Performance optimisation of 3DGAN training and inference on Intel architectures

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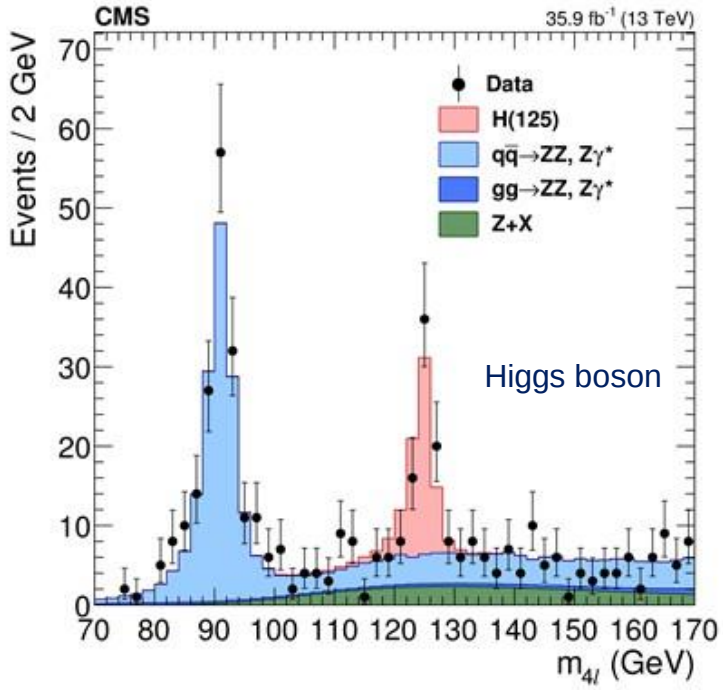
Outline

Monte Carlo Simulation

Essential for data analysis & detector design



Understand how detector design affects measurements and physics

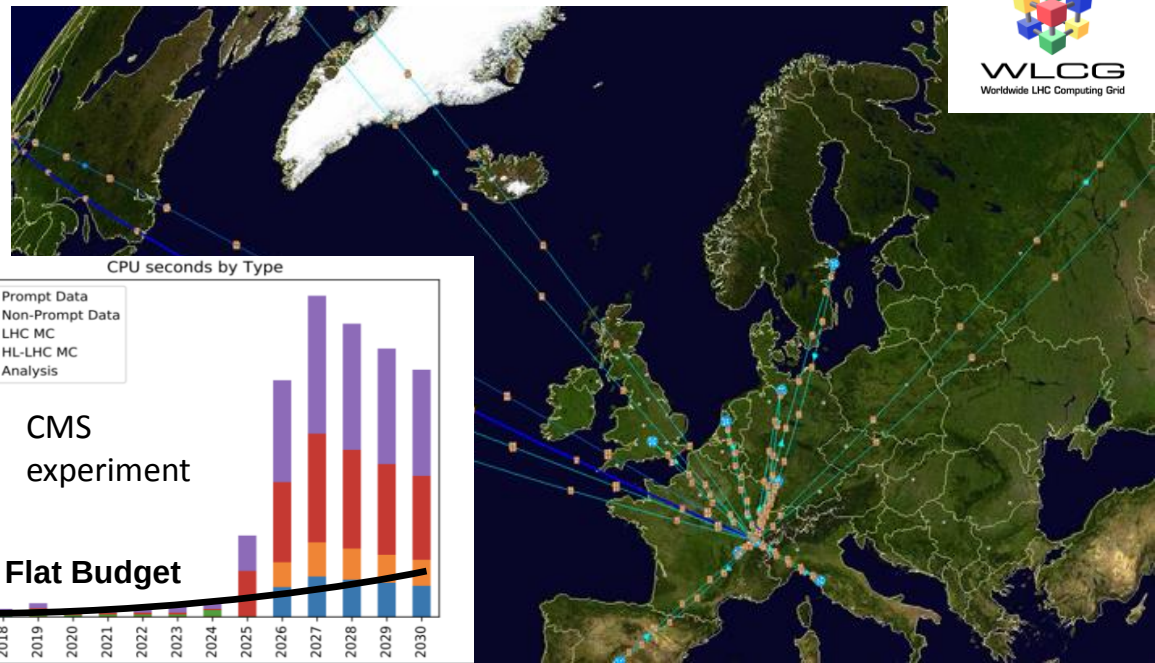
- Correct for inefficiencies, inaccuracies, …
- Compare theory models to data

It requires complex physics and geometry modeling

- >50% of **Worldwide LHC Computing Grid (WLCG)** power today
- HL-LHC brings x100 increase in simulation need

Generative Models a **generic approach**

- Inference is much faster than Monte Carlo



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Deep Generative Models

Extract meaningful representations from data

Internal representations learned by shallow systems are simple (Bengio & LeCun 2007, Bengio 2009)

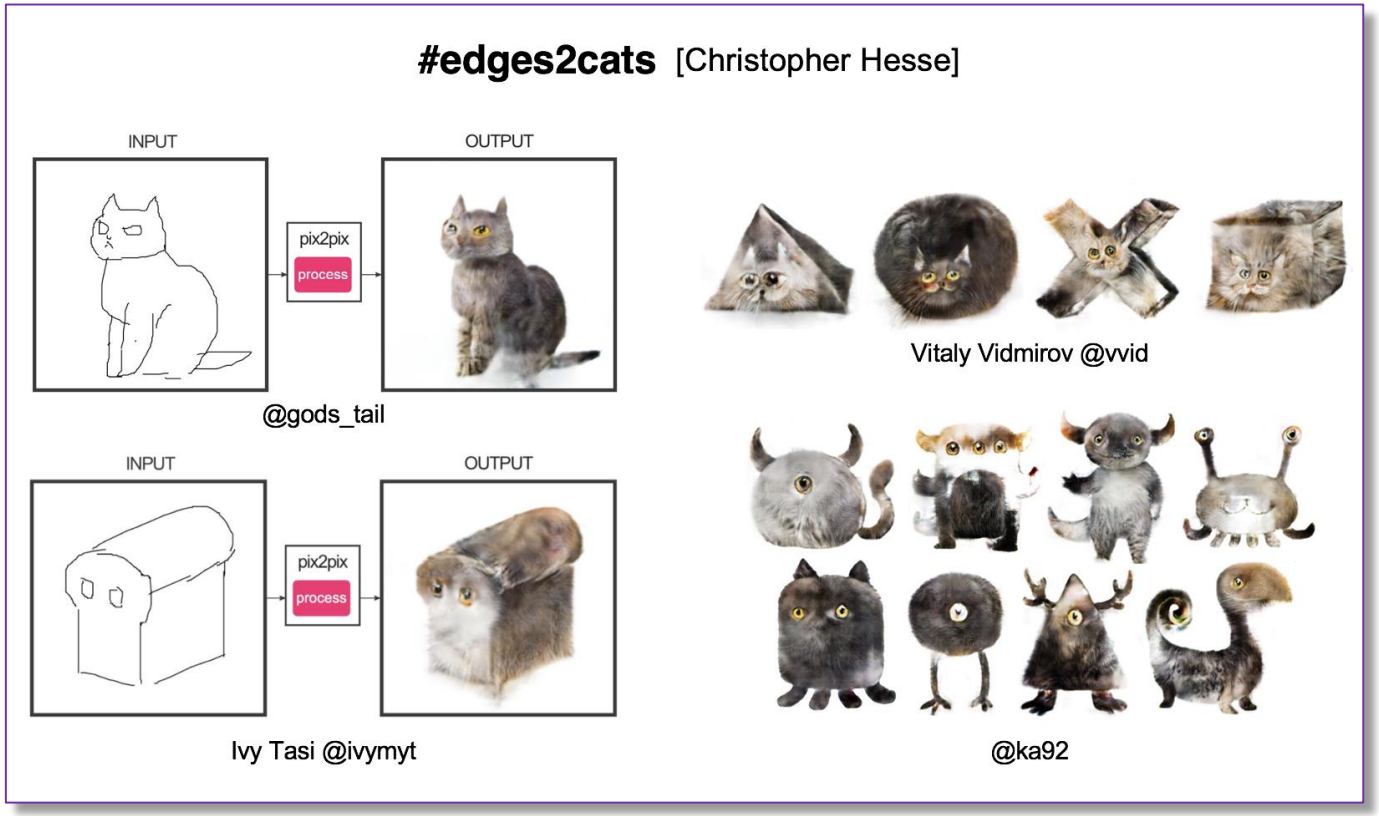
- Incapable of learning complex hidden structures
- Require large amounts of labeled data

