Distributed Training of Generative Adversarial Networks for Fast Simulation

HPC and AI in High Energy Physics

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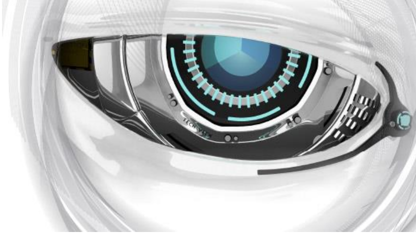
24/9/2019

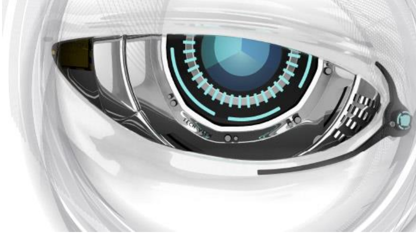


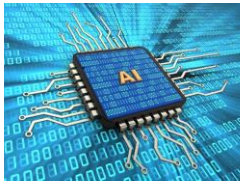
Overview

- Introduction
  - HPC and AI in HEP
  - Fast simulation
  - 3DGAN
- Distributed Training
  - Distributed training initial optimization
  - Scaling up to 256 nodes
  - Inference time
- Summary

HPC and AI

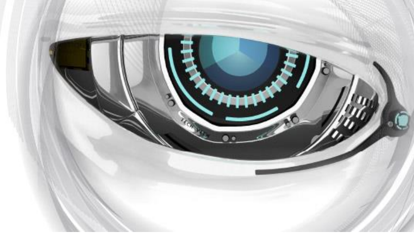
Main driving forces………...





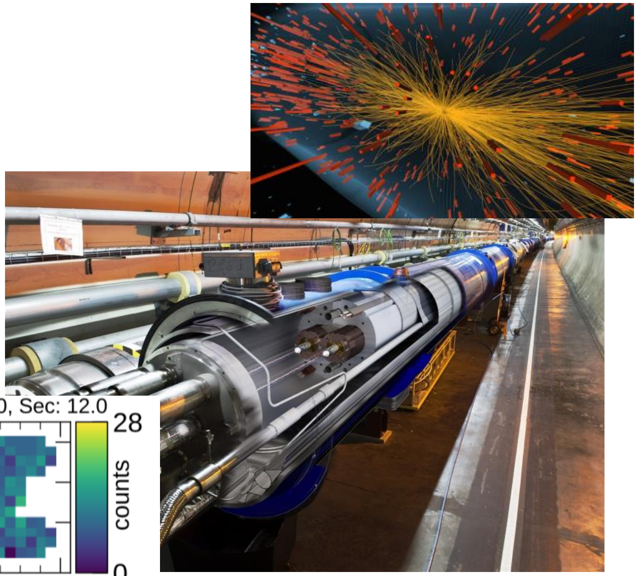
- Deeper models
  - Deep Neural Networks often have millions of parameters
- Big data
  - More complex problems require more data
- Faster
  - Training speedup
  - Inference speedup
- Parallelizable processes
  - Parallelism can be implemented at different levels

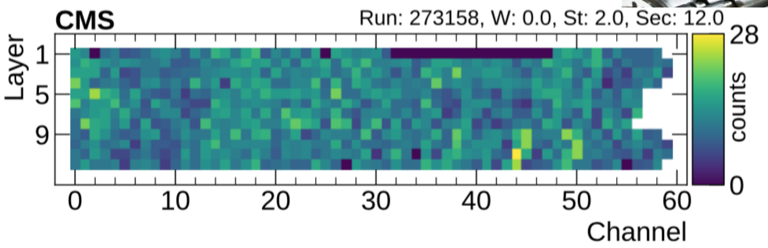
High Energy Physics



AI applications in HEP

- All venues of science are benefitting from AI for problems where..
    - Underlying processes are difficult to model
    - Require high computational sources
    - Time consuming
    - Noisy data
- High Energy Physics
    - Applications
        - Reconstruction and Analysis
        - Trigger optimization
        - Simulation
- AI crucial for HEP experiments
    - HPC hardware
        - Maximize performance
        - Fast time-to-model





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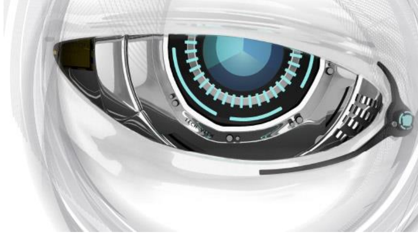
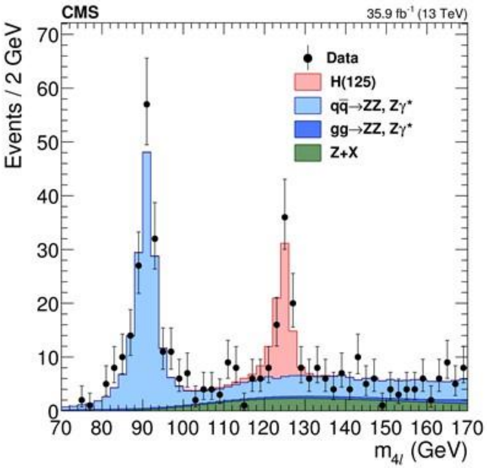
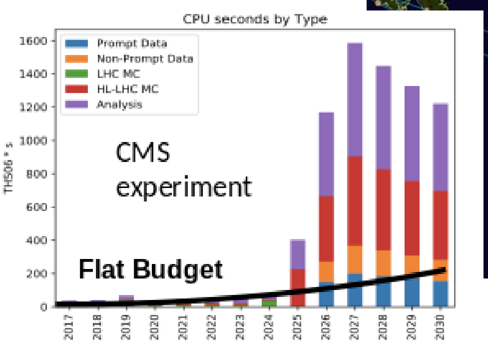
HEP Simulation

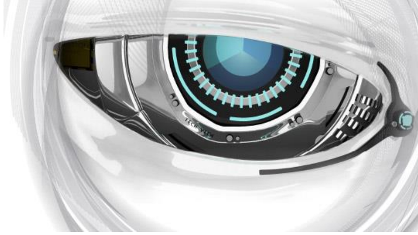


Essential for data analysis & detector design

- Understand how detector design affects measurements and physics
  - Correct for inefficiencies, inaccuracies, unknowns
  - Compare theory models to data
- Complex physics and geometry modeling
  - >50% of Worldwide LHC Computing Grid (WLCG) power today
  - Increase by 100x by 2025!



