3D convolutional GAN for fast simulation

HSF Fast Simulation topical meeting

F. Carminati, G. Khattak, S. Vallecorsa

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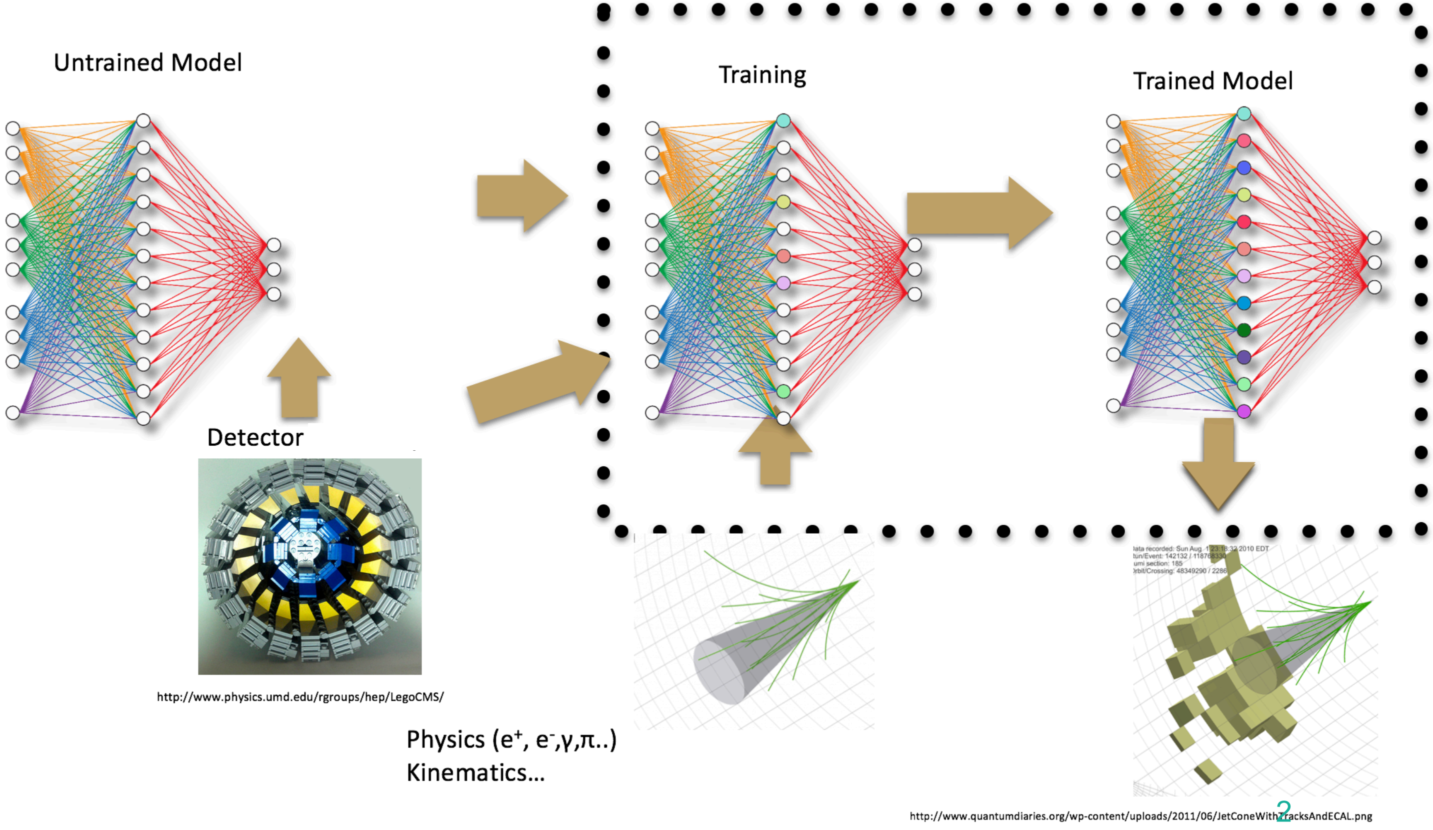
A DL engine for fast simulation

Provide a tool that can be configured and trained for different detectors

- Start with time consuming detectors
  - Next generation highly granular calorimeters
- Train on Monte Carlo data
- Optimise training time



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Our plan

- Are generative models accurate enough?
- Can we sustain the increase in detector complexity?

→

- A first proof of concept
- Understand performance and validate accuracy

- How generic is this approach?
- Can we “adjust” architecture to fit a larger class of detectors?
- What resources are needed?

→

- Prove generalisation is possible
- Understand and optimise computing resources

- Can it be integrated in a “standard” simulation workflow?

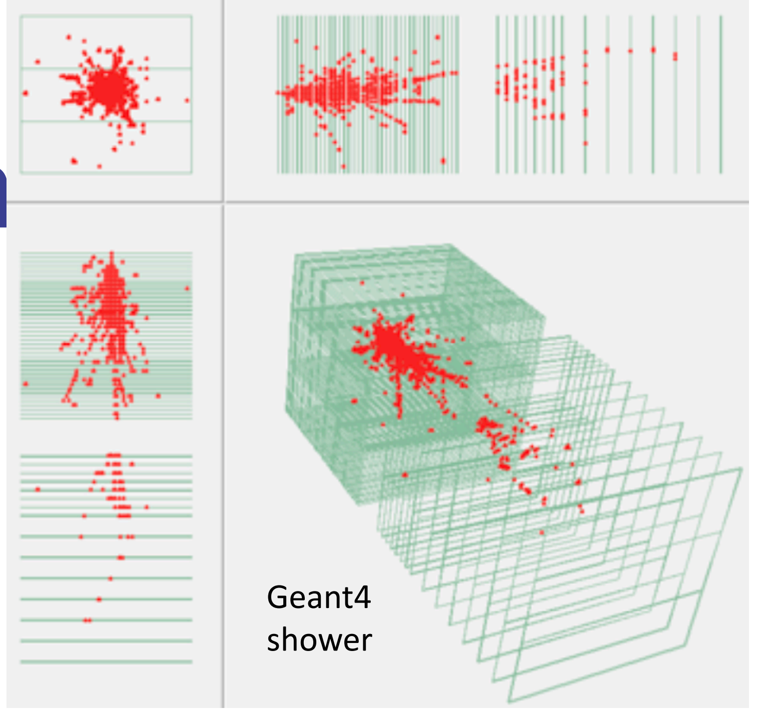
→

- Pre-processing
- Interfaces to simulation engine

Collaboration with CERN SFT group

Proof of concept, benchmarking and validation

CLIC calorimeter simulation



Data is essentially a 3D image

Electromagnetic calorimeter detector design(*)

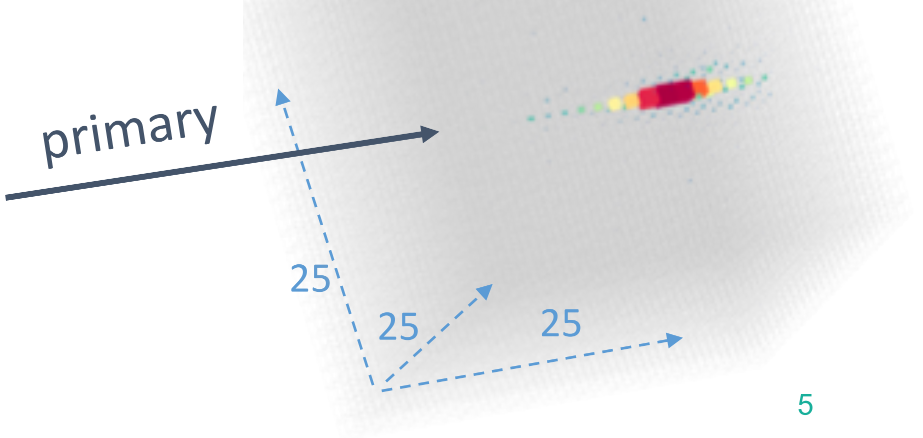
(Linear Collider Detector studies)

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

1M single particle samples (e,γ,π) with flat energy spectrum (10-500) GeV

1. Orthogonal to detector surface (25x25x25 pixels)
2. +/- 30° random incident angle (51x51x25 pixels)

Highly segmented
Sparse.



(*) http://cds.cern.ch/record/2254048#

3D convolutional GAN

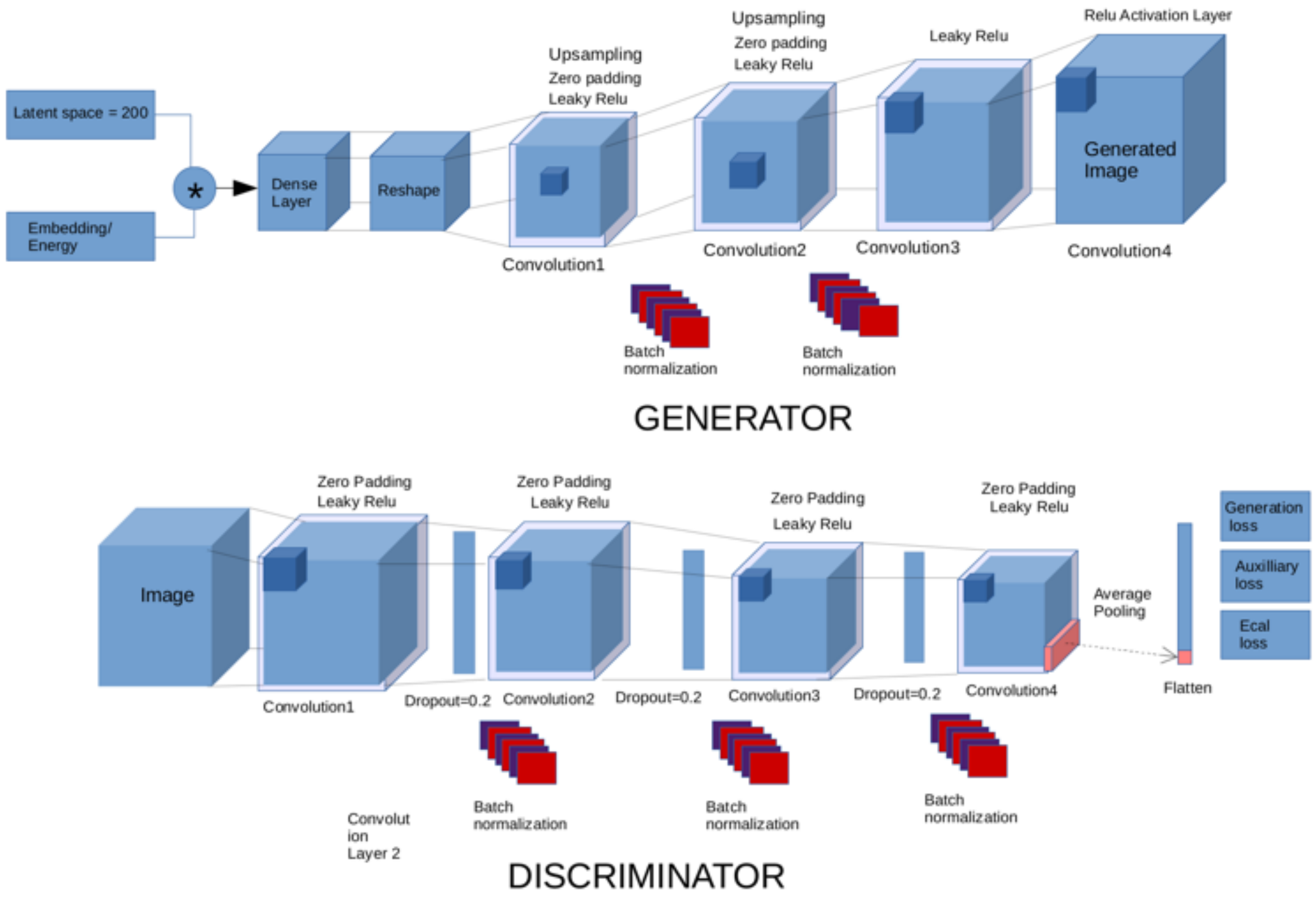
Similar discriminator and generator models

