

# GANs for (fast) simulation



Sofia Vallecorsa for the GeantV team

# Outline

- ▣ Introduction
- ▣ A generic framework for fast simulation
- ▣ GANs for calorimeter showers
- ▣ Summary & Plans

# Simulation in HEP

▣ Detailed simulation of subatomic particles is essential for data analysis, detector design

- ▣ Complex physics and geometry modeling
- ▣ Heavy computation requirements, massively CPU-bound

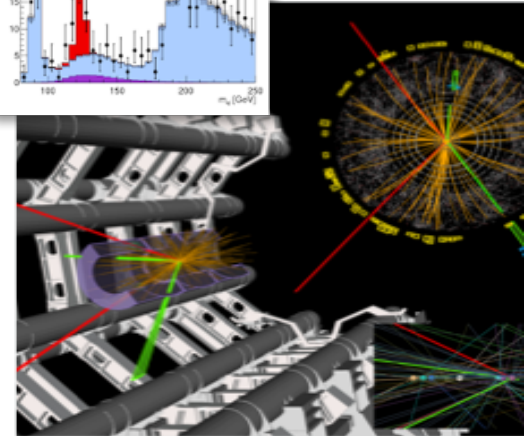
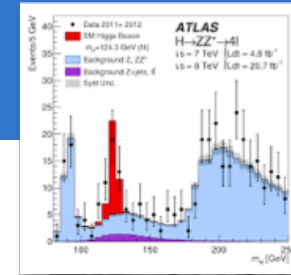
More than 50% of WLCG power is used for simulations



200 Computing centers in 20 countries: > 600k cores

@CERN (20% WLCG): 65k processor cores ; 30PB disk + >35PB tape storage

@HL-LHC needs x100 speed-up in simulation



# Speeding up simulation

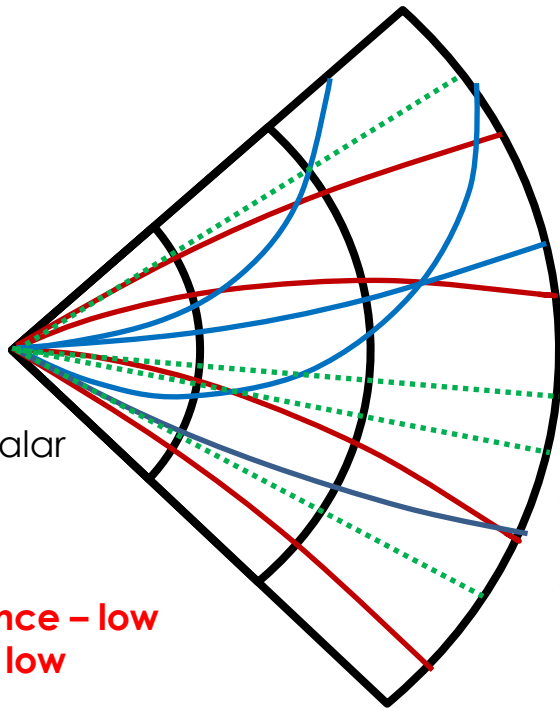
- ▣ State of the art software is Geant4
  - ▣ All particle MonteCarlo transport program
  - ▣ C++ open source simulation toolkit
  - ▣ Capable of handling extremely complex geometries
  - ▣ Large spectrum of applications
  - ▣ Massive and extensive validation
- ▣ Event level multi-threading



# GeantV: Adapting simulation to modern hardware

## Classical simulation

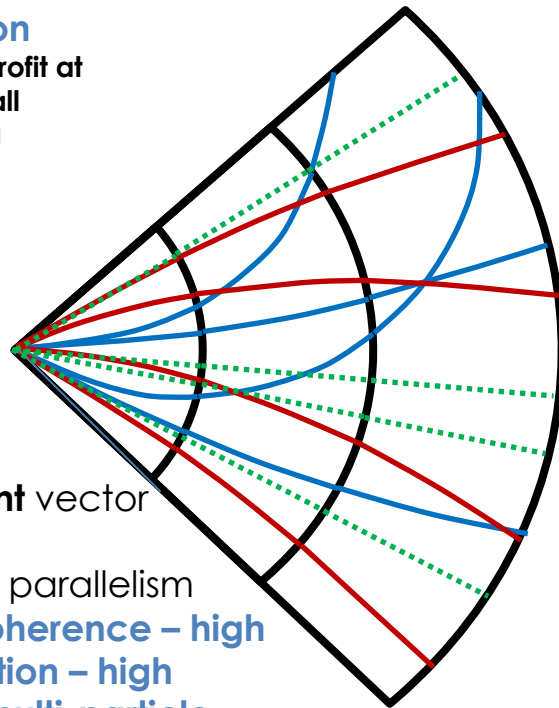
hard to approach the full machine potential