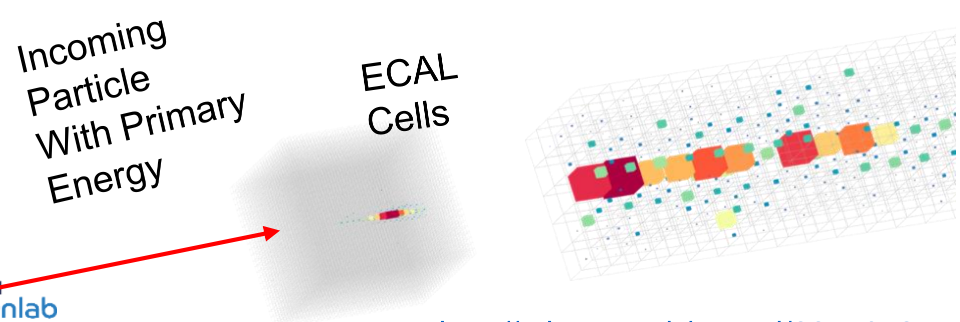


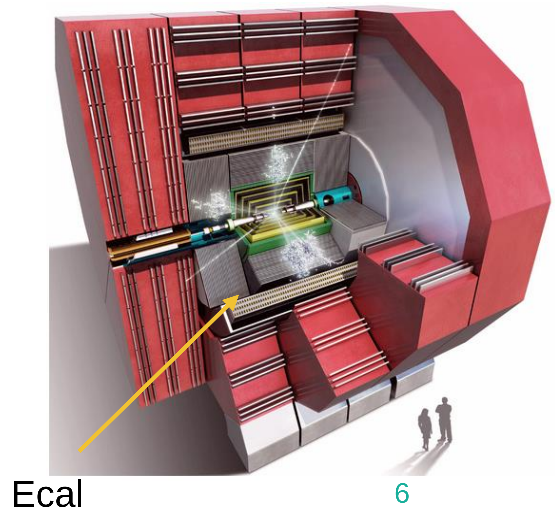


Data set

Compact Linear Collider CLIC

- **Proposed** linear particle accelerator
- **Calorimeter data set** developed for ML applications
- Events as selected cells around the barycenter of particle showers simulated using Geant4
- Primary particle energy 10-500 GeV (electrons)
  - Event → 25 x 25 x 25 image → 15, 625 cells
    - 200,000 events
- Detector response as 3D images
  - Highly segmented (pixelized)
    - critical for particle identification and energy determination
  - Highly sparse
    - only ~20% cells with energy deposition
  - Large dynamic range
    - > seven orders of magnitude





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

http://clicdp.web.cern.ch/

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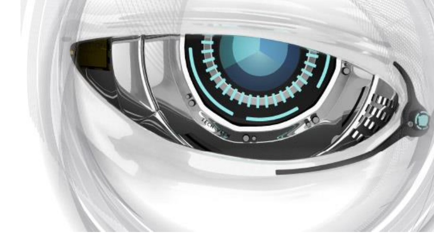
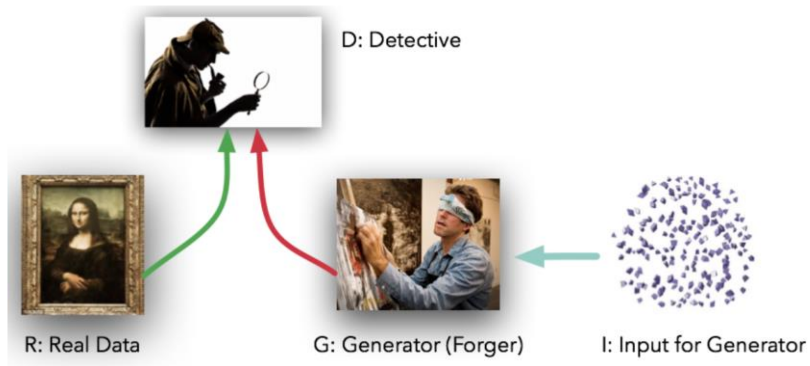
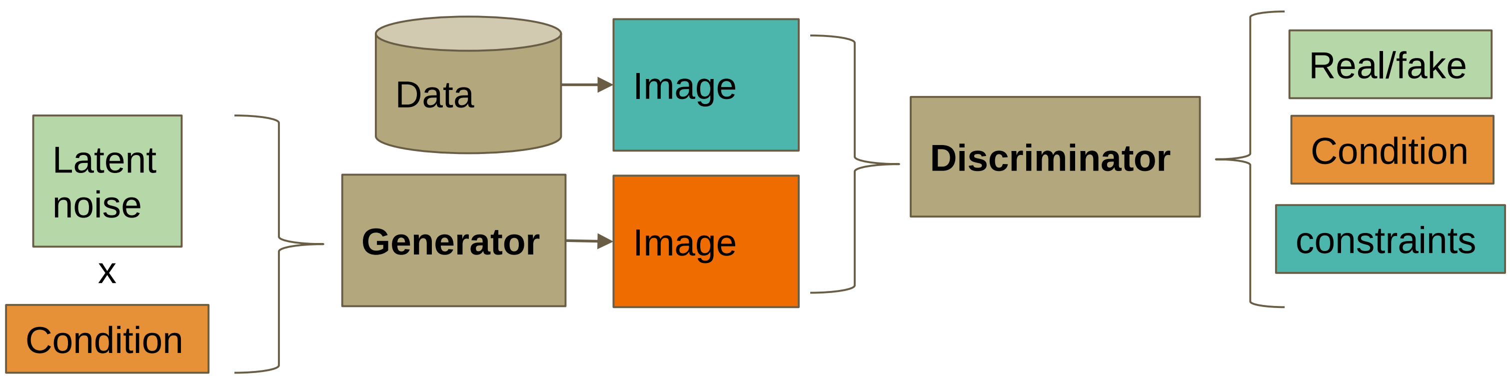


3DGAN

Generative Adversarial Network

- Simultaneously train two networks that compete and cooperate with each other
  - Discriminator
  - Generator