- **3D convolutions** (keep X,Y symmetry)
- ~1M parameters total

Condition training on input variables (energy, angle)

Auxiliary regression tasks assigned to the discriminator: cross check

- **Custom losses**



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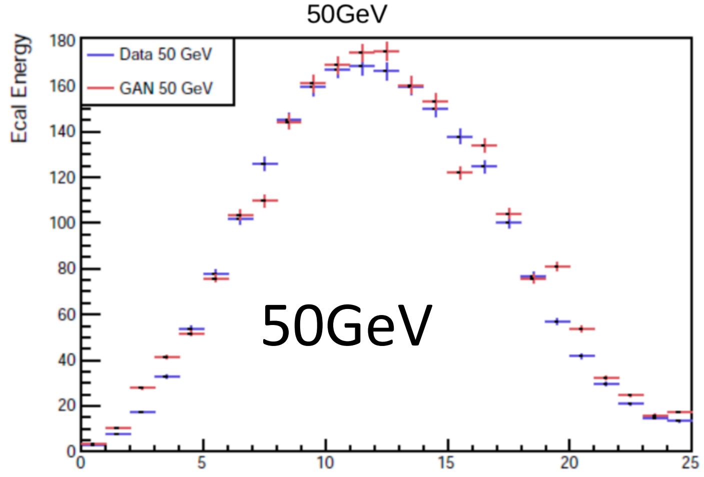
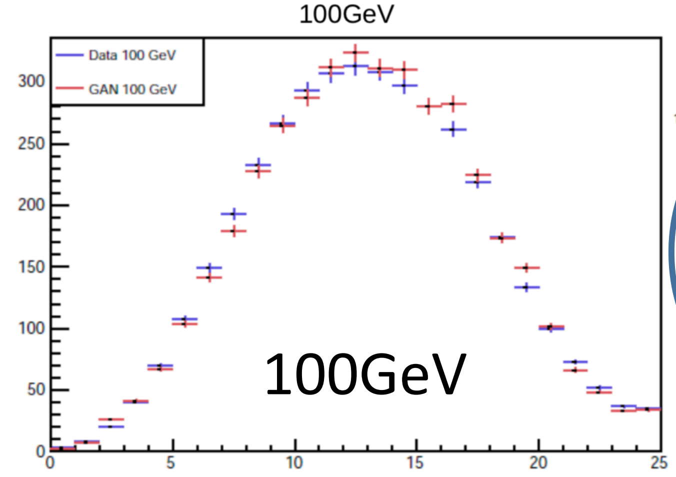
Validation and optimisation

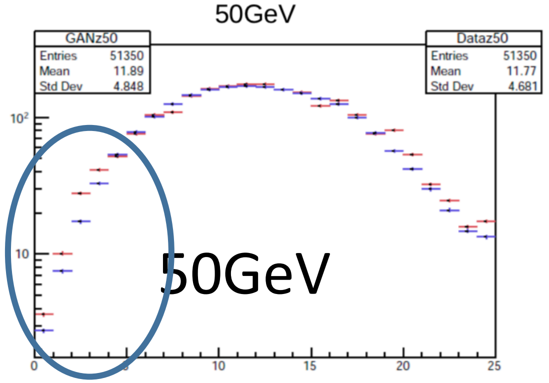
- Detailed GAN vs GEANT4 comparison (More than 200 Plots!)
  - High level quantities (shower shapes)
  - Calorimeter response (single cell response)
  - Particle properties (primary particle energy)
- Optimisation on
  - Network Architecture (Layers, filters, kernels, initialisation)
  - Losses definition
  - Data pre-processing
- Results agree within a few % to Geant4 (sometimes labelled “DATA” in next slides ☺)
- Run TriForce classification and regression engine on GAN generated data
  - (Matt Zhang, https://github.com/BucketOfFish/Triforce_CaloML)

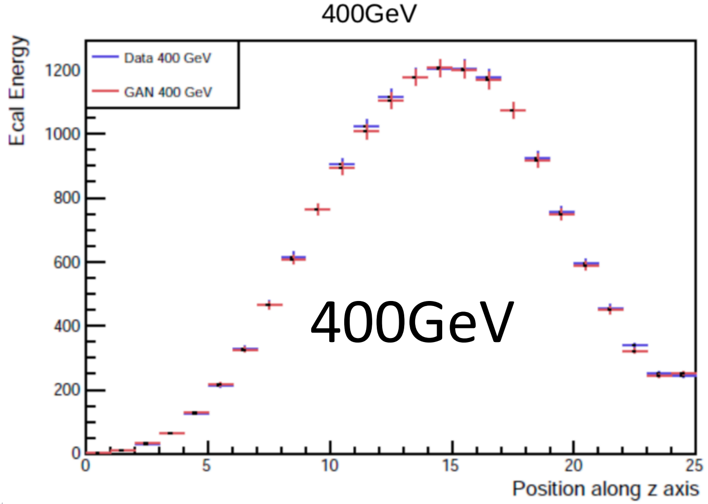
We run on Caltech ibanks GPU cluster thanks to Prof M. Spiropulu