→ Deep Generative Models

- → Allow higher levels of abstractions
- → Improve generalisation and transfer

→ Multiple applications

- Find Underlying Factors (**Discovery**)
- Detect Rare events (**Anomaly Detection**)
- Predict future events (**Planning**)
- Find Analogies (**Transfer Learning**)



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arXiv:1406.2661v1

Generative Adversarial Networks

Simultaneously train two networks that compete and cooperate with each other

Generator G generates data from random noise

Discriminator D learns how to distinguish real data from generated data

https://arxiv.org/pdf/1701.00160v1.pdf

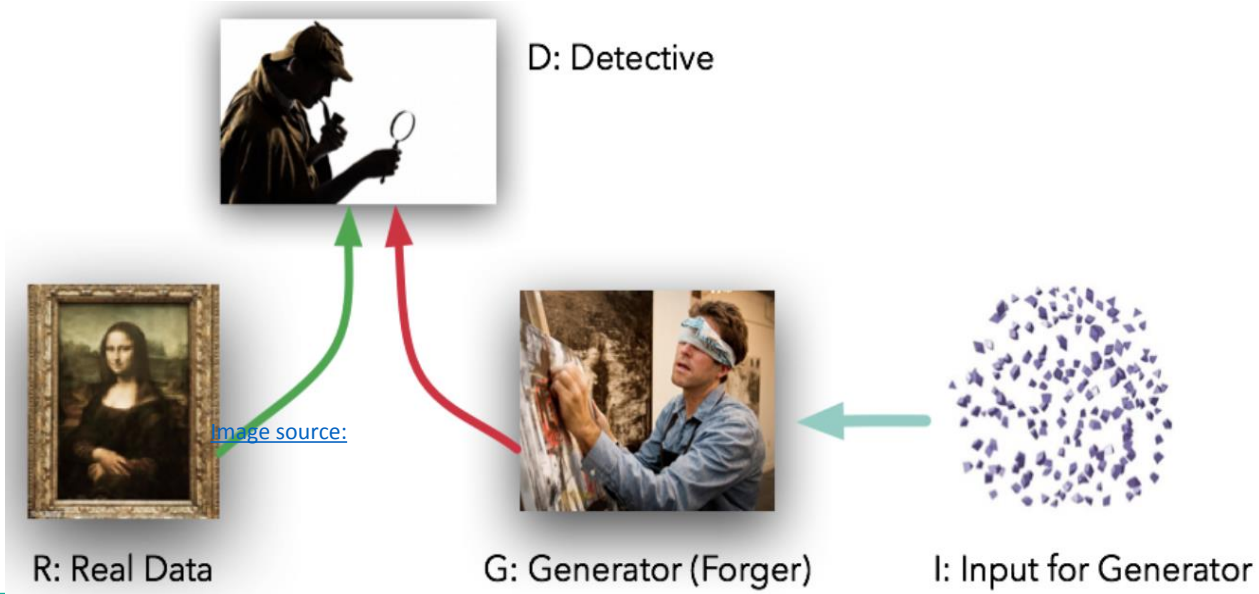


Image source:

The counterfeiter/detective case

Counterfeiter shows its Monalisa to the detective

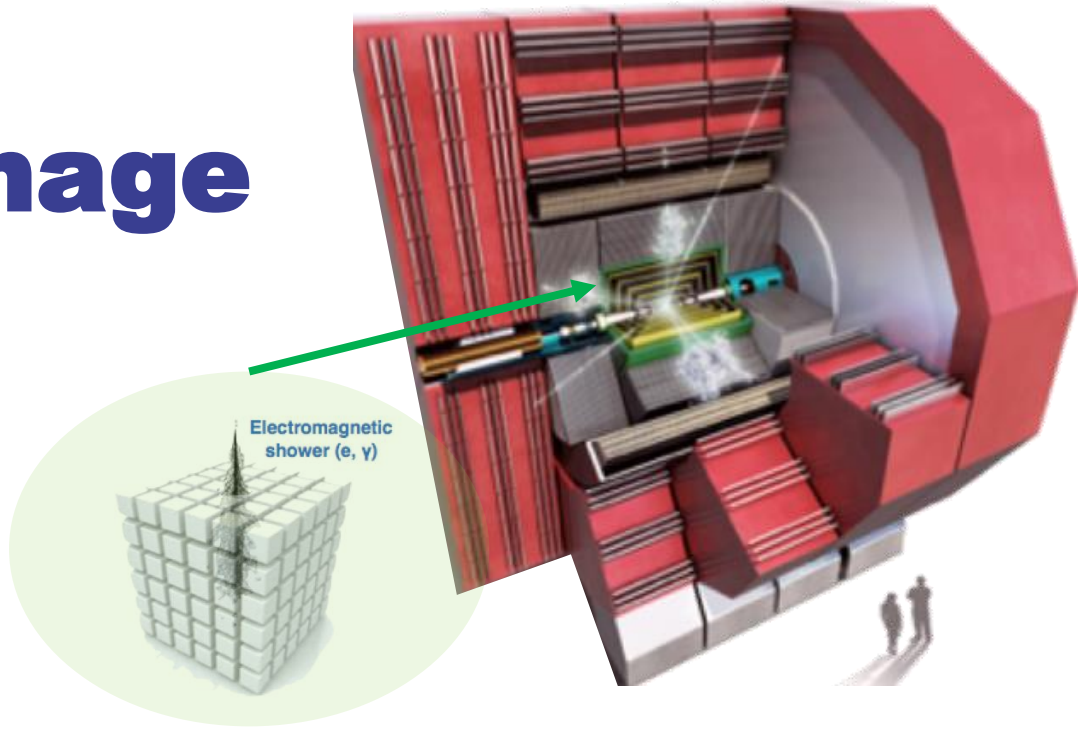
Detective says it is fake

Counterfeiter makes new Monalisa-style based on feedback

Iterate until detective is fooled

Detector output as 3D image

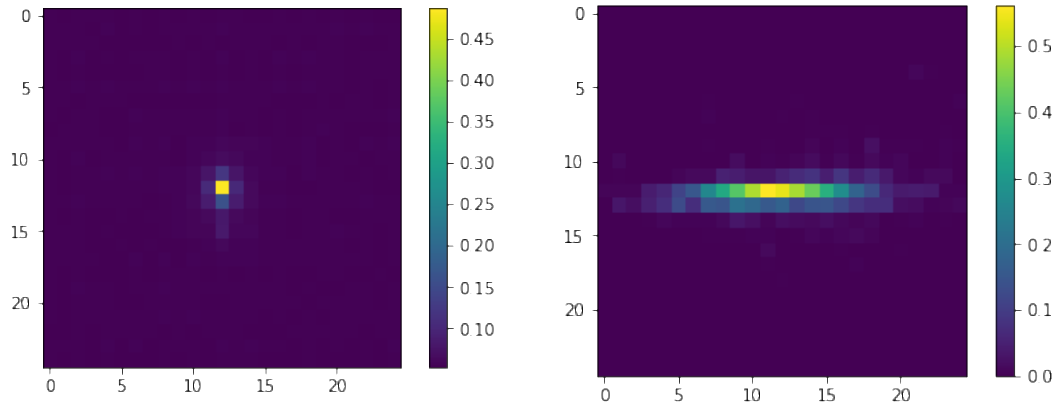
Array of absorber material and silicon sensors

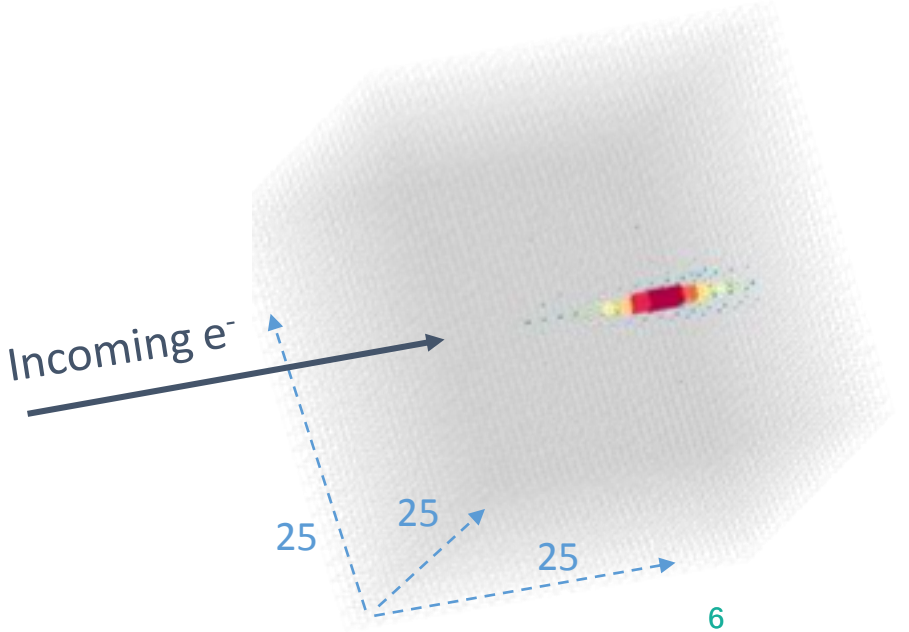


CLIC is a CERN project for a linear accelerator of electrons and positrons to TeV energies