A generalized view of 3DGAN

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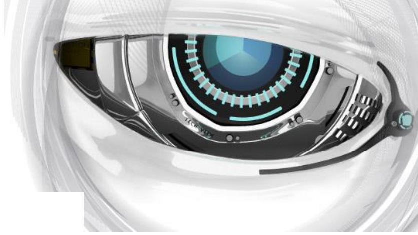
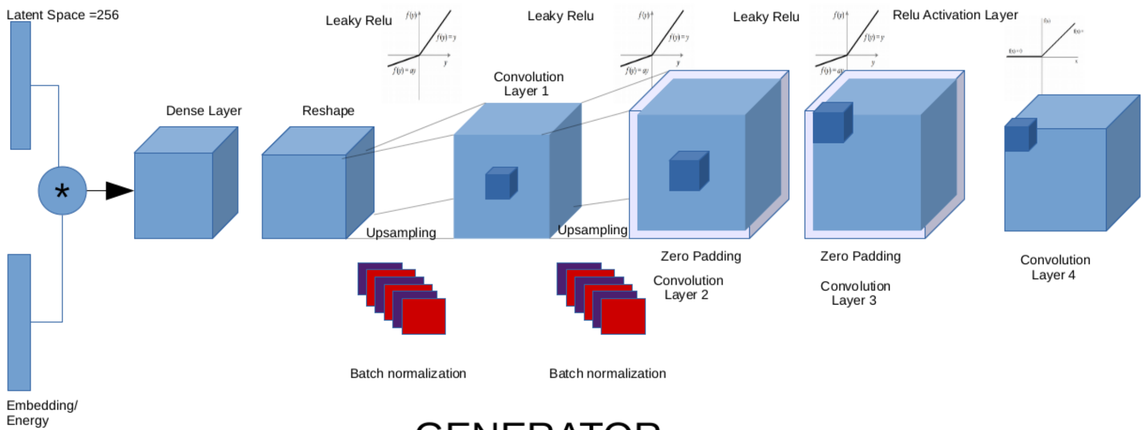
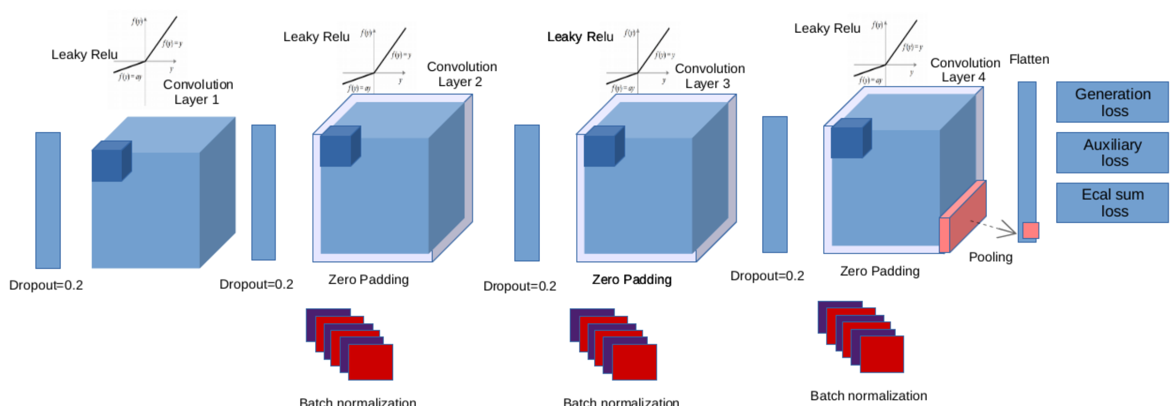
3DGAN Architecture





GENERATOR



DISCRIMINATOR

~1 M parameters
Total model Size 3.8MB

Evaluating the performance by agreement to labels and Physics related constraints

"Caltech ibanks GPU cluster thanks to Prof M. Spiropulu"

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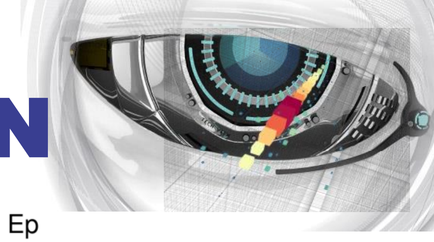
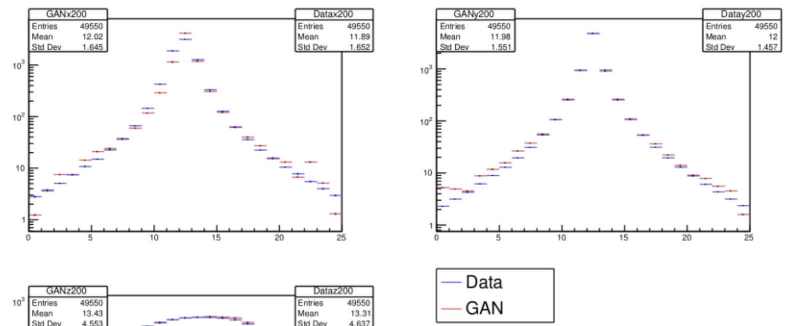
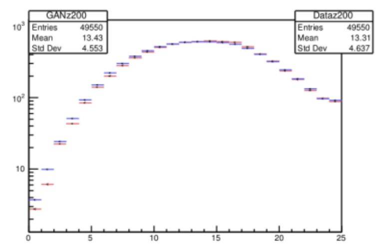
Physics Simulation with 3DGAN

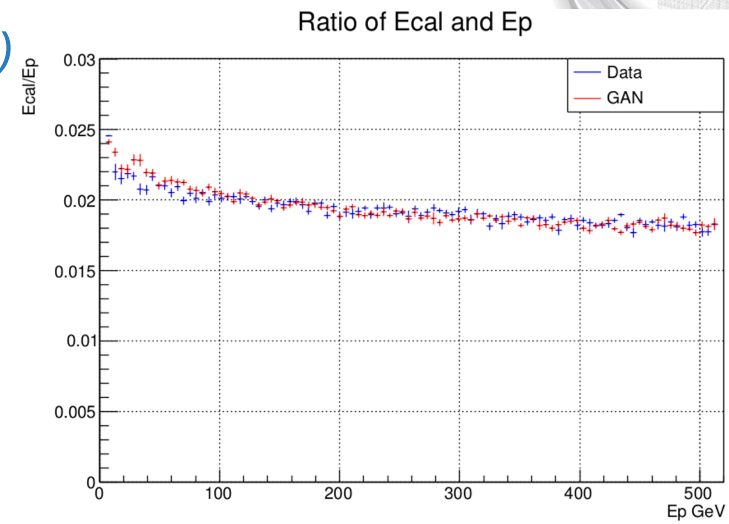


Comparison to Monte Carlo (>300 plots)