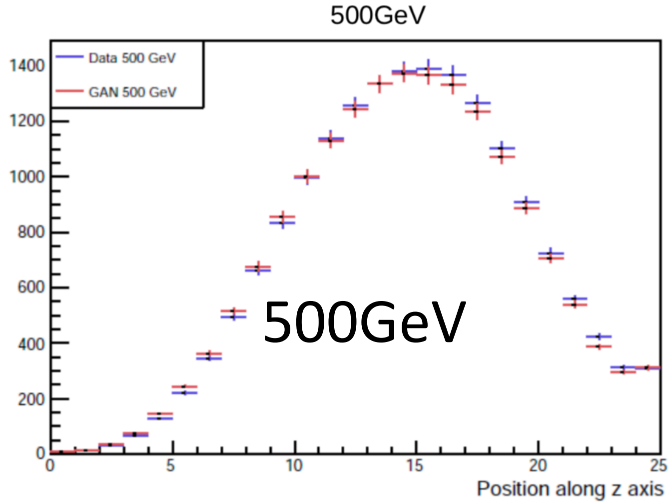
Electrons shower shapes

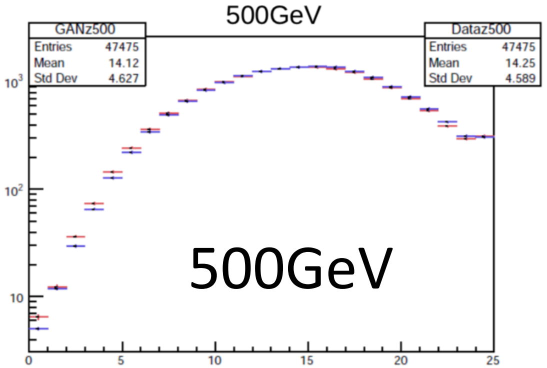






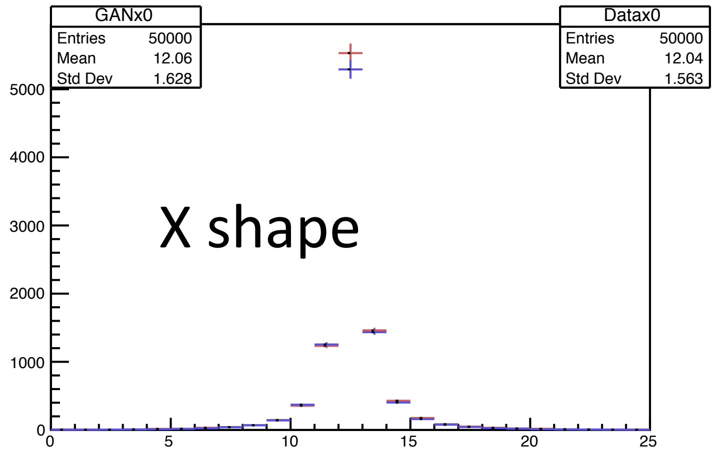


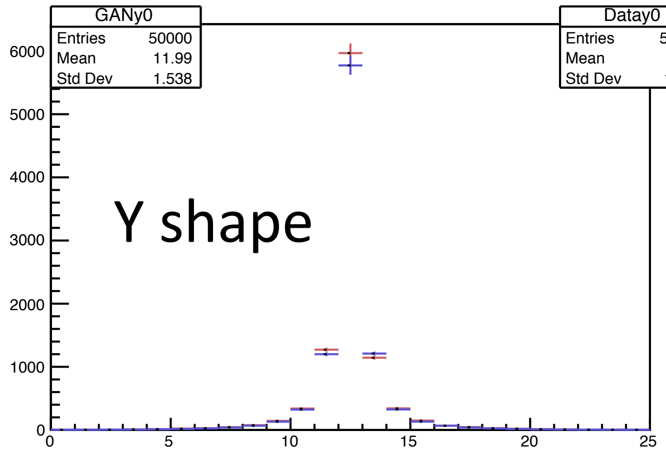


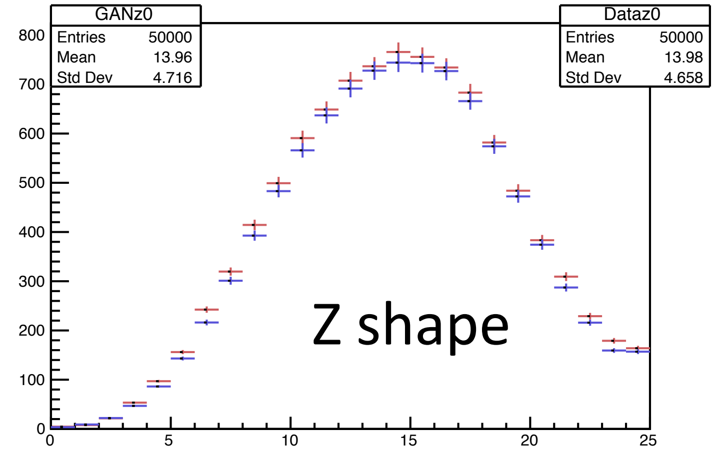


Neutral Pions

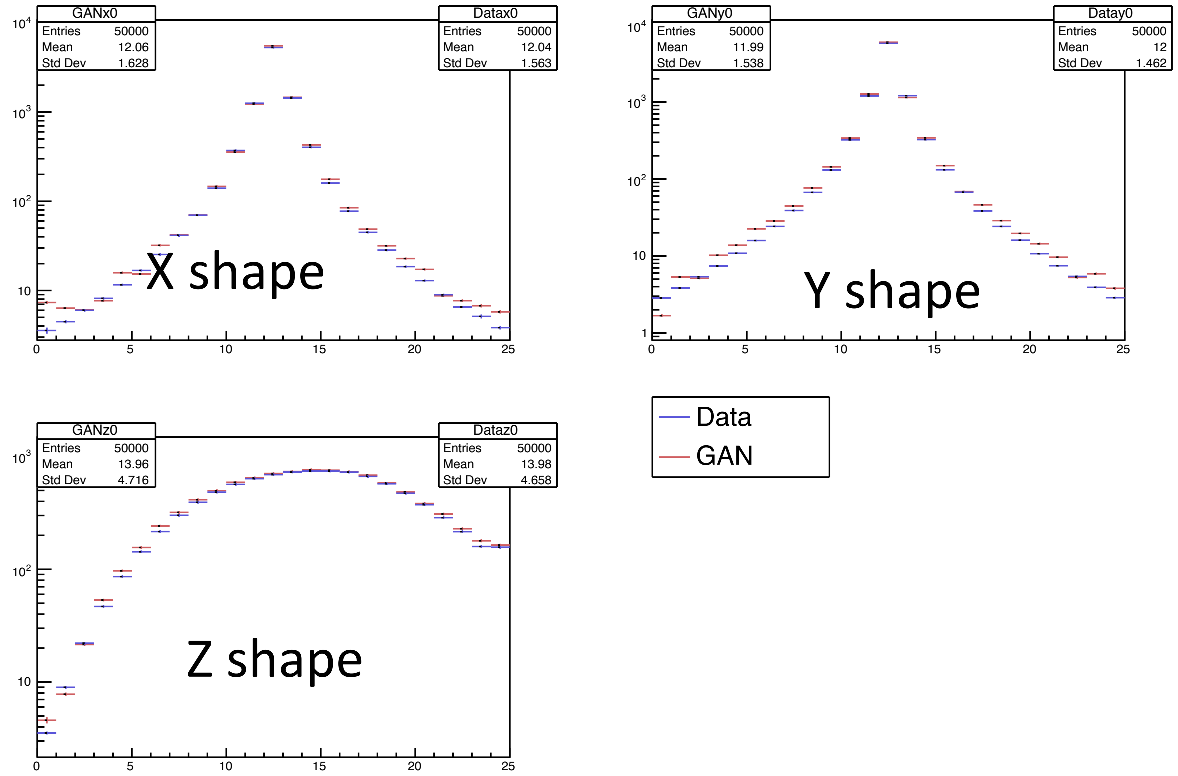
10-500 GeV







Log scale



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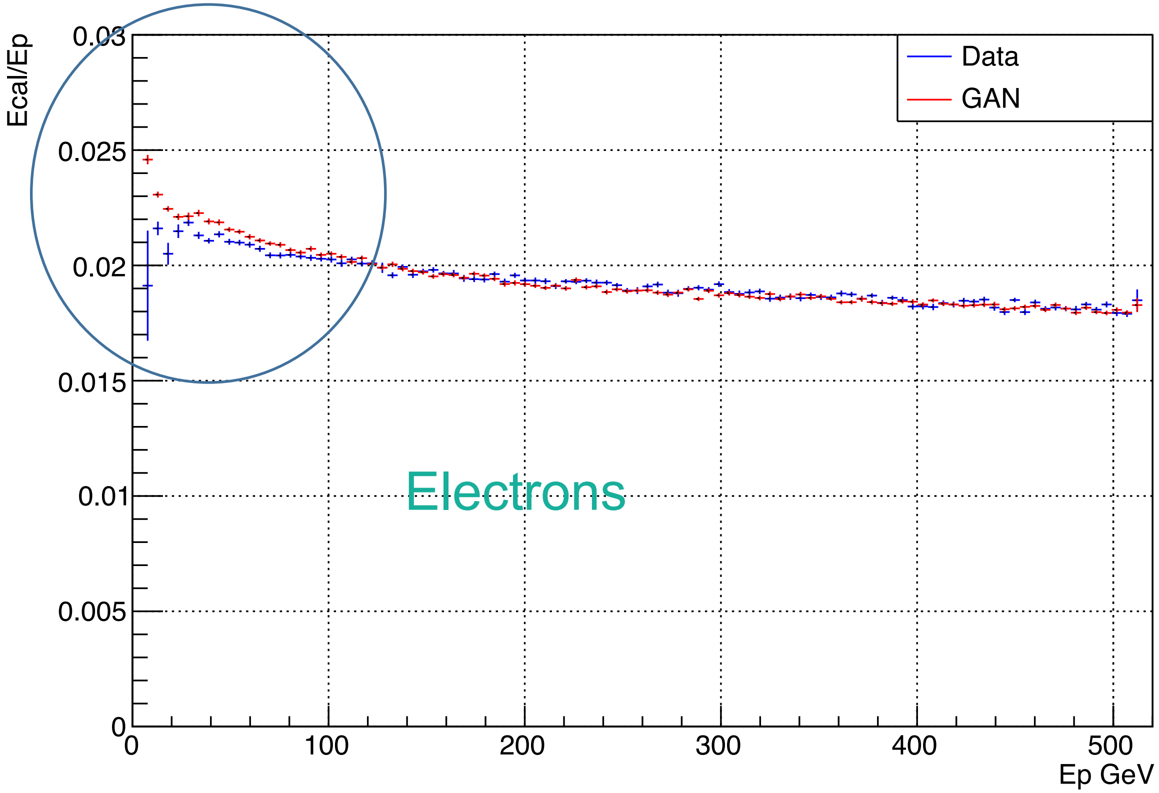
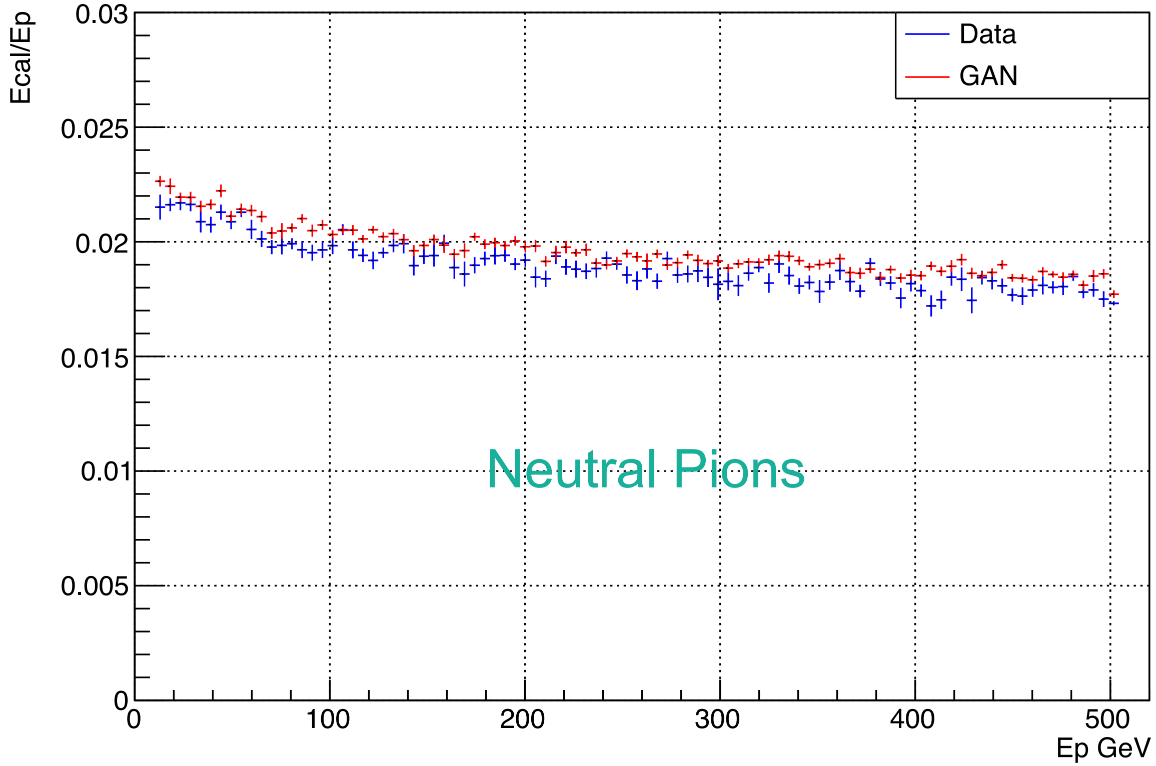
Deposited energy and sampling fraction





GAN seems to slightly overestimate slightly neutral pions energy deposits

Computing resources & Generalisation

Distributed training

Hyper-parameter scans

Computing performance

Distributed training is needed

Inference:

Geant4: 17 s/particle **vs** 3DGAN: 7 ms/particle

➔ speedup factor > 10000!!

➔ Testing inference on accelerators (GPUs, FPGAs) and dedicated hardware

Training:

45 min /epoch on Tesla P100

Introduce **data parallel** training based on MPI

Test several libraries

Run on HPC clusters and Cloud (HNSciCloud providers)

