AutoML for fast simulation

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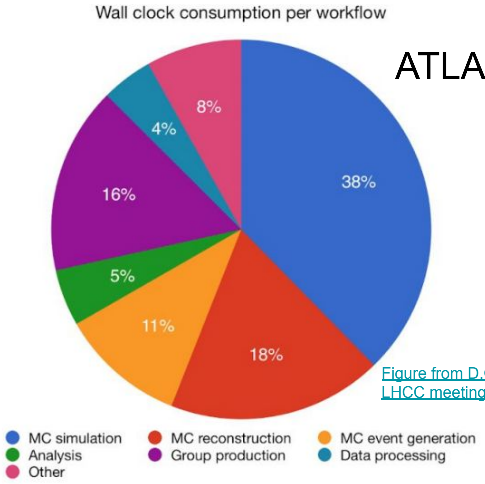
Motivation

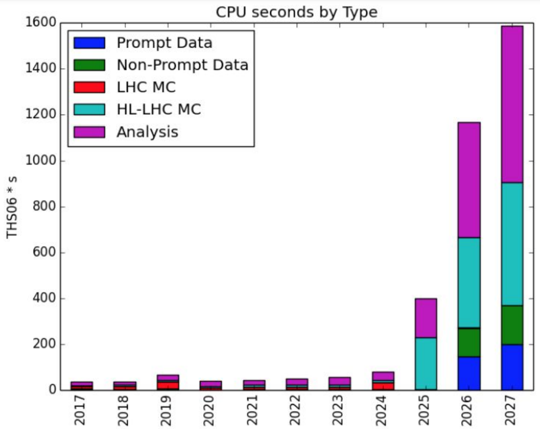
- Successful physics programs depend on the availability of Monte Carlo simulated events;
- Simulations, and shower simulation in the calorimeter in particular, are a large part of CPU consumption in the experiments;
- An alternative: fast simulation approach using Machine Learning;
- **Challenge**: How to optimize the hyperparameters of these models automatically.

[Reference: A. Zaborowska, Fast Simulation]



ATLAS

[Figure from D.Costanzo, J.Catmore, LHCC meeting]



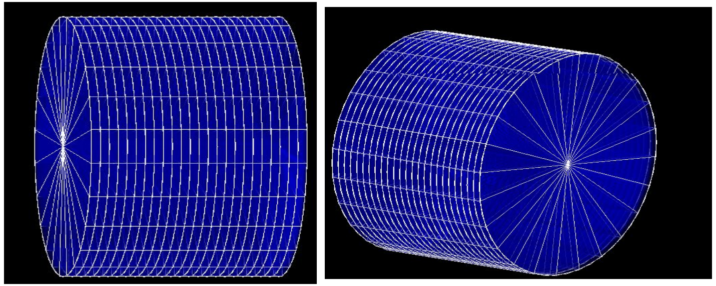
CMS

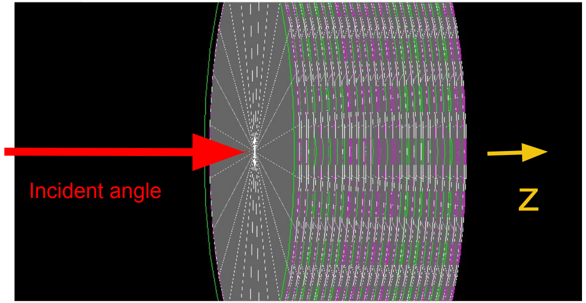
[Figure from J.Phys.:Conf.Ser.1085 022006]

Context - Shower Simulations

- The **calorimeter** is segmented into layers (z), and in radial (r) and azimuthal angle (phi);
- Incoming particle hits the calorimeter and generates **secondary particles**;
- Showering process: Cascade of **energy deposition** along the calorimeter layers;
- For the simulation, one shower in a layer can be seen as an **image**;
- Currently, the main method used is the Geant4 Monte Carlo simulation.

