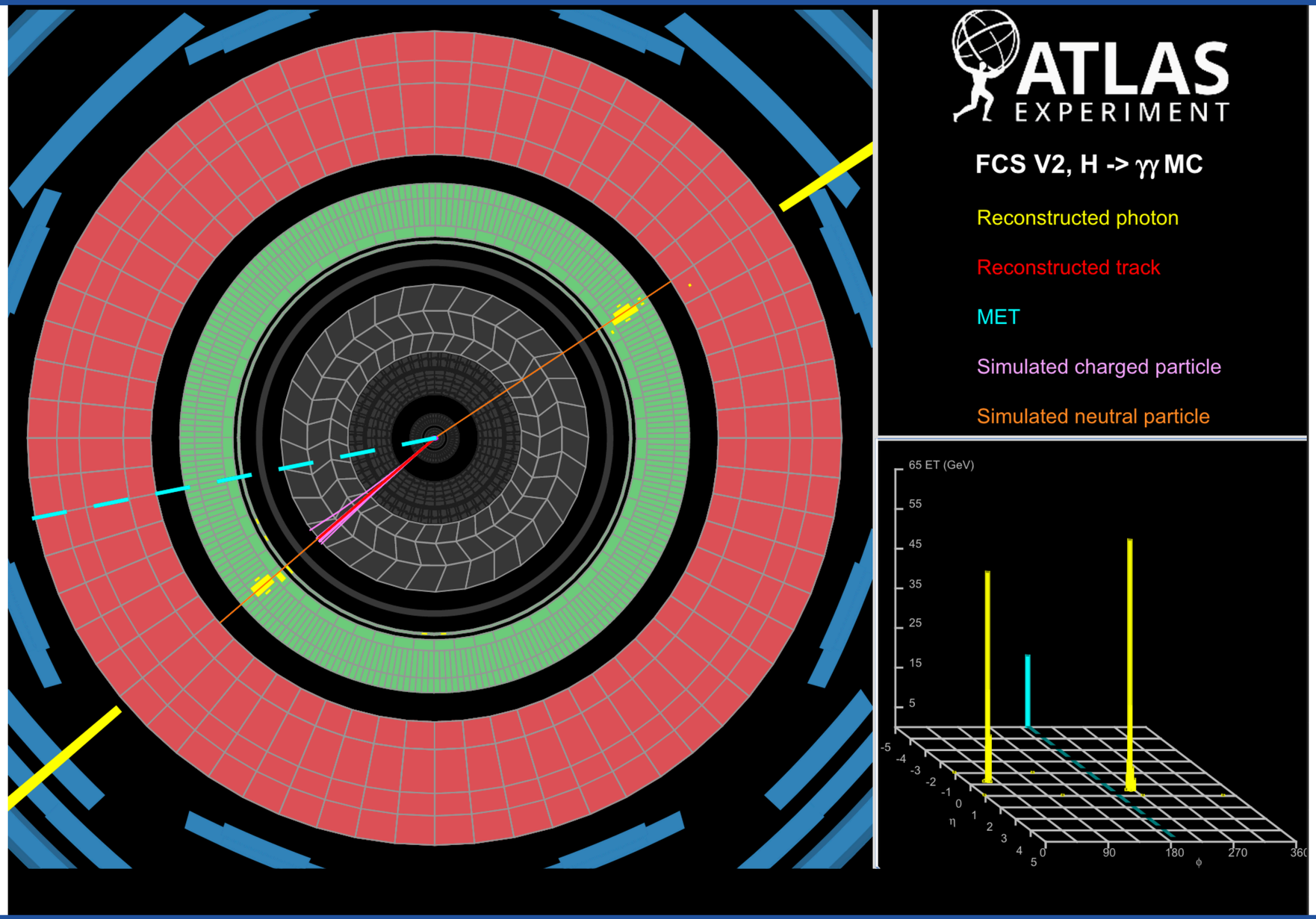




### Streamlining full+fast simulation techniques



# Future fast simulation



# Future fast simulation

## Fast Digitisation for Inner Detector

ATL-SOFT-PROC-2017-022

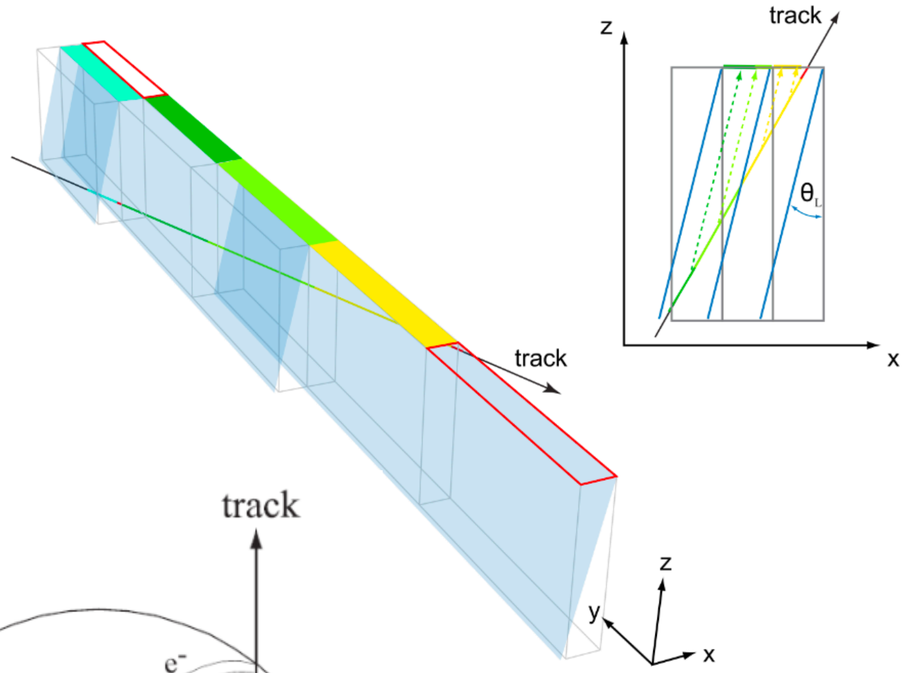
- Most time-consuming (~50%) due to high density of hits
- Implemented for Pixel, SCT, and TRT detectors

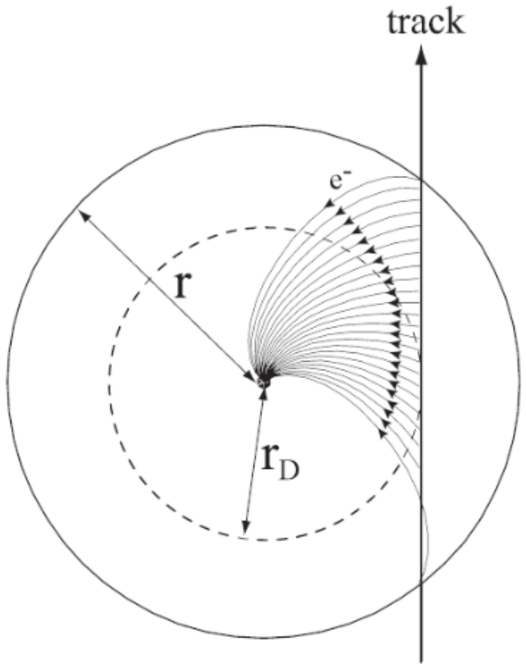
### *Pixel and SCT*

- Estimate charge by projecting simulated track length onto readout surface (for each readout channel)
  - Corrections made for Lorentz angle drift
- Charge and track lengths smeared to account for multiple scattering
- Form clusters directly from track information (no cluster-finding algorithms)

### *TRT*

- Emulate response using distance of nearest approach
- Smear for uncertainty estimate
- Parameterisation allows for particle ID



# Future fast simulation

## Fast(/truth-assisted(/seeded)) Reconstruction (/Pseudo-tracking)

- Build particle trajectories from digitised hits
  - Combinatorial in nature, exponential increase with increasing pile-up
    - Dominated by Inner Detector

### *Methodology*

- Emulate effect of standard algorithms using MC generator (*i.e.* truth) information
  - Skip time-consuming pattern recognition
- Manipulate hit content and efficiency
  - Apply similar selection on criteria used in standard tracking