- **Single event** scalar transport
- Embarrassing parallelism
- **Cache coherence – low**
- **Vectorization – low (scalar auto-vectorization)**

## GeantV simulation

needs to profit at best from all processing pipelines

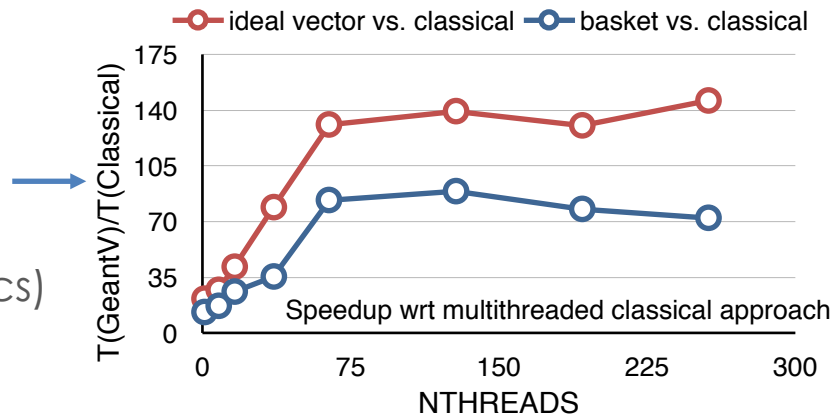
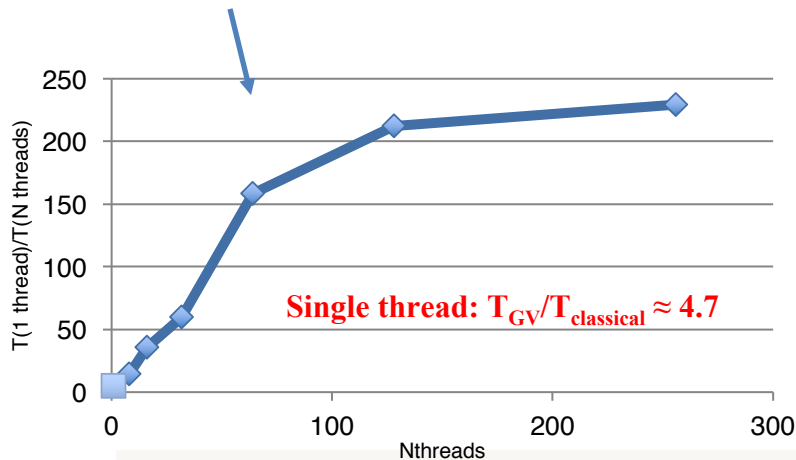


- **Multi-event** vector transport
- Fine grain parallelism
- **Cache coherence – high**
- **Vectorization – high (explicit multi-particle interfaces)**

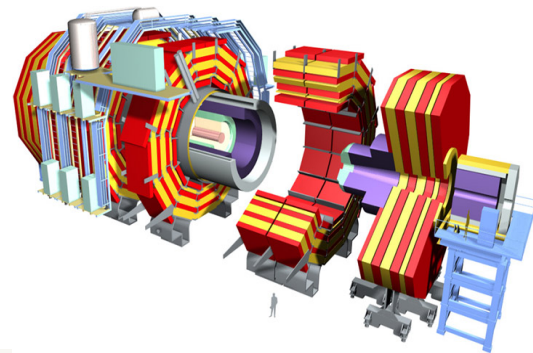


# Some benchmarks on multi-cores

- GeantV delivers already a part of the expected performance
- Testing new geometry navigation performance wrt classical (ROOT)
- CMS detector simulation (tabulated physics)