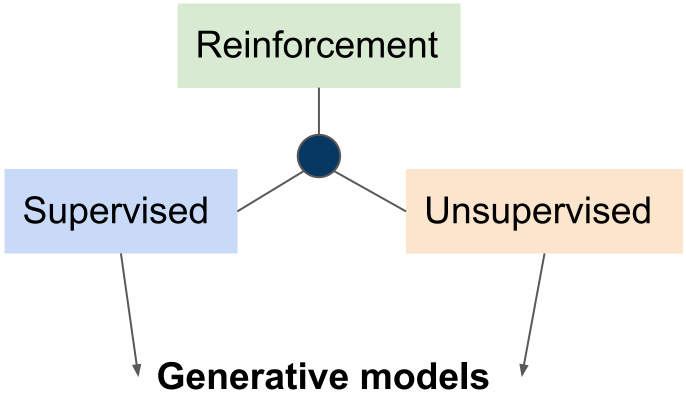
PBWO4 Geometry with 24x24x24 cell segmentation

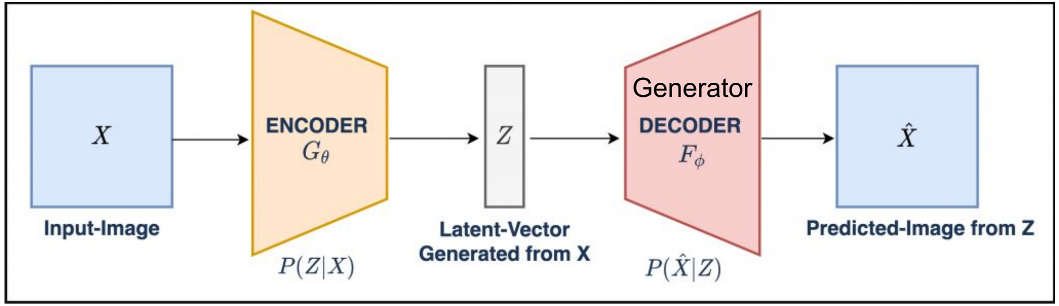




Context - Machine Learning Techniques

- Machine Learning: Learns to improve performance by experience;
- Generative Models
  - Learn the true data distribution of the training set to reproduce it;
  - From noise, generate new data;
- Variational Autoencoder (VAE)





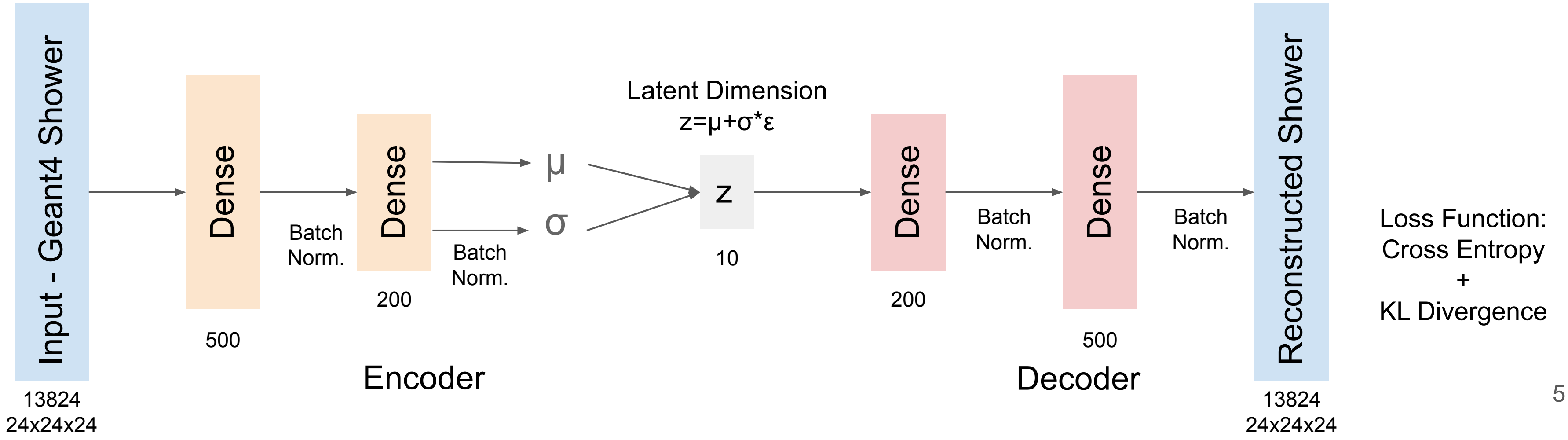
Reference

Implementing VAE for shower simulation

- Training data (Geant4):
  - 10k events;
  - Incident particles
    - Energy: 60 GeV
    - Direction: perpendicular to the surface of the calorimeter
- Model: learns to simulate the energy deposited in the (24, 24, 24) calorimeter.