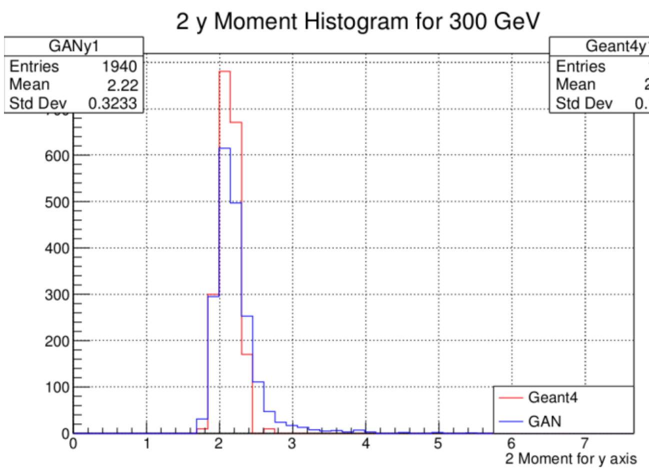




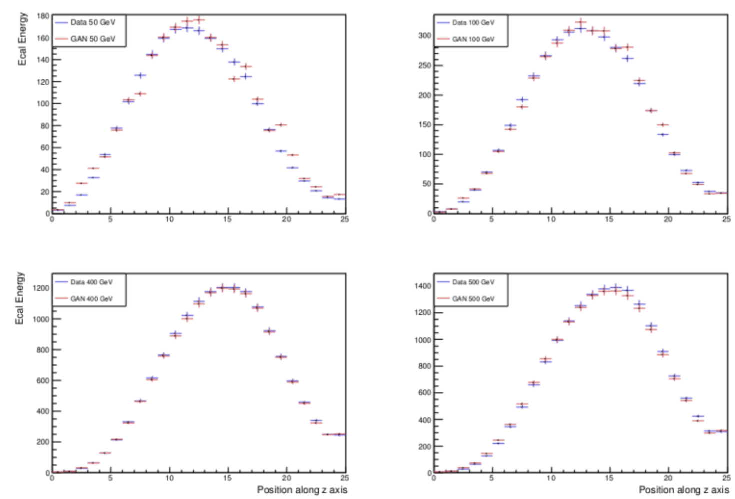
Energy Deposition along x, y, z axis for 200 Gev



Sampling Fraction (Ecal sum/Ep)

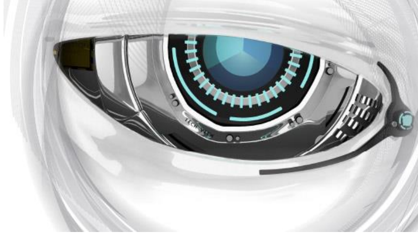


Y moment (width)



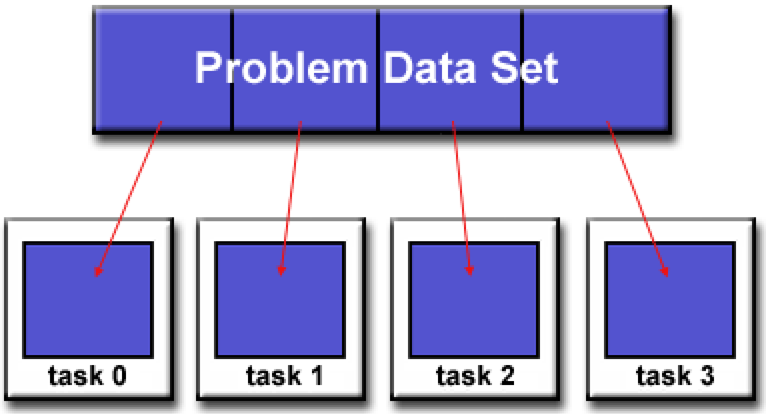
Energy deposition in transverse direction for 50, 100, 300 and 400 GeV

Distributed training



3DGAN

- Training time ~ **1hour/epoch** on GeForce GTX 1080
- 30 to 50 epochs for complete training taking **days**
- Reducing training time is essential for:
  - Hyper parameter scans
  - Detector design studies
- Distributed training with Horovod
  - Data parallelism
  - Synchronous update

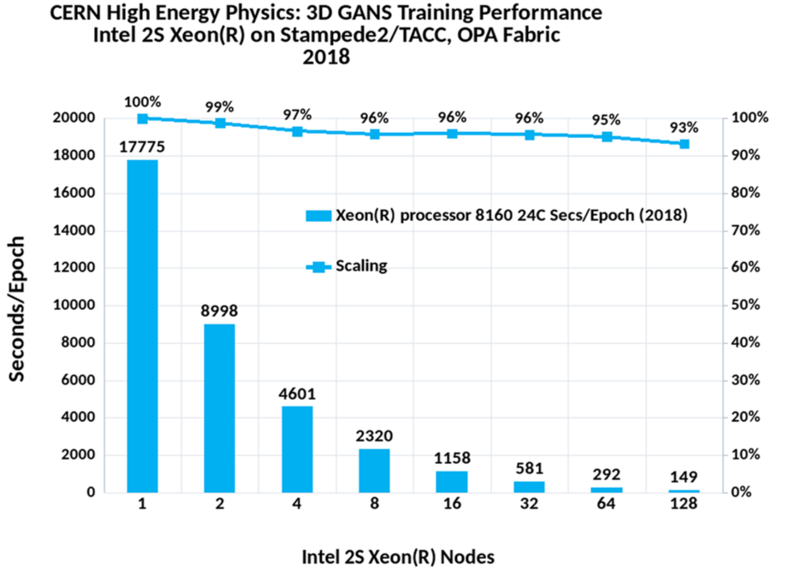


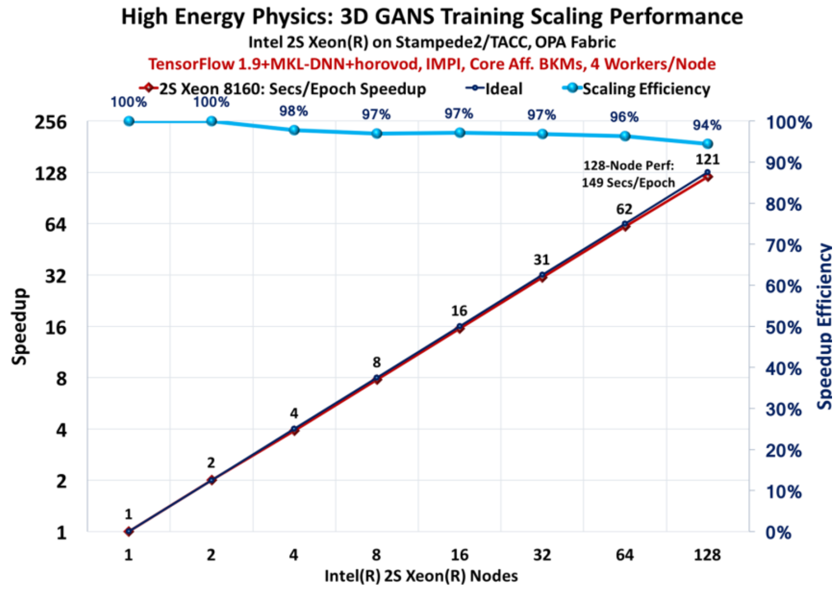
Distributed Training initial optimization

TACC Stampede 2 (2018)

- Stampede 2 cluster
  - Dual socket Intel® Xeon® **8160**
  - 2x 24 cores per node, 192 GB RAM
  - Intel® Omni-Path Architecture
- Software
  - **Tensorflow 1.9** (Intel optimized)
  - Keras 2.13
  - Horovod 0.13.4
- Single Node Optimization:
  - Replace Eigen with **MKL-DNN**
  - Optimize number of **convolution filters**
- Parallelize:
  - 4 workers/node

