Fast simulation with Machine Learning

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Outline

Introduction

Introduction to Machine Learning and some info about its evolution and ecosystem

Need for FastSim

How and why experiments will need more and more fast simulations approaches

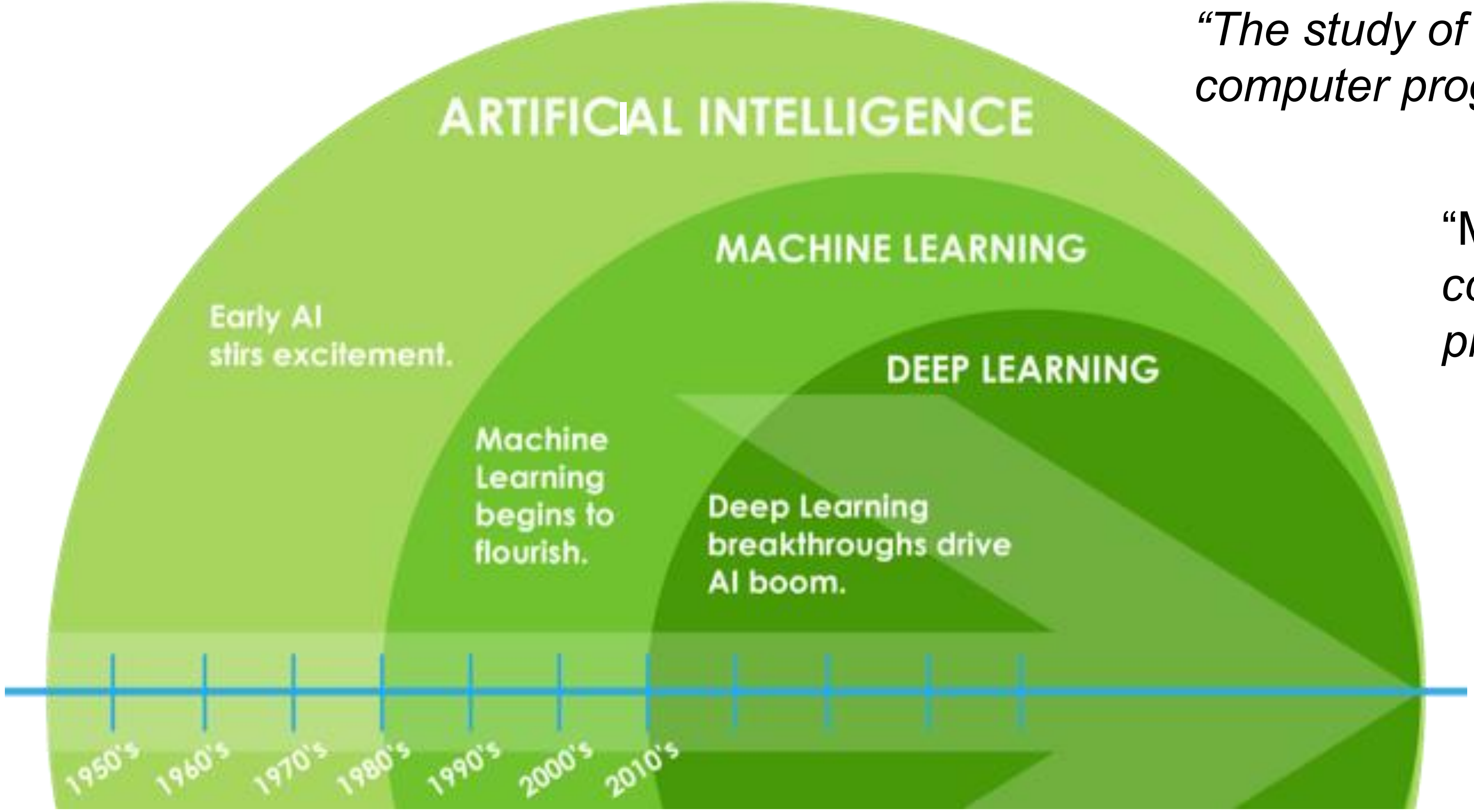
Fast Simulation in the experiments

Different approaches to fast simulation in LHC experiments

A Generic Fast Simulation approach

To what extent these approaches can be generalized?

AI, ML and DL

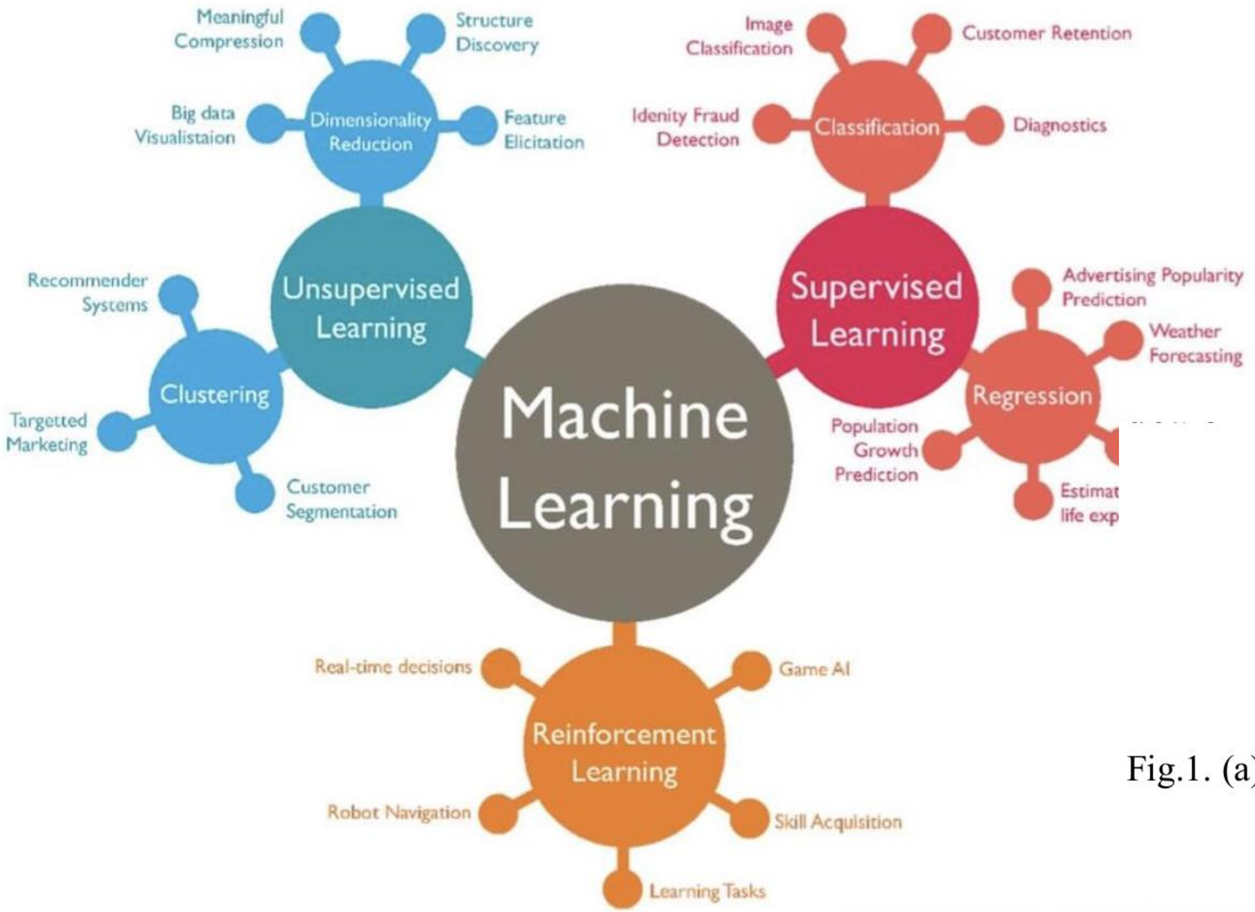


"The study of the modelling of human mental functions by computer programs."—

"Machine learning is the sc*ience of getting computers to act without being explicitly programmed."—*

"Deep Learning is a subfield of machine learning concerned with algorithms inspired by the structure and function of the brain called artificial neural networks".—Machine Learning Mastery

Variety of ML/DL algorithms



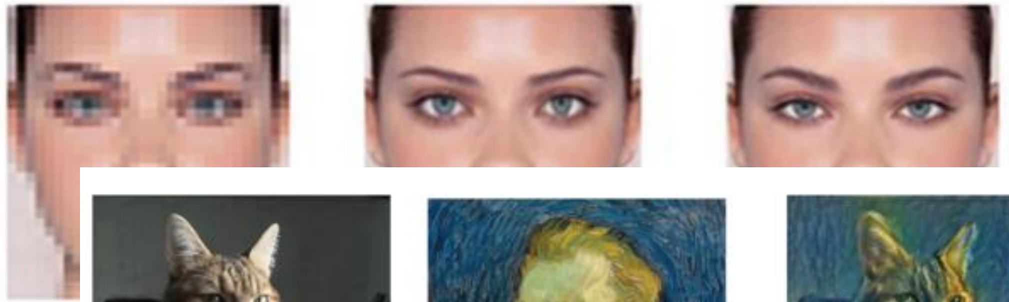
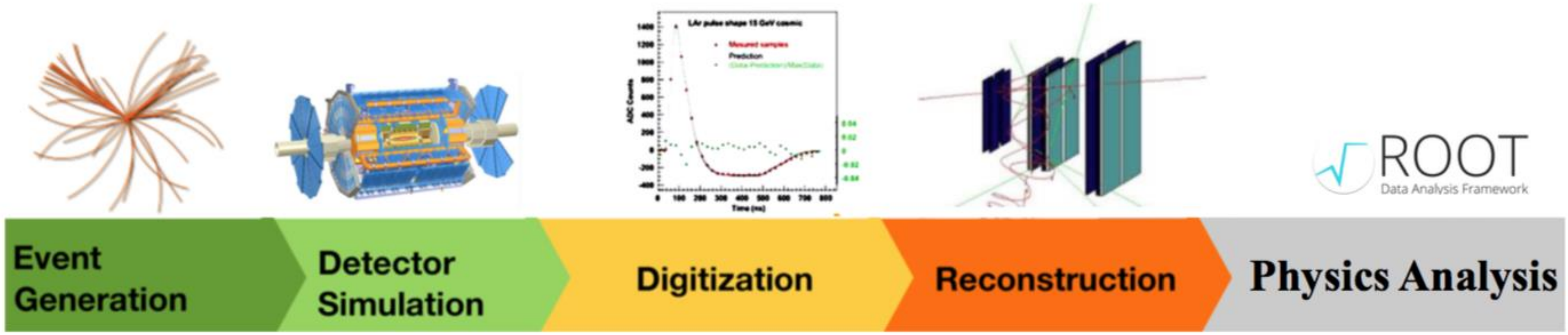
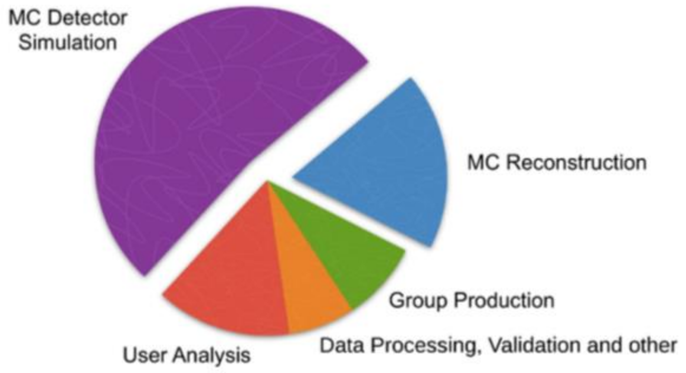