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**

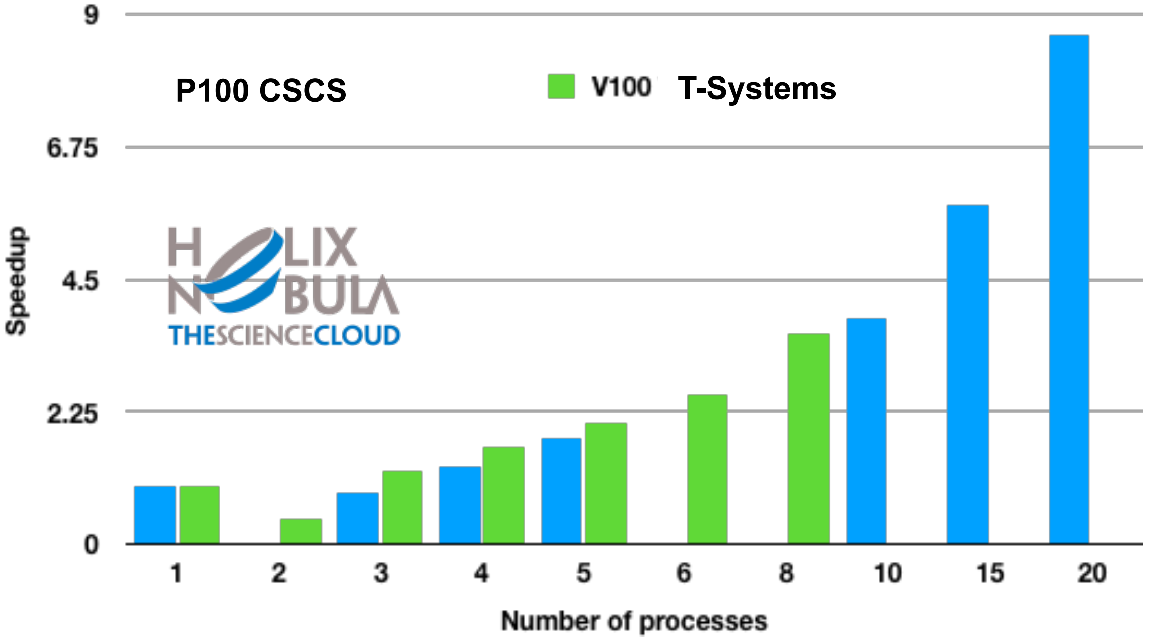
Optimisations in TF (1.2) + MKL-DNN

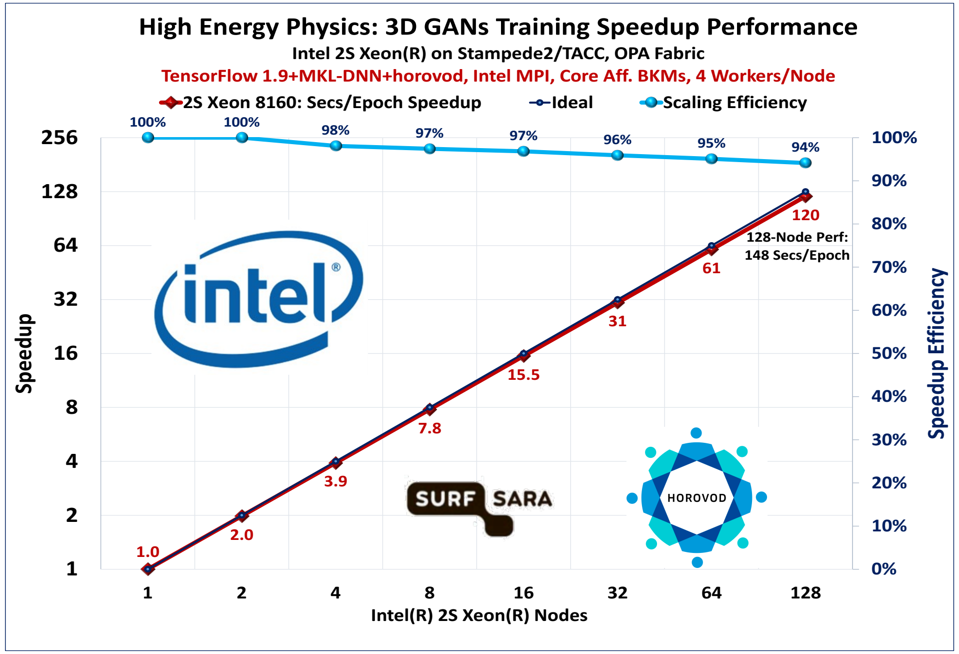
1 msec/shower

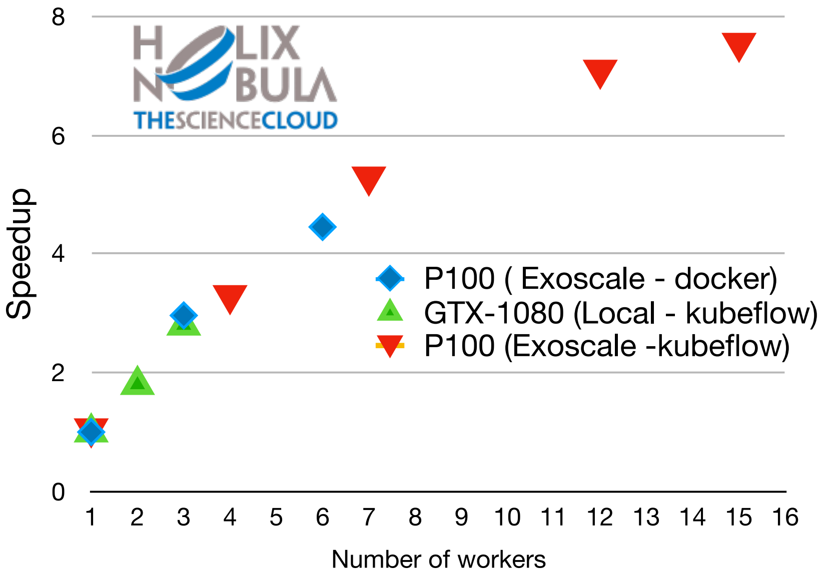
→ Speedup factor >10000

Distributed training

- Cloud deployment via docker + Kubernetes/Kubeflow (R. Rocha CERN IT-CM)
- Frameworks
  - Horovod
  - mpi_learn
- Hardware resources
  - Cloud (HNSciCloud)
  - HPC centers (Oakridge – TACC)







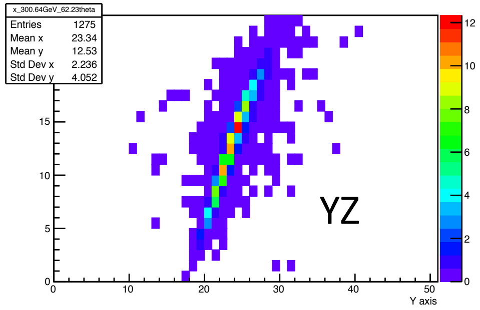
Generalisation

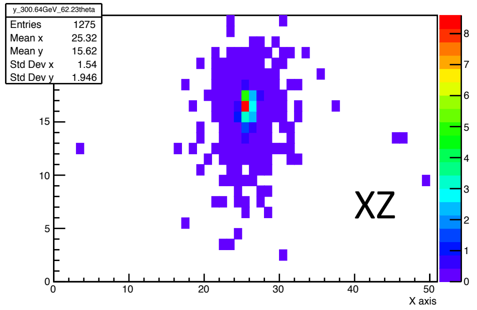
Electrons enter the calorimeter within a 60°-120° angle range

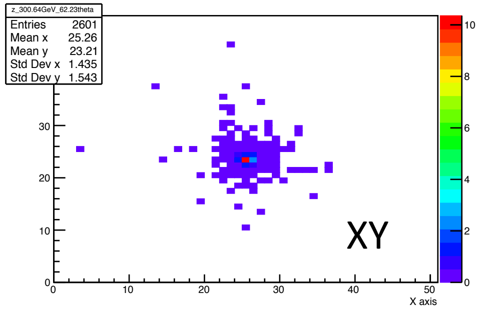
Wider/asymmetric image size (51x51x25)

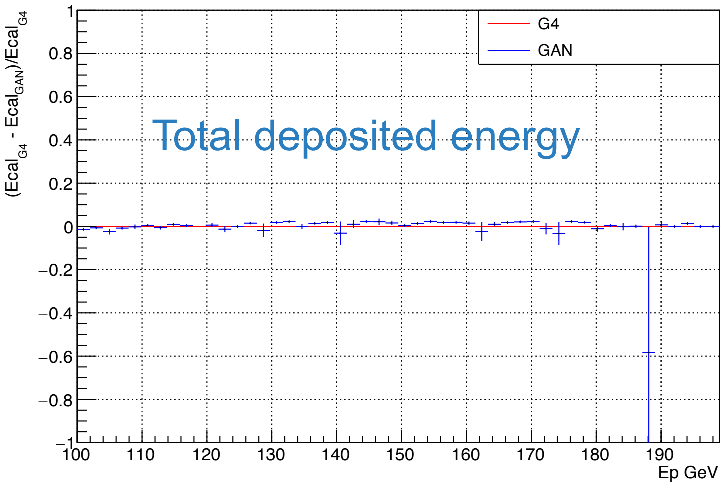
Minimal architecture changes “by hand”

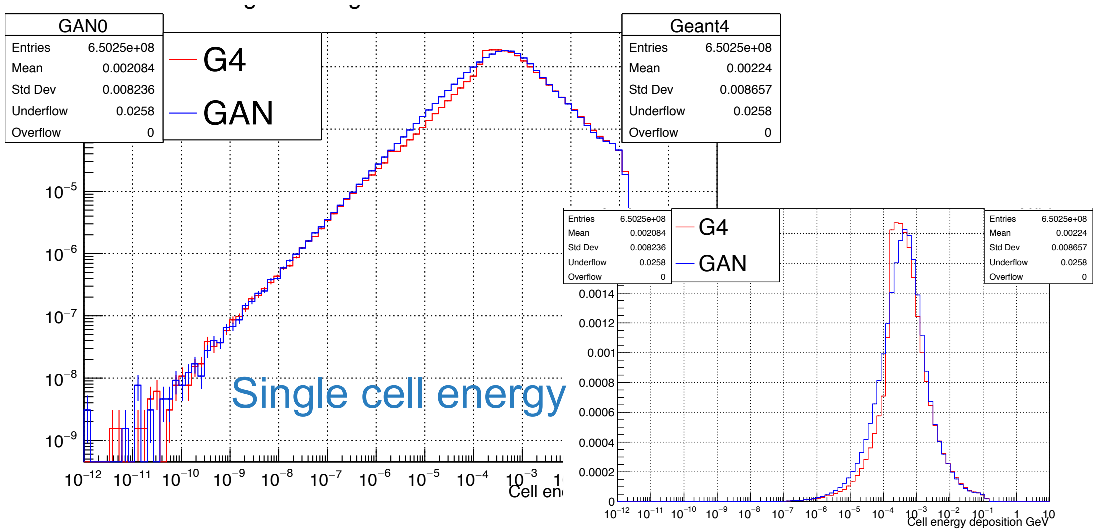
- Adjust convolution parameters
- Additional terms in the loss function:
  - Angle-related term
  - Constrain energy spectrum











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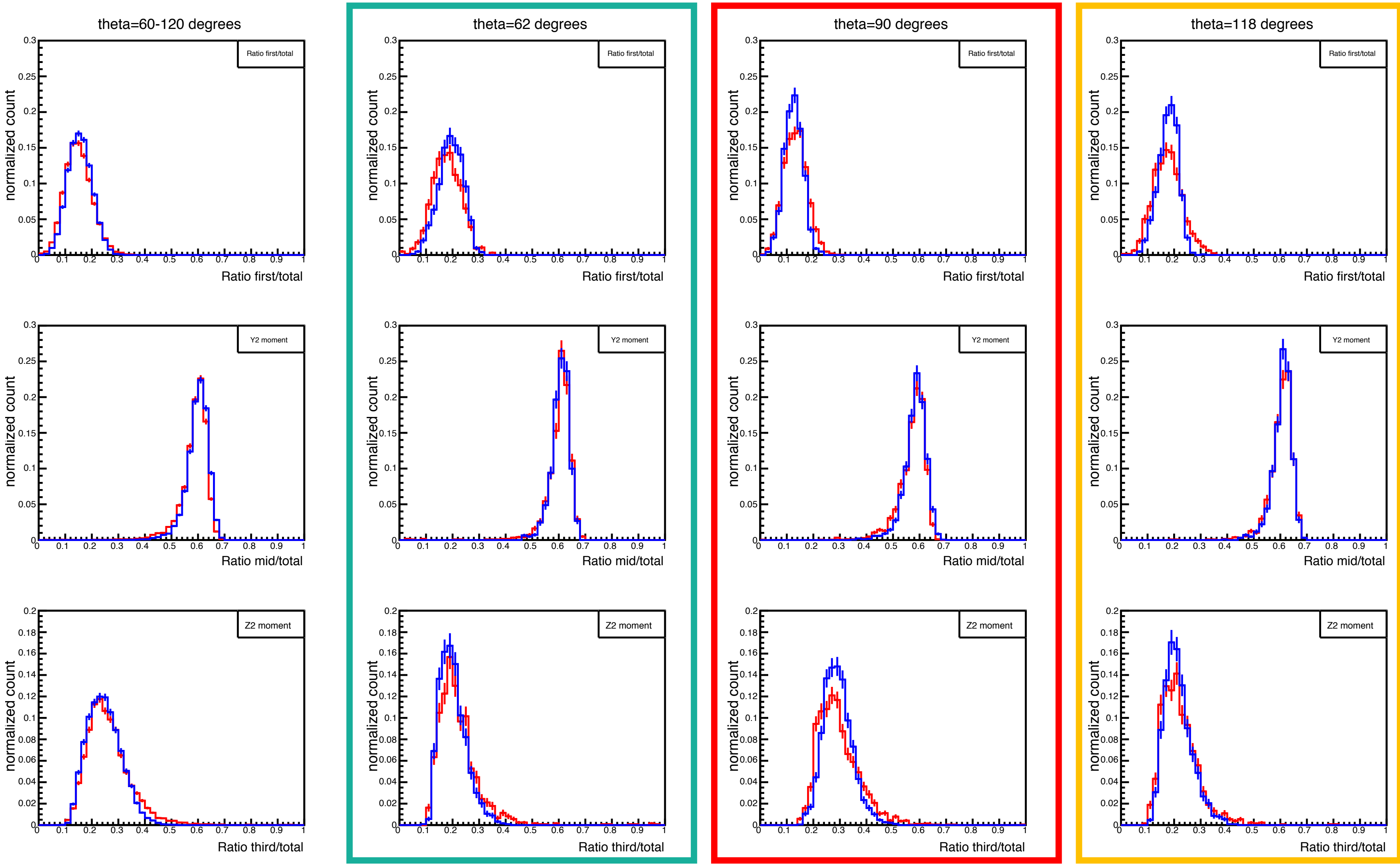
Angle dependence (I)

Spit calorimeter in 3 layers along its depth (cells: 1-8, 8-16, 24-25)