IXPUG 2018





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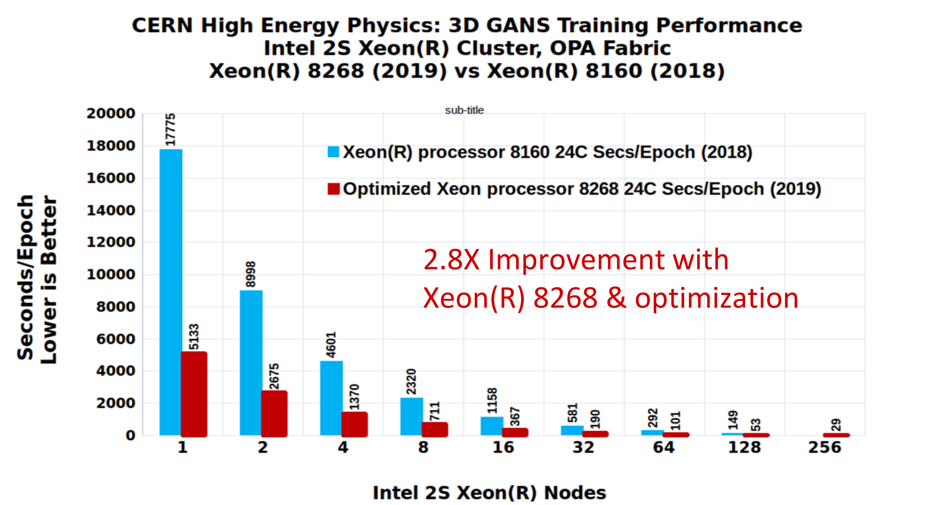
Scaling up to 256 nodes

Xeon 8268 (2019)

- Intel Endeavour cluster:
  - **NASA** Advanced Supercomputing Division (NAD)
  - Named after spaceship Endeavour
  - Xeon® **8268 Cascade Lake**
  - 2 Sockets /node
  - 24 cores per socket
  - Intel® Omni-Path Architecture
- Software:
  - **Tensorflow 1.14** (Intel optimized)
  - MKL-DNN 0.18
  - Horovod 0.16.4
  - Keras 2.2.4



- For 128 2CPU Xeon Nodes
  - 2018: < **2.5 Mins**/Epoch Xeon 8160 (Skylake CPUs)
  - 2019: < **1 Min**/Epoch Xeon 8268 (Cascade Lake CPUs) – **2.5X**
    - Time to Train to Accuracy: **14.4 minutes** on 256 Nodes

2019

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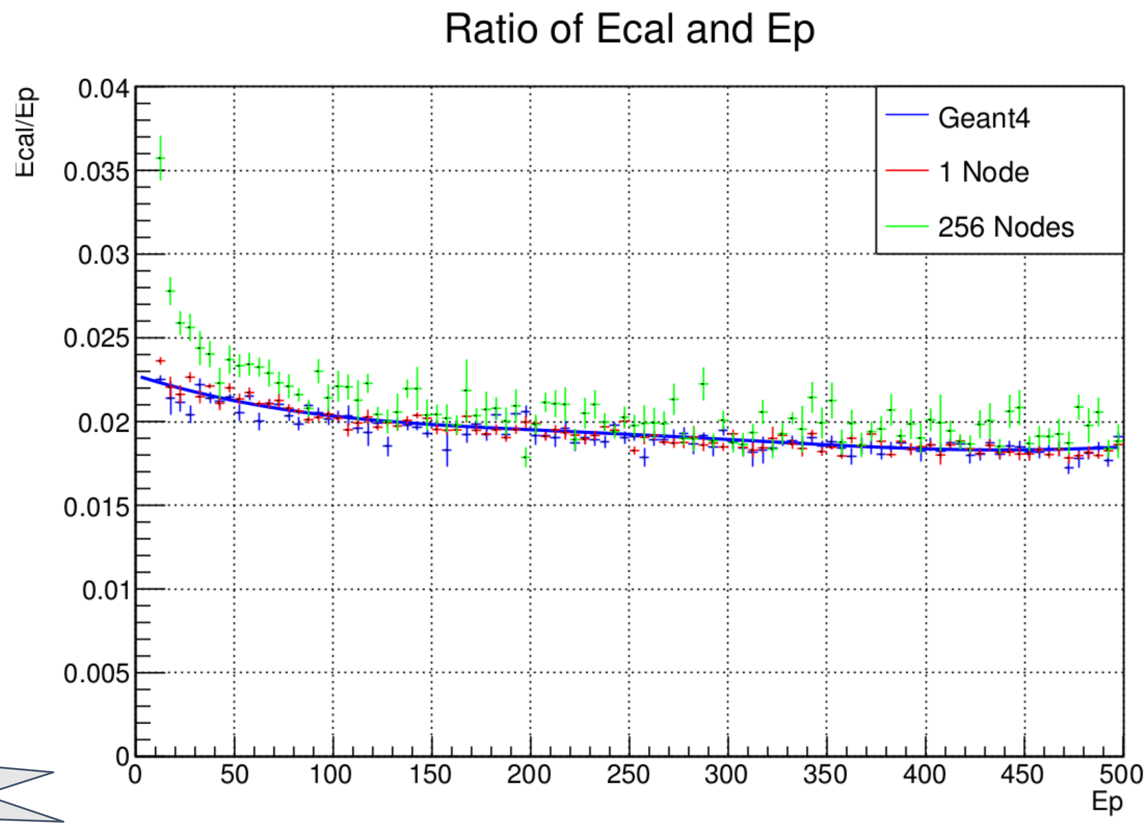
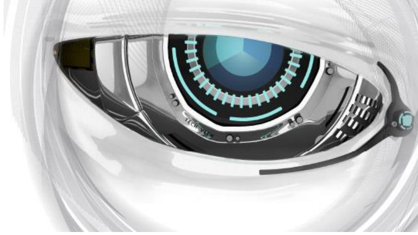
Physics Performance

Sampling Fraction



2019

Inference time



Tensorflow 1.9

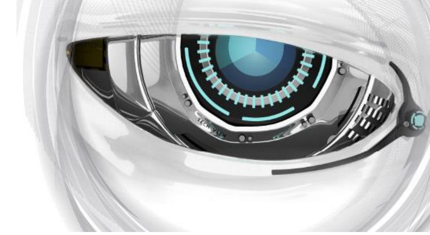
Method	Platform	Time/Shower (ms)	Speedup
Classical Monte Carlo (Geant4)	2S Intel Xeon Platinum 8180	17000	1.0
3DGAN (BS=128) 1-stream		16	2500

Baseline (TF 1.4)