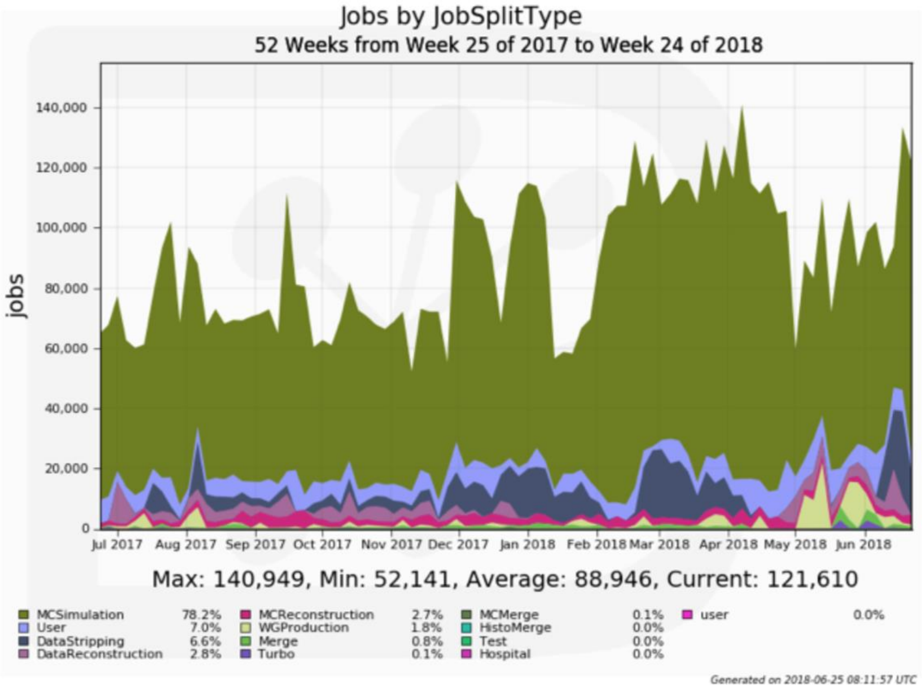
Fig.1. (a) Low I ... ace.

Need for Fast Sim

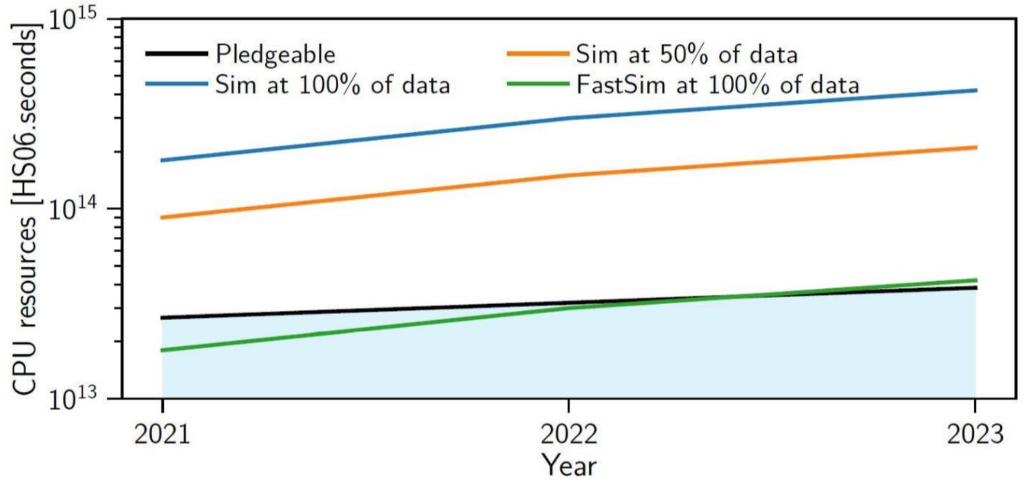




ICHEP2018, Hasib Ahmed (Atlas)



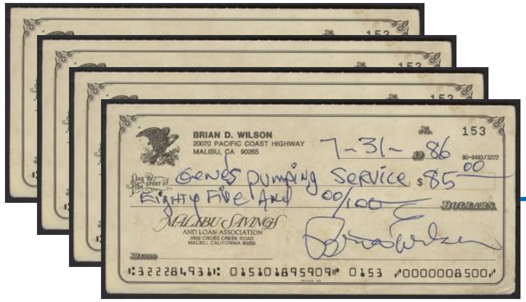
Legend: "Sim at 50% of data" = FullSim sample is 50% the datasize, FastSim sample is 50% the datasize



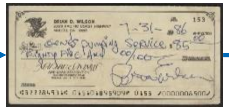
FastSim assumed to be 1/10 faster than FullSim

HSF workshop 2018, G. Corti (LHCb)

Generative Adversarial Netwoks



https://33milesinnewaygocounty.files.wordpress.com



Generator

https://giphy.com/gifs/leonardo-dicaprio-catch-me-if-you-can-5leocharacters-t1h4nnWEWKfn2

Discriminator

https://thechive.files.wordpress.com

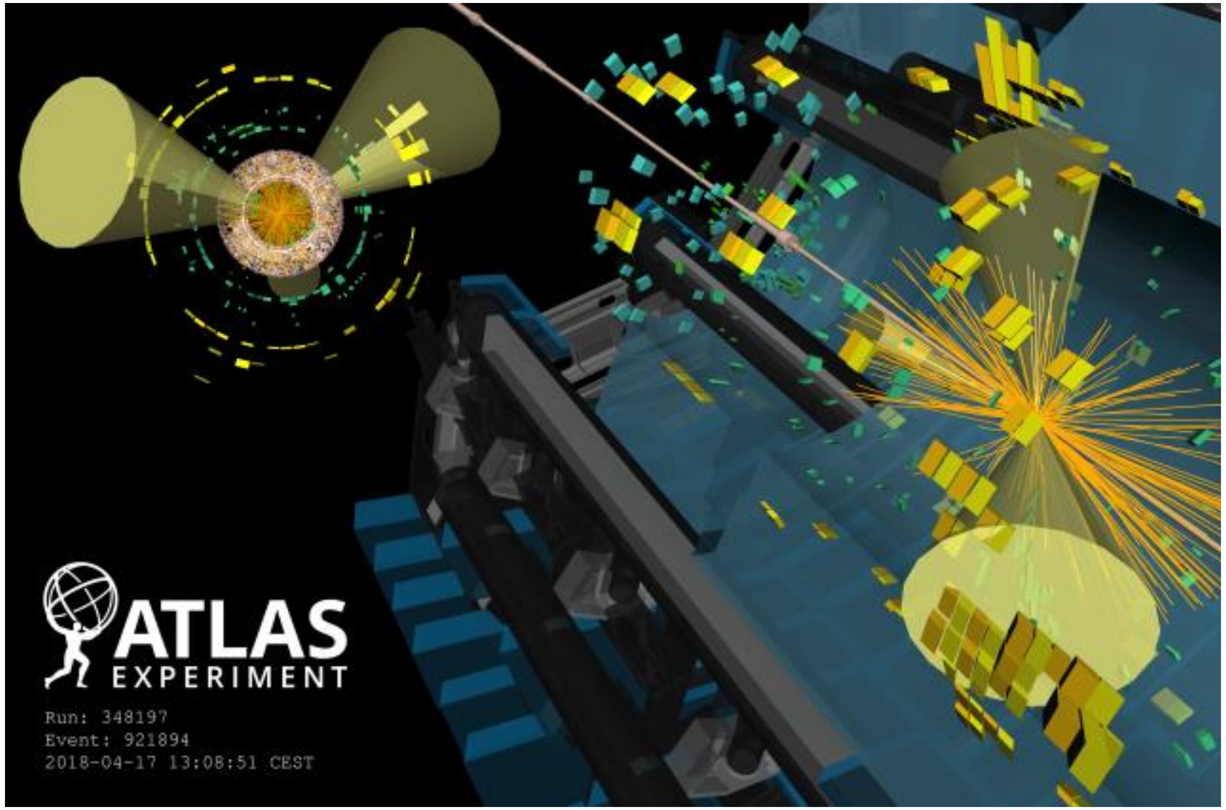
**First example of simplified calorimeter simulation, CaloGan: M. Paganini et al. arXiv:1712.10321*

FastSim Atlas

During Run 1 and 2 of the LHC, a fast calorimeter simulation (FastCaloSim) was successfully used in ATLAS.

An improved version of FastCaloSimv2 that incorporates the experience gained with the Run 1 version is currently under development.

The new FastCaloSim makes use of machine learning techniques, such as **principal component analysis** and **neural networks**, to optimise the amount of information stored in the ATLAS simulation infrastructure.



PCA

The longitudinal energy parametrization is based on a principal component analysis (PCA), to decorrelate deposited energies in the various calorimeter layers

GAN

Generative Adversarial Network. The main concept behind this unsupervised generative model is to train two neural networks to play a min-max game between each other.

