CERN openlab

Generative Models for Simulation

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CERN openlab Technical Workshop 2023

Content

In this talk – **projects in collaboration with Intel Corp. and SURF B.V.**

- Introduction and motivation
- 3DGAN quantization with Intel® Neural Compressor
- 3DGAN integration with Geant4

Following talk

- Foundation Models

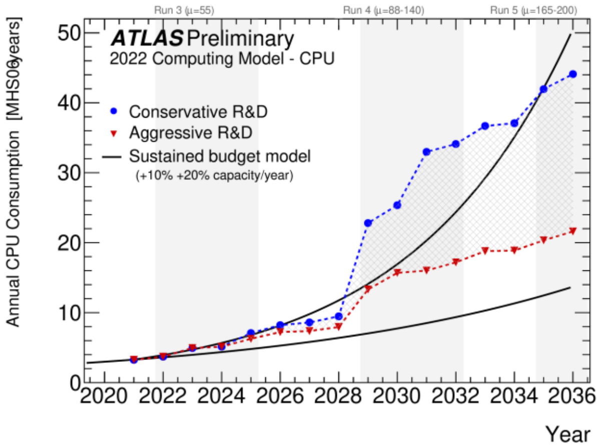
Introduction

Detector simulations

- Monte Carlo-based toolkits (Geant4) – particles interacting with matter
- HEP experiments – specific software frameworks using Geant4
- Computationally intensive
  - 50 % WLCG resources used for simulations[1]
  - E.g. ATLAS – aggressive R&D approach required for HL-LHC

Faster alternatives

- Deep learning models of different types
  - GANs, VAEs, NFs, GNNs, …
  - Development in experiment groups, Geant4, Openlab (IT)
- Focusing on electromagnetic calorimeters (ECAL)
  - High granularity -> most time demanding step in simulation (> 50 %[2])



ATLAS (2022)

[1] The HEP Software Foundation. A Roadmap for HEP Software and Computing R&D for the 2020s. Comput. Softw. Big. Sci 2019.

[2] M. Rama. Fast Calorimeter Simulation in the LHCb Gauss Framework.CHEP 2018.

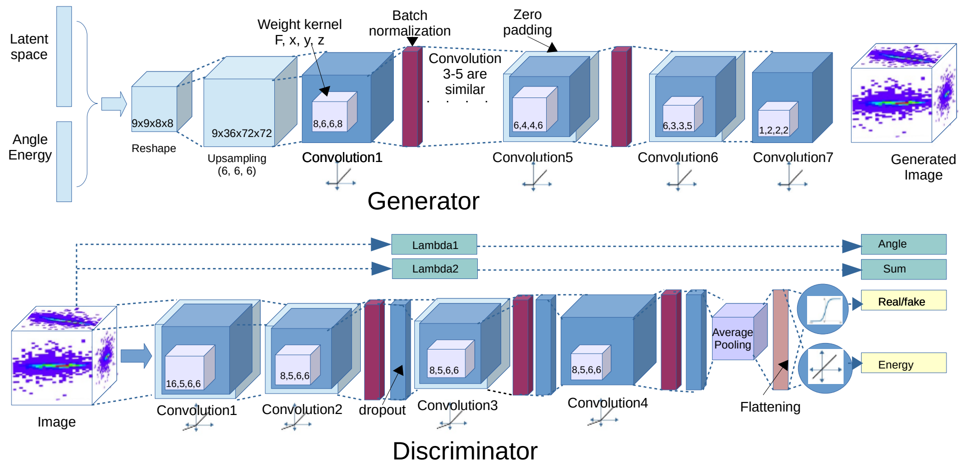
3DGAN and ECAL dataset

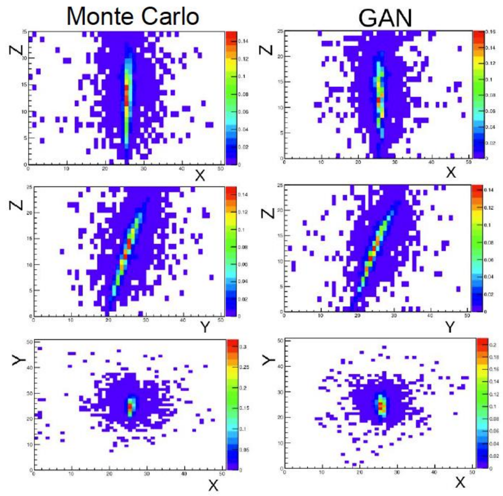
3DGAN model

- 7x 3DConv layers in generator
- Generator output conditioned by primary energy E_p and incident angle θ