Keras

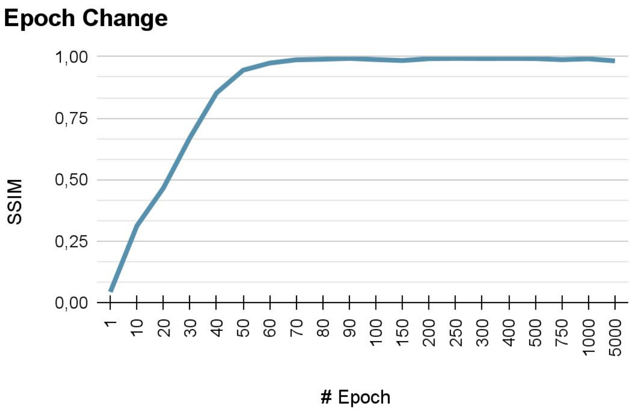
TensorFlow



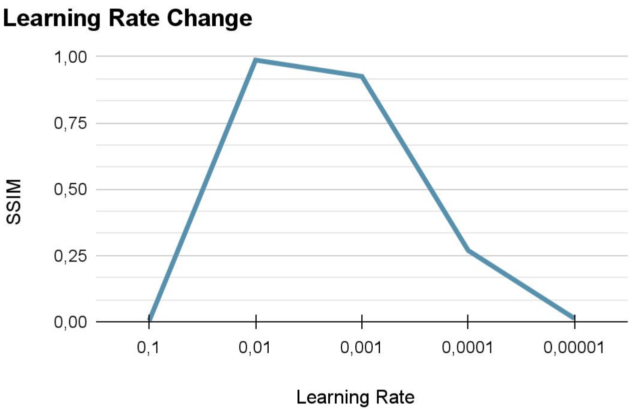
Tuning the hyperparameters

- Hyperparameters: parameters of the model that are used to control the learning process;
- We can try to tune it by changing one value at a time and seeing the impact in the model by hand;
- Metric: SSIM

Fixed Hyperparameters:
latent_dim:10;
ki:RandomNormal;
bi:Zeros;
batch_size:100;
dense_layers:2;
int_dim1:500;
int_dim2:200;
epochs:varies;
activ:relu;
outActiv:sigmoid;
val_split:0.1;
wkl:0.5;
opt:Adam;
lr:0.001;



Fixed Hyperparameters:
latent_dim:10;
ki:RandomNormal;
bi:Zeros;
batch_size:100;
dense_layers:2;
int_dim1:500;
int_dim2:200;
epochs:50;
activ:relu;
outActiv:sigmoid;
val_split:0.1;
wkl:0.5;
opt:Adam;
lr:varies;



AutoML

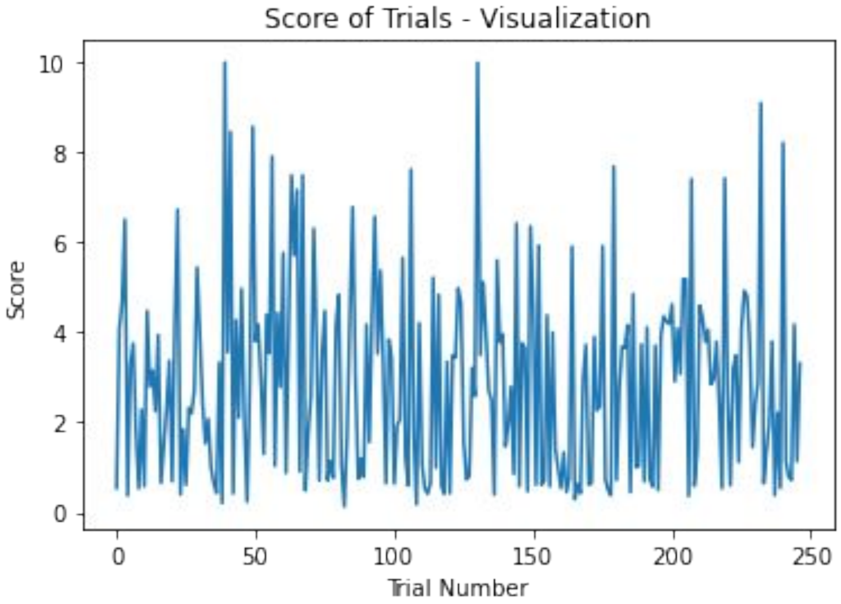
- Automatically search the best hyperparameters according to a certain metric;
- Has the advantage of changing more than one at the same time;
- Multiple ways of tuning: Random Search, Bayesian Optimization, Hyperband Algorithm;
- AutoKeras and Keras Tuner;

