Fast simulation of the HGCAL with generative models

A newly started project - Preparation and first results on energy regression

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HamGen

Terascale, 23.11.2021

The DeGeSim Project
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RWTH AACHEN UNIVERSITY

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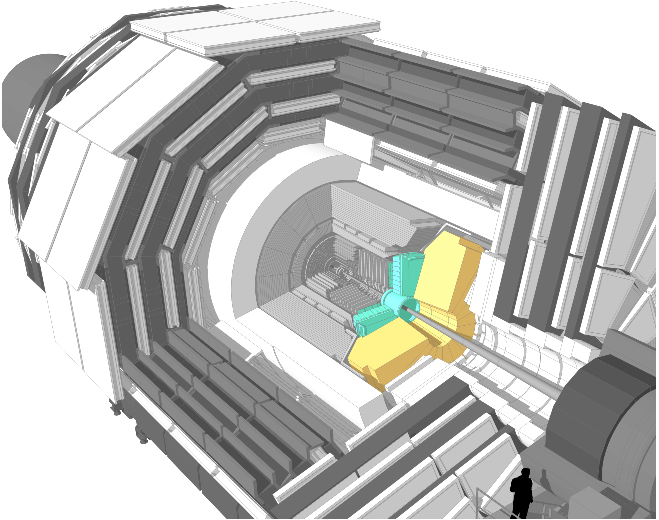
DESY.

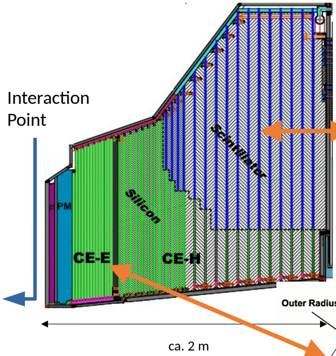
The HGCAL

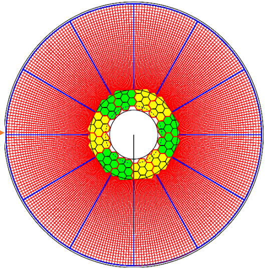
Upgrade for the High-Luminosity LHC in the endcap region

- > Replacing the present forward calorimeter (right) to meet the challenges of the HL phase
- > A high granularity imaging calorimeter
- > Greatly improved spatial resolution and timing
    - Better discrimination of pileup
    - Better shower separation etc.

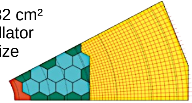


The Geometry of the HGCAL



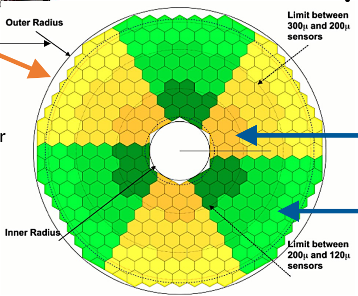


4 to 32 cm² scintillator cell size



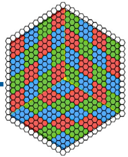
One mixed layer of scintillator and silicon detectors in CE-H (left). Each hexagon represents a wafer with multiple detector cells (pictures below).

- The outer scintillator tiles form a square grid with different edge sizes.
- Note the cut hexagons that define the outer/inner borders (above).

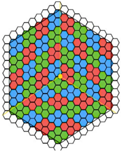


One silicon layer in CE-E (right).

- Each hexagon represents a wafer with multiple detector cells (pictures to the right).
- Higher number of cells in the inner sections.



0.52cm² silicon cell size

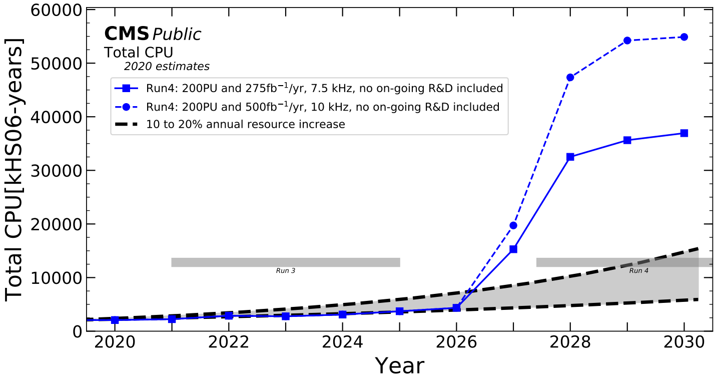


1.18cm² silicon cell size

All Pictures: CMS-TDR-019

Computing Challenge

- High Luminosity phase
  - More particles to simulate
- HGCAL – More cells and channels
  - Complex and time-consuming simulations



CPU time requirements (link)

⇒ Increase in computing time beyond the expected increase in resources.