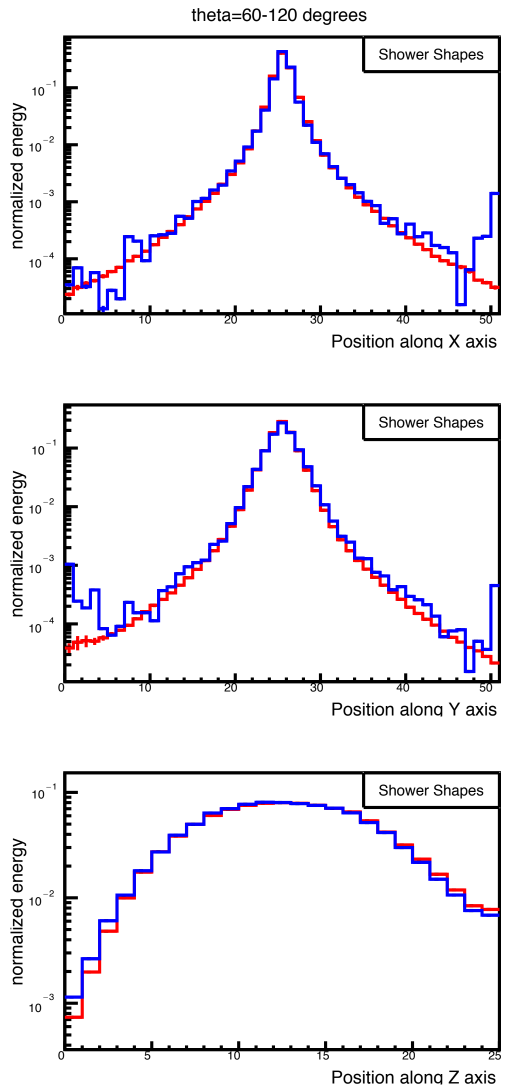
Measure energy deposited in layers wrt total

inclusive | 60° incident angle | Ortogonal | 120° incident angle

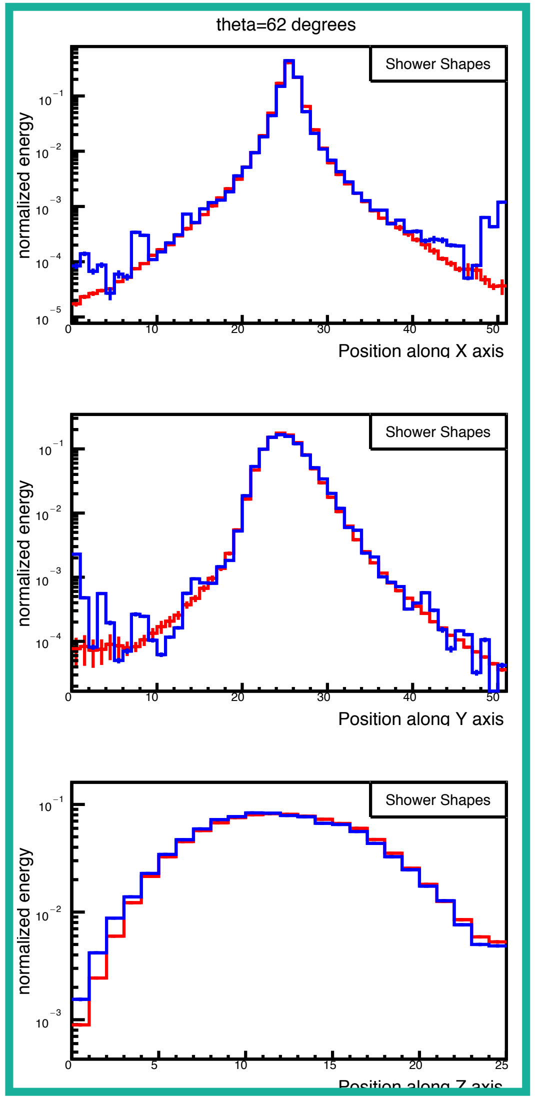


Angle dependence (II): shower shapes

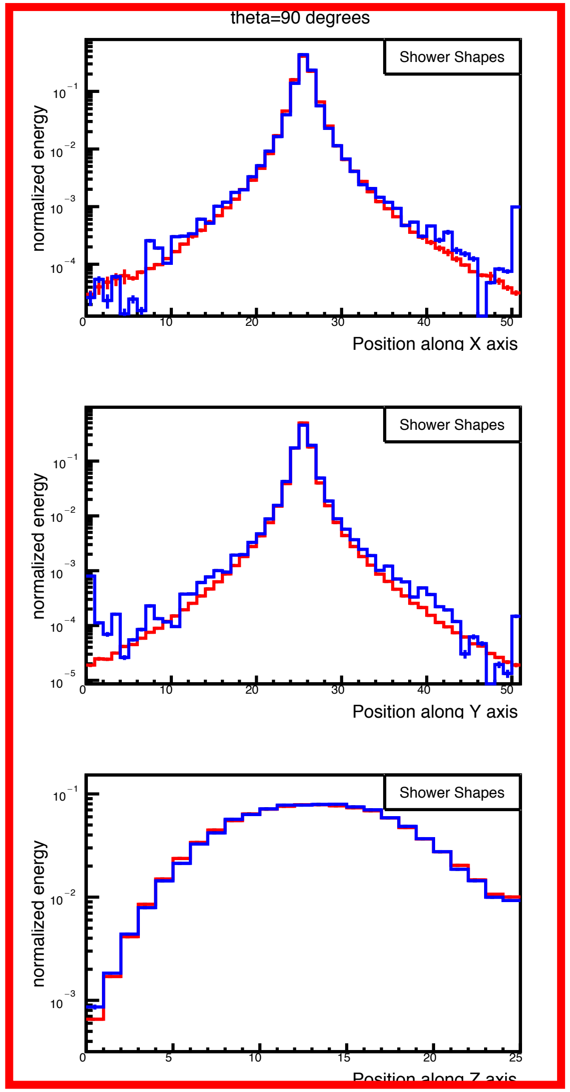
inclusive



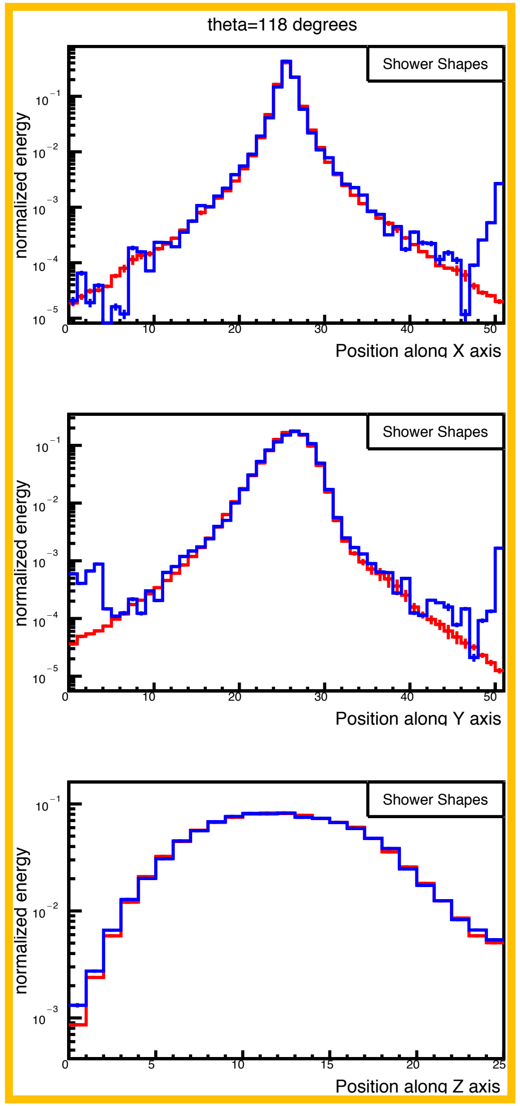
60° incident angle



Ortogonal



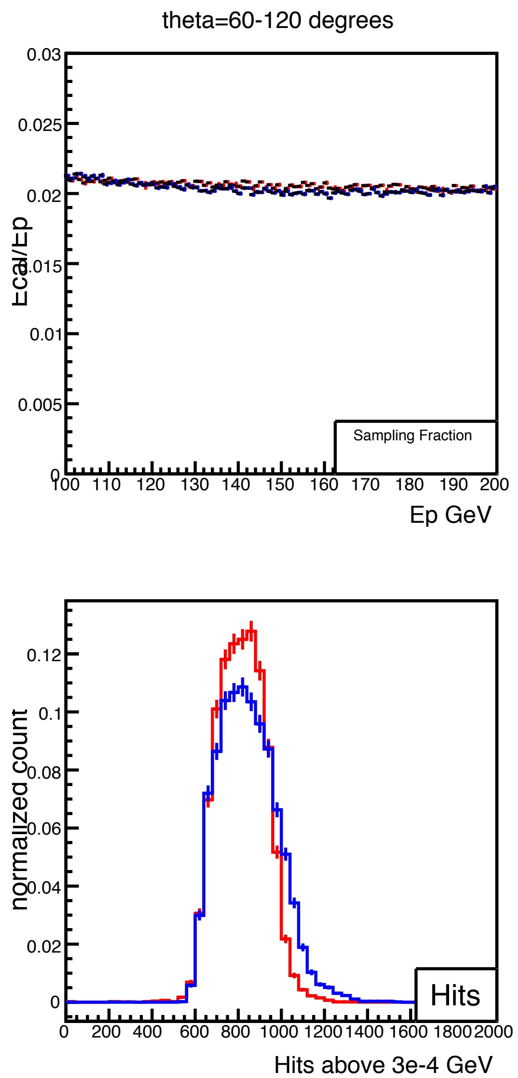
120° incident angle



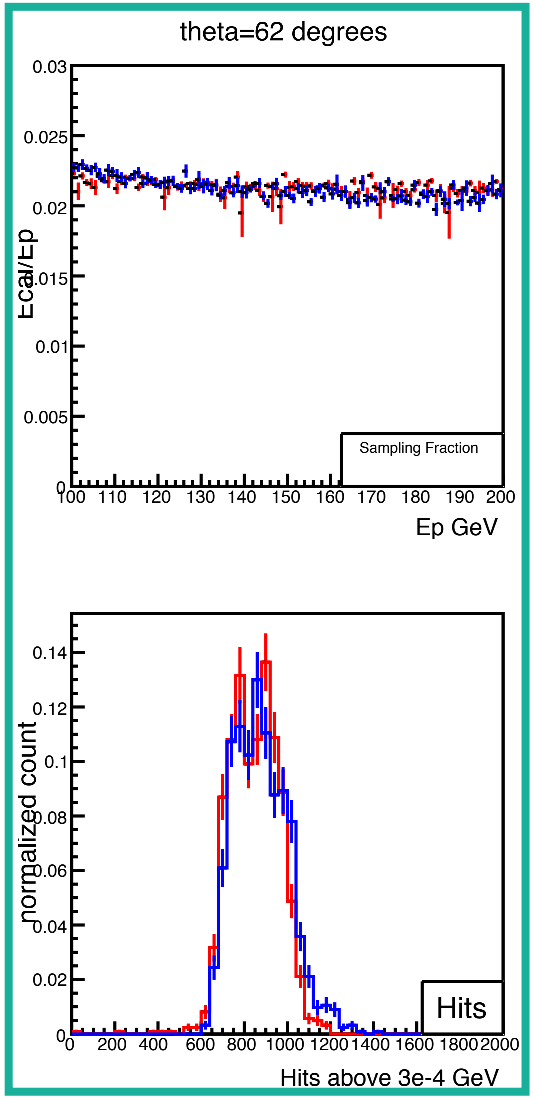
Angle dependence (III)