Electromagnetic calorimeter design

- Sparse images
- Highly segmented (pixelized)
- Large dynamic range

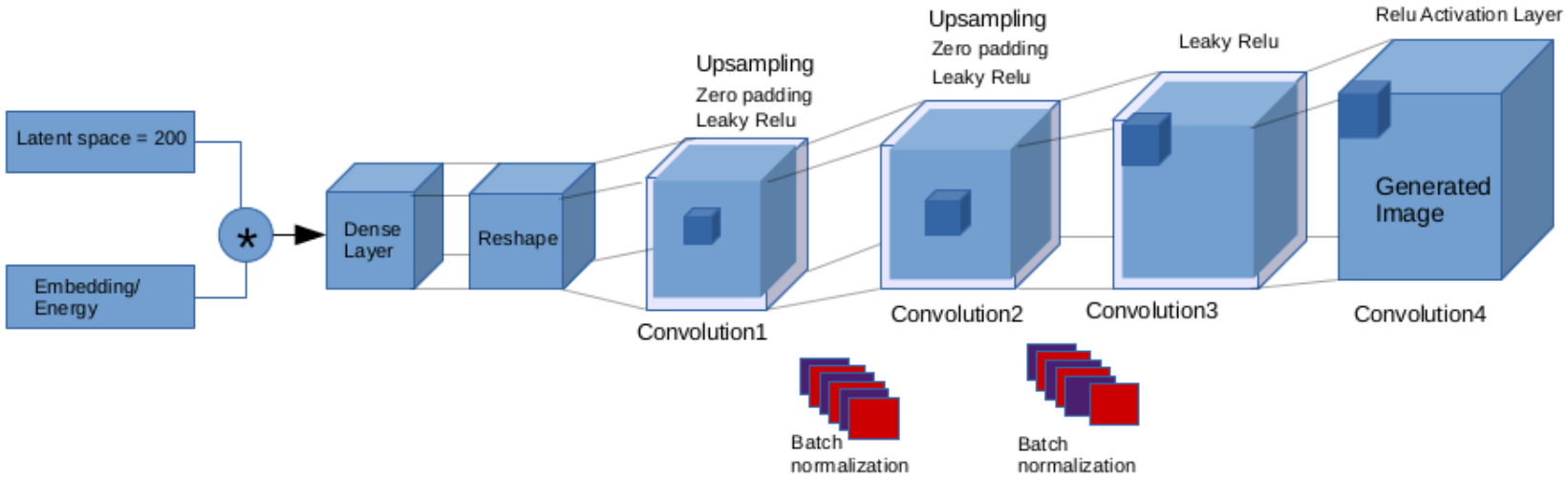




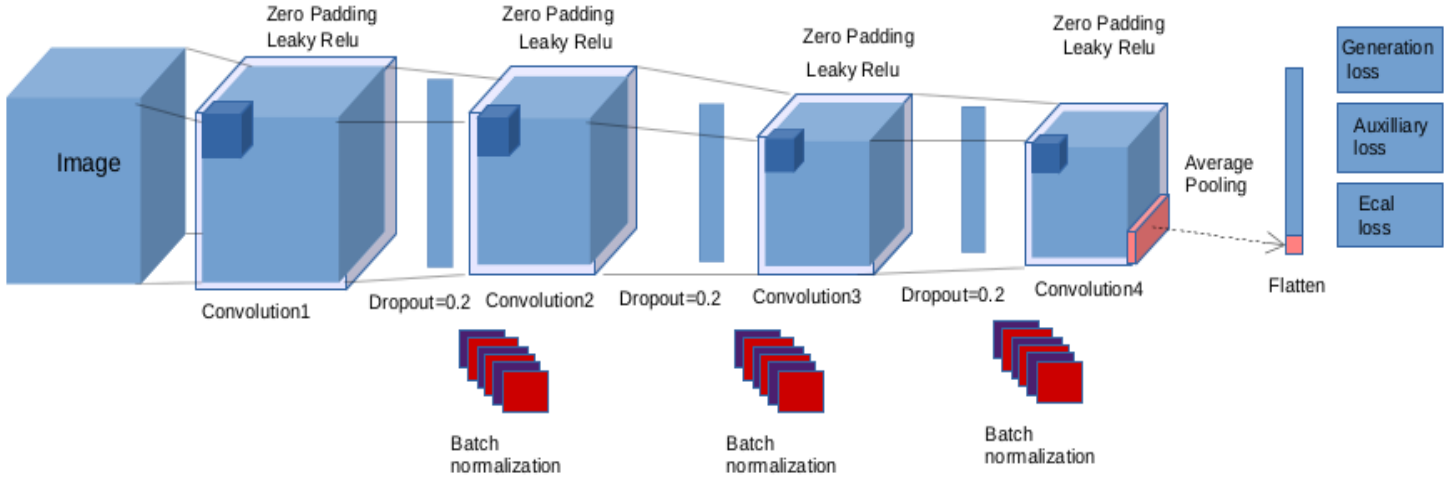
http://cds.cern.ch/record/2254048#

Our model: 3D convolutional GAN

Generator



Discriminator



~1M parameters

Total model Size: 3.8MB

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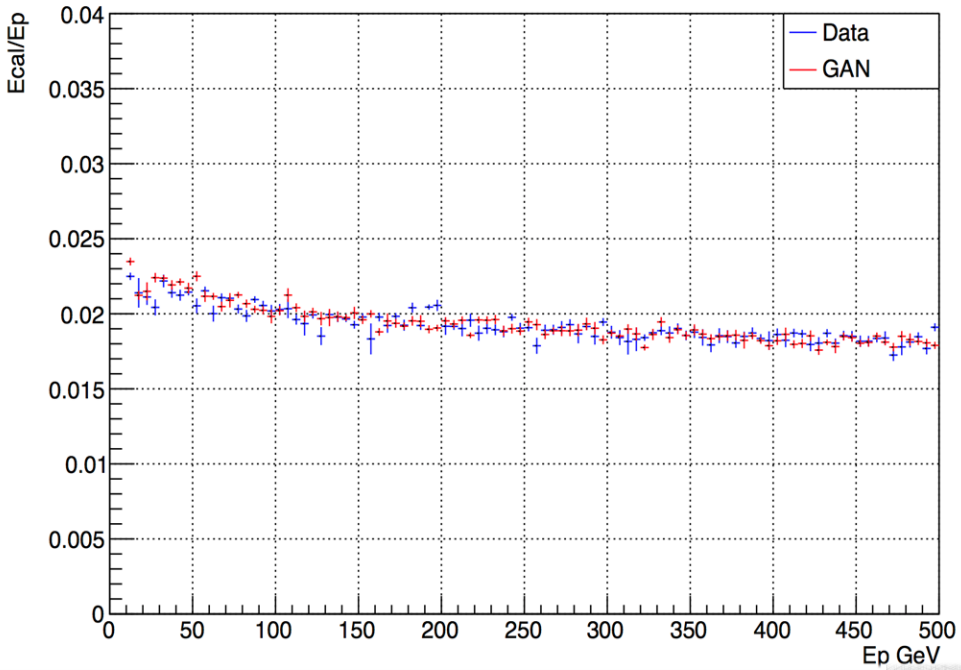
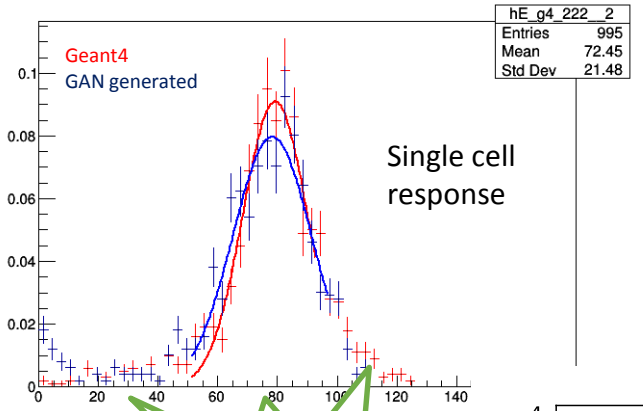
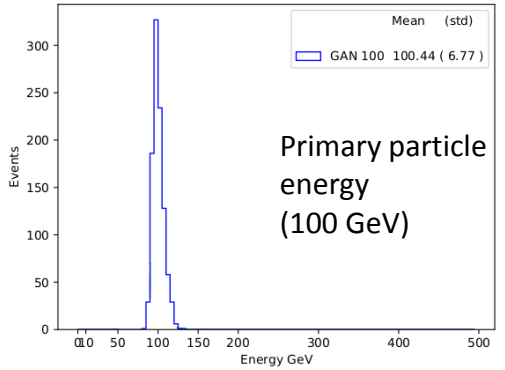
Physics simulation with GANs

Comparison to Monte Carlo





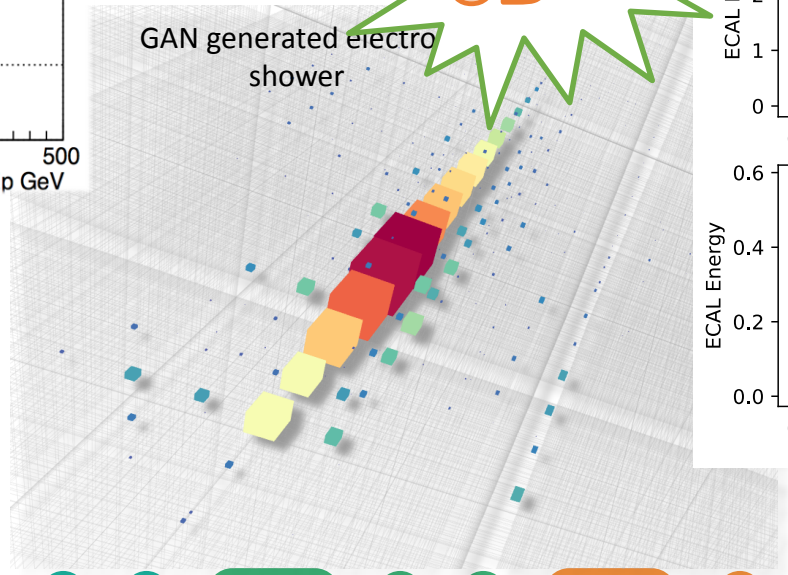
Single cell response

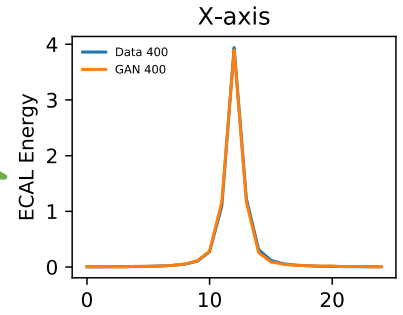


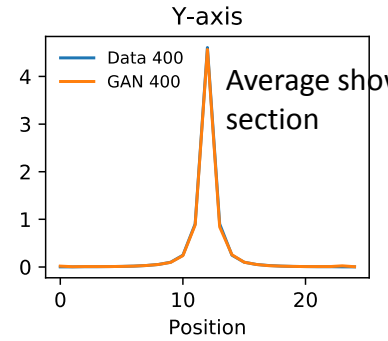
Primary particle energy (100 GeV)