Vision

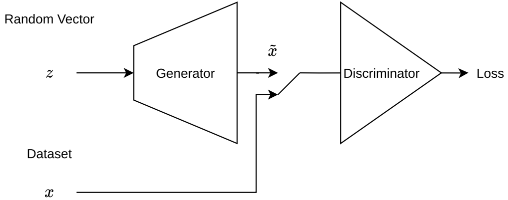
Save CPU time by using a **Neural Network** to simulate the **HGCAL**.

Vision

Save CPU time by using a **Neural Network** to simulate the **HGCAL**.

- Multiple proof-of-principle demonstrations for GAN/VAE-based fast calorimeter simulation
- But no working CMSSW implementation yet
- Use Graph Neural Networks (‘GNNs’) to deal with sparsity and irregular geometry

Generative Adversarial Networks



Loss eg. Minmax:

$$\mathbb{E}_x\left[\log D(x)\right] + \mathbb{E}_z\left[\log\left(1 - D(G(z))\right)\right]$$

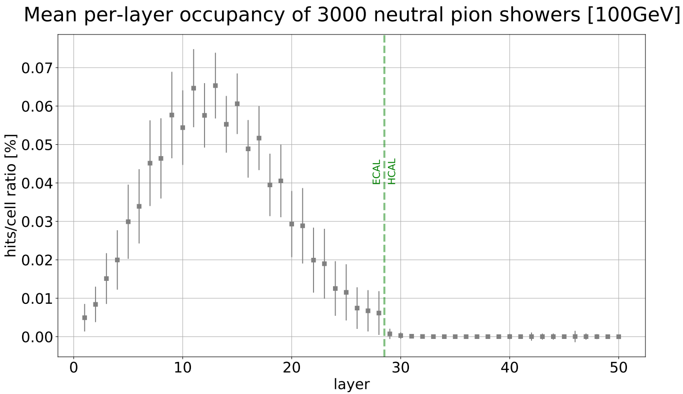
Maximize for the generator, minimize for the discriminator

First proposed by Goodfellow et al (`arXiv.org` 1406.2661)

Necessary Steps

Starting the project

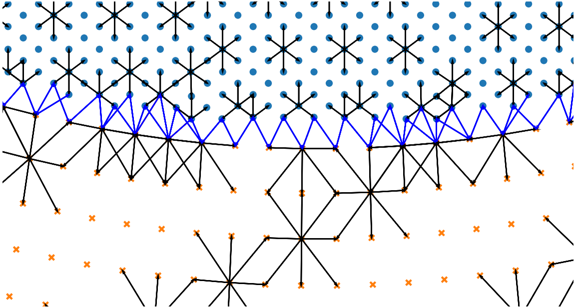
- Training sample production
  - Training will be on single particles (photon, leptons, hadrons)
  - Downside of high granularity $\Rightarrow$ **Sparse data** (right)
- Make the geometry and cell properties accessible to the deep learning frameworks
  - Construct the neighborhood between the cells for the graph representation
- Eventually, development of a generative model to handle sparse data and large graphs



Geometry Extraction

Make the HGCAL geometry available to the Deep Learning frameworks

- CMSSW provides
  - Cell positions
  - Cell properties, e.g. type
    - Silicon
    - Scintillator
  - Neighboring cells within silicon or scintillator
- Full detector neighborhood construction only once
  - Min. distance (x, y) neighbors beyond subdetector borders
  - Nearest cell in $\pm z$ direction



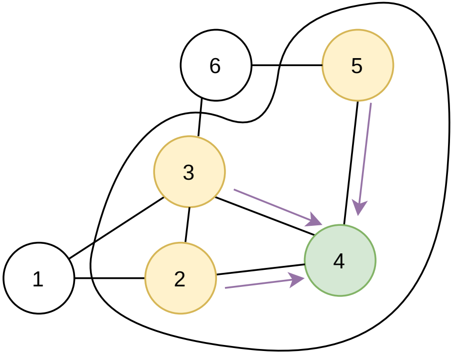
Part of a layer in the hadronic part of the HGCAL

- Black: Some connections within the silicon/scintillator parts
- Blue: The connections between silicon and scintillator cells
- Max distance 0.5 cm between the corners of the cells

ML on graphs

Message Passing: Information propagation for GNNs

Update Node 4
(w/ Neighbors, Messages)



1 Message:

$$\mathbf{Msg}_{j\to i} = \mathrm{Msg}\left(\mathbf{x}_i, \mathbf{x}_j, \mathrm{edge}_{j\to i}\right)$$

2 Aggregate:

$$\mathbf{Aggr}_i = \underset{j\in\mathcal{N}(i)}{\mathrm{Aggr}}\, \mathbf{Msg}_{j\to i}$$

3 Update:

$$\mathbf{x}_i \leftarrow \mathrm{Upd}\left(\mathbf{x}_i, \mathbf{Aggr}_i\right)$$