Longitudinal and lateral energy parameterization

CHEP 2018, Jana Schaarschmidt *(ATLAS)*

The Longitudinal Energy Parametrisation

Energy deposit in each calorimeter layer along the shower axis and total energy

Problem: The energy deposits in the various layers are correlated with each other

Transformation to uncorrelated set of variables with principal component analysis, to reduce complexity

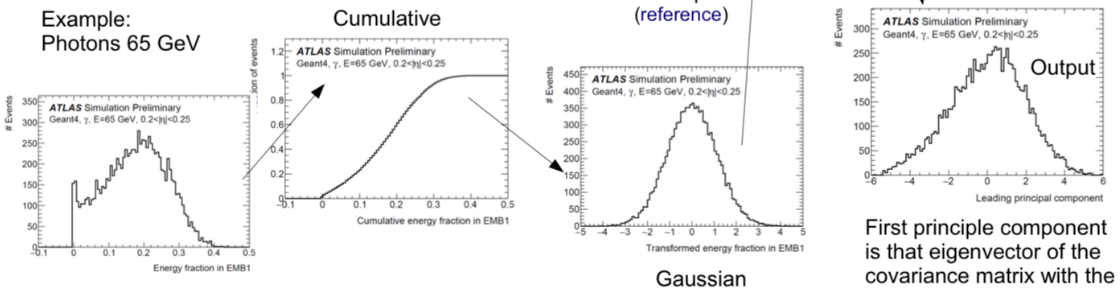
1st PCA chain:

G4 Inputs: Energy fractions, Total energy → N inputs → **N Cumulative distributions** → Inverse error function → N Gaussians → **PCA** → **PCA output data** N components

TPrincipal (reference)

N outputs

Example: Photons 65 GeV

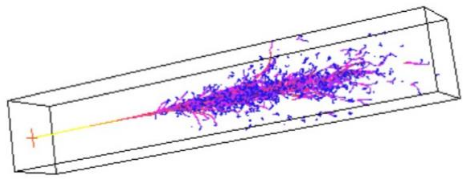


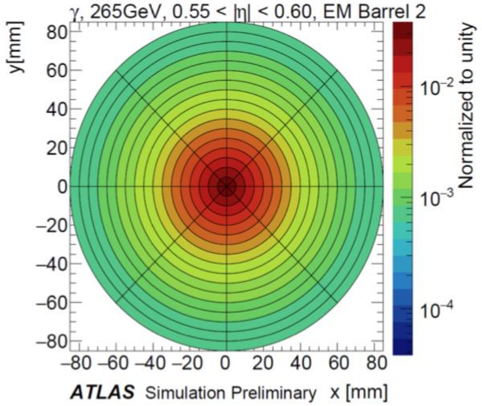
First principle component is that eigenvector of the covariance matrix with the largest eigenvalue (variance)

During simulation, this chain is performed back-wards:

Gaussian random numbers → **Inverse PCA** → Inverse PCA output (Gaussians) → Error function → Uniform numbers [0,1] → **Inverse Regression Or Histogram** → **Simulated Inputs**

The Lateral Energy Parametrisation („Shape“)





- Shower shape:

  - Most energies in the center (close to the shower axis)
  - Energy tails extending perpendicular to the axis

- The shape parametrisation is based on Geant4 HITs.

  - Close-by hits merged to reduce computation time
  - Hits saved in ntuple format to be used to derive histograms

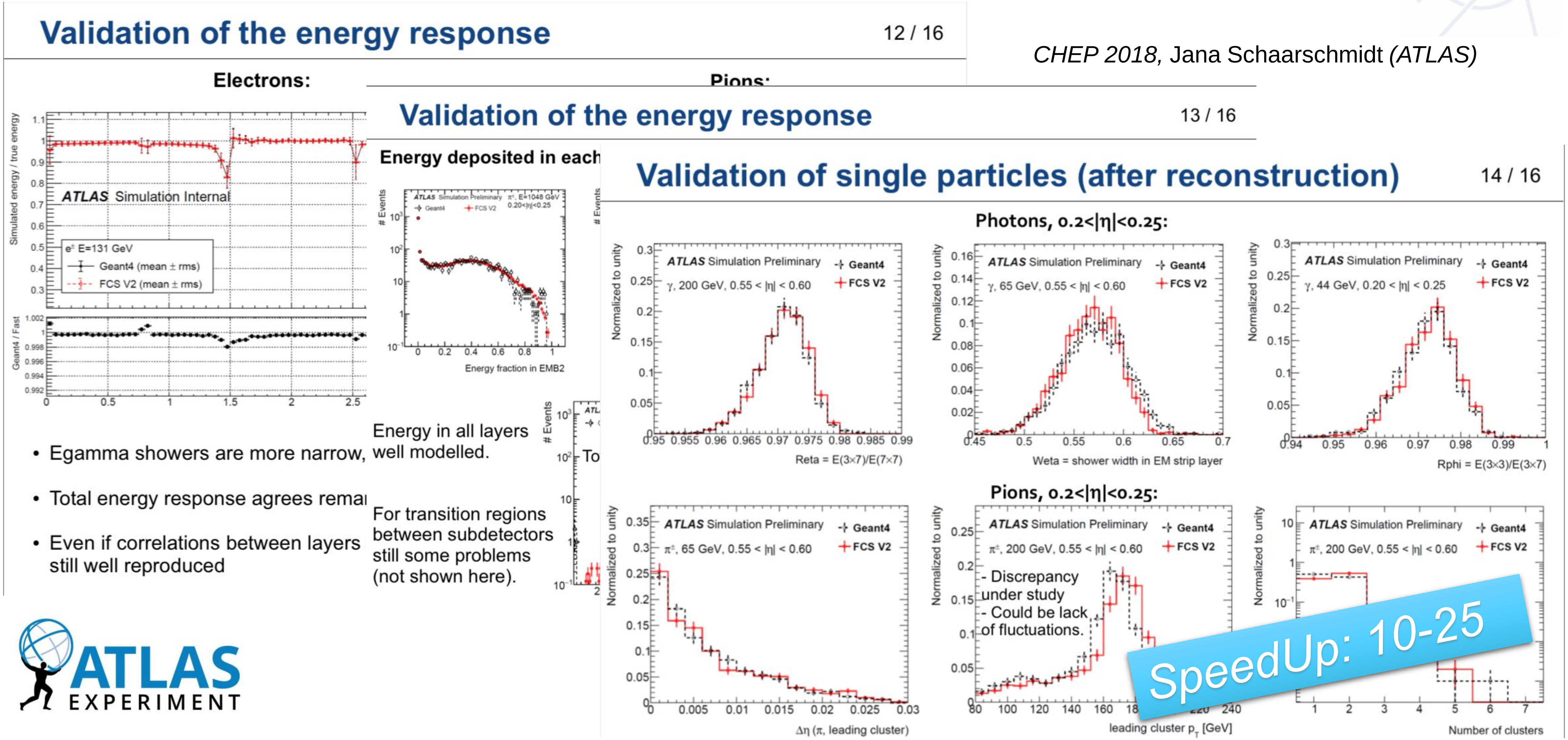
- These 2D histograms act as **probability density functions** during the fast simulation: Fast sim hits are randomly sampled from it

- 2D histogram stored per layer and per PCA bin
- Spline and regression techniques can be used to reduce memory

ATLAS EXPERIMENT

Validation of the energy response

CHEP 2018, Jana Schaarschmidt *(ATLAS)*



DNNCaloSim*

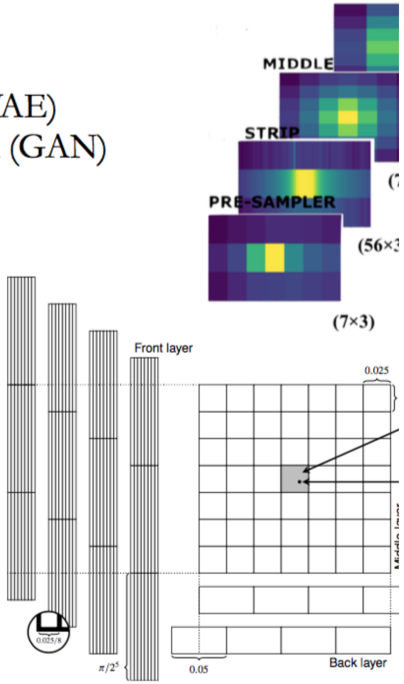
ICHEP 2018, Hasib Ahmed (ATLAS)

New approaches of fast simulation: *DNNCaloSim*

Deep generative networks to generate EM showers

Networks investigated:
Variational Auto Encoder (VAE)
Generative Adversarial Network (GAN)

- Only photons in EM calorimeter (< 1% leakage to hadronic calorimeter)
- Energies [1, 260] logarithmically spaced
- Pseudo rapidity $0.20 < |\eta| < 0.25$
- The energy deposits are voxalized into rectangular shapes
- A total of 266 cells are considered for energy deposits
- The networks are trained with energies normalized to the energy of the incident particle

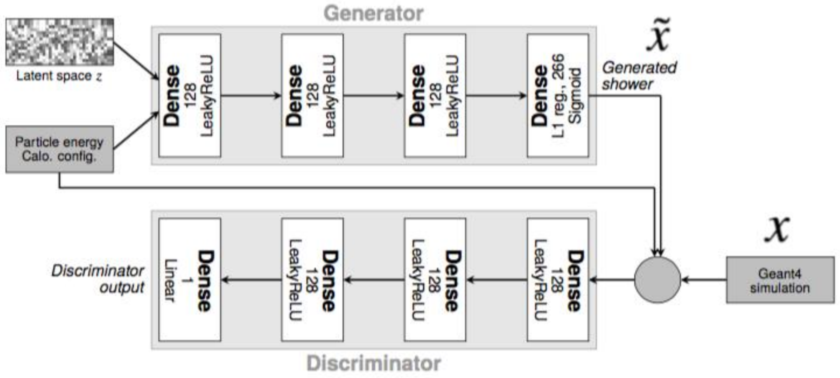


Hasib Ahmed(U Edinburgh)

Generative Adversarial Network

DNNCaloSim

Generative network with a feedback from a Discriminator network



Improve the robustness of training by calculating Wasserstein loss with a two sided gradient penalty

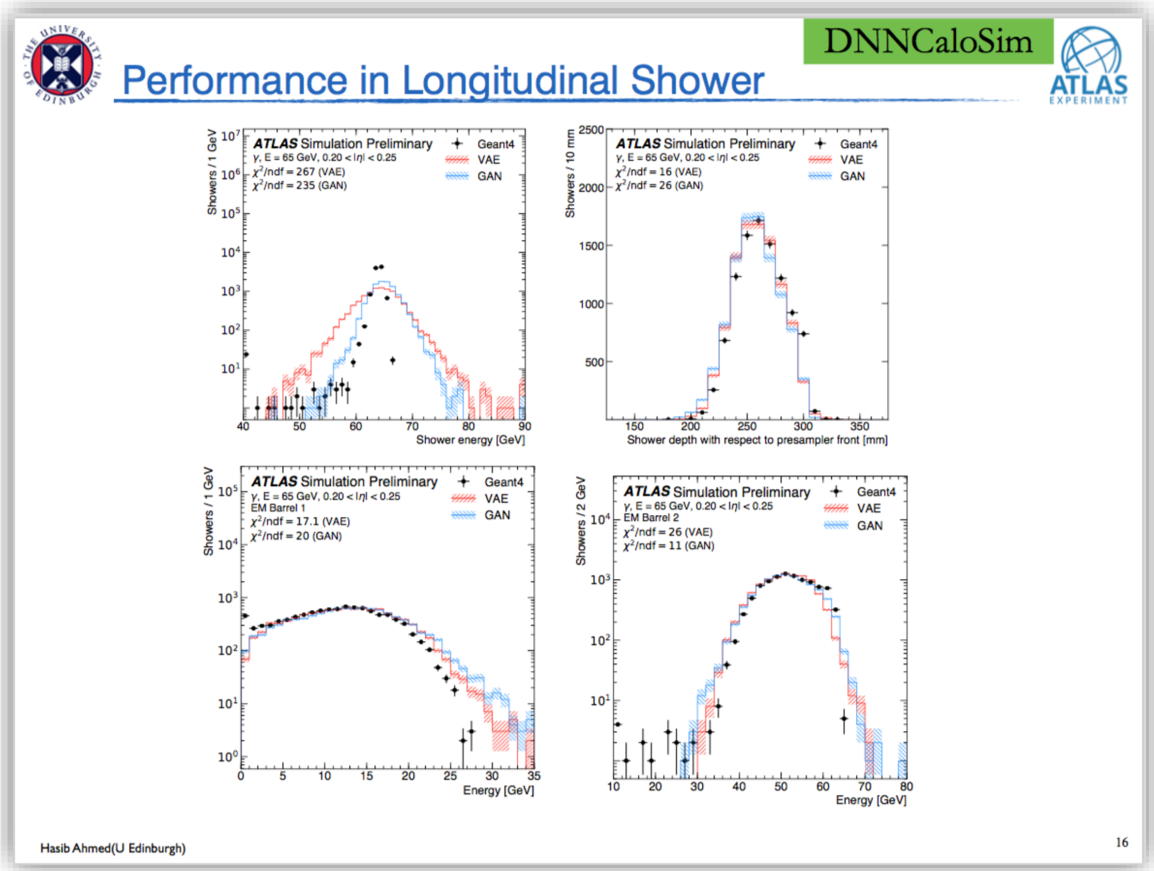
$$L_{\mathrm{GAN}} = \underbrace{\underset{\tilde{x}\sim p_{\mathrm{gen}}}{E}[D(\tilde{x})]}_{\text{ability to identify generated shower correctly}} - \underbrace{\underset{x\sim p_{\mathrm{Geant4}}}{E}[D(x)]}_{\text{ability to identify Geant4 shower correctly}} + \lambda \underbrace{\underset{\hat{x}\sim p_{\hat{x}}}{E}[(||\Delta_{\hat{x}} D(\hat{x})||_2 - 1)^2]}_{\text{penalizes by calculating Wasserstein loss}}.$$