Sampling fraction annd number of hits

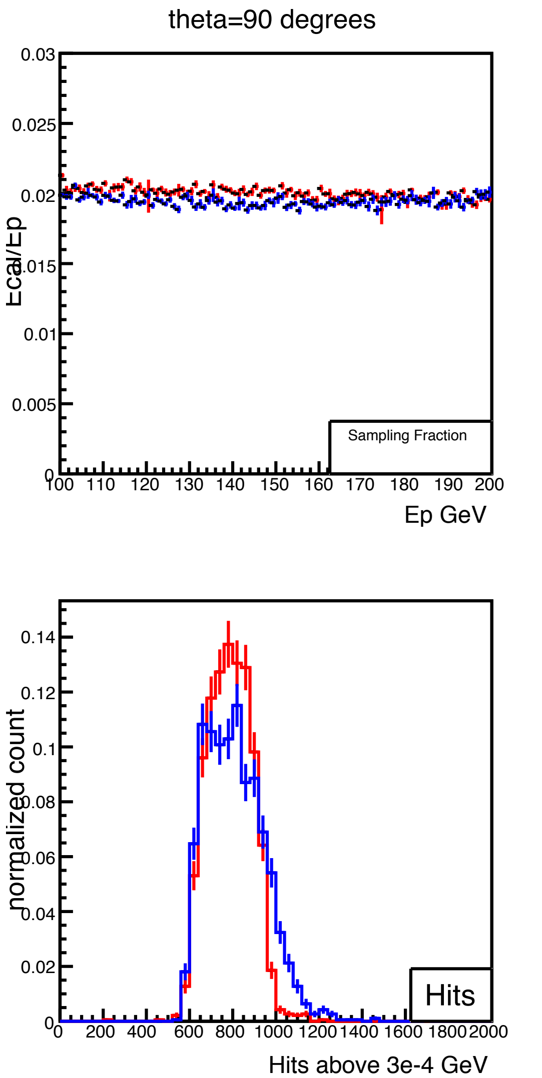
inclusive



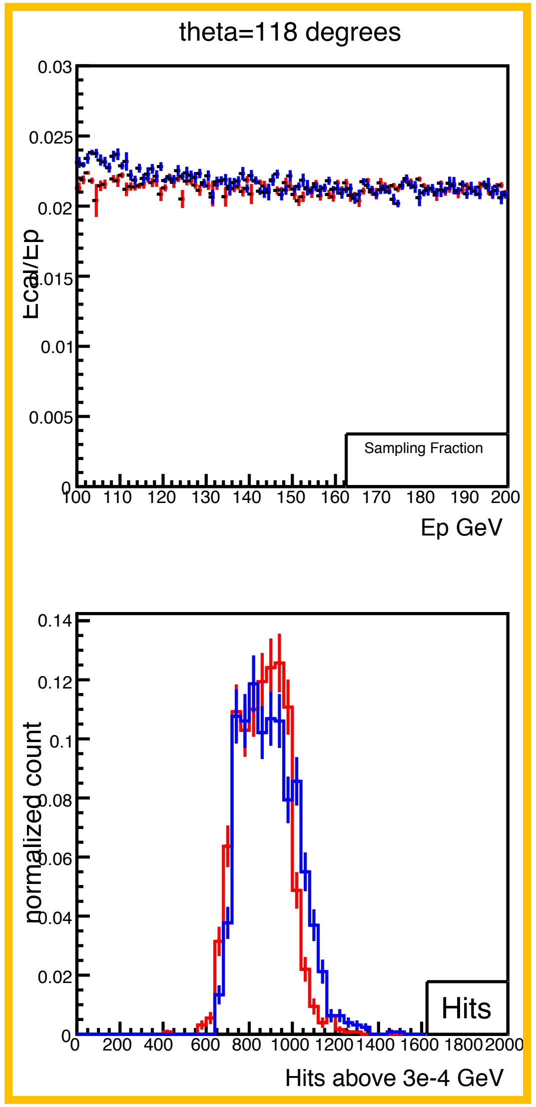
60° incident angle



Ortogonal



120° incident angle



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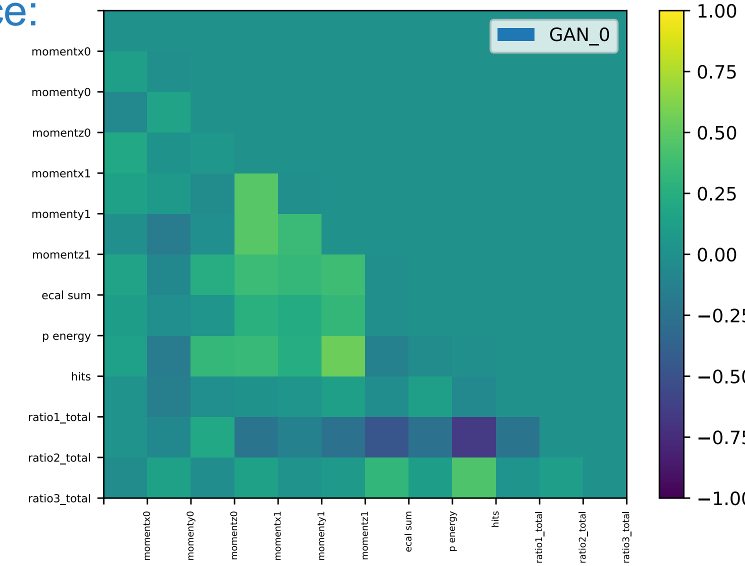
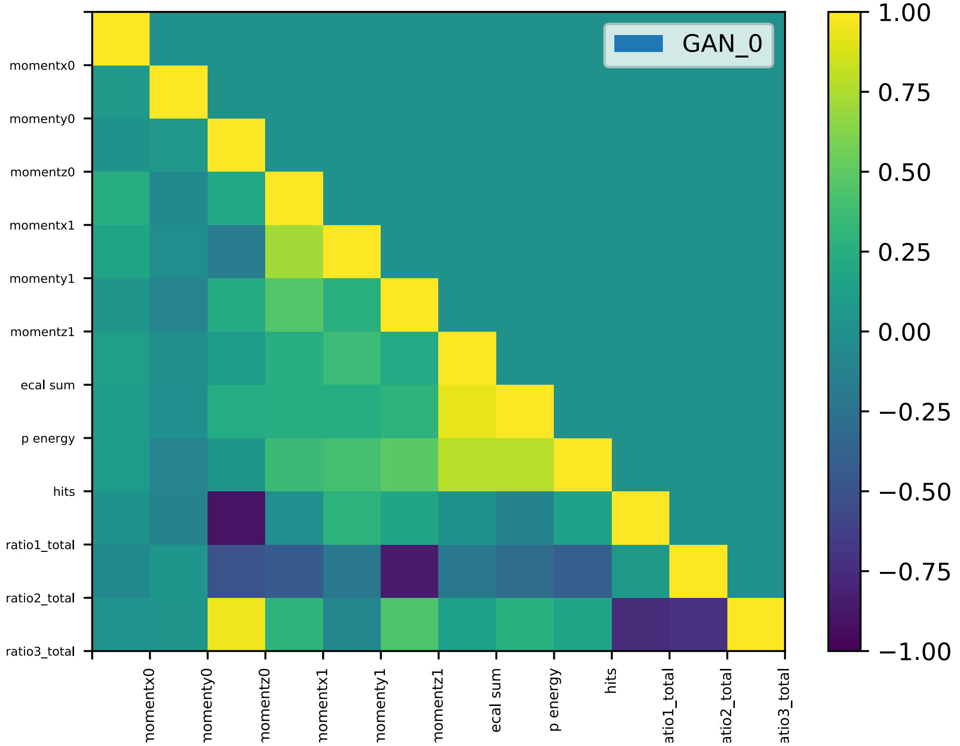
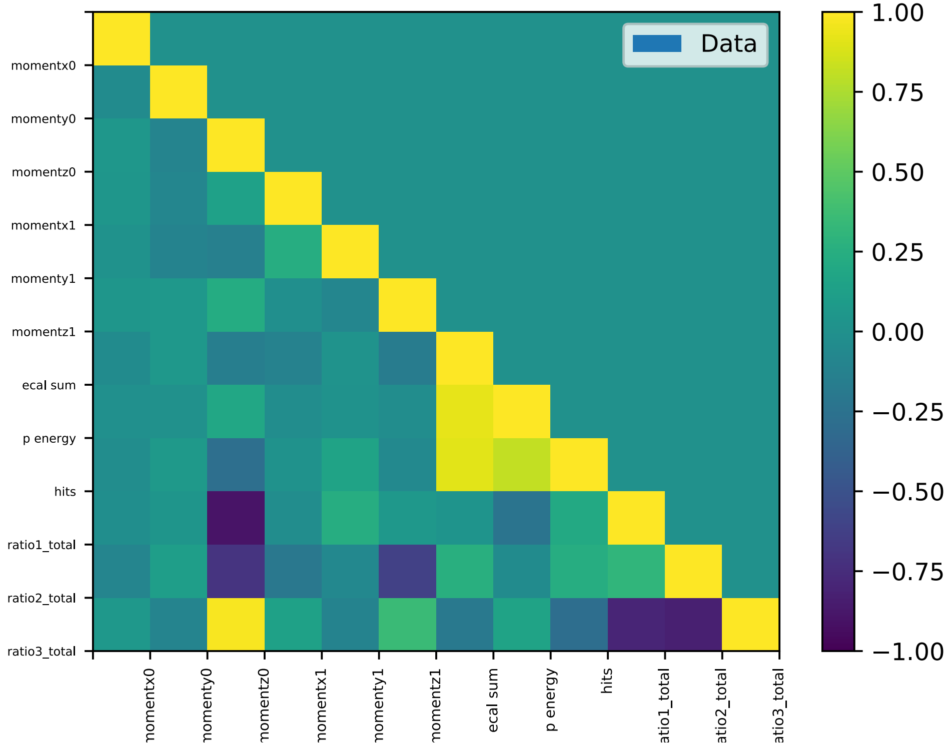
Internal correlations

3DGAN can correctly reproduce most G4 internal correlations

Difference:







Generalisation

Training and architecture hyper-parameters optimisation

How much can we generalise our network to other calorimeters?

- Different geometries, read-out patterns, energy scales

Tuning the right architecture cannot be done by hand

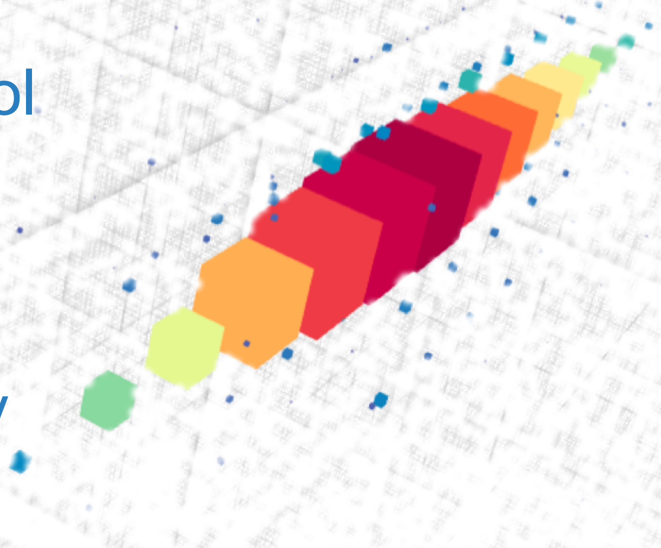
- Full parameter scan is resource/time consuming.

Test different optimisation approaches:

- Sequential Model-Based Optimization
  - Optimize intial architecture candidate, defining a finite set of states to explore
- Reinforcement Learning
  - Network accuracy is the **reward function**. Architecture or hyper-parameter modification are **actions**
- Evolutionary Algorithms
  - Can allow simulataneous weights training and architecture optimisation

mpi-learn integrates a optimisation engine (mpi-opt)

Summary & Plans



3D GAN: first step towards customizable simulation tool

- Agreement to Monte Carlo within few percent
- Work in SFT to test integration in simulation framework

Meta-optimization and hyper-parameters scans are key

- Test of several distributed training approaches
- Understand / optimize performance at scale

We are working heavily on “technological/computing” aspects in collaboration with industry (Intel, IBM, Google)

Test different platforms for inference and training: CPUs, accelerators (GPUs, FPGAs)

Questions?

Sofia.Vallecorsa@cern.ch

Thanks!