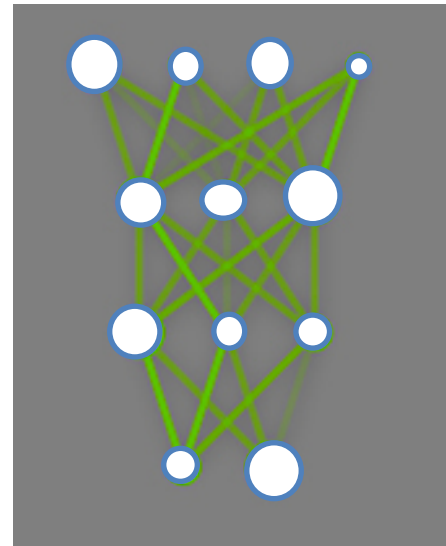
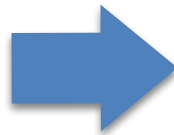
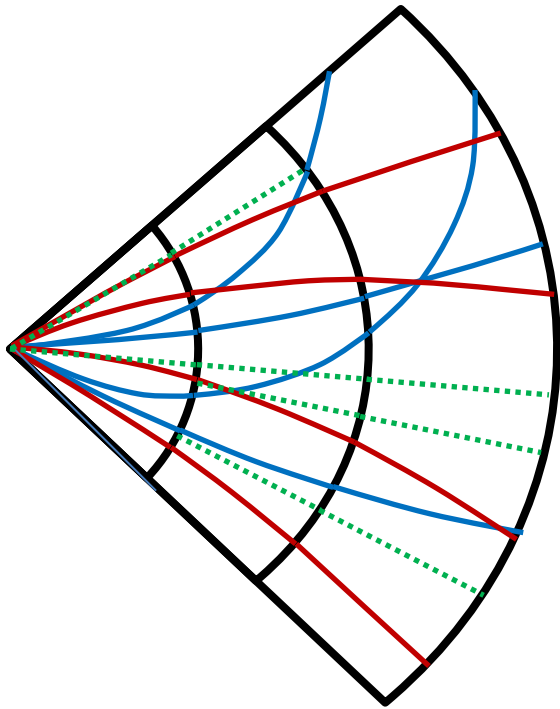
Intel Xeon Phi 7210  
@1.30 Hz – 64 cores



# Going beyond x10: fast simulation

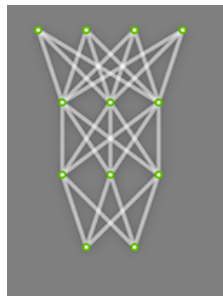
- In the best case scenario GeantV will give  $O(10)$  speedup
  - Not enough to cope with HL-LHC expected needs
- Improved, efficient and accurate fast simulation
  - Currently available solutions are detector dependent
- A general fast simulation tool based on Machine Learning techniques
  - Fully configurable interface embedded in GeantV

# Going beyond x10: fast simulation

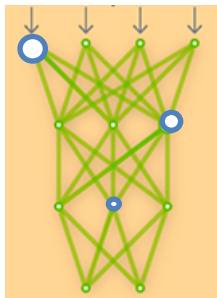


# ML engine for fast simulation

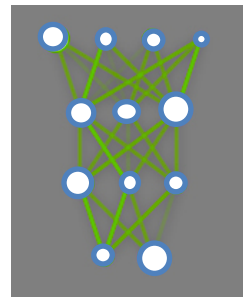
Untrained Model



Training

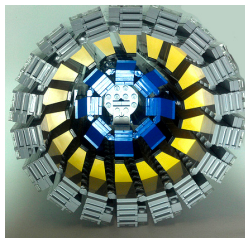


Trained Model

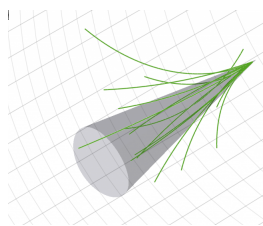


GeantV

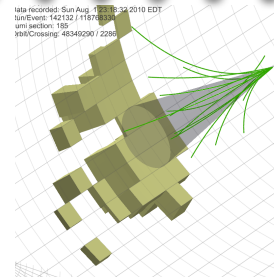
Detector



<http://www.physics.umd.edu/rgroups/hep/LegoCMS/>

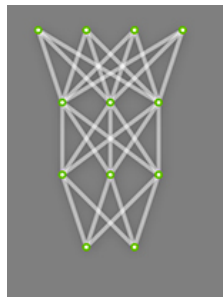


Physics ( $e^+$ ,  $e^-$ ,  $\gamma$ ,  $\pi^+$ ...)  
Kinematics...