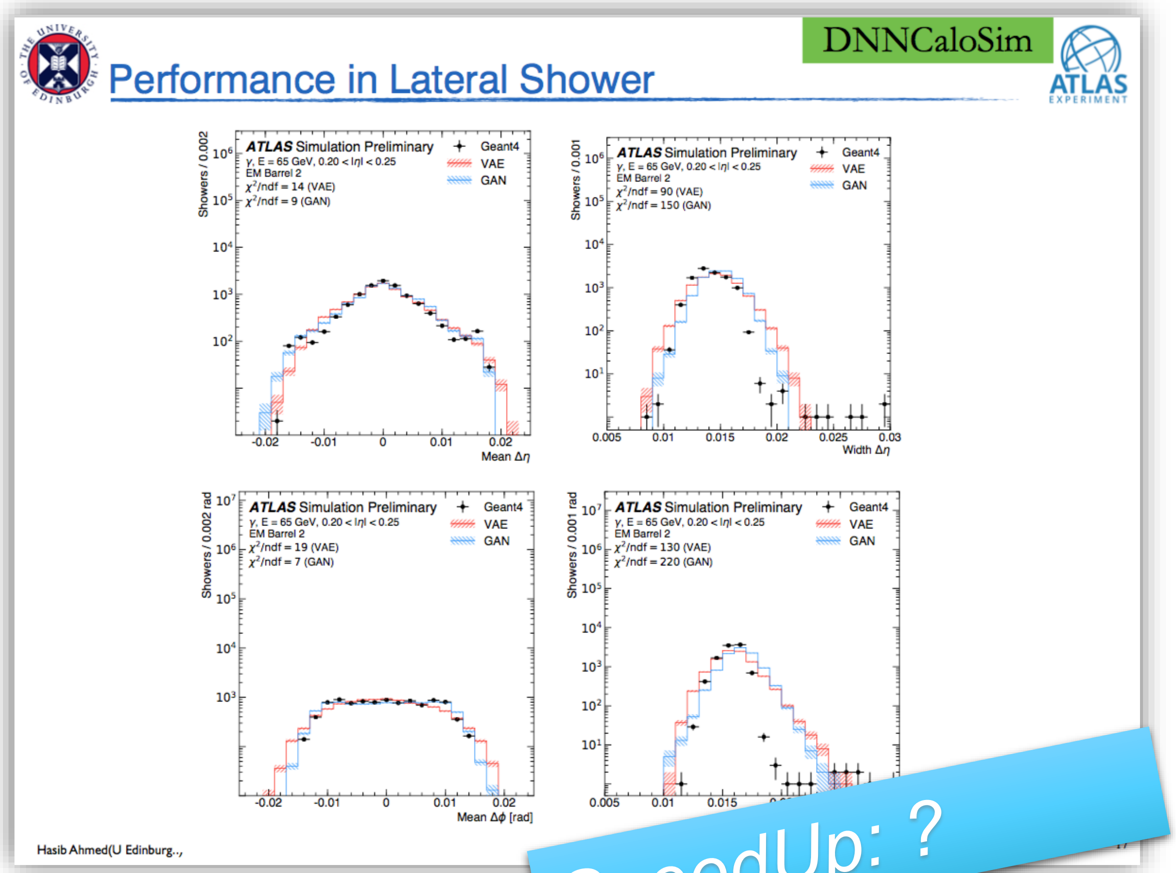
Hasib Ahmed(U Edinburgh) 15

*Based on CaloGan: M. Paganini et al. arXiv:1712.10321

DNNCaloSim

ICHEP 2018, Hasib Ahmed (ATLAS)





SpeedUp: ?

FastSim Alice

Using generative models for fast simulations in the TPC (Time Projection Chamber) detector for the ALICE Experiment

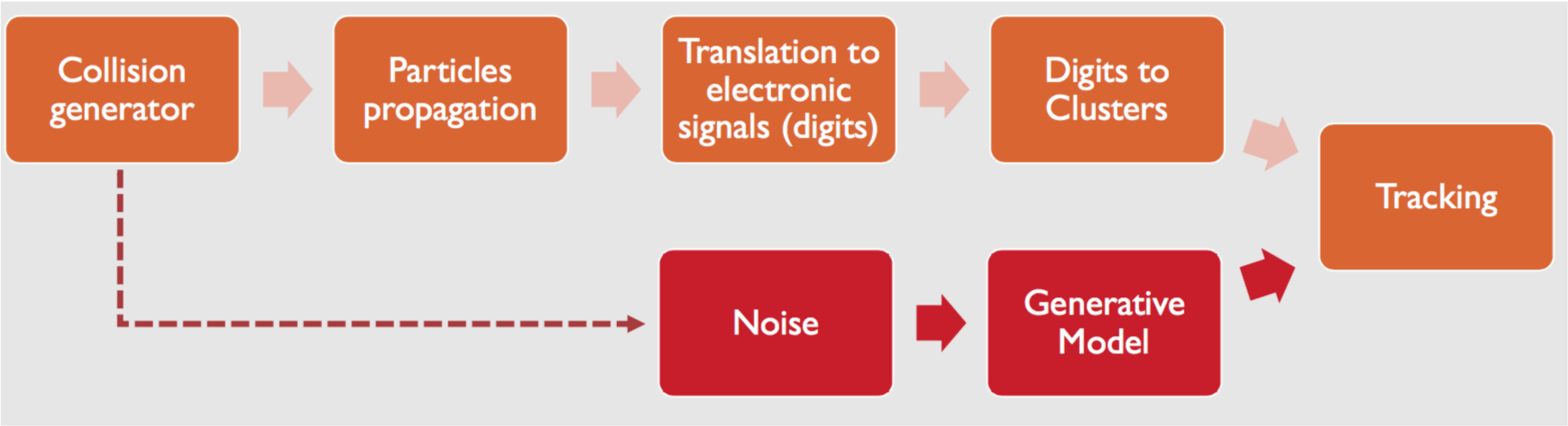
Substitute part of the simulation pipeline, namely particle propagation and translations to digits and clusters, with a generative model, initialized with noise.

Cluster Simulation

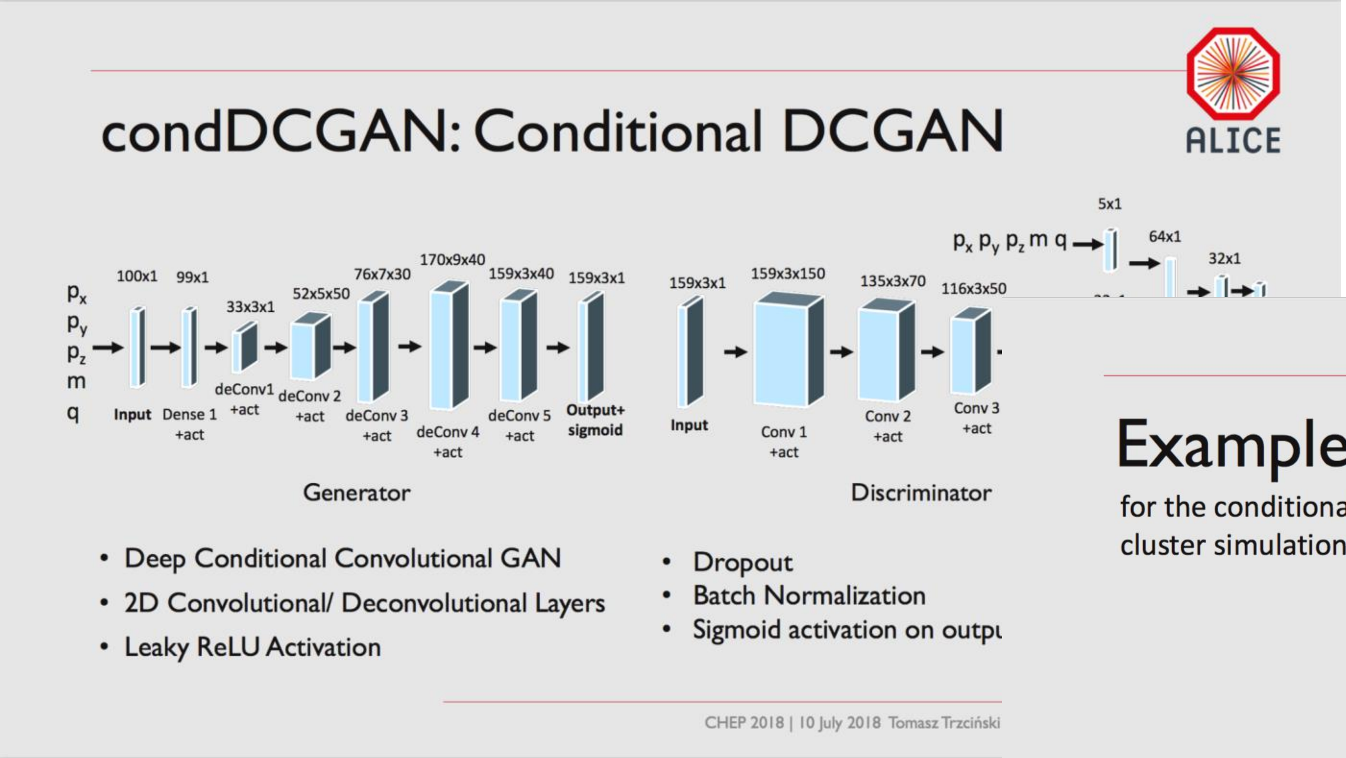
The dataset consists of 3D trajectories of particles after collision generated using Monte Carlo simulation