AutoKeras

```
Trial 99 Complete [00h 02m 11s]
val_loss: 1631254.0

Best val_loss So Far: 14444.9970703125
Total elapsed time: 07h 45m 14s

Search: Running Trial #100

Hyperparameter    |Value          |Best Value So Far
latdim            |150            |30
lr                |0.001          |0.0001
activ             |softsign       |gelu
wkl               |0.005          |0.5
opt               |2              |3
ki                |LecunNormal    |LecunUniform
bi                |Zeros          |VarianceScaling
enc_layers        |4              |5
intdim_enc0       |750            |750
dec_layers        |4              |5
intdim_dec0       |200            |100
batch_size        |200            |50
epochs            |90             |50
intdim_enc1       |250            |750
intdim_enc2       |50             |1000
intdim_enc3       |500            |100
intdim_dec1       |100            |1000
intdim_dec2       |350            |500
intdim_enc4       |50             |1000
intdim_enc5       |200            |50
intdim_dec3       |750            |50
intdim_dec4       |350            |50
intdim_dec5       |100            |500
```

AutoML - RandomSearch

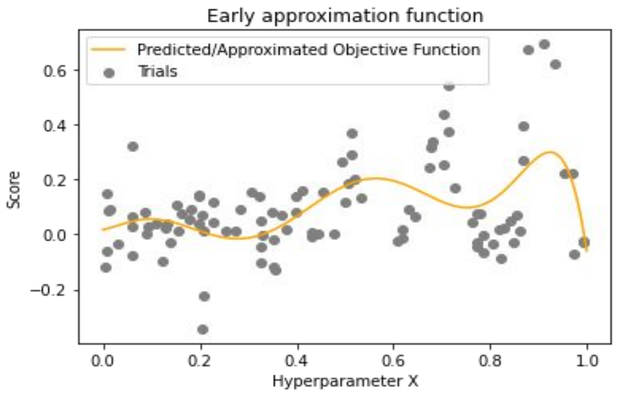
- Input
  - Model;
  - Number of trials;
  - Range of each hyperparameter;
  - Metric (for scoring the trials);
- Randomly pick a new set of hyperparameters (hp) at each trial;
- Train the model using these hp;
- Calculate a score using the input metric;
- Compare the score to previous trials;

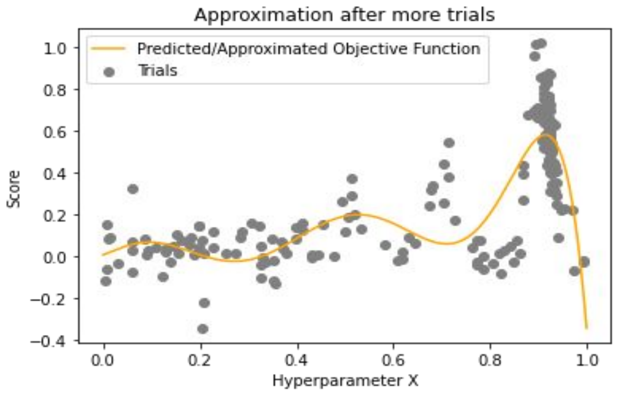


AutoML - Bayesian Optimization

It optimizes the tuning process by trying to calculate an approximation of the objective function for the tuning (score as a function of the hyperparameters):

- Pick a random set of hp, calculate the score;
- Estimate the objective function with a Gaussian process from the values of previous trials;
- Predict the score of N random sets of hp with this approximated objective function;
- Get the best set and train the model with it;
- Use this trained trial to better estimate the objective function.





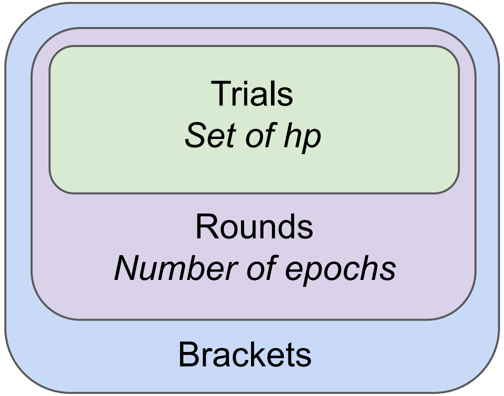
Illustrative Example with one parameter:
[Reference]

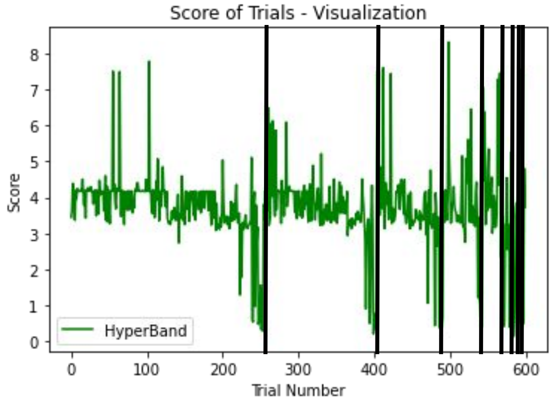
AutoML - Hyperband

Improves the Random Search by exploring a bigger space in less time (running on fewer epochs) and **keeping the best trials to develop** further:

- Input
  - Maximum number of epochs to train (m)
  - Factor (n) for which to increase the number of epochs;
- For each round i, train the m/n^i of sets on n^i epoch.
  - Choose the best trials to run for more epochs.
- To explore more of the space, we have brackets (black lines).