Energy Regression

Discriminator and a regressor have similar tasks:

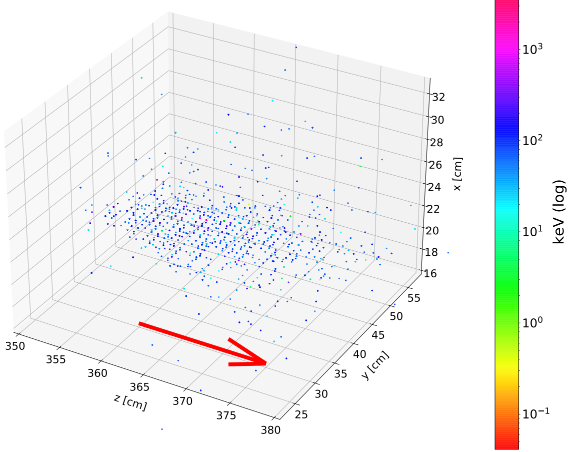
- > Discriminator maps the graph to a probability
- > Regressor maps the graph to a regressed variable

⇒ Technical implementation similar

⇒ Capabilities of GNN architectures measurable in a regression task

Idea : Test technical capabilities and the power of GNN architectures with energy regression on simplified datasets.

3D development of a 100GeV neutral pion shower

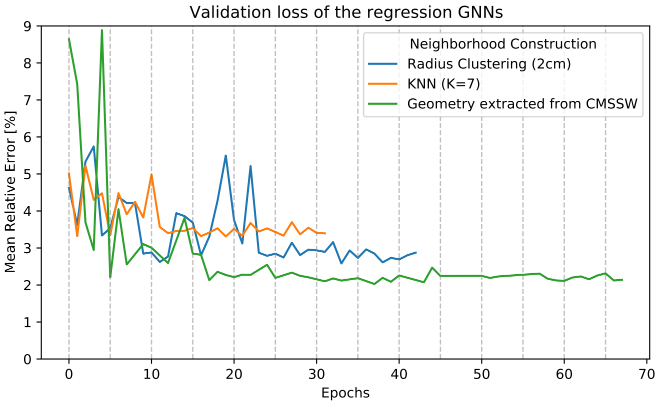


W. Korcari

Energy Regression GNN on HGCAL showers

Collaboration with W. Korcari, G. Kasieczka (UH)

- Simulate only the relevant part of the HGCAL
- Photons with $[50, 100]\,\mathrm{GeV}$ and $\eta = 2$
- Loss: $L = \frac{1}{n}\sum_i \left|1 - \frac{\hat{y}_i}{y_i}\right|$
- Early stopping



⇒ Technical capabilities proven

⇒ GNN shows very promising performances

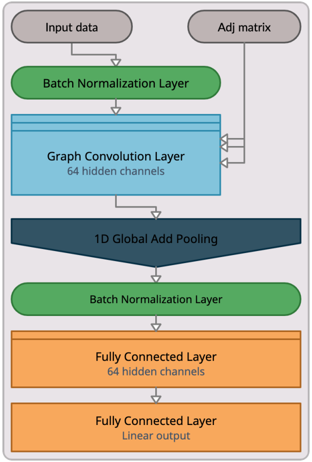
⇒ Geometry extracted from CMSSW leads to the best results

Architecture of the GNNs on HGCAL showers

Collaboration with W. Korcari, G. Kasieczka (UH)

- PyTorch implementation:
  - 3 GCNConv layers
  - 2 fully connected layers
  - 2 Batch normalization layers
- Hyperparameters:
  - Learning rate 0.001
  - Batch size 64
  - 300 epochs