DCGAN

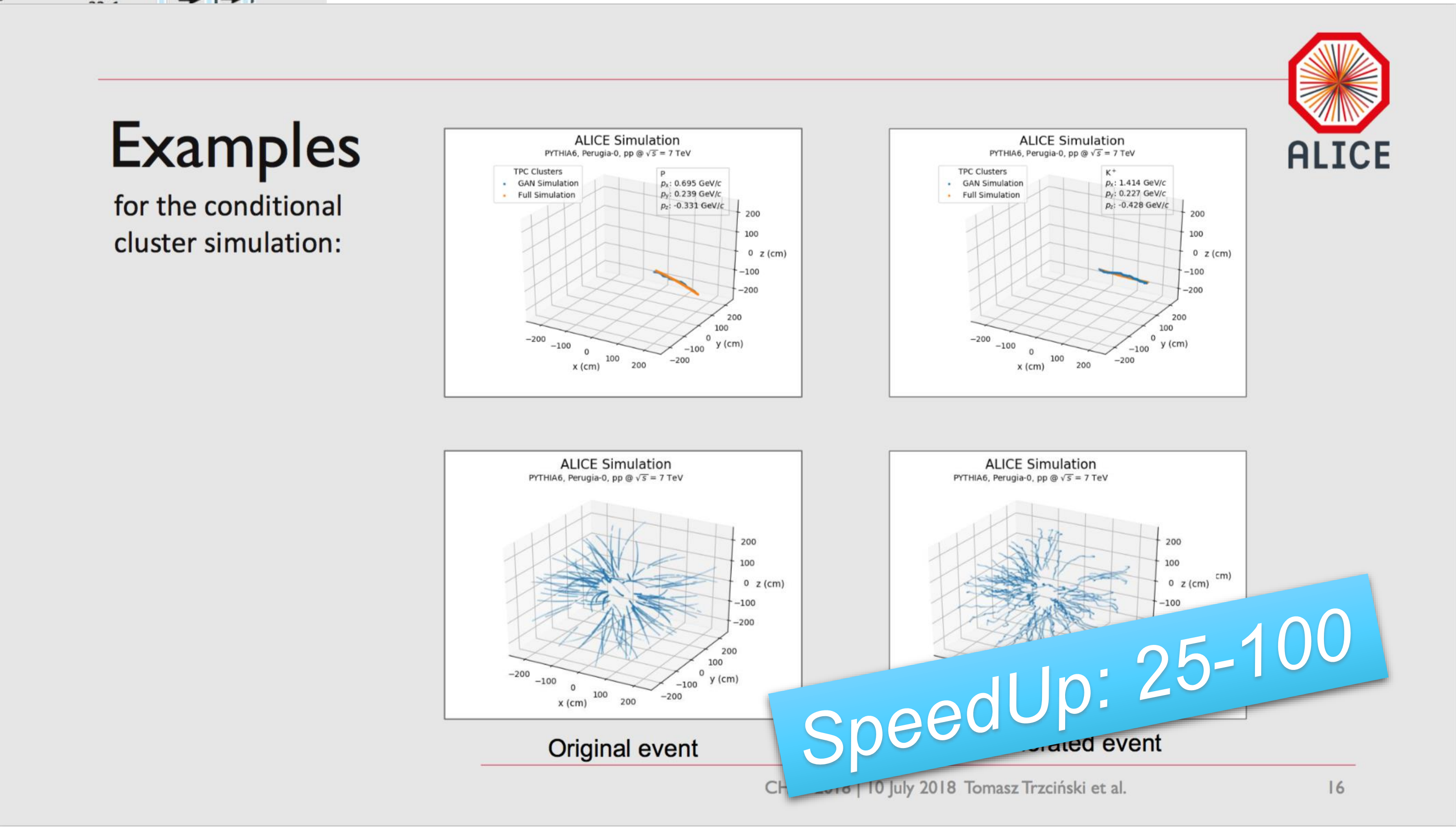
Class of networks that use convolutional and de-convolutional layers to seek for and produce meaningful patterns



Deep Conditional Convolutional GAN

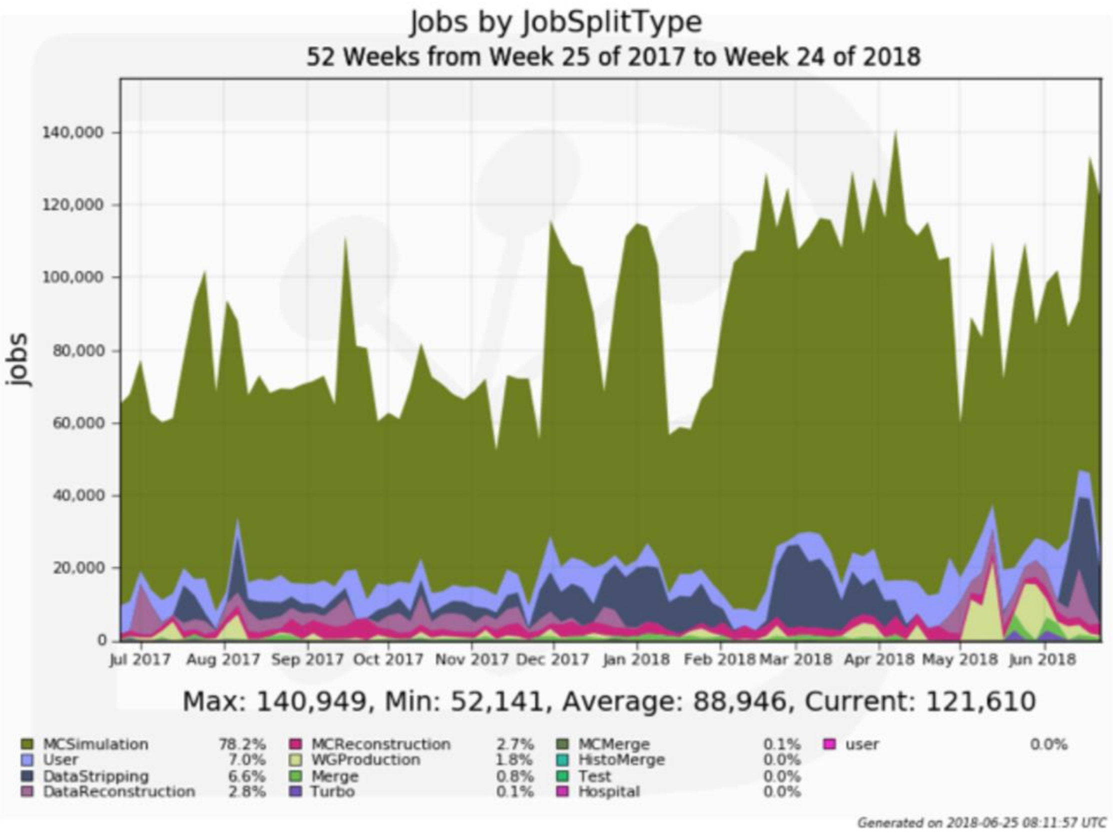


CHEP 2018, **Tomasz Trzcinski** *(ALICE)*



FastSim LHCb

- The simulation application for the LHCb experiment is *Gauss*
    - Particle generation and transport in the detector Based on the Gaudi framework
    - Depends on a number of external libraries, including Geant4 for particle transport
    - A separate application, Boole, takes care of the digitized detector’s response
- Simulation takes most of the LHCb CPU resources



Run III

Collecting more interesting events in Run III – and further – will require more events to be simulated

FastSim need

Need to shift towards a scenario where a significant fraction of LHCb MC events is fast-simulated

A palette of fast simulations in LHCb

ICHEP2018, **Mark Whitehead (LHCb)**

01 Simplified detector simulation

- Reduced detector: RICH-less or tracker-only. *In production*
- Calorimeter showers fast simulation. *Under development*
- Muon low energy background, used with full muon detector simulation. *In production*

02 Simulation of partial events

- Simulate only particles from signal decay. *In production*
- ReDecay, e.g. use N-times the non-signal decay part of the event. *In production*

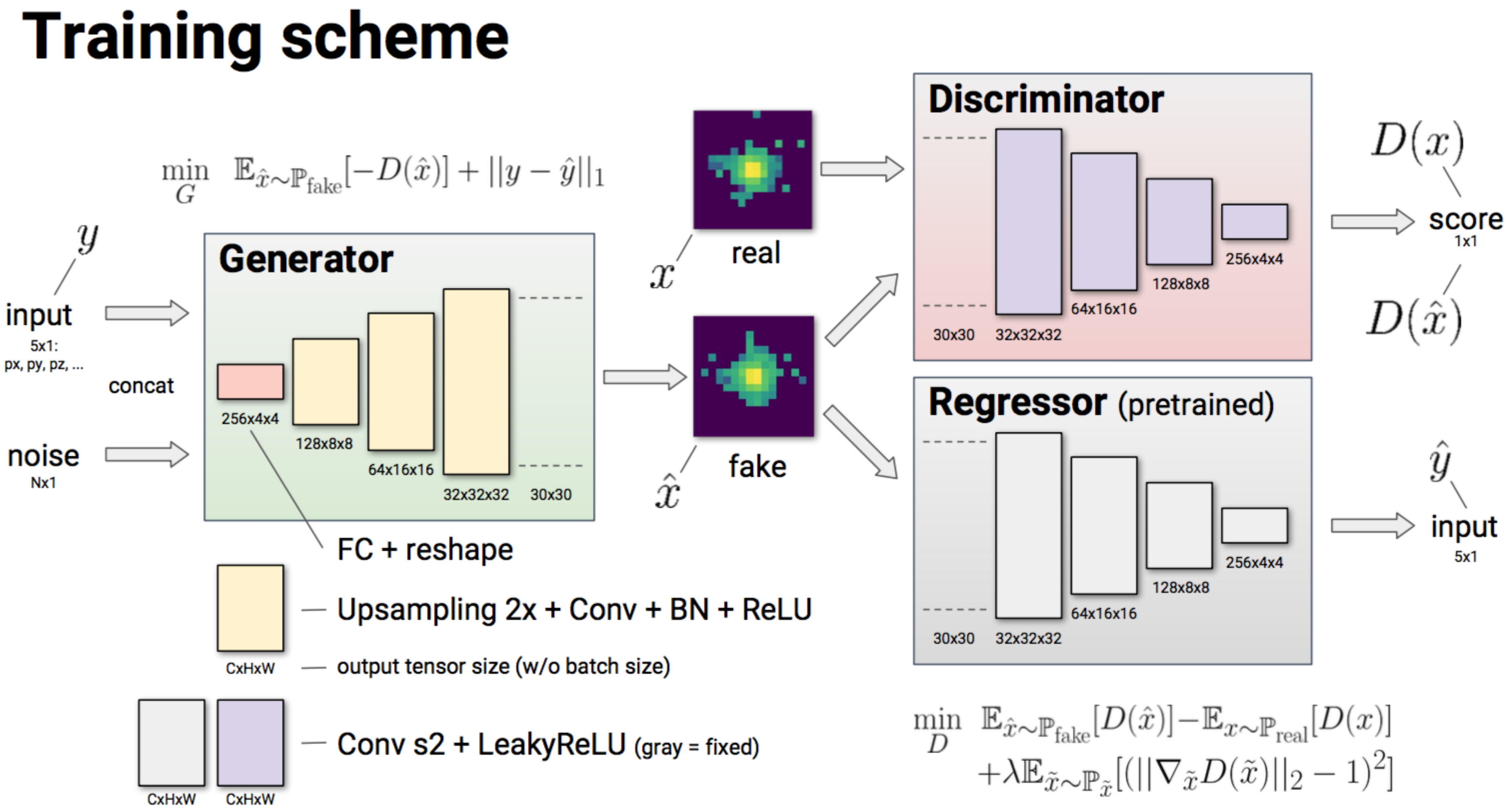
03 Fully parametric simulation

- Parametrized tracking, calorimeter and particleID objects with a DELPHES-based infrastructure. *Under development*