Hyperband Scheme



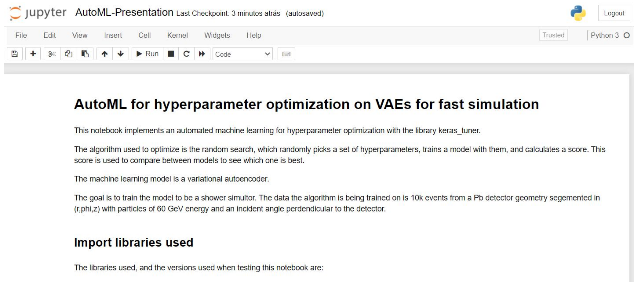


AutoML - Code Details

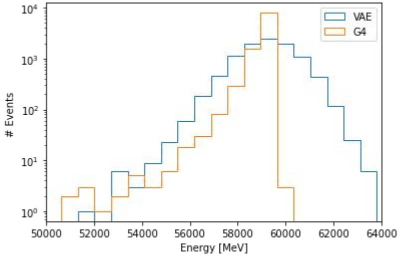
- Implementation of the VAE for each method using Keras Tuner.
- Jupyter Notebook - [Link]

```python
def build_model(hp):
    vae = VAEBlock(hp)
    vae.compile(optimizer=vae.optimizer, loss=[vae.my_loss()])
    return vae
```

```python
tuner_rs = MyTuner(
    build_model,
    objective= keras_tuner.Objective('val_all',  direction='min'),
    max_trials=250,
    #overwrite=True,
    directory='automl',
    project_name='metrica_bonita')
```

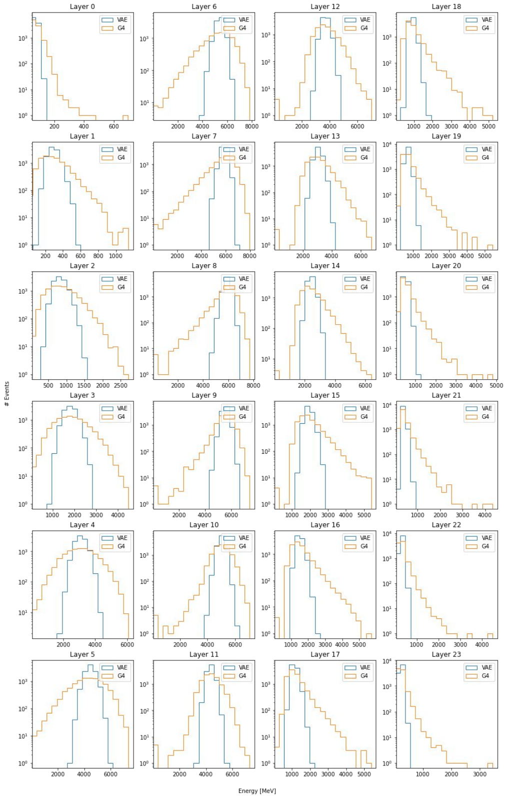


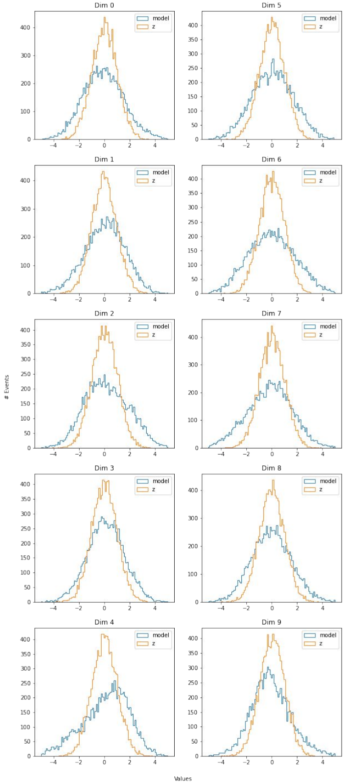
AutoML - What we want the model to be good at