W. Korcari (UH)

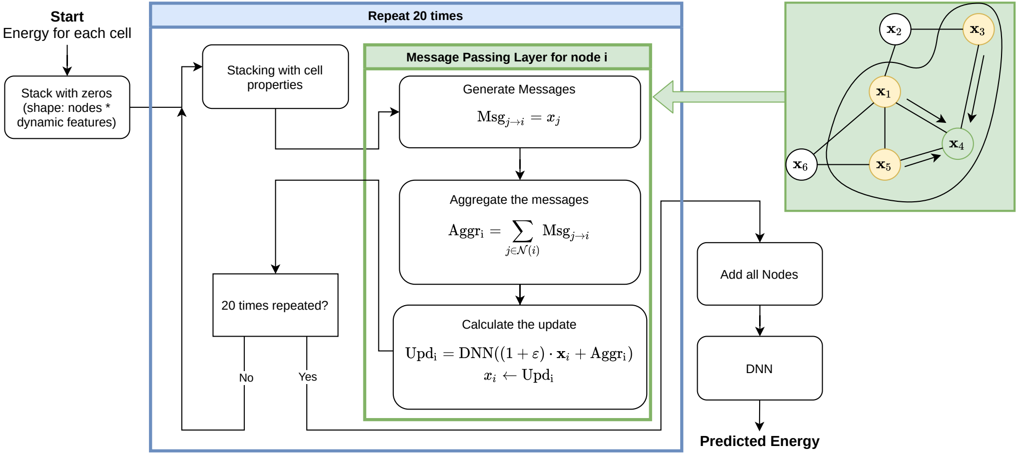


Energy Regression GNN on a Toy Dataset

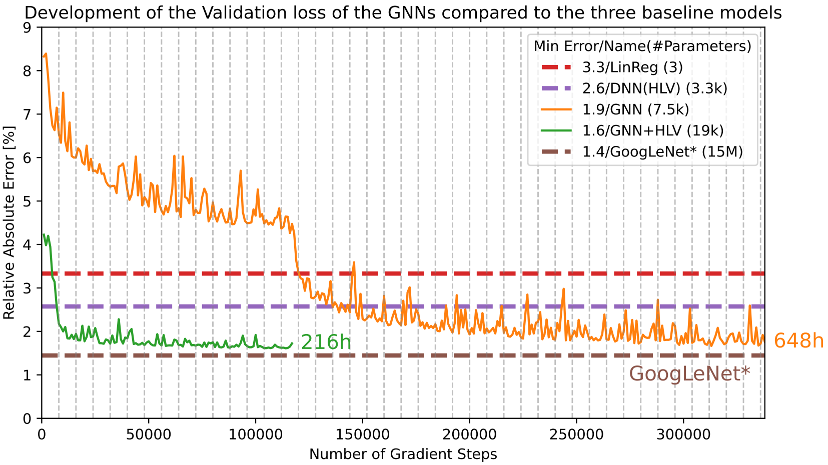
Simplified dataset for Performance Studies

- A CLIC inspired toy dataset (`arXiv.org` 1912.06794):
  - ECAL: 25 layers of 51 × 51 cells
  - HCAL: 60 layers of 11 × 11 cells
  - Electron showers, $p_\mathrm{T} \sim \mathrm{U}_{[0\,\mathrm{GeV},500\,\mathrm{GeV}]}, \varphi \sim \mathrm{U}_{[0,0.35\mathrm{rad}]}, \eta \sim \mathrm{U}_{[-0.524\mathrm{rad},0.524\mathrm{rad}]}$
- Some Models are provided with following variables ("High Level Variables"):
  - E_elmag Sum of cells in the electromagnetic part
  - E_hadron Sum of cells in the hadronic part
  - η (Energy weighted average)
  - ϕ (Energy weighted average)
- Loss is the mean relative error: $L = \frac{1}{n}\sum_i \left|1 - \frac{\hat{y}_i}{y_i}\right|$
- Early stopping

The Architecture of the GNNs on the Toy Dataset



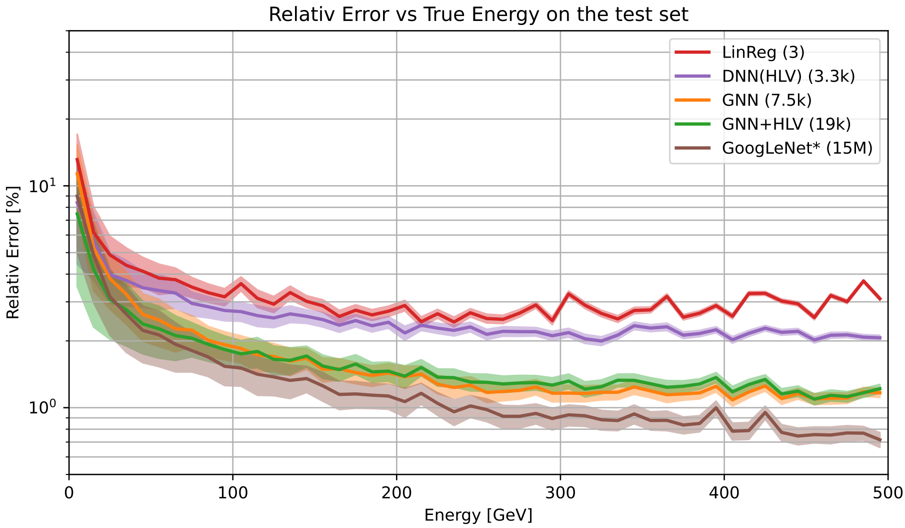
Training of the Energy Regression GNNs on the Toy Dataset



⇒ GNNs approach the performance of state-of-the-art Models

⇒ HLV help convergence and shorten training time

Performance Comparison



Summary

- Geometry was extracted from CMSSW
- Technical infrastructure has been set up
- GNNs show good performance in a regression task
- Studies on generator architectures ongoing

Thank you!

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