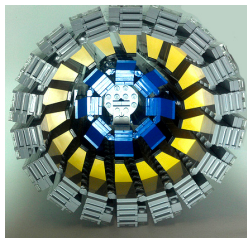


# ML engine for fast simulation

Untrained Model

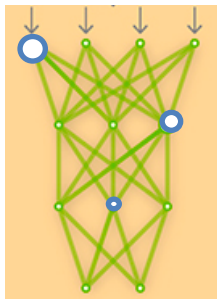


Detector

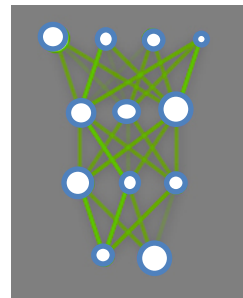


<http://www.physics.umd.edu/rgroups/hep/LegoCMS/>

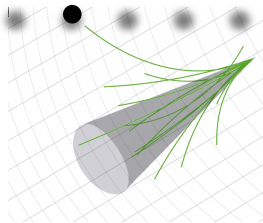
Training



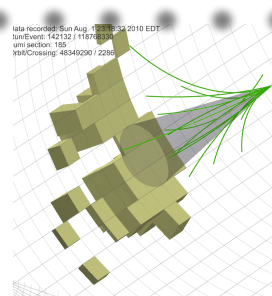
Trained Model



GeantV



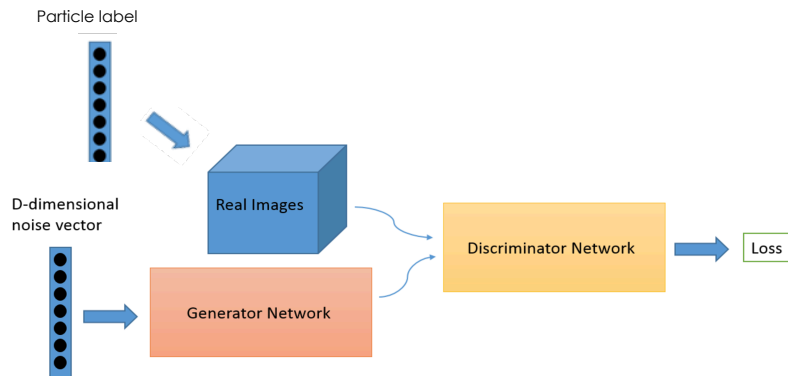
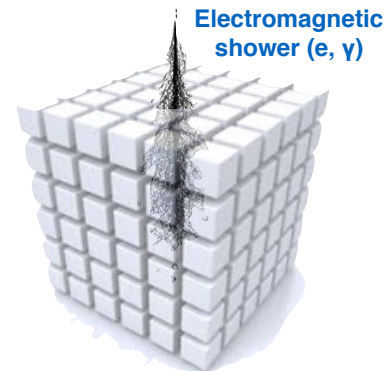
Physics ( $e^+$ ,  $e^-$ ,  $\gamma$ ,  $\pi^+$ ...)  
Kinematics...



lata recorded: Sun Aug 16 10:33:34 2010 EDT  
lun(Event: 142132 / 1187801)  
lun(section: 155  
lun(Crossing: 48346290 / 2289)

# Testing GANs for calorimeter images

- ▣ Calorimeters simulation is time consuming
- ▣ Treat energy deposits in cells as 3D image
- ▣ Use LCD ECAL dataset<sup>(1)</sup>

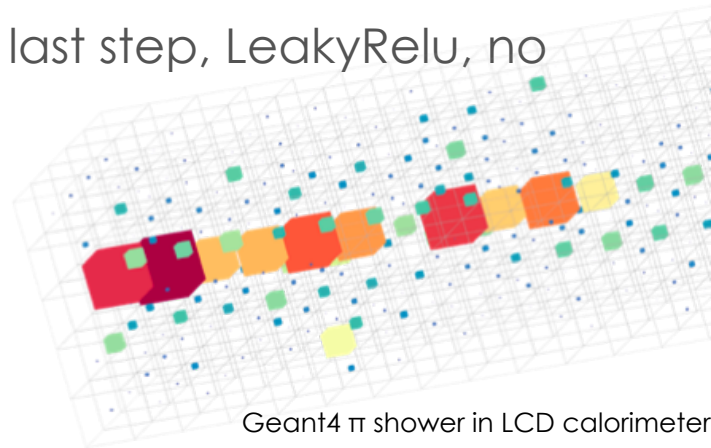
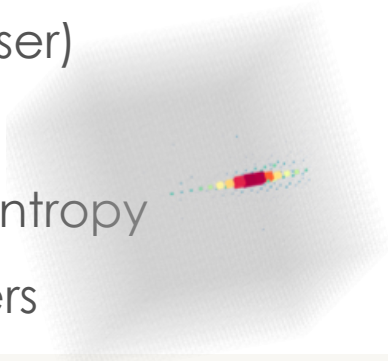