No single solution for all needs, but different options organized under the unique *Gauss* framework

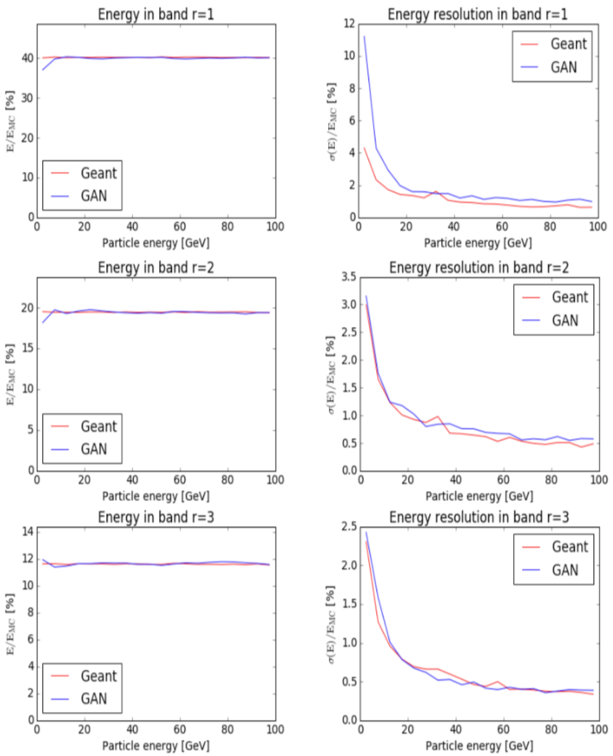
Deploy solutions when mature for physics

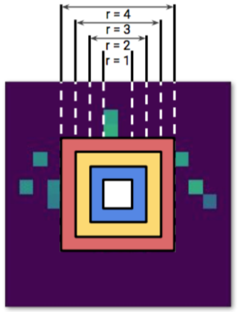
Wasserstein Conditional GAN

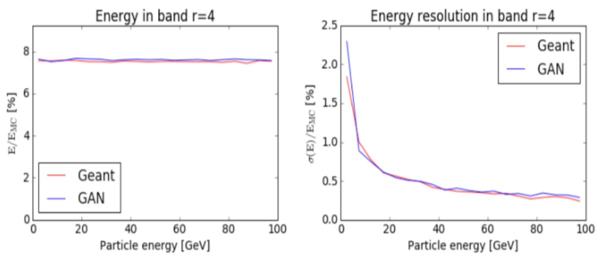


$$\min_D \; \mathbb{E}_{\hat{x}\sim\mathbb{P}_{\text{fake}}}[D(\hat{x})] - \mathbb{E}_{x\sim\mathbb{P}_{\text{real}}}[D(x)] + \lambda\mathbb{E}_{\tilde{x}\sim\mathbb{P}_{\tilde{x}}}[(||\nabla_{\tilde{x}}D(\tilde{x})||_2 - 1)^2]$$

Performance

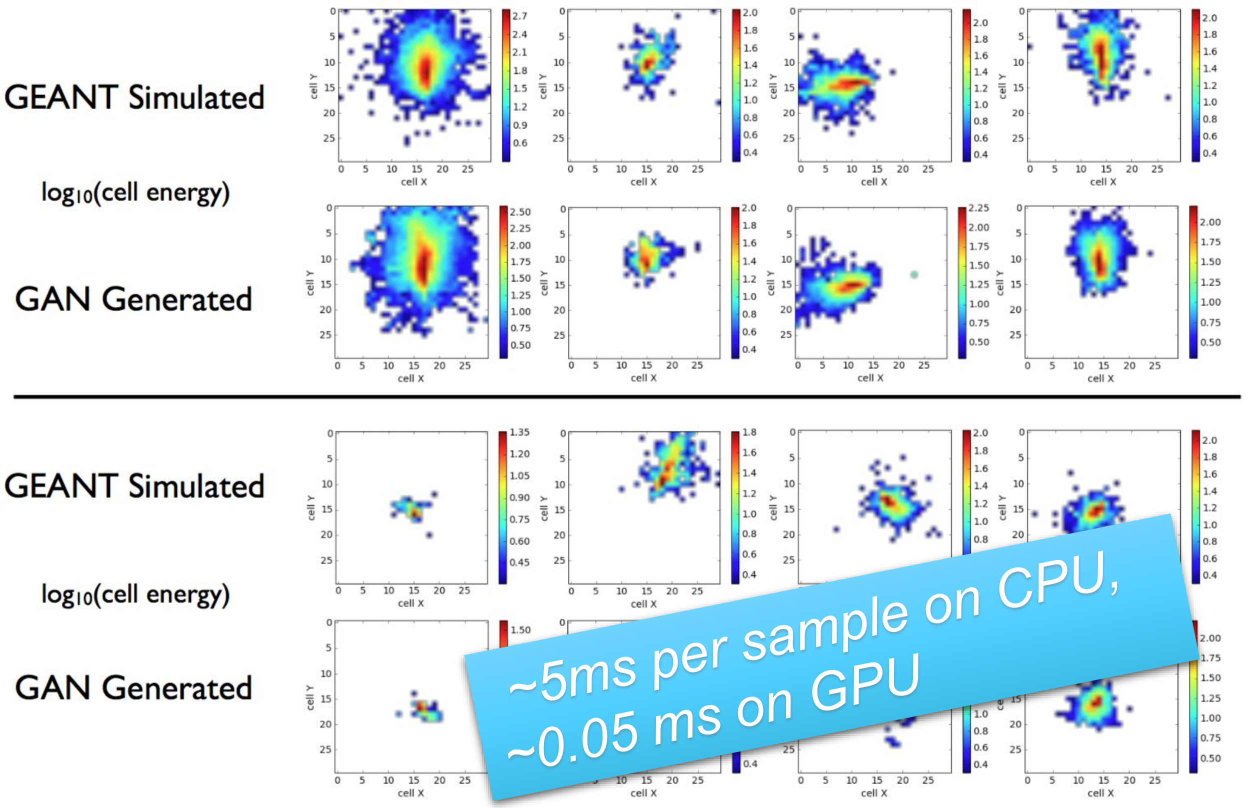






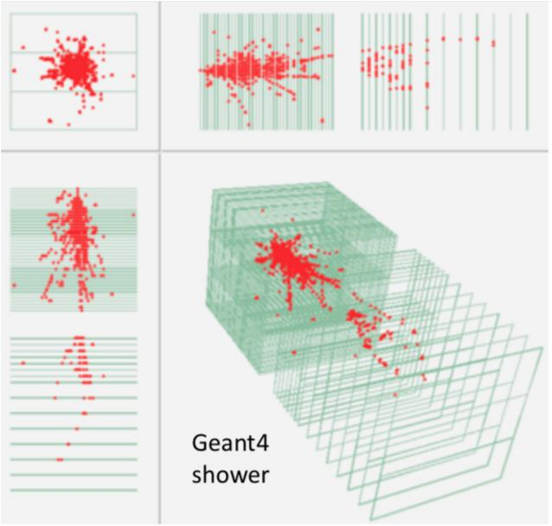
- Good reproduction of first and second moments for cluster shape

ICHEP2018, **Mark Whitehead (LHCb)**



~5ms per sample on CPU,
~0.05 ms on GPU

A generic FastSim approach



- CLIC calorimeter simulation for the proof of concept
    - Data is essentially a 3D image

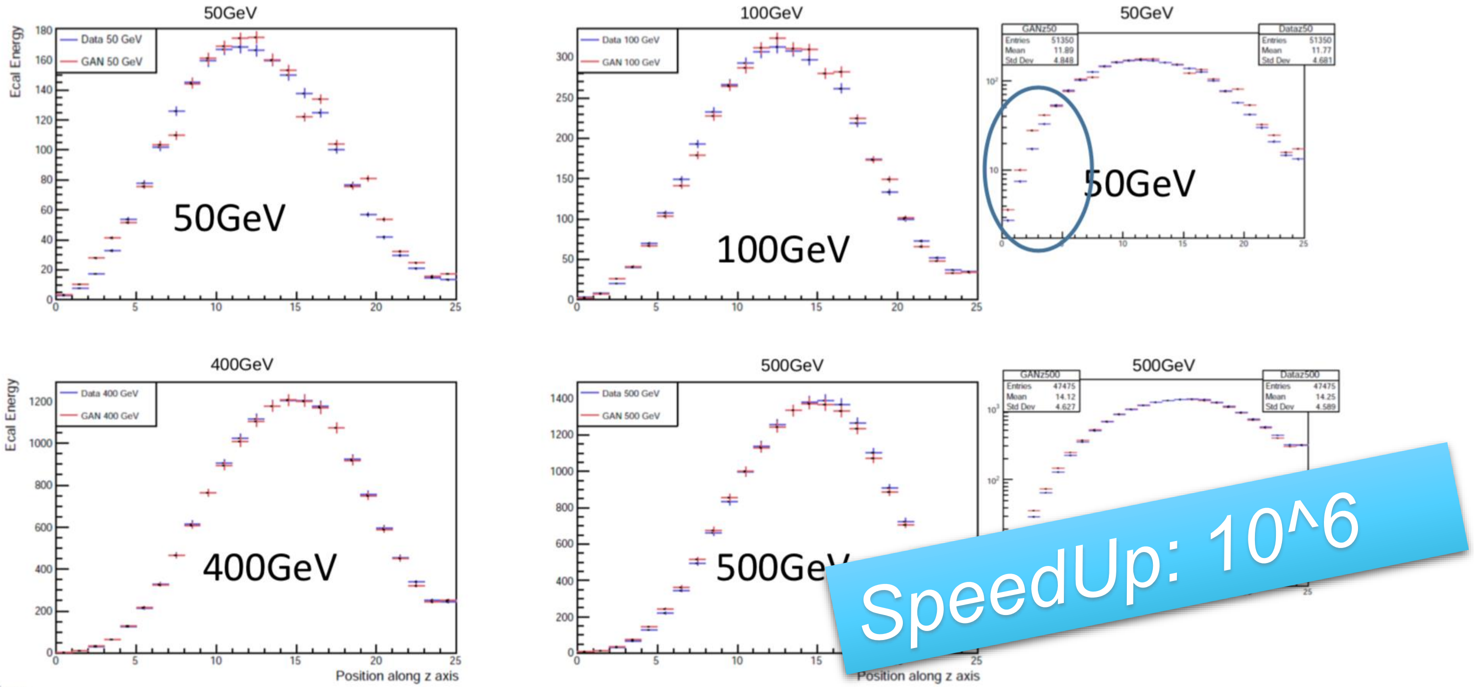
Electromagnetic calorimeter detector design(*)