Training dataset (MC samples, Zenodo)

- 3D image of a shower from single e^- entering ECAL
  - 51x51x25 cells (~ 65k)
- Primary energy E_p = 2 - 500 GeV
- Incident angle θ = 60° - 120°





G. Khattak *et al.* Fast simulations of a high granularity calorimeter by generative adversarial networks. *Eur. Phys. J. C*. 2022

Quantization with Intel® Neural Compressor

- Intel® Neural Compressor
  - Tool for model compression - quantization, pruning, knowledge distillation
  - Automated strategies for model quantization – to meet given accuracy goals
- Quantizing 3DGAN generator: FP32 → INT8
  - Post-training static quantization
  - Use generator loss as accuracy metric for quantization
    - Based on mean and variance of the shower shapes

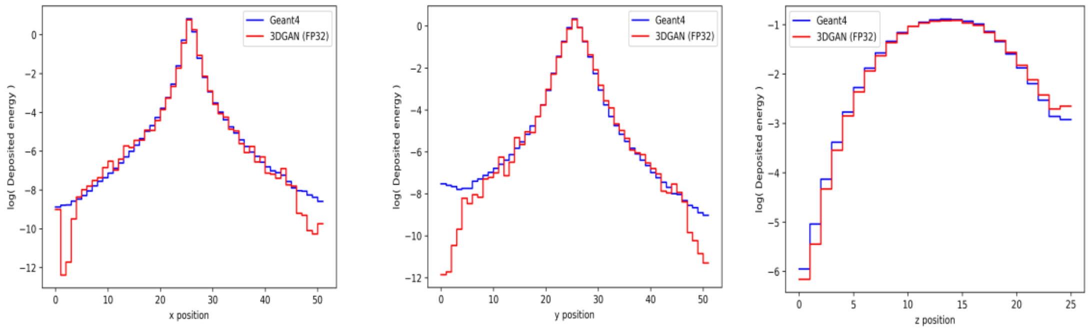


Image: Shower shapes in *x*, *y*, *z* axis (Geant4 vs. 3DGAN)

Generator loss for quantization

- Squared error on mean values and variance on the shower shapes

$$D = \text{dataset}$$
$$I = \text{network input}(D)$$
$$O = 3DGAN(I)$$

$$A_x = \text{mean}(D,\ \text{axis} = x), A_y, A_z$$
$$\widetilde{A}_x = \text{mean}(O,\ \text{axis} = x), \widetilde{A}_y, \widetilde{A}_z$$
$$V_x = \text{var}(D,\ \text{axis} = x), V_y, V_z$$
$$\widetilde{V}_x = \text{var}(O,\ \text{axis} = x), \widetilde{V}_y, \widetilde{V}_z$$

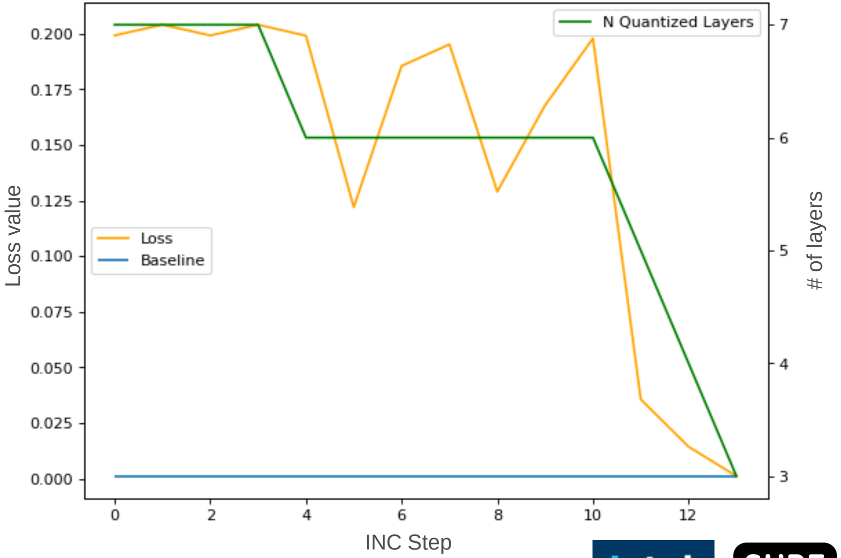
$$\text{loss}\,(D, O) = \sum_{x,y,z} \text{MSE}(A_., \widetilde{A}_.) + \sum_{x,y,z} \text{MSE}(V_., \widetilde{V}_.)$$

Quantization with Intel Neural Compressor

- Quantize all layers → step by step reverse the process until the accuracy target is met.