Method	Platform	Time/Shower (ms)	Speedup
Classical Monte Carlo (Geant4)	2S Intel Xeon Platinum 8180	17000	1.0
3DGAN (BS=128) 1-stream	2S Intel Xeon Platinum 8160	1.25	13600
3DGAN (BS=128) 2-stream		0.93	18279
3DGAN (BS=128) 4-stream		0.85	20000

TF 1.9 (optimized)

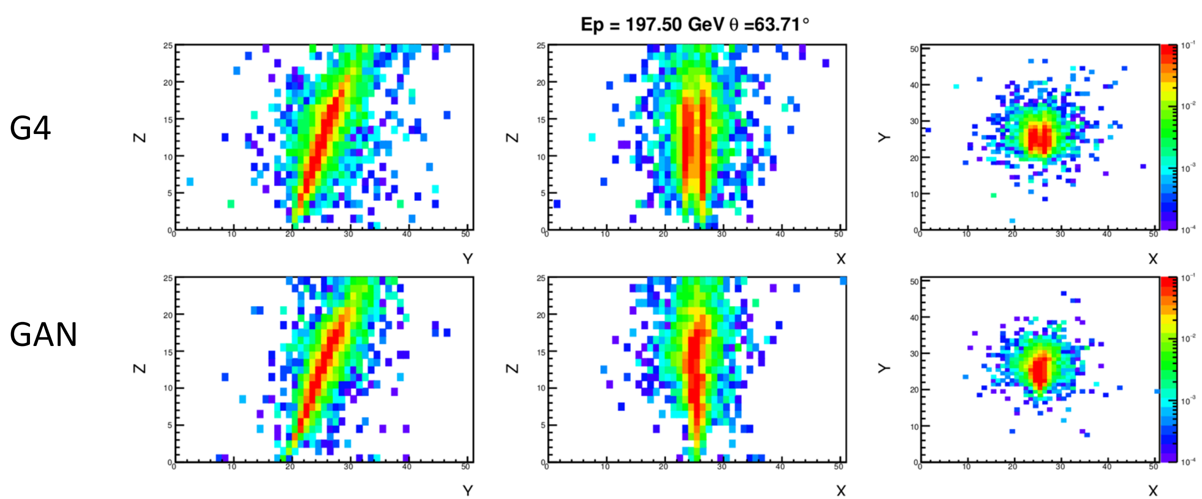
TF 1.14(WIP)



More complex 3DGAN

Larger images with incident angle 60° to 120°

- A more **realistic scenario** where image is generated condition on both:
  - Primary particle energy
  - Incident angle
- Variable angle data (electrons)
  - Event → **51 x 51 x 25 image → 65, 025 cells**
    - **400,000** events from 2 to 500 GeV
- Event size is more than **4x** larger
- Thus training data size is also larger
- Network is deeper (**~1.2 M parameters**)



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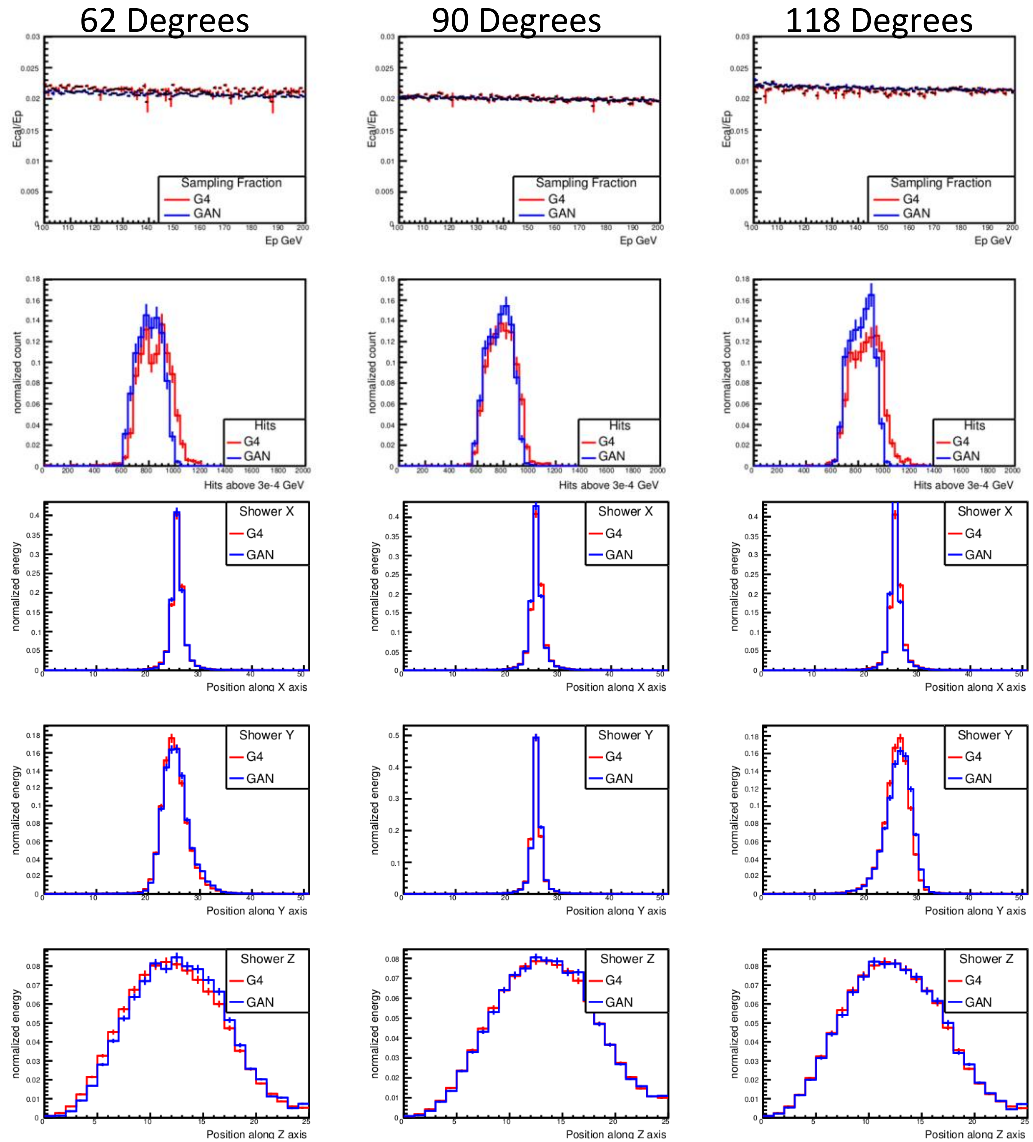
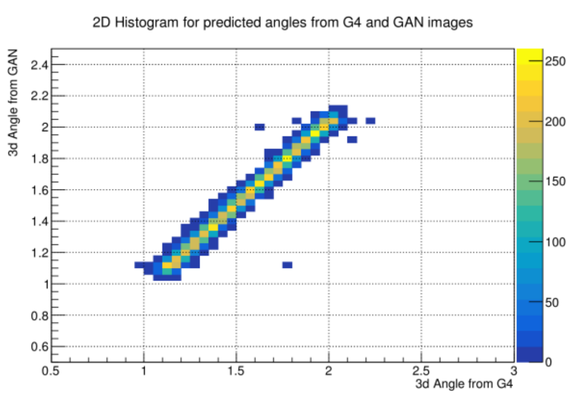
Physics performance