3D

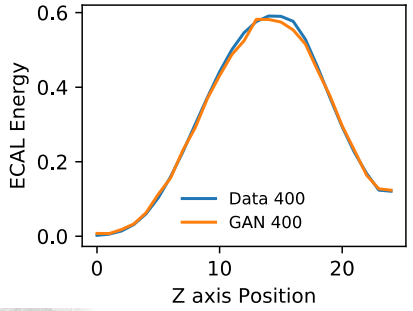
GAN generated electro shower

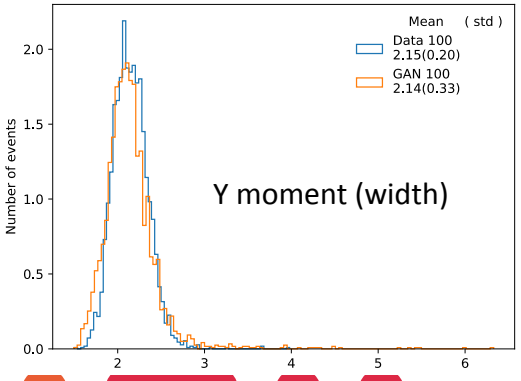






Average shower section





Y moment (width)

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Parallelizing Training

A fast training process requires a distributed approach

Distribute training via Horovod

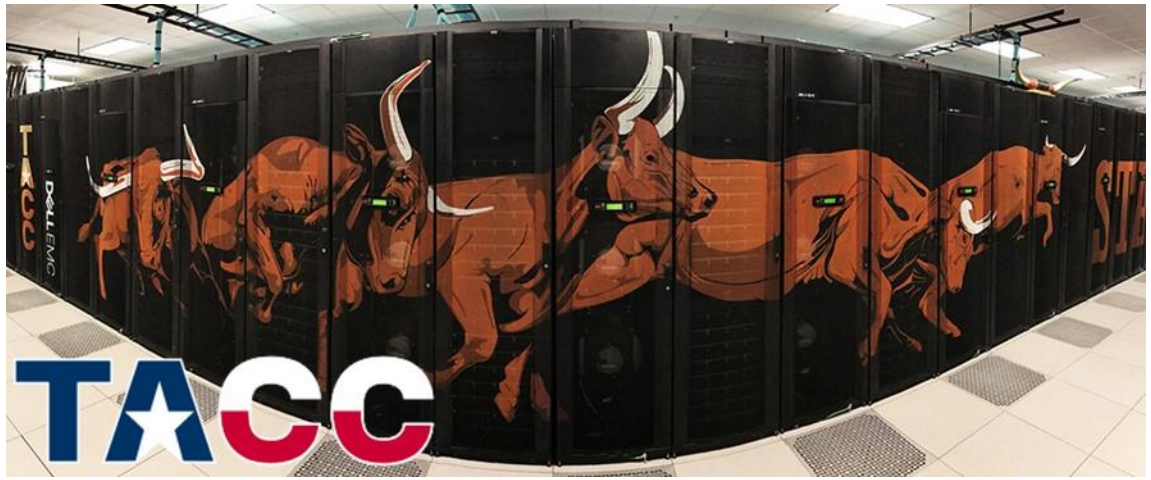
- Ensure data is loaded in parallel

Use Keras, TensorFlow + MKL-DNN

- MKL-DNN includes 3D Conv Support

Run on Stampede2 cluster

- Dual socket Intel® Xeon® 8160
- 2x 24 cores per node, 192 GB RAM
- Intel® Omni-Path Architecture



Single-Node optimisation

Training performance

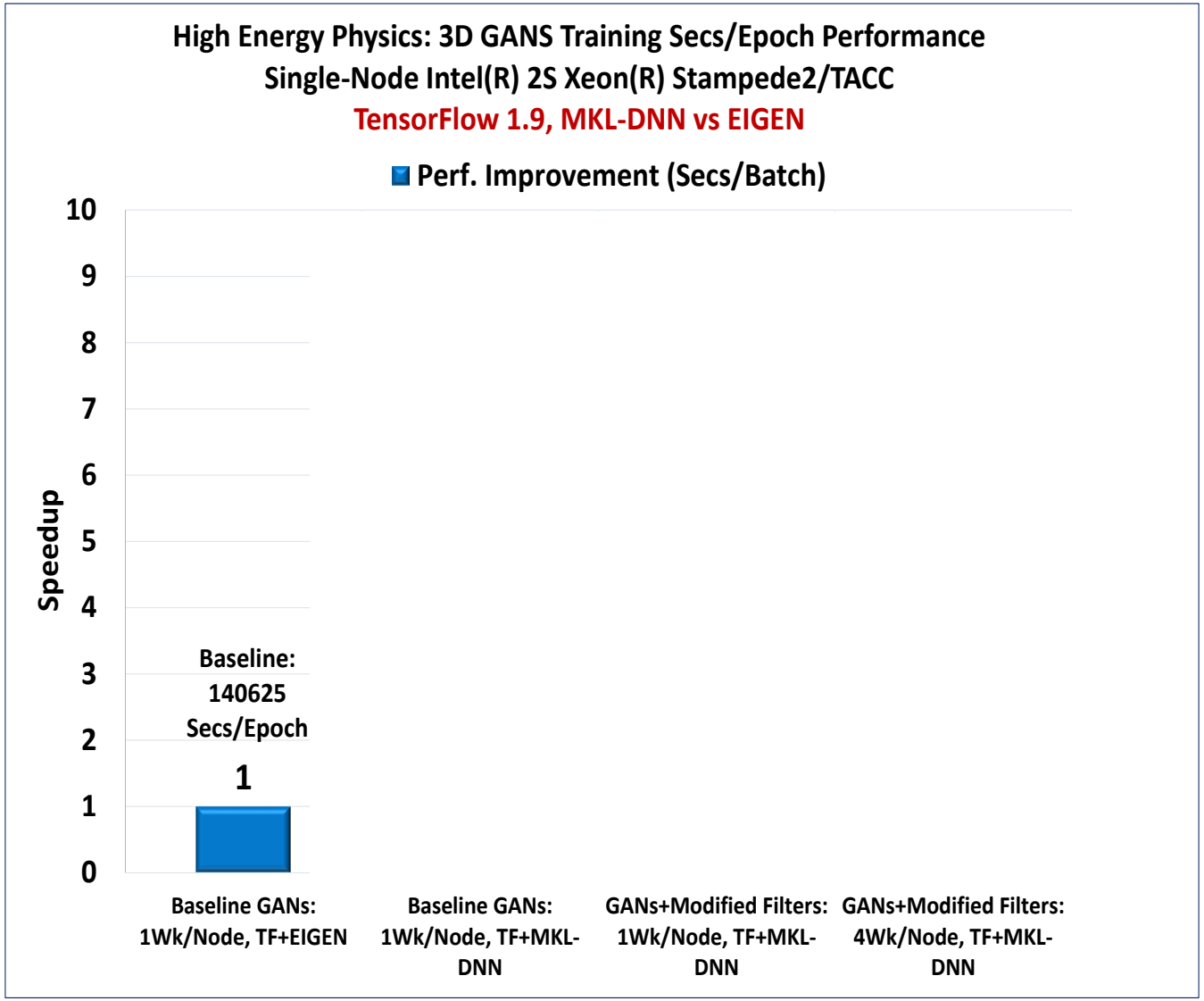
Our baseline:

1 worker/node TF + Eigen

Replace Eigen with MKL-DNN

+ Optimize number of convolution filters

+ Parallelize to 4 workers/node



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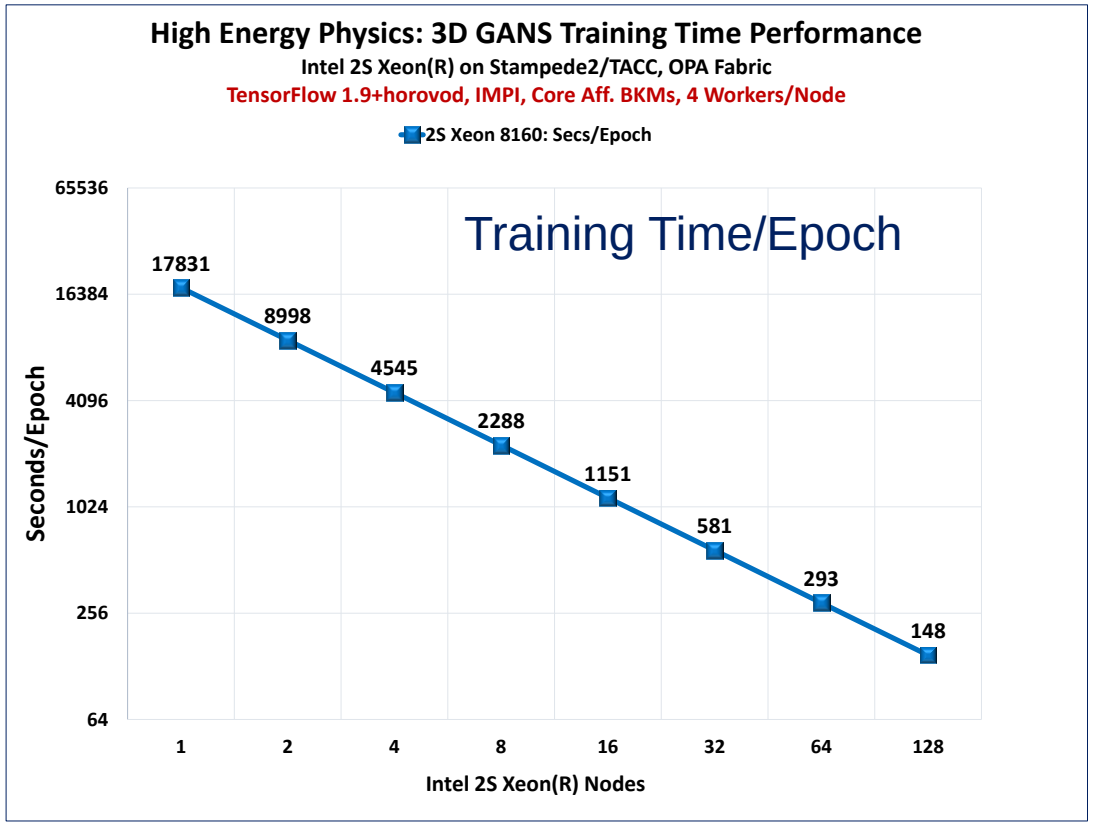
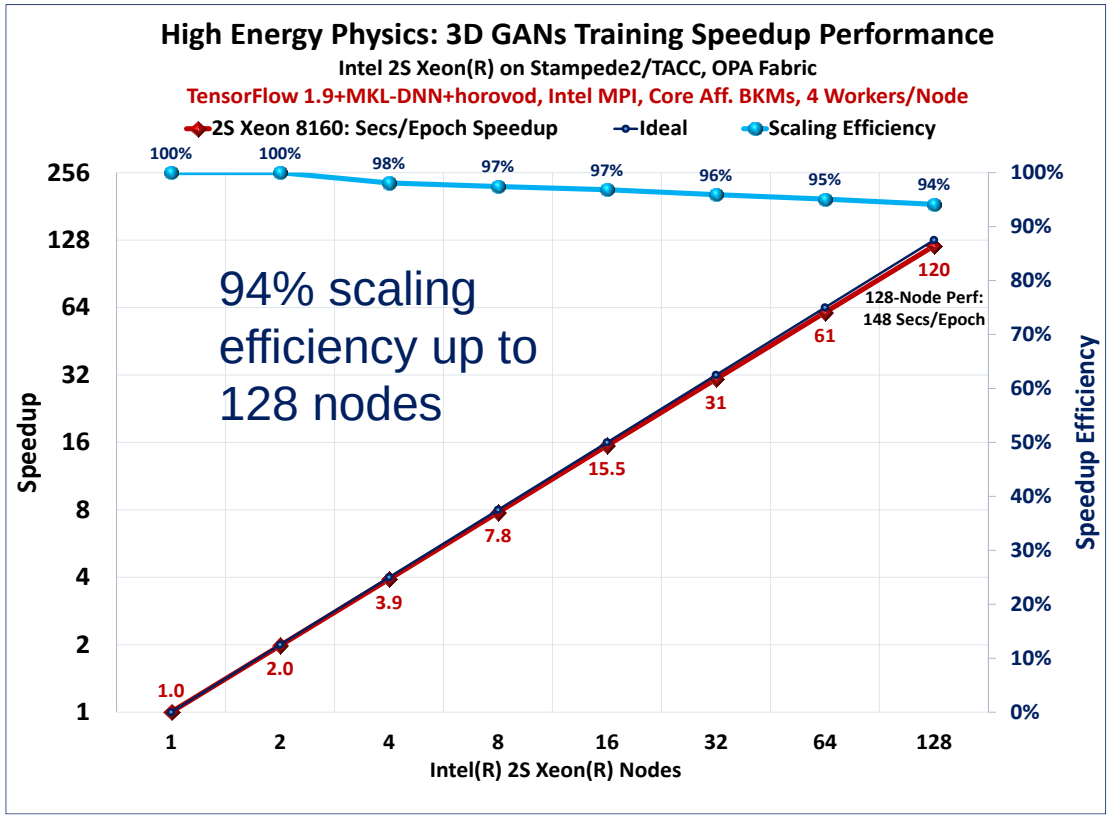
Multi-Node Scaling Performance