- ▣ Use particle flags to condition the training
- ▣ 3D convolutions using Keras + Tensorflow

(1) See Amir's talk and tutorials

# Testing GANs for calorimeter images

- ▣ Similar discriminator and generator models
  - ▣ 3D conv layers with different x,y,z filter sizes
- ▣ Implemented several tips&tricks found in literature
  - ▣ Some helpful (no batch normalisation in the last step, LeakyRelu, no hidden dense layers)
  - ▣ Some not (Adam optimiser)
- ▣ Batch training
  - ▣ Loss is combined cross entropy
  - ▣ Tested different optimisers

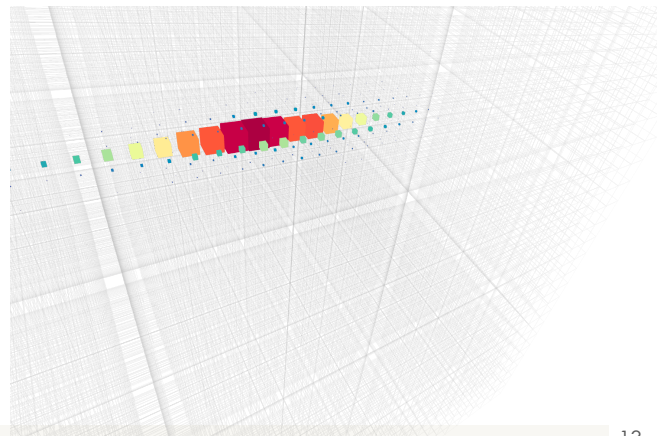
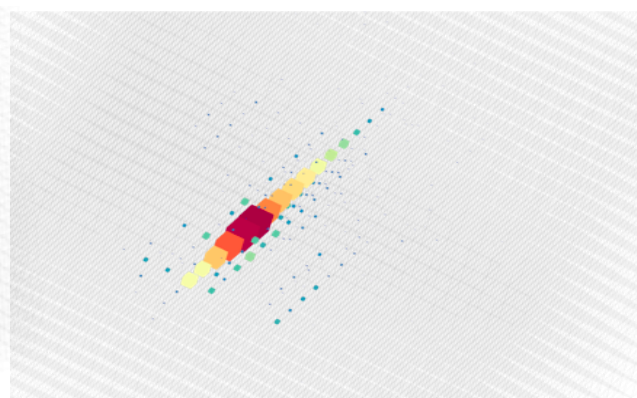
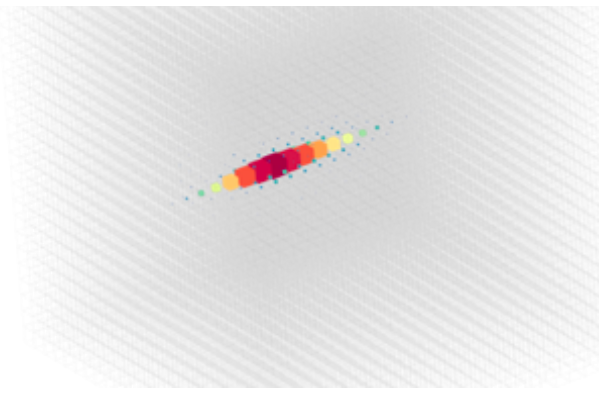
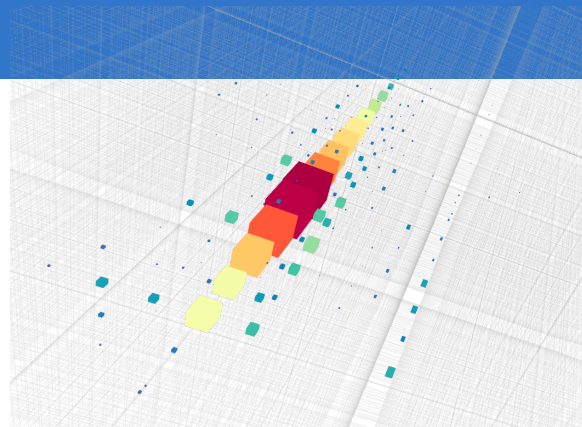