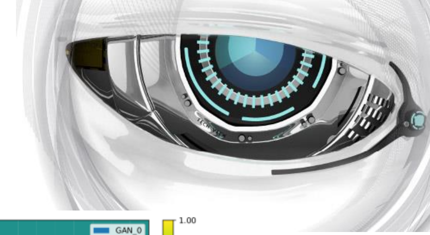
For primary particle energy 100-200 GeV and angle in bins around 62, 90 and 118 Degrees

- Sampling Fraction
- Hits
- Shower Shapes:
  - Energy deposited along x, y and z axis
- Measured Angle

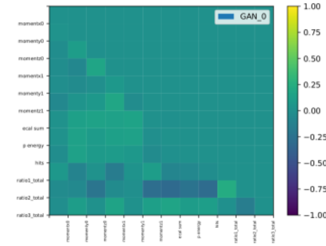


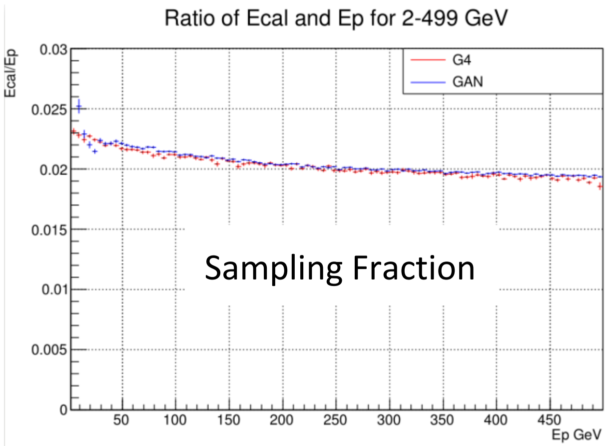


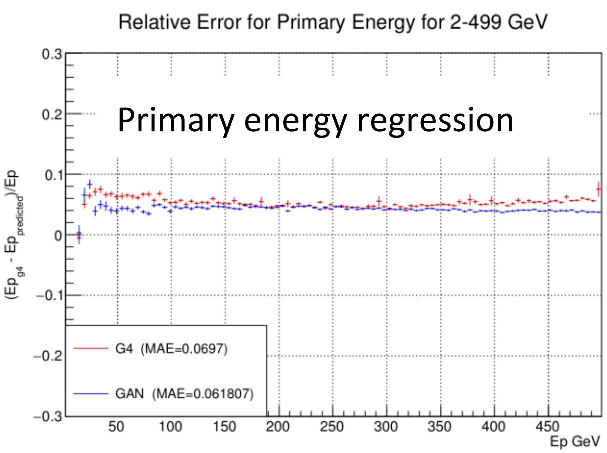
Transfer Learning



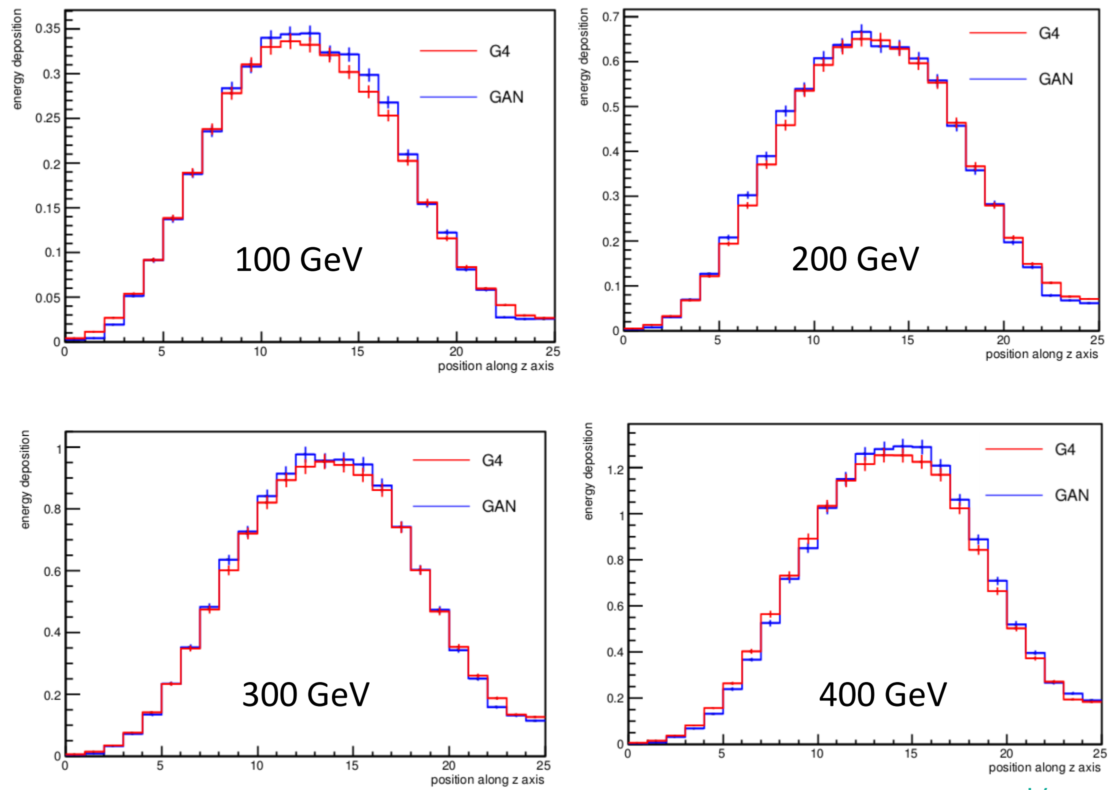
- Training for 2-500 GeV spectrum
  - Starting from pretrained weights (trained for 100-200 GeV)



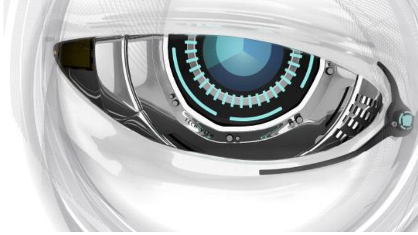




Shower shapes in the longitudinal direction for Different Primary energies



Generalisation



Training and architecture hyper-parameters optimisation

- 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 simultaneous weights training and architecture optimisation