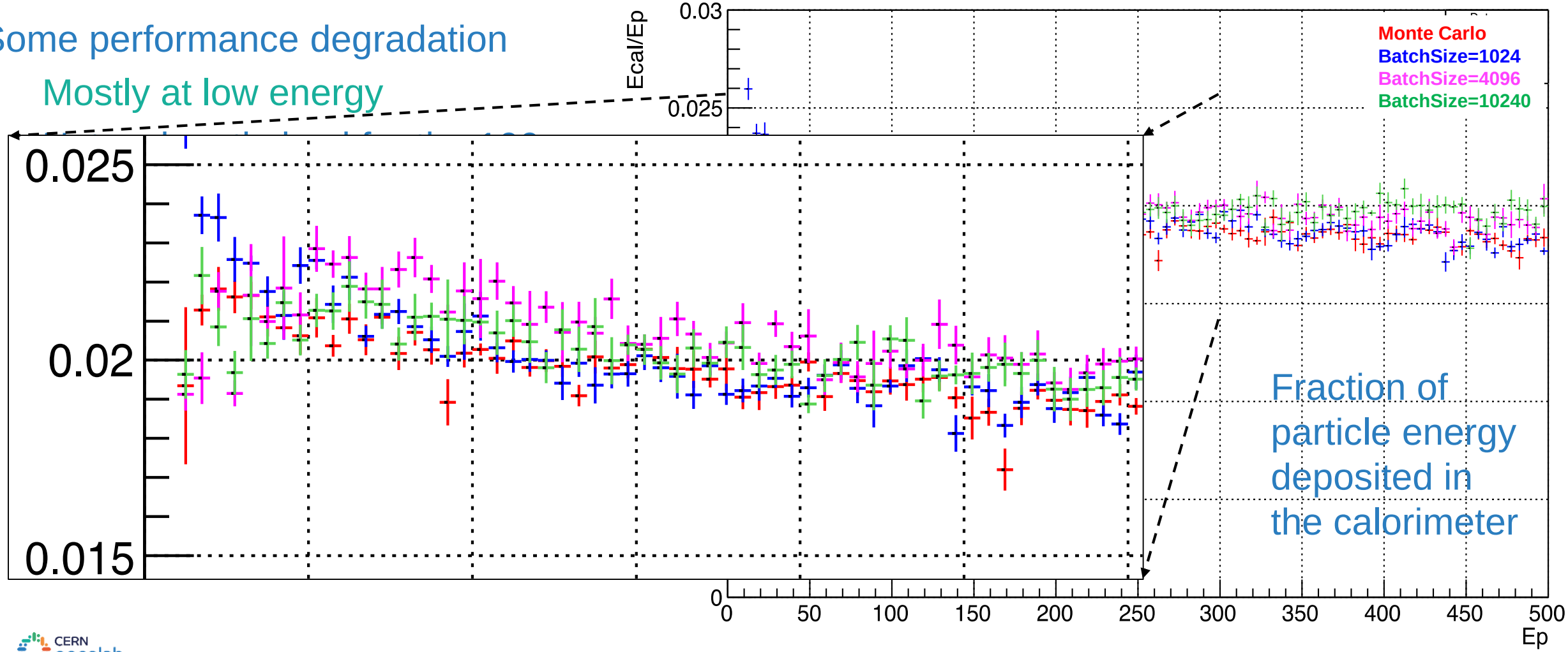




Physics performance

Some performance degradation

Mostly at low energy



Inference time

Inference:

Classical Monte Carlo simulation requires 17 s/shower

3DGAN (TF 1.4) takes 7 ms/shower

➔ speedup factor > 2500

Time to create an electron shower		
Method	Machine	Time/Shower (msec)
Classical Monte Carlo	2S Intel® Xeon® Platinum 8180	17000
3D GAN (batch size 128)	**2S Intel® Xeon® Platinum 8180**	**7**

Further optimsation (TF 1.9 + MKL-DNN with 3D/conv)

+ adjust TF (interop/intraop) parameters ~ **1 - 4 ms/shower * on a Intel Xeon Platinum 8160:**

+ use of multiple data streams:

1 stream 1.25 ms/shower

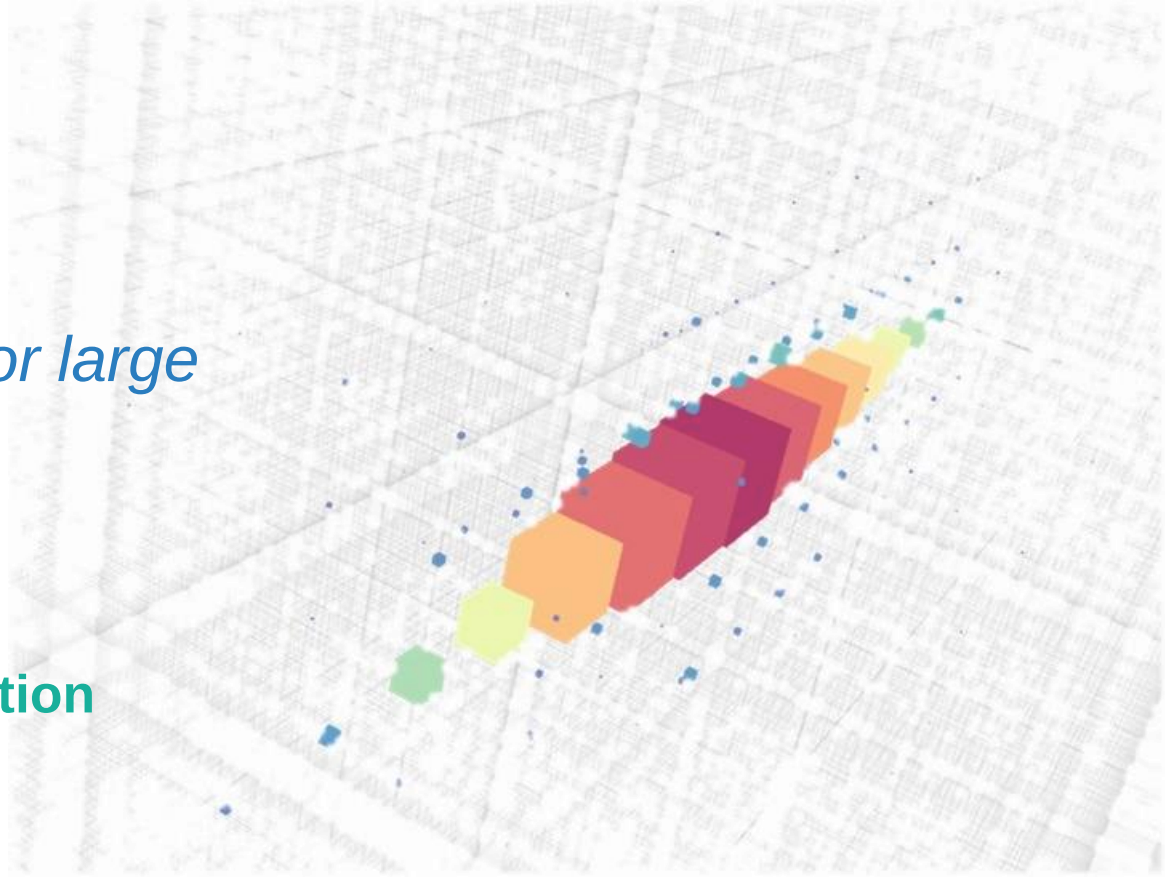
2 streams 0.93 ms/shower

4 streams 0.85 ms/shower

https://ark.intel.com	Intel Xeon Platinum 8180	Intel Xeon Platinum 8160
# cores	28	24
# threads	56	48
Base Frequency	2.5 GHz	2.1 GHz

*measured on 10000 showers

Summary



Extensive NN training will be a new workflow for large HEP experiments

Distributed training and HPC optimization is critical

- Enables **architecture optimization** and **generalization**
- **Increase the size of the problems** we can solve

Initial results on 3DGAN optimisation are very promising

- **Reduced training time by 8x on single node**
- Linear scaling brings down training time to ~2min/epoch on 128 nodes
- **Inference time is reduced by a factor 7x**

Preliminary results hints at better performance removing keras layer: we are investigating

Thank you

Questions?