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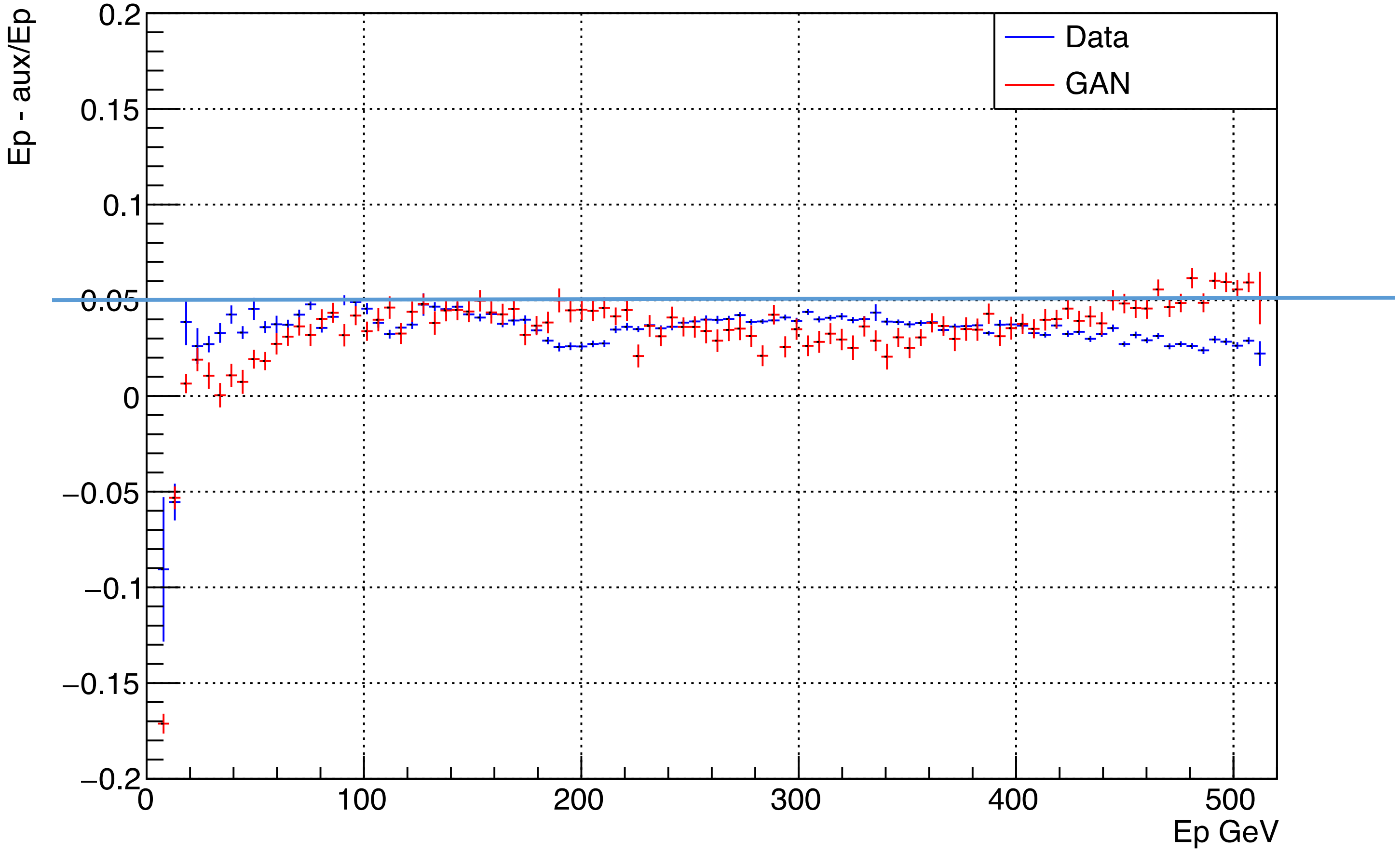
Discriminator regression on input energy

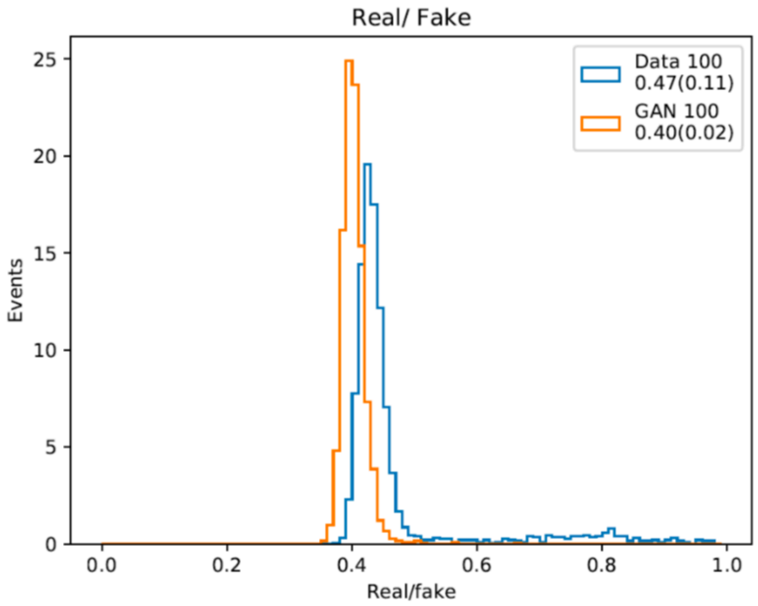


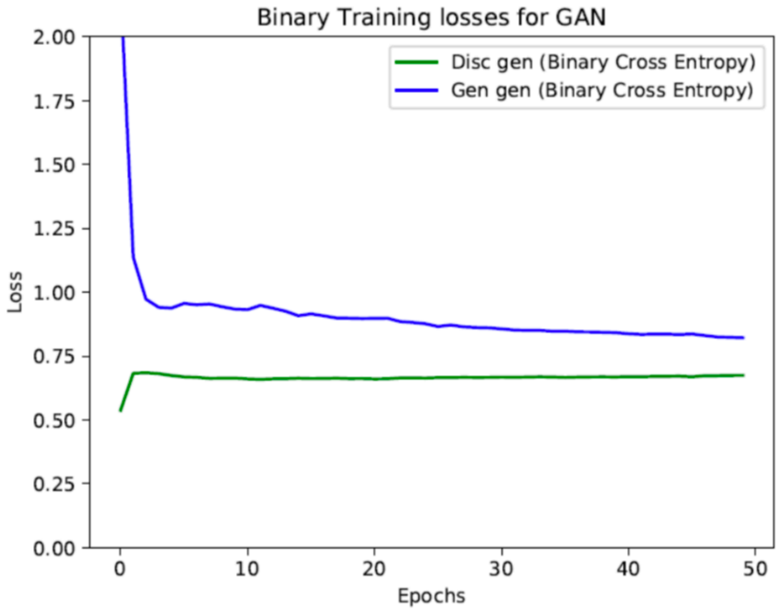
5% error on auxiliary energy regression

Conditioning and auxiliary tasks

Loss is linear combination of 3 terms:

- Combined cross entropy (real/fake)
- Mean absolute percentage error for regression tasks