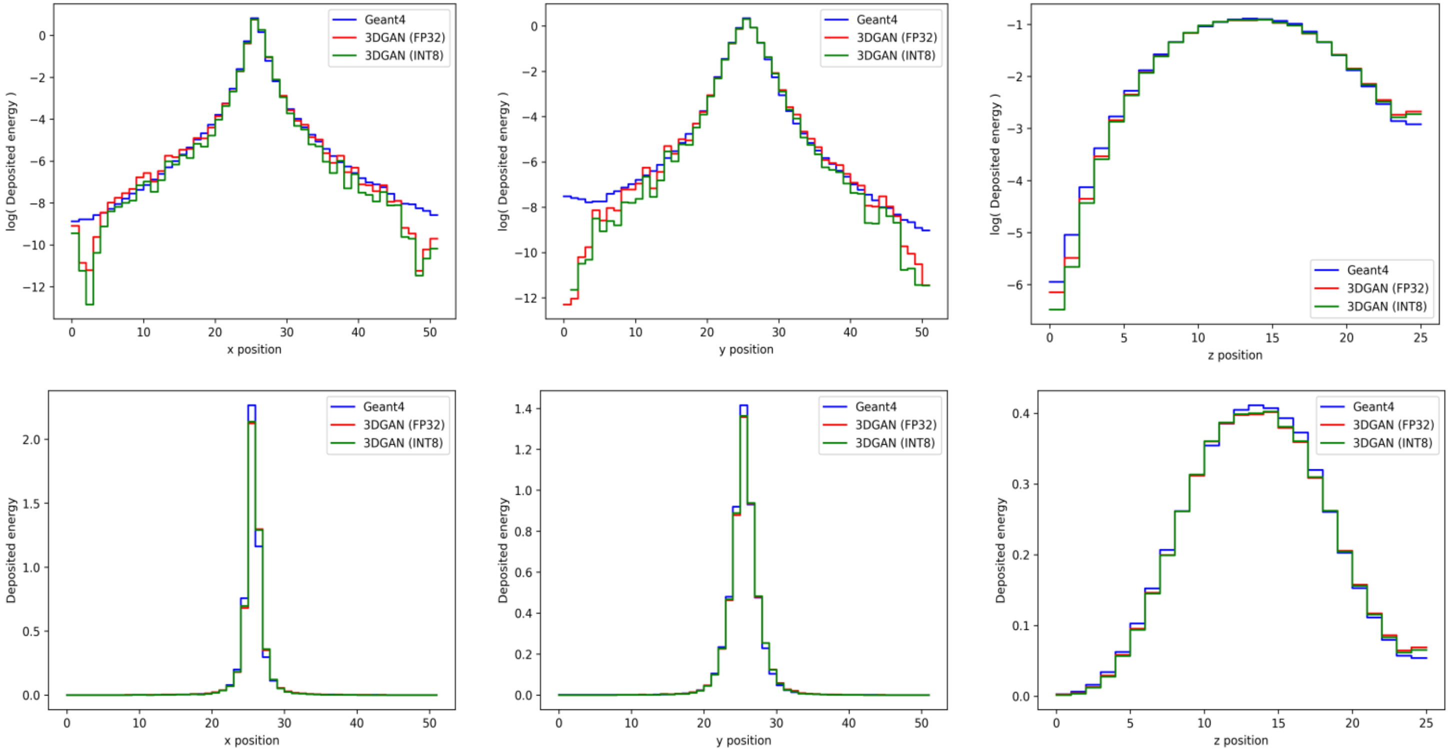
step_id	Num Quantized Layers	Loss
Baseline	**0**	**0.0011**
INC Steps		
0	7	0.1992
1	7	0.2040
2	7	0.1992
3	7	0.2040
4	6	0.1991
5	6	0.1220
6	6	0.1855
7	6	0.1952
8	6	0.1290
9	6	0.1678
10	6	0.1979
11	5	0.0356
12	4	0.0143
13	**3**	**0.0011**

- One data file - 5 000 samples
  - Training – 540k samples
- 10 minutes to quantize the model (13 iterations)



Duncan Kampert, SURF B.V. Code: https://github.com/sara-nl/QuantizedGAN

Quantization: Shower shapes



Quantization: Inference Throughput Performance

- On all platforms:
  - Applier Intel® Neural Compressor Graph Optimizations
  - Intel® optimized Tensorflow 2.10

- **Baseline:** 3rd Gen Intel® Xeon® Scalable Processor 8360 – FP32
- 3rd Gen Intel® Xeon® Scalable Processor 8360 – INT8
- Intel® Xeon® Max Series – FP32
- Intel® Xeon® Max Series – AMX/TMUL INT8

Up to **4.3x speed up** compared to baseline.