(Linear Collider Detector studies)

- 1.5 m inner radius, 5 mm×5 mm segmentation: 25 tungsten absorber layers + silicon sensors

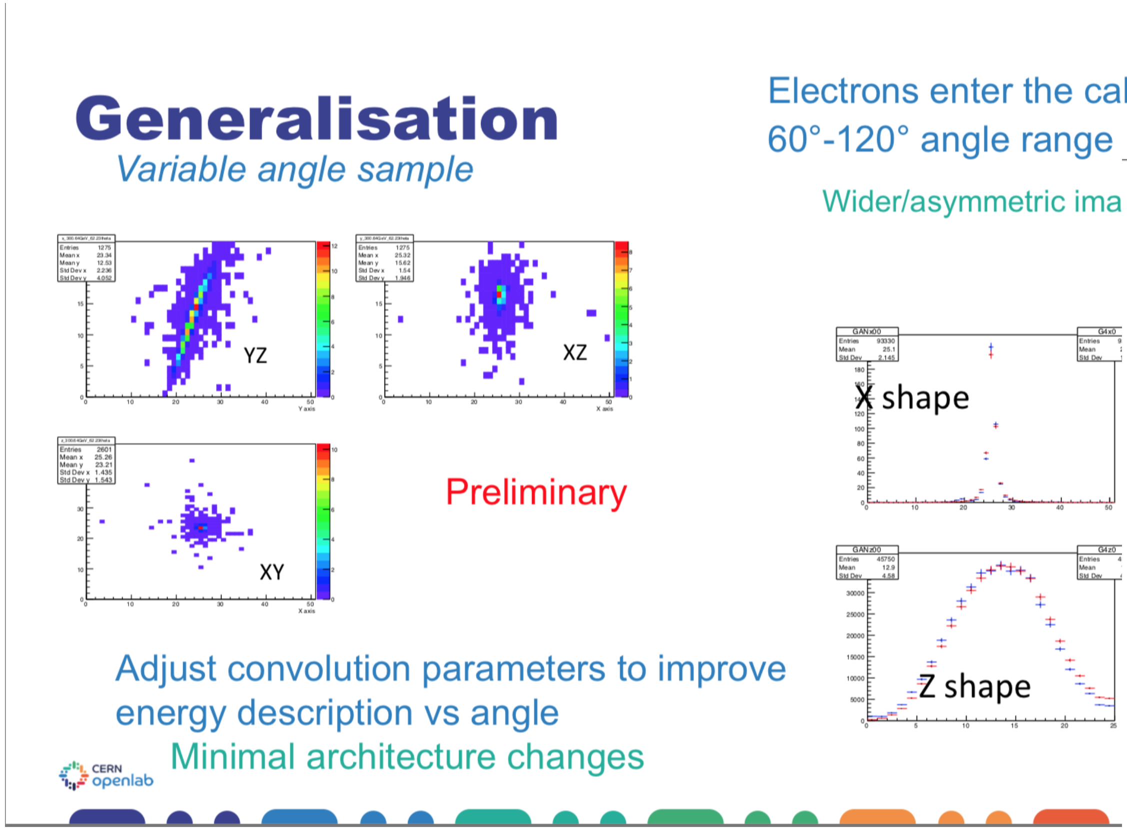
1M single particle samples (e,γ,π)

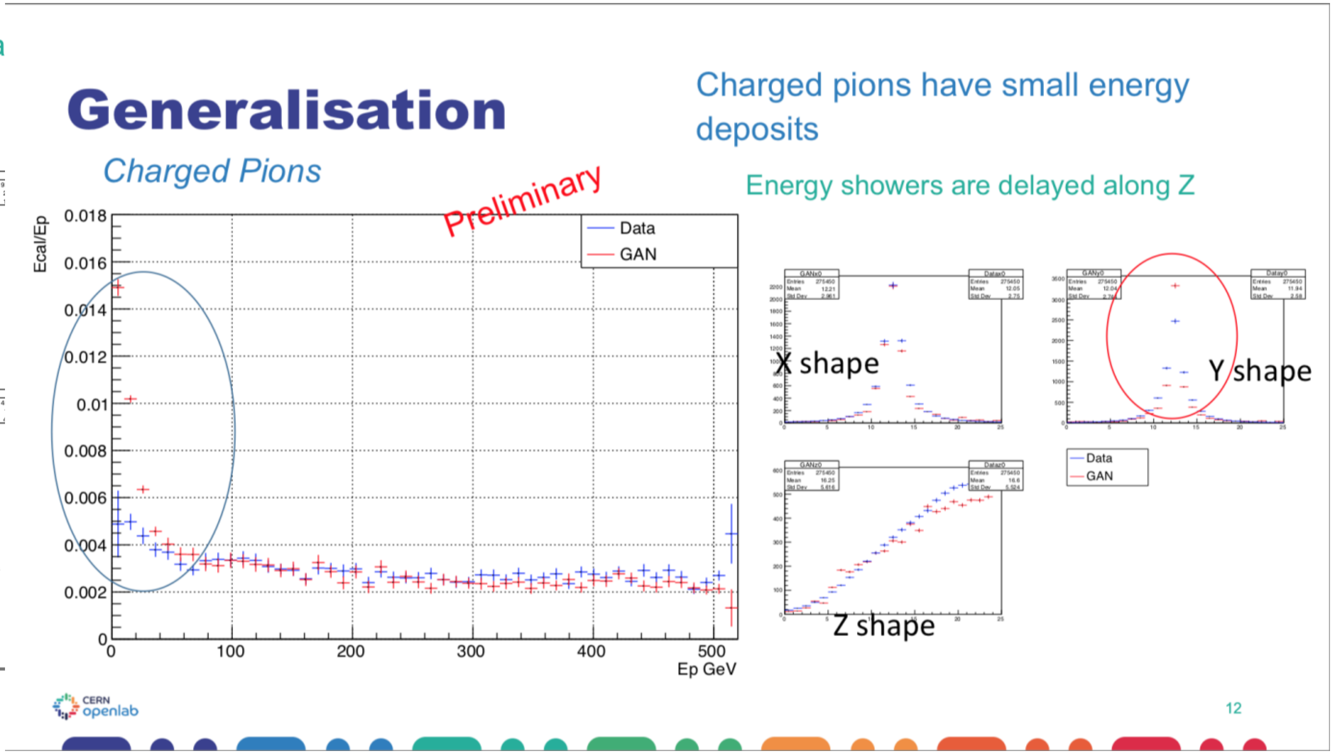
- Flat energy spectrum (10-500) GeV
- Orthogonal to detector surface
- +/- 10° random incident angle



CHEP2018, **Sofia Vallecorsa (OpenLab)**

A generic FastSim approach





Machine learning to empower physics modeling

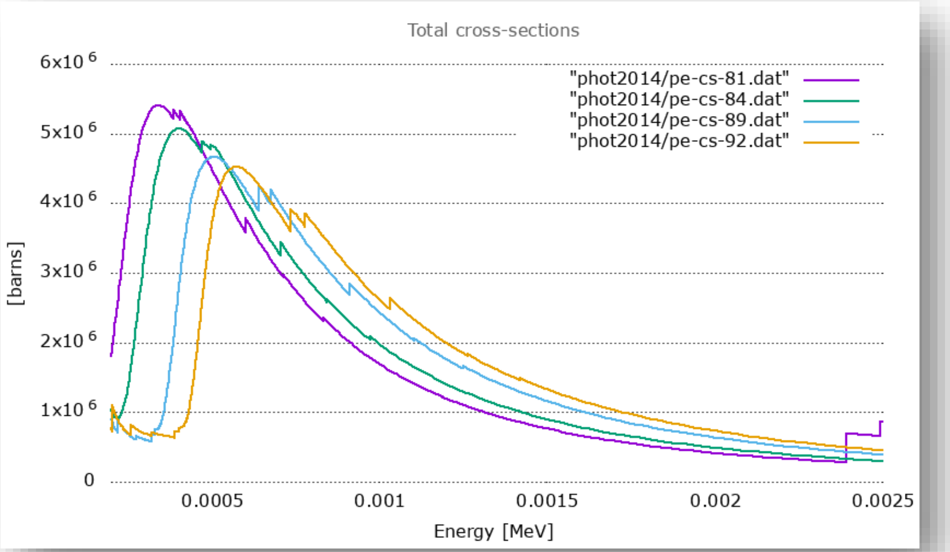
- Machine learning applied to FASTSIM looks very promising

- What if we go one level beyond and we replace computationally expensive physics models with ML blocks
  - Able to learn complex cross-sections shapes (total, differential)?
  - Able to directly generate the final-state?

→ From "physics-agnostic" to "**physics-aware**" neural networks

Training Physics-aware supervised neural networks[1][2]

- Embed physical-laws underlying the process
- To be used to infer physical quantities (momenta, directions, energies..)
- Both for continuous and discrete processes



[1] "QCD-Aware Recursive Neural Networks for Jet Physics", Kyle Cranmer et Al, https://arxiv.org/abs/1702.00748 - Feb 2017

[2] Physics Informed Deep Learning: Data-driven Solutions of Nonlinear Partial Differential Equations, Maziar Raissi et Al, https://arxiv.org/abs/1711.10561 - Nov 2017

Thanks for your attention.