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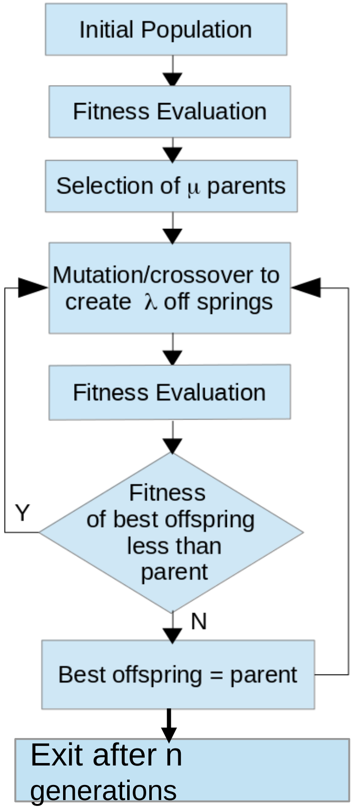
Evolutionary Approach

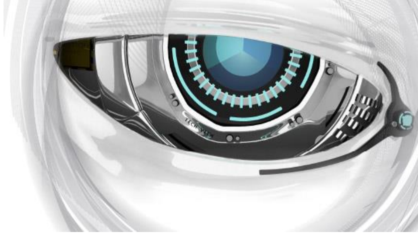
Genetic Algorithm to train and optimize neural networks simultaneously

- **GA** can train Neural Network
  - **Global** instead of local minima
  - **Complex and indirect cost** functions are possible
  - **Highly Scalable**
- Currently used in hyper-parameter scans
  - Architectures are encoded as a chromosome
  - Weights are trained by gradient descent for evaluation of each individual
  - Time and resource intensive



Challenges

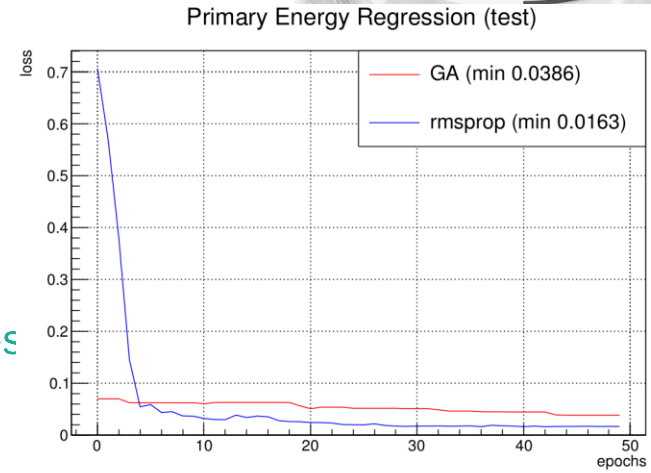
GA for GAN

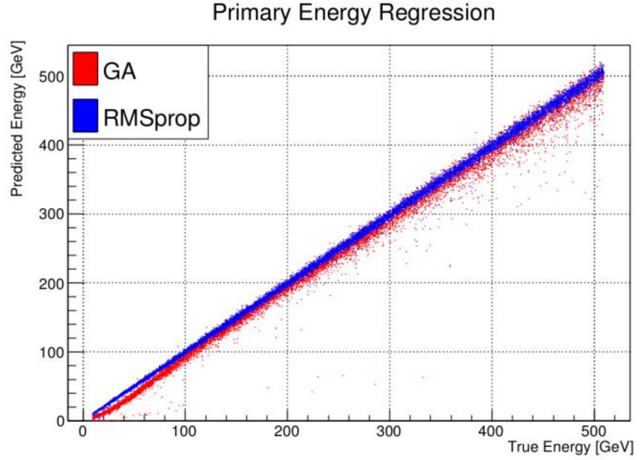


- Network Size:
  - Trainable parameters in **millions** for 3DGAN model
- Large Computing resources?
- Architecture Optimization:
  - Flexible and stable
- Adversarial Training:
  - Simultaneous training of **two networks**
- Inexact solution:
  - A **hybrid approach** can incorporate SGD as a callback

Initial Implementation

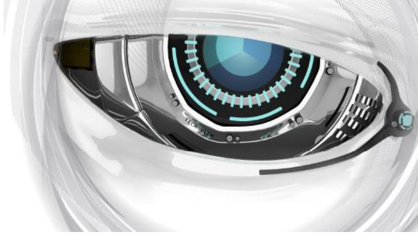
GA with pytorch





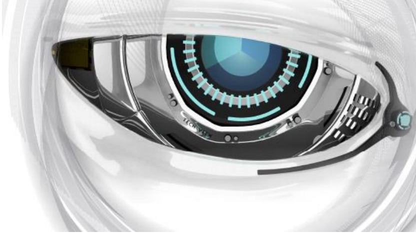
- Reduced complexity:
  - Simplified discriminator regression on 2D images
  - Weight update
- Implement evolutionary algorithm
  - Testing batch training with GA
    - Smaller batches resulted in better training
  - Random updates vs. random weights
    - Random weights allow faster convergence
  - 6-8 optimal number of offsprings
  - No Bias
  - Comparison to RMSprop (lr=0.01)
    - Faster convergence
    - Lower accuracy
- Update weights and architecture at the same time is faster than GA based hyper-parameter scan
- Improve accuracy by adding gradient descent steps

Summary & Plans



NN training will be a new workflow for large HEP experiments

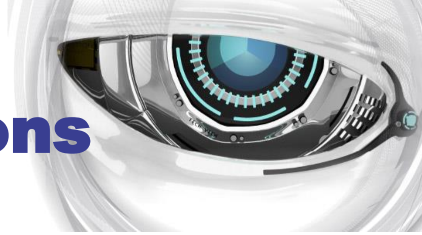
- Distributed training and HPC optimization is critical
    - Enables **architecture optimization** and **generalization**
    - Increase the size of the problems we can solve
- Results on 3DGAN optimisation are very promising
    - Reduced training time by **8x** on single node
    - Linear scaling brings down training time to **< 0.5 min/epoch** on **256** modes of 2CPU Xeon 8268
    - Inference time is **x20000** faster than Monte Carlo approach
- Implement GA based combined architecture and training search Estimate performance and needs in terms of computing resources
    - Several techniques can be explored (indirect weight encoding and asynchronous update)
- Increase complexity (network, dataset, …)



Thank you

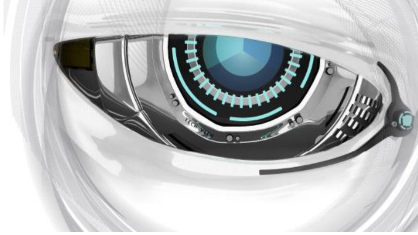
Questions ?

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

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 (256 Nodes):
  - 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

Training time