Total Energy

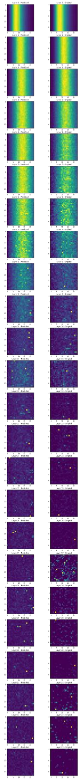
Energy per layer





How gaussian the latent representation is

Representation



AutoML - Metrics to choose the best model

- Loss?
    - Problem - different weights for the reconstruction part and the gaussianity of the latent space;
- Loss, but with same weight and order of magnitude for both parts?
    - Problem - the value for the cross entropy wasn't a good measure to look at similarities capturing the high and low energetic parts in the reconstruction;
- SSIM for the reconstruction?
    - Problem - Didn't take into account the gaussianity of the latent space;
- MSE as a metric to compute the distance between the gaussian distribution and the learned latent space distribution?
    - Problem - Didn't take into account the reconstruction part;
- Combine MSE and SSIM?
    - Worked well for the results on the evaluations!!
    - **But....**

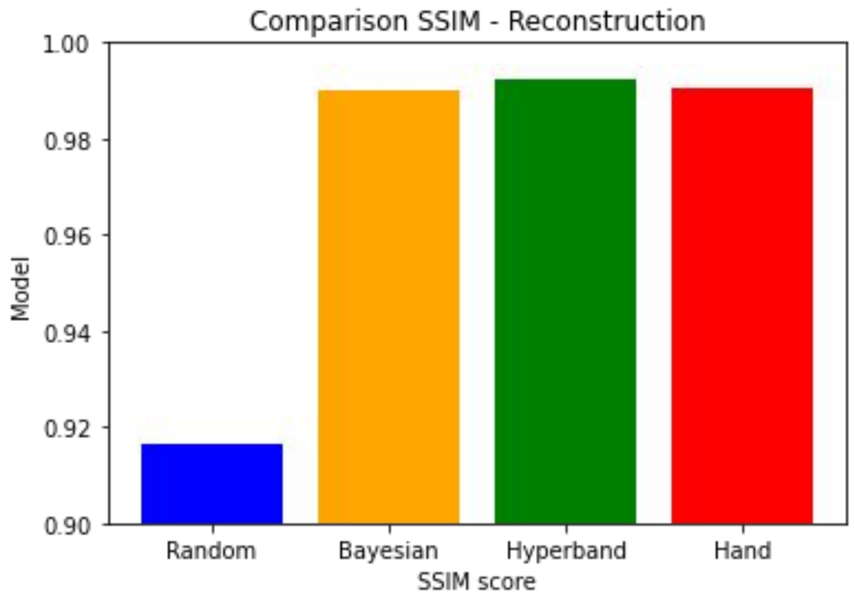
AutoML - Metrics to choose the best model

- What about the generation, that takes into account the physics properties of the simulation?
  - Problem: The best models scored from those metrics didn’t do well with the generation
- Solution: Combined metric - the Machine Learning part and the Physics part.
  - The SSIM for the reconstruction;
  - MSE as a metric to compute the distance between:
    - gaussian distribution and the learned latent space distribution
    - total energy deposited in the calorimeter, comparing the Geant4 and the generation with VAE from random values;
  - Mean of the MSE of the energy deposited in each layer, comparing the Geant4 and the generation with VAE;