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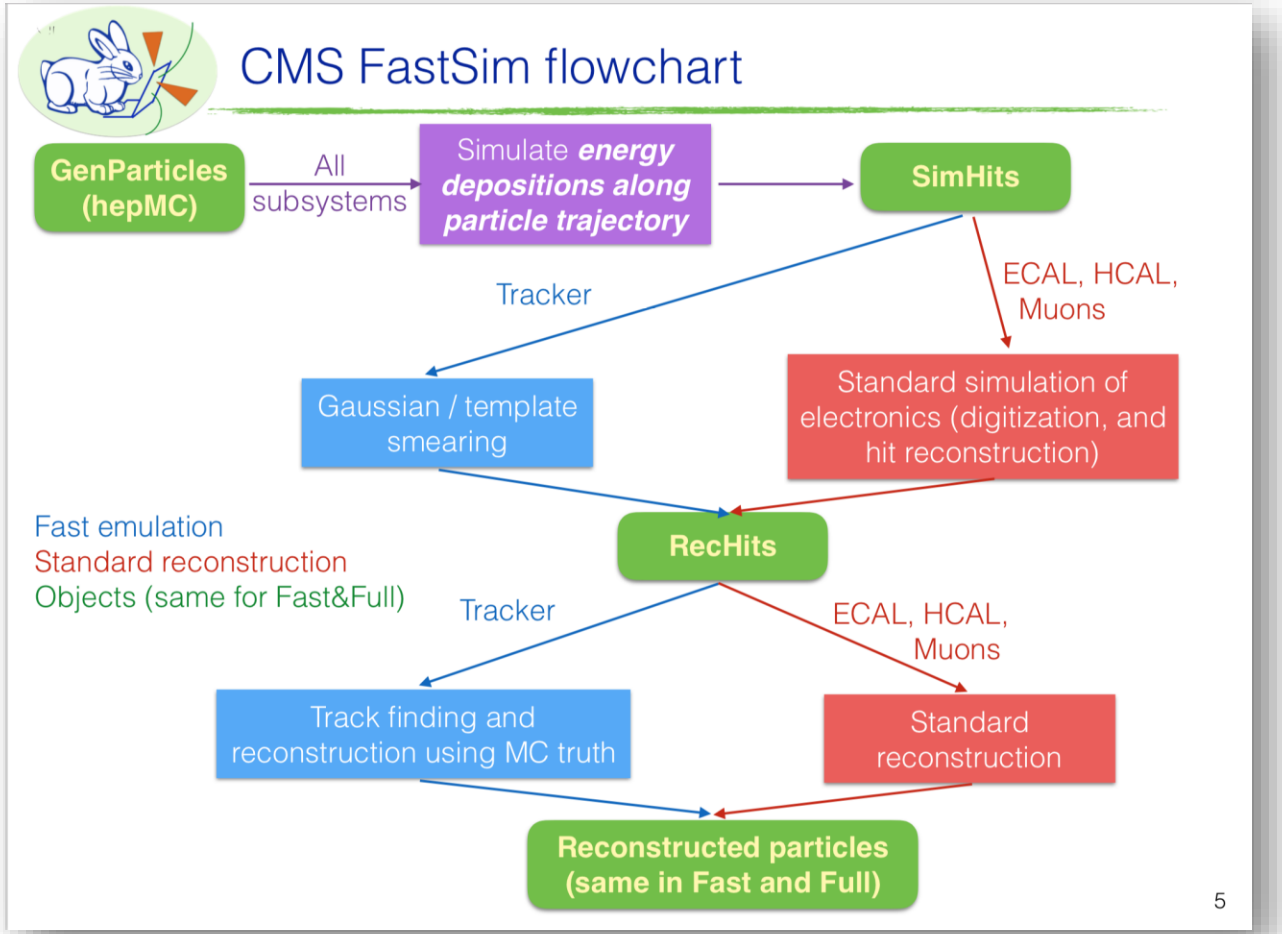
FastSim CMS

LPCC 2017, **Sezen Sekmen** (CMS)



Fast simulation (FastSim) is an integral part of CMS physics studies and the CMS software framework.

- Speeds up CMS event simulation ~100 times and CMS event simulation+reconstruction ~20 times.
- Regularly validated within the official CMS software release validation framework.
- Mainly validated against FullSim. Reproduces FullSim mostly by about 10%.

- Actively maintained by ~15 developers working part time on different aspects of the framework.

- Mainly validated against FullSim. Reproduces FullSim mostly by about 10%.

CMS Fast Sim

Why is FastSim fast?

CMS FastSim concept: CMS FastSim is a single, uniquely-defined framework (as opposed to e.g. ATLAS, which consists of several different levels of simulation).

Main difference wrt FullSim is in the simulation step. Low level quantities are parametrized.

- Geometry is simplified.
- Material interactions are simplified and parametrized.
- Calorimetric showers are parametrized.

Hit reconstruction (RecHits) mostly follows standard reconstructi
(applied to FullSim and data). Exception:

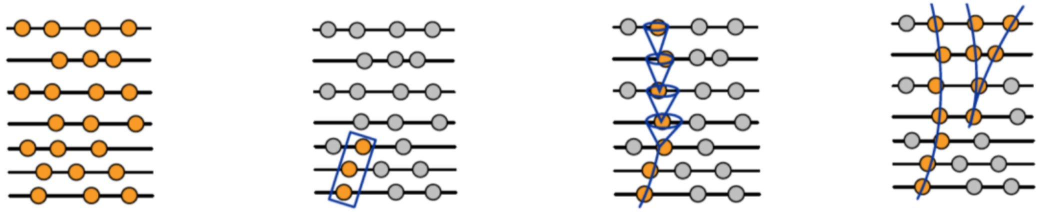
- Tracking RecHits: No digitization and local reco in tracker. RecHits emulated by smearing SimHits.

Object reconstruction mostly follows standard reconstruction (applied to FullSim and data). Exception:

- Track reconstruction / finding emulated with help from MC truth

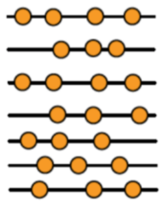
LPCC 2017, **Sezen Sekmen** *(CMS)*

Data/FullSim: Combinations of hits need to identified from a nearly infinite number of hit permutations created by charged particle trajectories, bent by the B field.



RecHits from charge deposits | seeding: find start of potential trajectories | trajectory finding: add hits to the seed that supports trajectory hypothesis | trajectory fit: global fit to estimate track parameters.

FastSim track reco: Restrict seeding and trajectory finding to only a local subset of hits using MC truth information. Large speed up by skipping permutations.



RecHits from charge deposits

Look up particle trut
information

- create seeds
- build a track candidate
- fit a track.

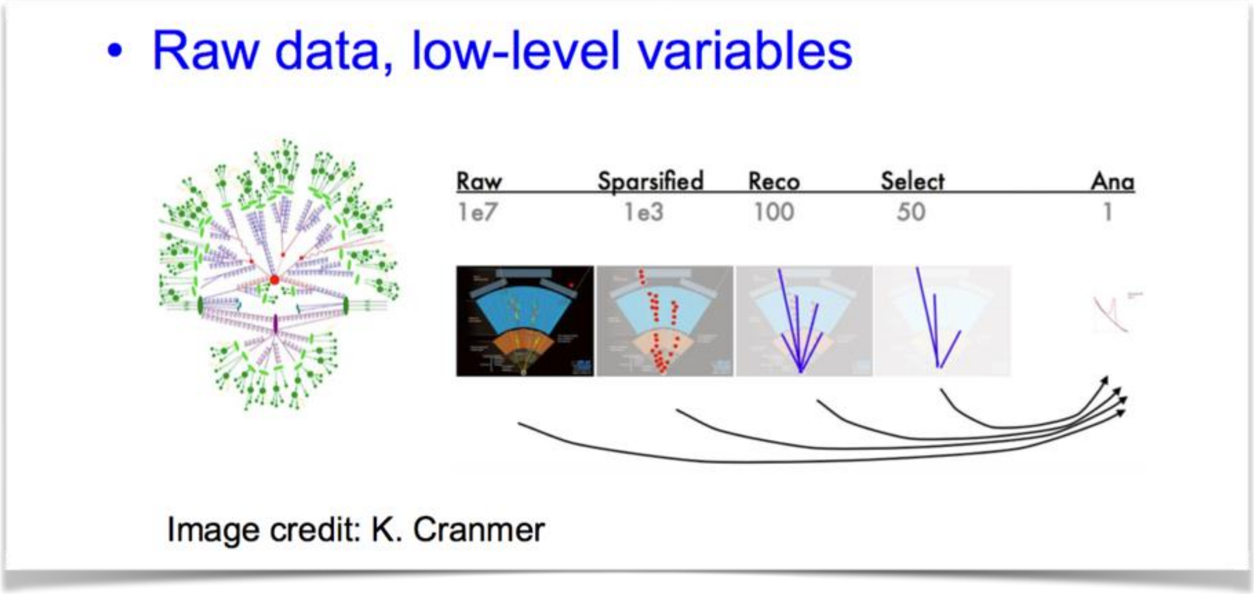
Iterative t

Create subsets of consistent RecHits

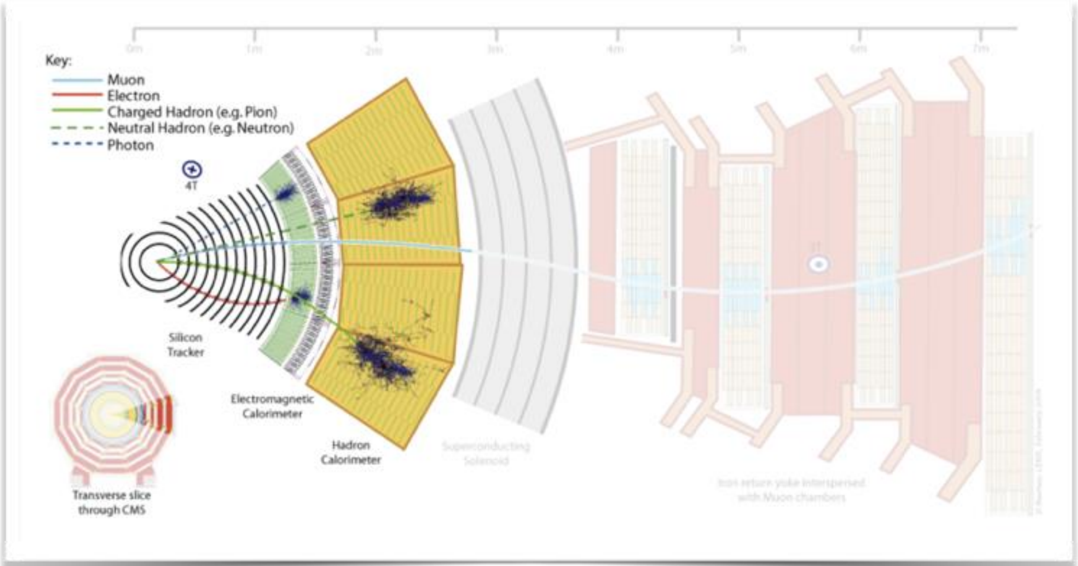
SpeedUp: ~100

End-to-end learning

- ➢All varieties of deep learning gaining traction
  - ➢Convolutional, Recurrent, LSTM, GANs
  - ➢Tree-based methods (XGBoost) still maintain some competitiveness
- ➢Machine learning models increasingly used together with low-level information



End-to-end learning



- PARTICLE AND EVENT ID CLASSIFIER WITH CNN
  - Able to learn particle kinematics and shower shapes
  - Classifier output can be de-correlated from mass of signal resonance
  - Well-suited to decays where particles can't be fully resolved/ reconstructed
  - Can tackle arbitrary decays: train on whole Standard Model on same network