Geant4  $\pi$  shower in LCD calorimeter

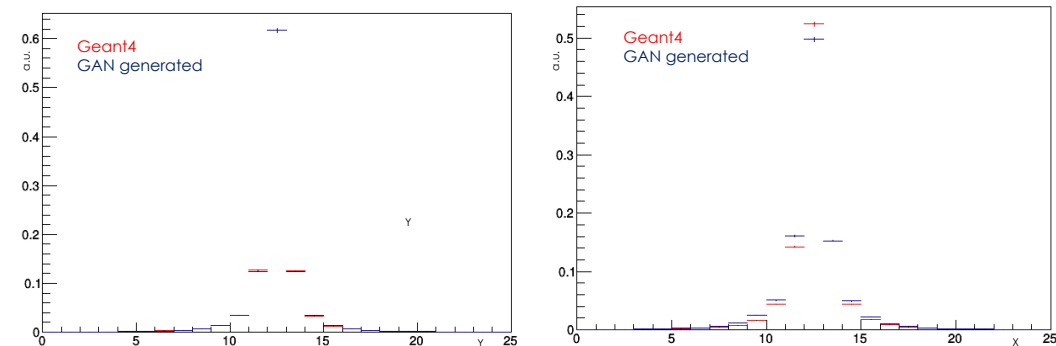
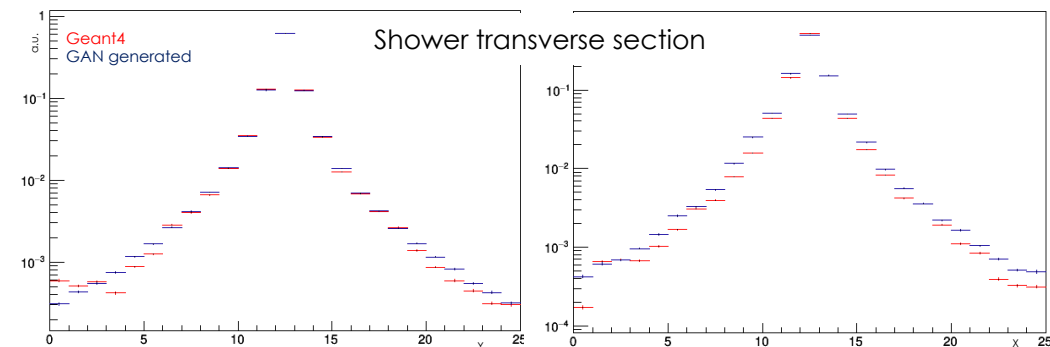


# Some images

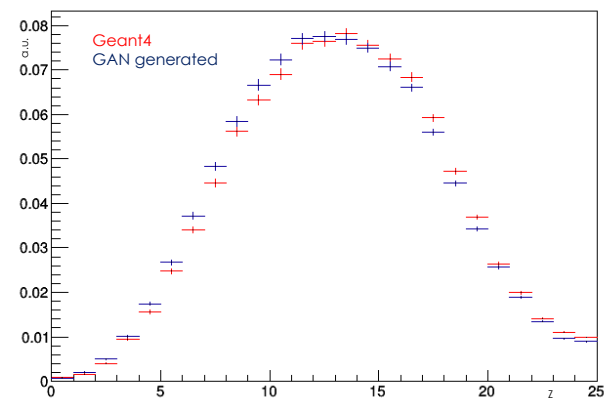
- ▣ Slice energy spectrum
- ▣ Start with photons & electrons