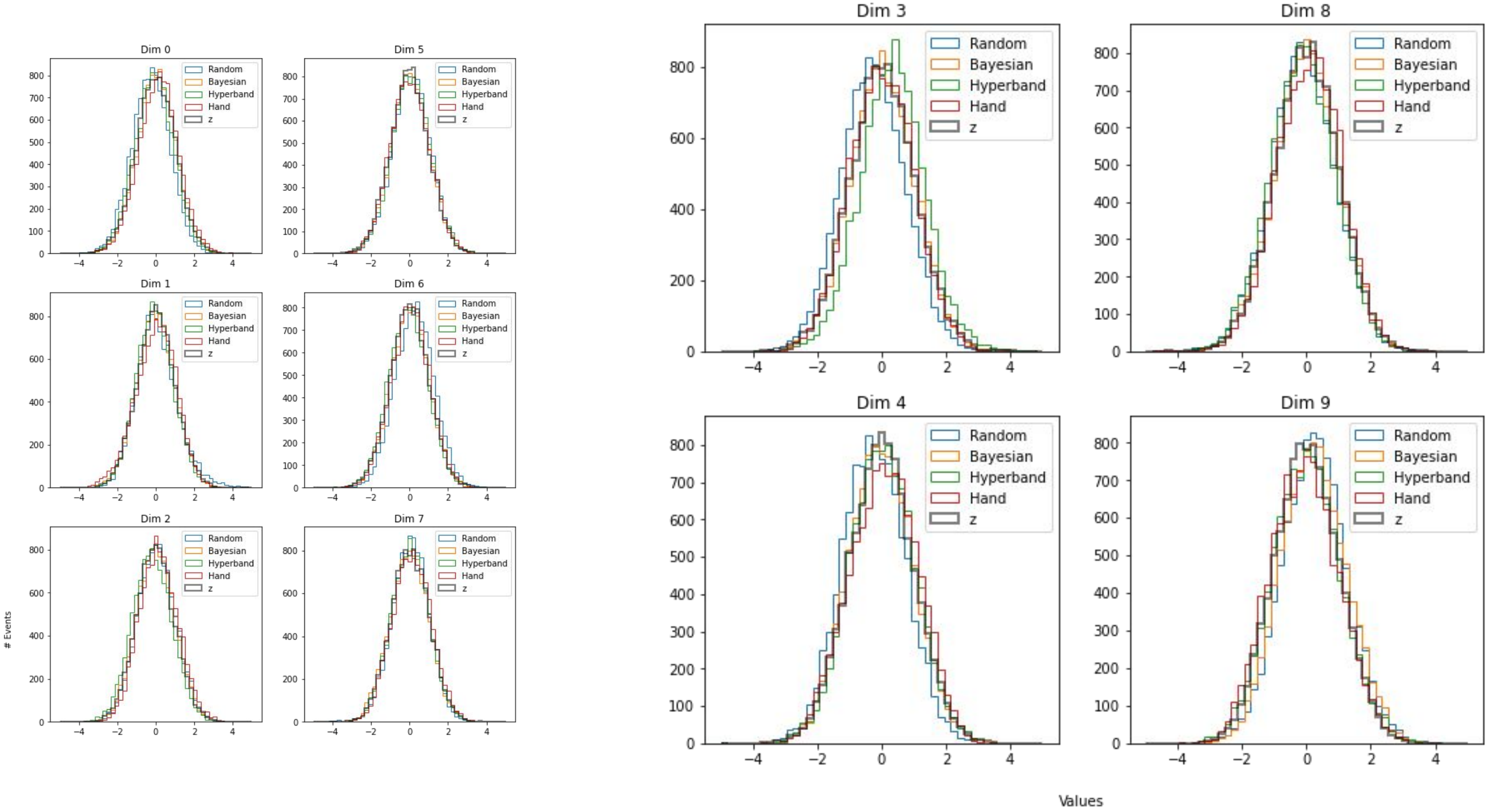
AutoML - Comparison

- Random - Best model using the Random Search.
  - 250 trials - 10h50min
  - The best model took 13 minutes to train (150 epochs);
- Bayesian - Best model using the Bayesian Optimization.
  - 250 trials - 13h14min
  - The best model took 9 minutes to train (90 epochs);
- Hyperband - Best model using the Hyperband.
  - 610 trials - 7h34min
  - The best model took 6 minutes to train (64 epochs);
- Hand - Best model considering the 4 metrics when using the hand tuning.
  - The whole hand tuning process took 3-4 days - 130 models evaluated;
  - The best model took 34 minutes to train (1000 epochs);