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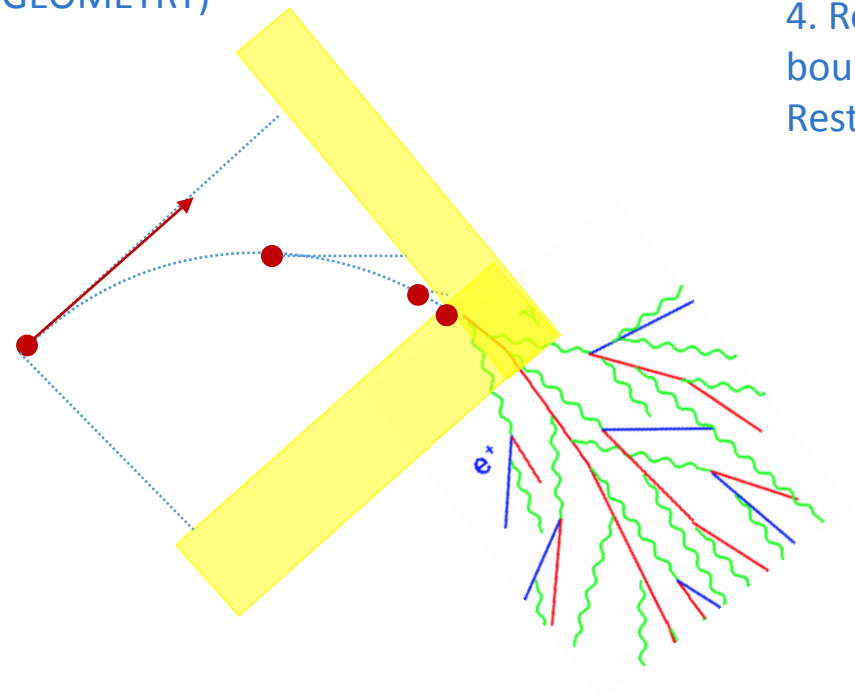
Classical Monte Carlo simulation

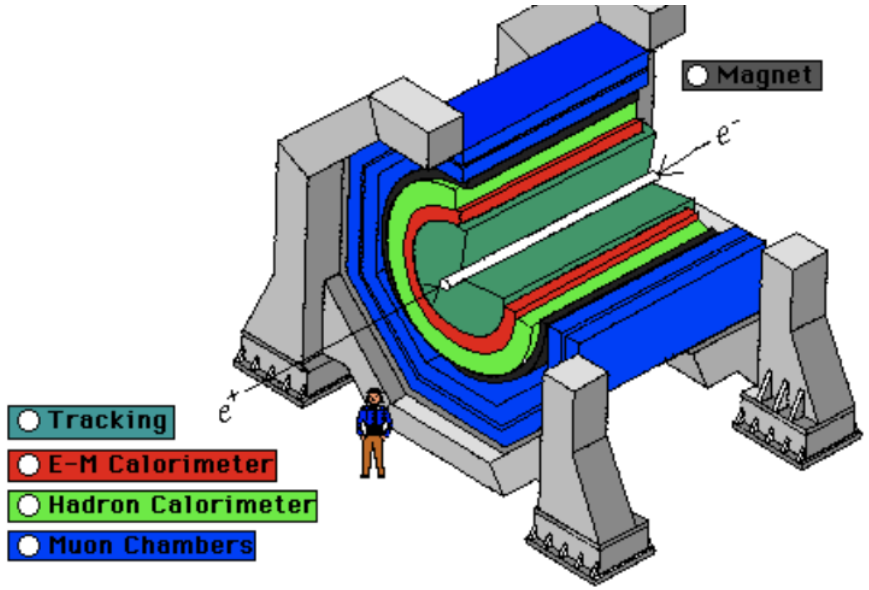
1. Calculate step particle could travel before doing a PHYSICS interaction

2a. Check if step is within volume boundaries(GEOMETRY)

3. Propagate with selected step

4. Repeat 2,3 until reaching volume boundary.
Restart from 1





Stampede2/TACC Configuration Details

Compute Nodes: 2 sockets Intel® Xeon® Platinum 8160 CPU with 24 cores each @ 2.10GHz for a total of 48 cores per node, 2 Threads per core, L1d 32K; L1i cache 32K; L2 cache 1024K; L3 cache 33792K, 96 GB of DDR4, Intel® Omni-Path Host Fabric Interface, dual-rail. Software: Intel® MPI Library 2017 Update 4Intel® MPI Library 2019 Technical Preview OFI 1.5.0PSM2 w/ Multi-EP, 10 Gbit Ethernet, 200 GB local SSD, Red Hat* Enterprise Linux 6.7.

TensorFlow 1.6: Built & Installed from source: https://www.tensorflow.org/install/install_sources

Model: CERN 3D GANS from https://github.com/sara-nl/3Dgan/tree/tf

Dataset: CERN 3D GANS from https://github.com/sara-nl/3Dgan/tree/tf

Performance measured on 256 Nodes with:
OMP_NUM_THREADS=24 HOROVOD_FUSION_THRESHOLD=134217728 export I_MPI_FABRICS=tmi, export I_MPI_TMI_PROVIDER=psm2 \
mpirun -np 512 -ppn 2 python resnet_main.py --train_batch_size 8 \
--num_intra_threads 24 --num_inter_threads 2 --mkl=True \
--data_dir=/path/to/gans_script.py --kmp_blocktime 1

https://portal.tacc.utexas.edu/user-guides/stampede2

Architecture, Dataset & Runtime Options

Optimise filter sizes

- **Conv Filters**: Multiple of 16 (MKL-DNN optimizations)

Dataset: 200000 electrons

- **Training Samples**: 180000 & **Validation**: 20000

Batch Size: 8/Worker, # Workers/Node=4/Node (Mapped to NUMA domains)

TF tuning: inter_op: 2 & Intra_op: 11 (Xeon® 8160 is 24C/CPU); **AVX512 –FMA support**

Learning Rate: 0.001, **Optimizer**: RMSprop

Warmup Epochs: 5 (Facebook Methodology), **Training Epochs:** 25