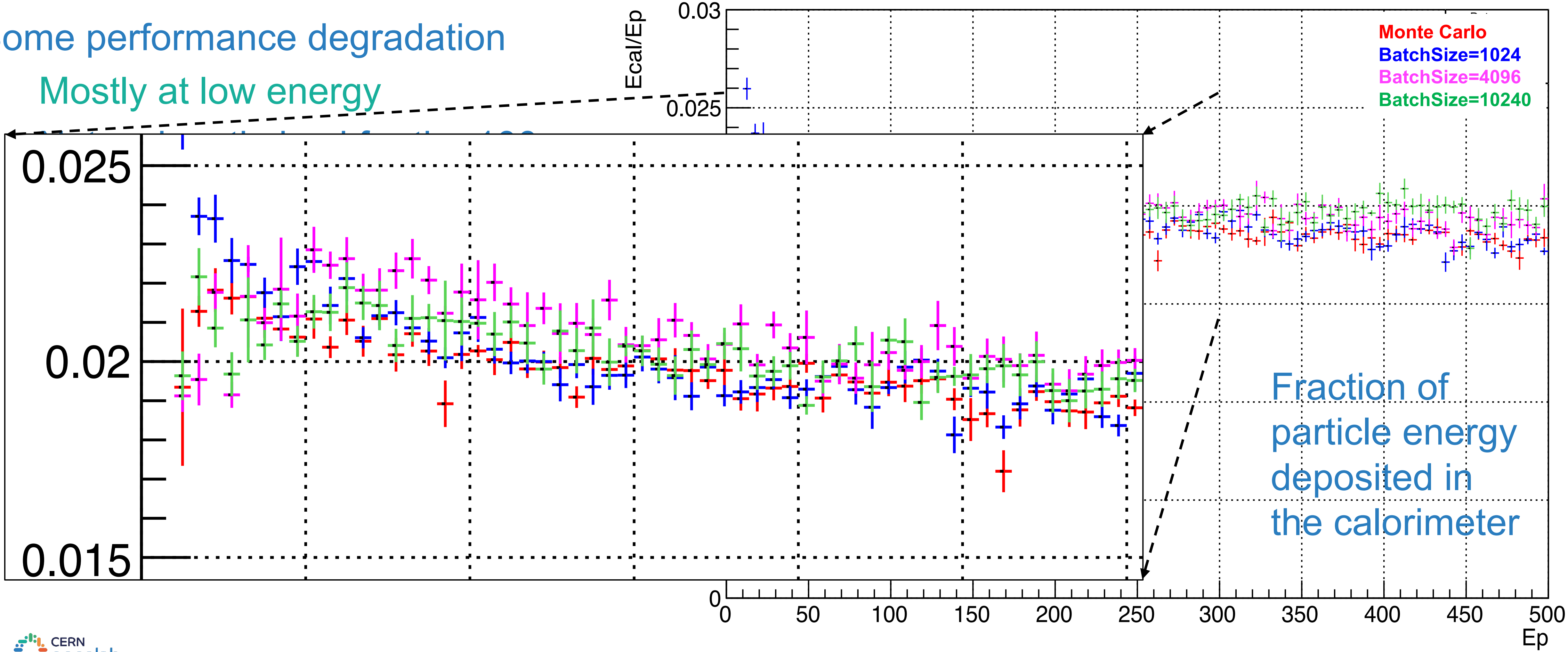




Physics performance

Some performance degradation

Mostly at low energy



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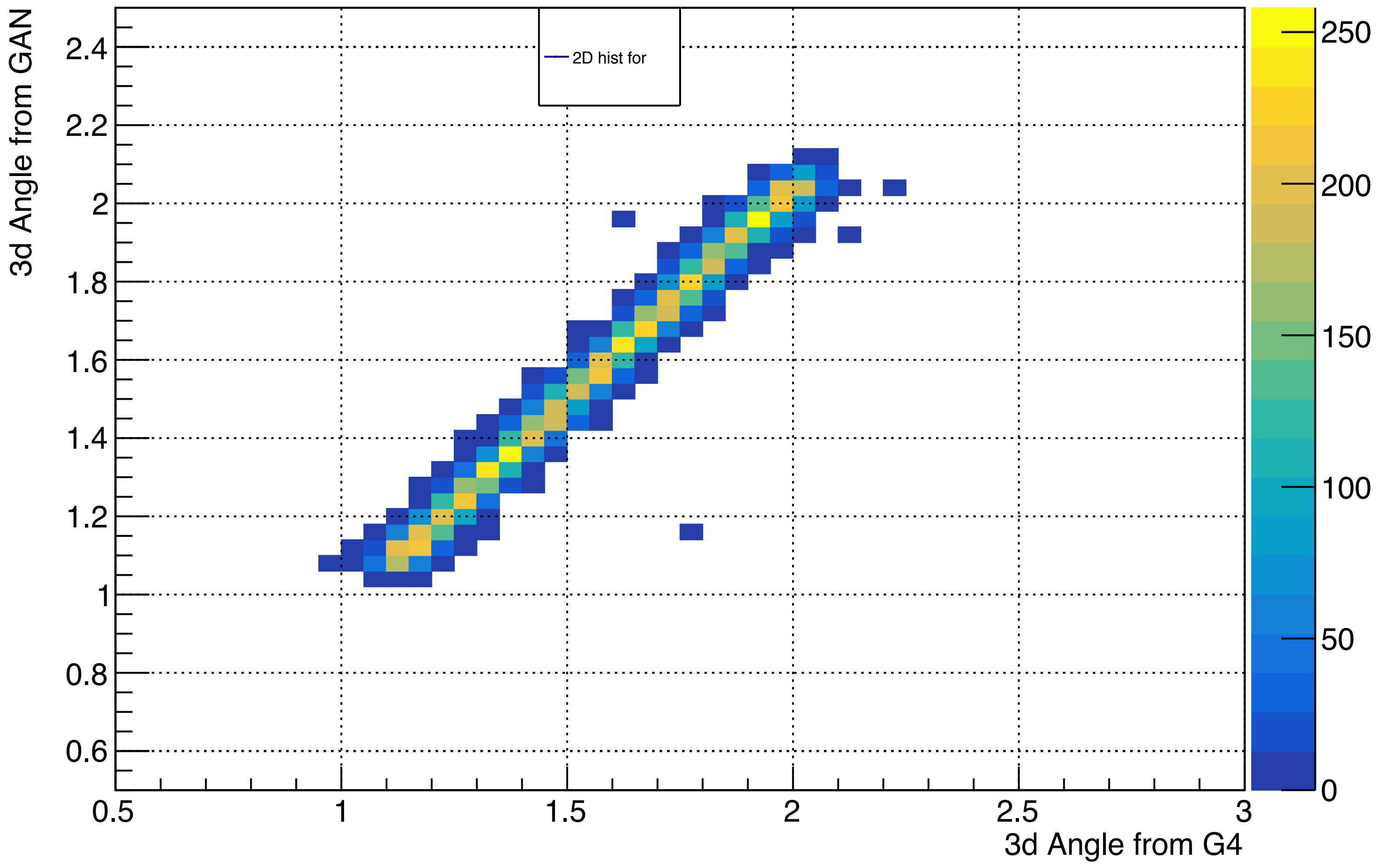
Angles


2D hist for
3d Angle from GAN
3d Angle from G4
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.5
1
1.5
2
2.5
3
250
200
150
100
50
0

https://github.com/vlimant/mpi_opt

https://github.com/vlimant/mpi_learn

mpi-opt

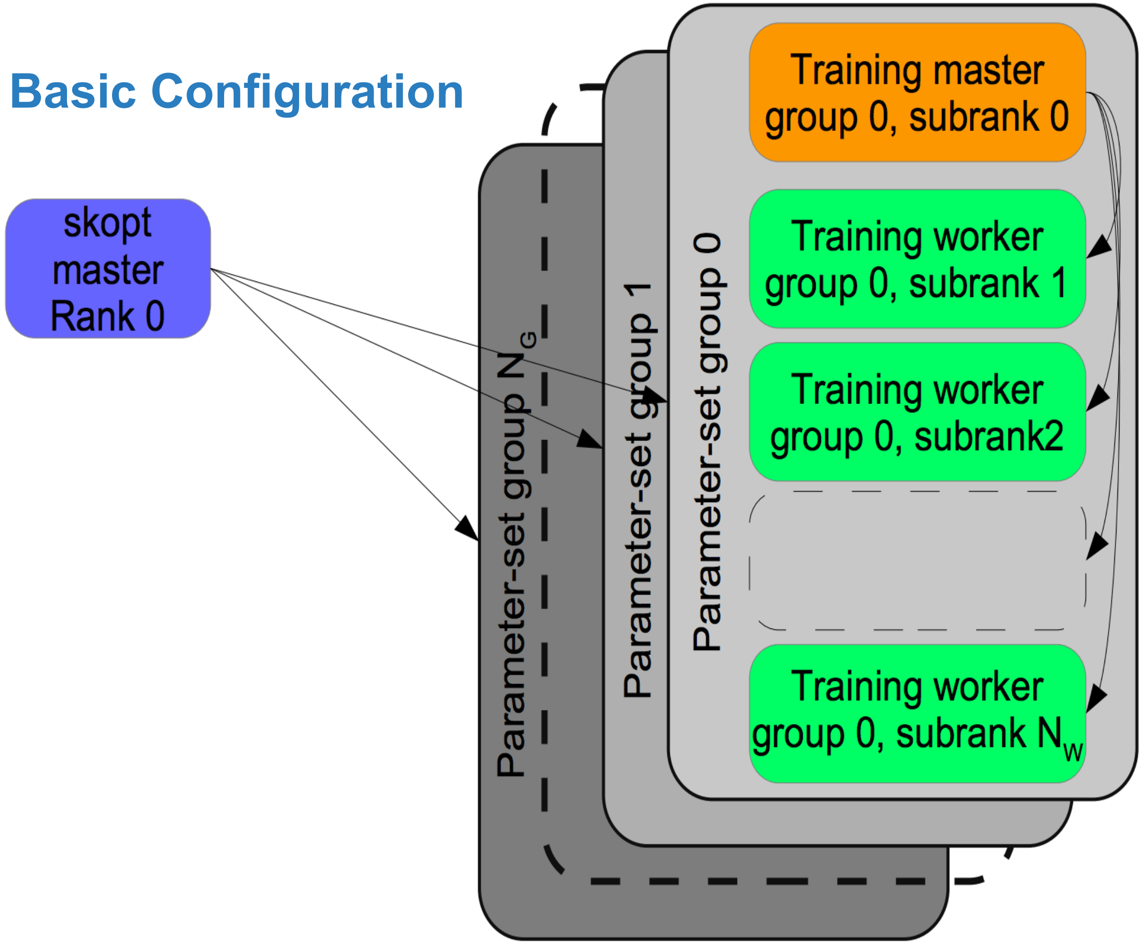
Parallelise optimisation with mpi-learn

Bayesian optimiser

Evolutionary approach

- One master runs optimisation (skopt)
- N_G groups of nodes train on a parameter-set
  - One training master
  - N_W training workers
- Can also run in “sub-masters mode¨
  - Sub-masters perform intermediate averaging

Basic Configuration



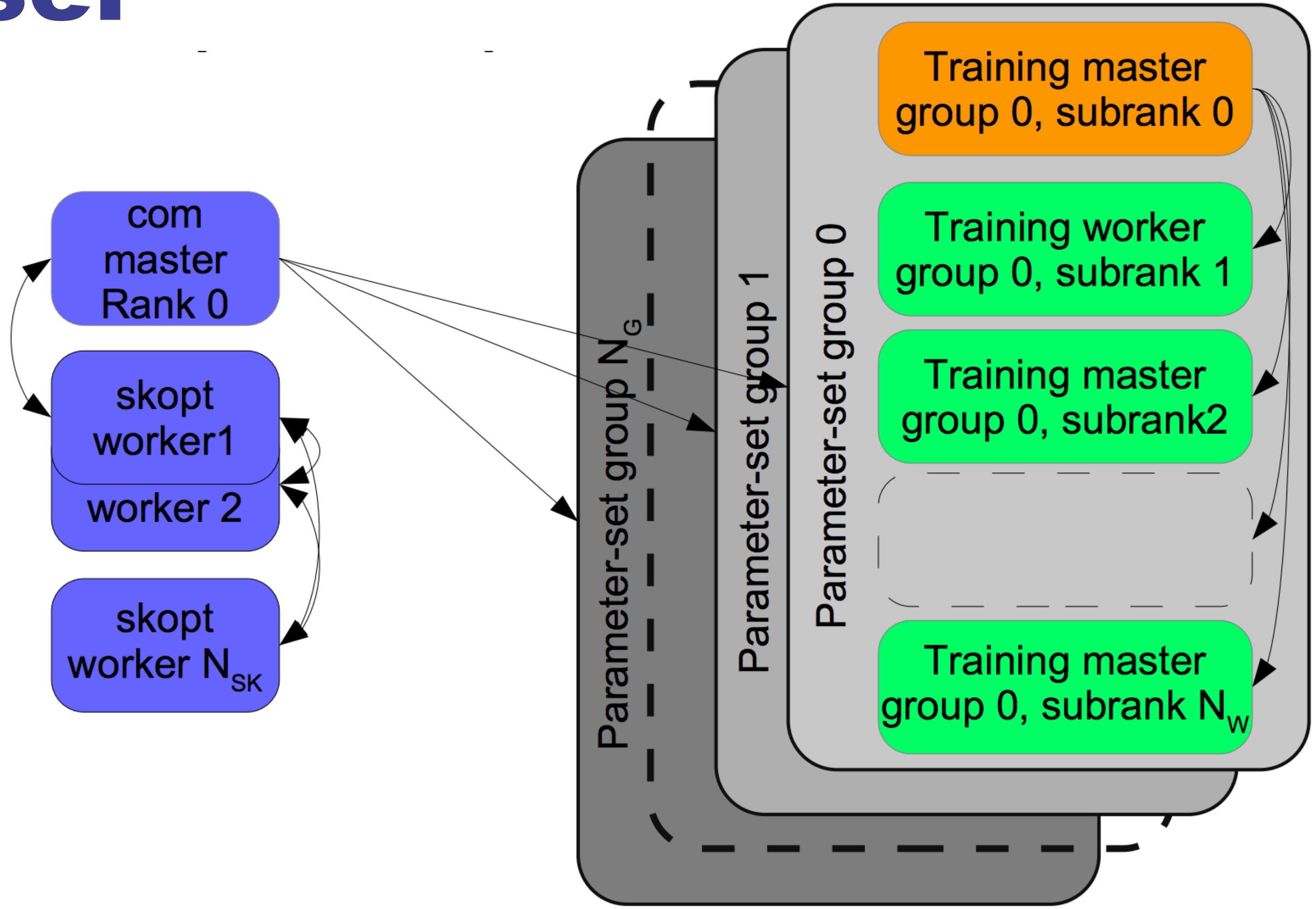
Parallel optimiser

One master running communication of parameter set

N_{SK} workers running the bayesian optimization

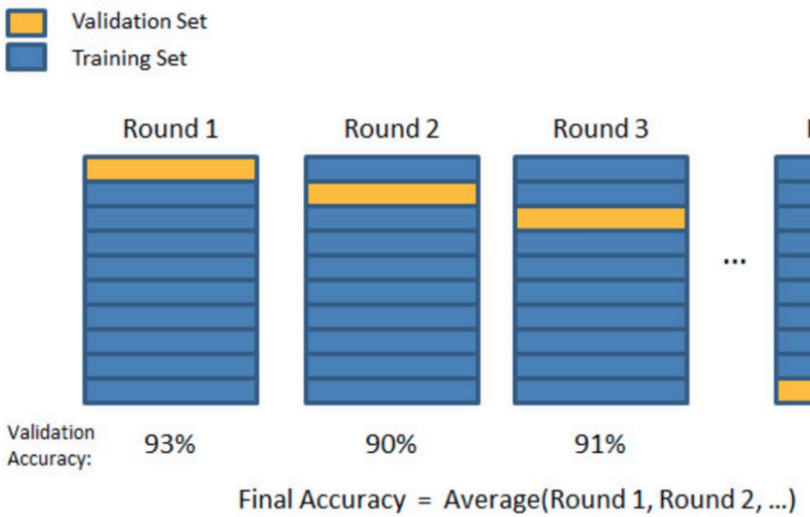
N_G groups of nodes training on a parameter-set on simultaneously

- One training master
- N_W training workers



prevent working groups to be idle while the optimisation fit is performed

K-folding cross validation



Estimate performance over different validation parts of the training dataset

Account for variance from multiple sources

- One master runs the bayesian optimization.
- Receives the average fom over N_F folds of the data
- N_G groups of nodes training on a parameter-set simultaneously
- N_F groups of nodes running one fold each
  - One training master
  - N_W training workers