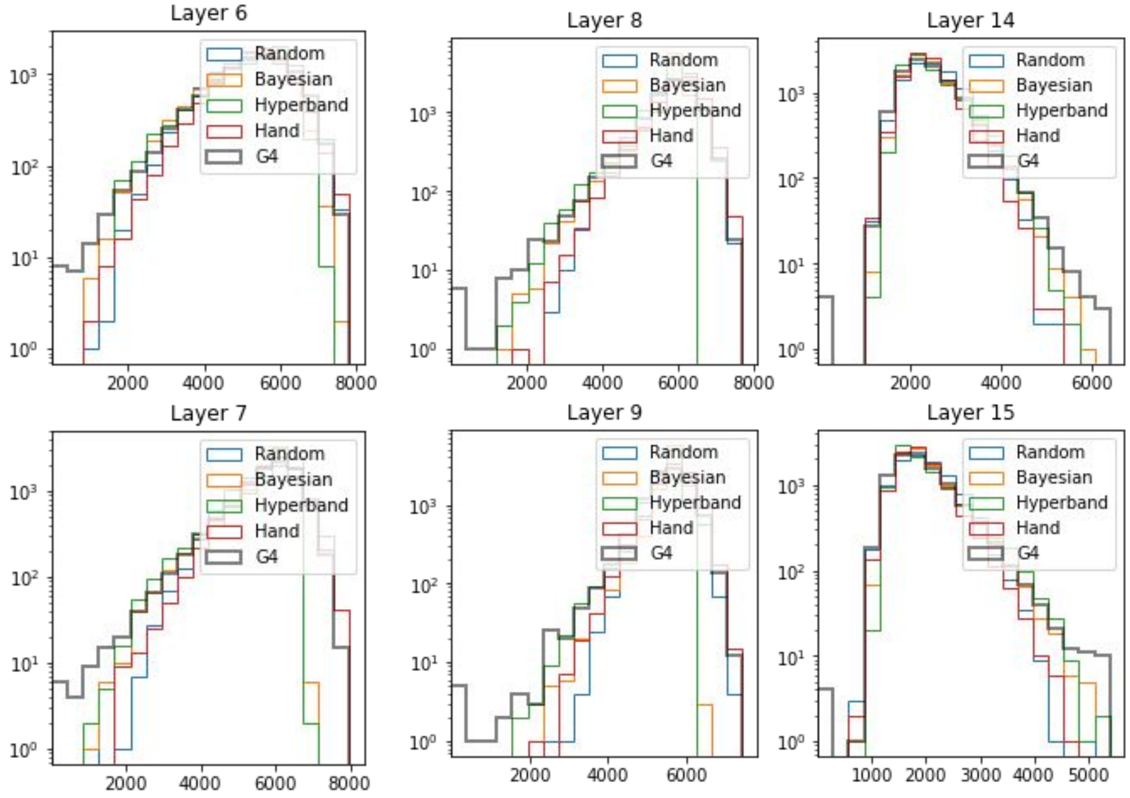
AutoML - Results - Reconstruction SSIM



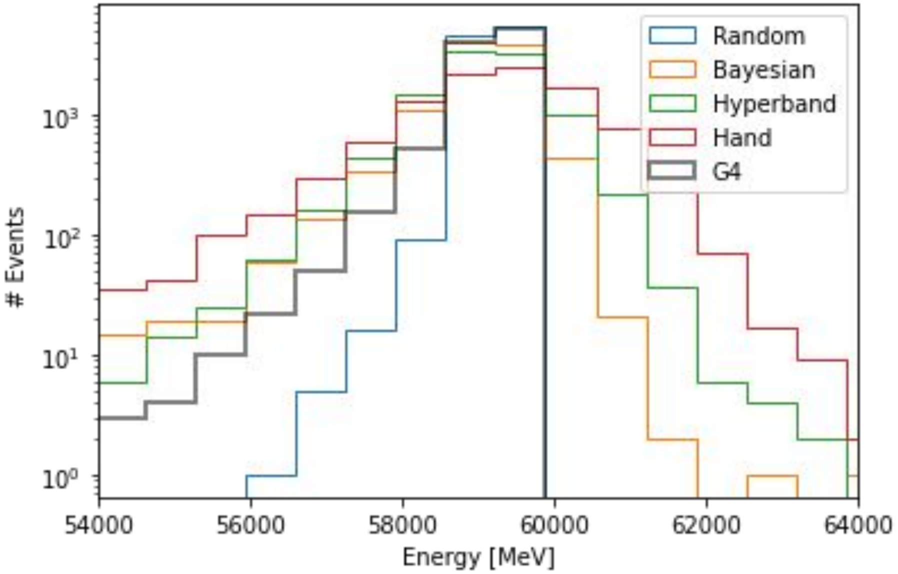
AutoML - Results - Gaussianity of the Latent Space



AutoML - Results - Energy per Layer



AutoML - Results - Total Energy



AutoML - Comparison

	Random Search	Bayesian Optimization	Hyperband
+	Simple	Tracking of the tuning process Approximate objective function for fast scoring	Fast Explore larger space Tracking of the tuning process
-	No control of the tuning process	Too long to approximate a good enough function	Discard some trials too fast

Summary and Conclusion

- Monte Carlo simulated events are a large part of **CPU consumption**;
- An alternative is to use **fast simulation** with Machine Learning;
- To improve the model, we have to **hand tune the hyperparameters**;
- **AutoML** can help to optimize those parameters automatically.
- To select the best model with the AutoML, it is important to have the right metric;
    - **Combined metric** (ML and physics) allow the tuner to choose the best considering all aspects of the problem

Summary and Conclusion

- This project is still in progress (2 weeks left)
  - The models from the AutoML are already better, and we are still training the tuner for longer;
    - Expanding the number of epochs will certainly help;
    - More trials will allow the algorithm to optimize better too.

Future

- Possibility to expand this algorithm to more complex problems!
- Never tried before in shower simulation context, and can help in different areas, besides using VAEs.