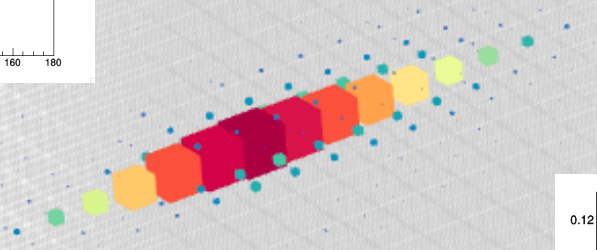
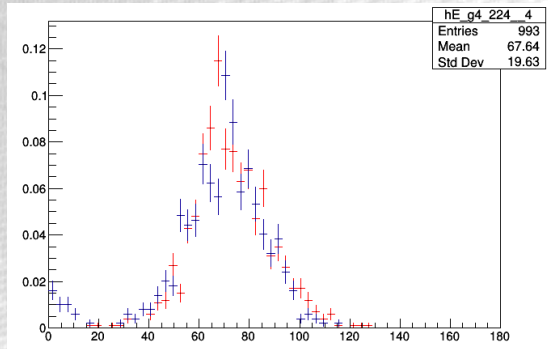
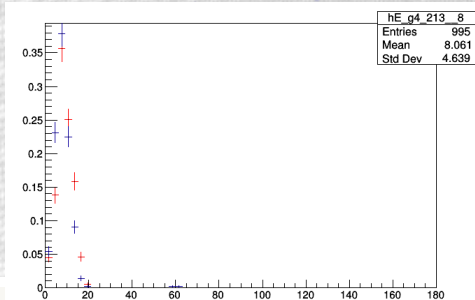
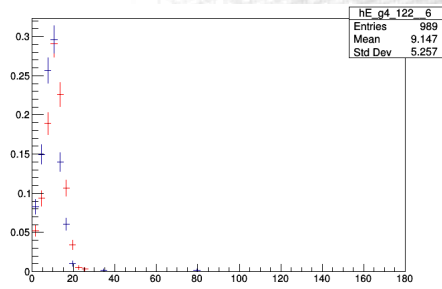
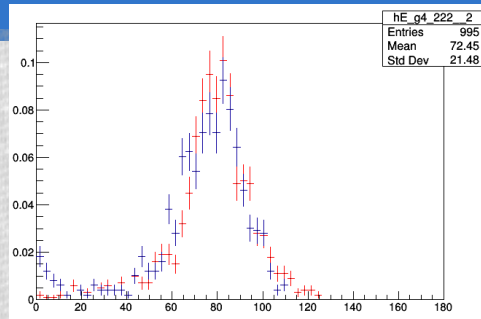
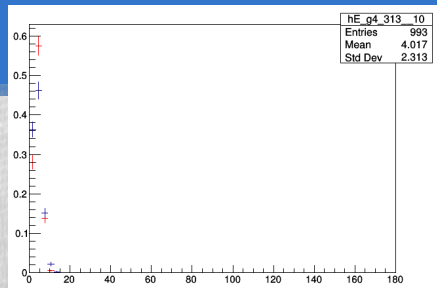
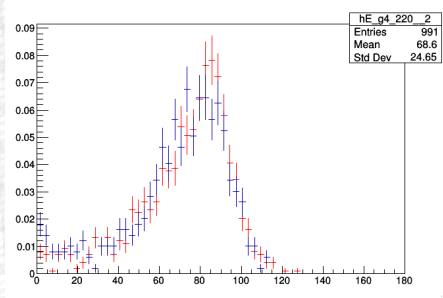
# GAN generated electrons



Shower longitudinal section

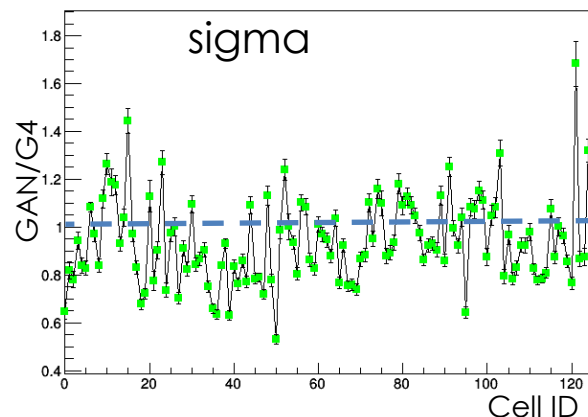
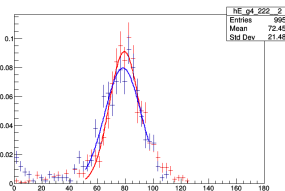
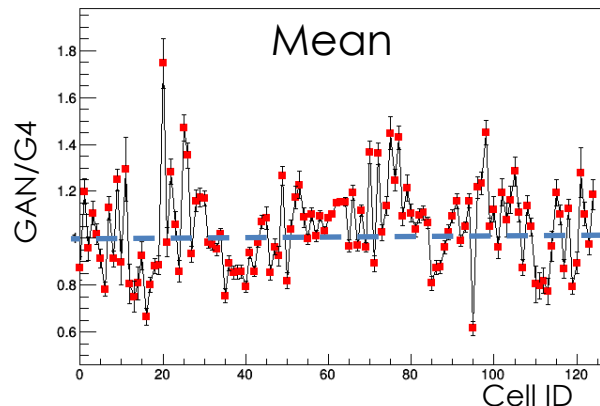


# Single cells



# Single cells

- Compare energy distribution mean and sigma per cell



- Cell energy sigma is underestimated by GAN
- Set up higher level criteria for image validation (reconstructed variables)

# Next steps

- ▣ Detailed study of calorimeter response and comparison to full sim and different fast sim tool
  - ▣ Testing different models to improve physics performance
  - ▣ Include energy info
- ▣ Use information available in the LCD dataset to compare to different techniques (i.e. MO regression)
  - ▣ Test different frameworks
- ▣ Test training on real data

# Training time ?

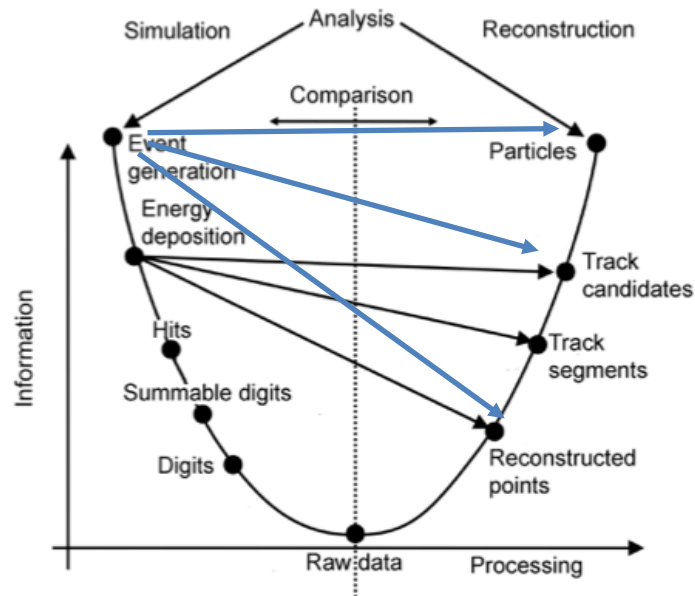
- ▣ Currently adversarial training takes a few hours on NVIDIA GTX1080
  - ▣ Work on the training algorithm
- ▣ Using DL techniques for fast simulation is profitable if training time is not a bottleneck
  - ▣ Depending on the final use case retraining the networks might be necessary
- ▣ Test different hardware & multi-node scaling

# Longer term...

- ▣ We want to provide a generic fully configurable tool
  - ▣ Optimal network design depends on the problem to solve
    - ▣ Embedded algorithms for hyper-parameters tuning and meta-optimization
    - ▣ Large hyper-parameter scans
  - ▣ Study parallelization on large clusters
    - ▣ Evaluate existing libraries
    - ▣ Optimize training strategy by reducing communication overhead

# Summary

- First images using GANs look very promising
  - Keep working on understanding and improving performance
- Insure computing efficiency and optimal performance on modern hardware
- Initial step of a wider plan to do ML based fast simulation with GeantV
- Even larger speedup gained by replacing digitization and reconstruction steps



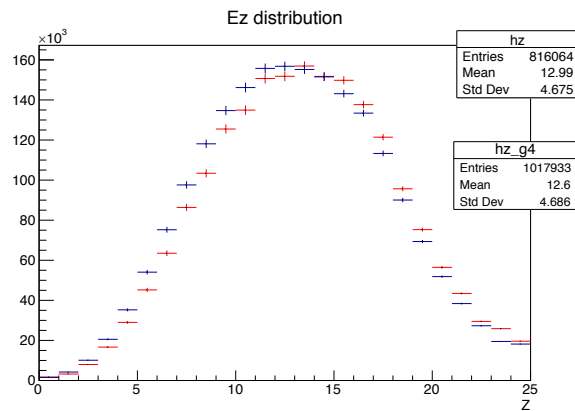




# Thank you

..many thanks to M. Pierini and J. Vlimant !

Z filter size = 8



Z filter size = 9