Credits:

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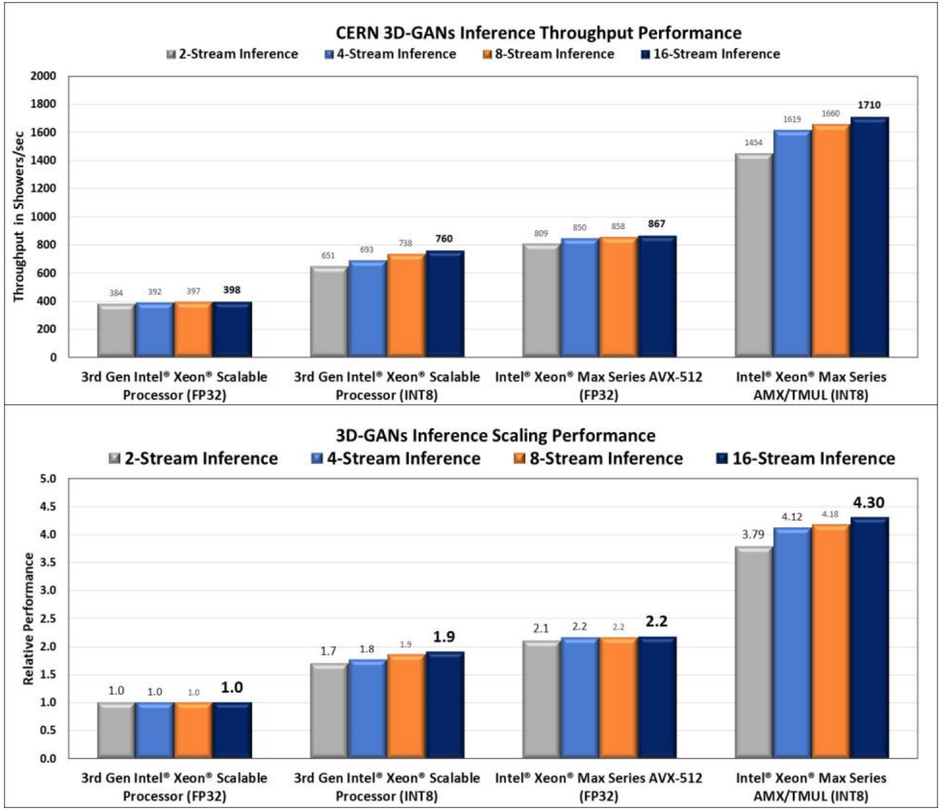
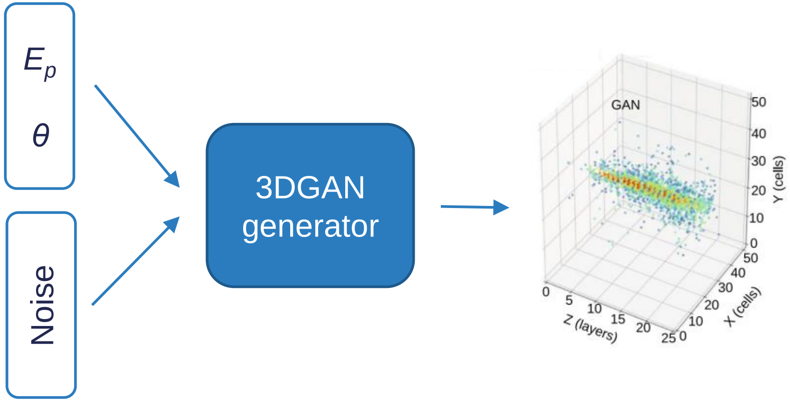


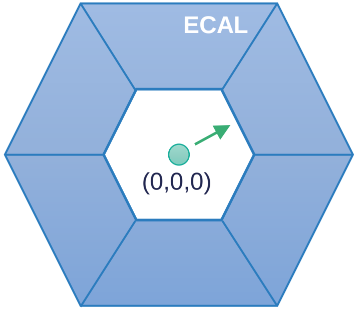
*AMX = advanced matrix extensions,TMUL = tiled matrix multiplication

3DGAN and Geant4 integration

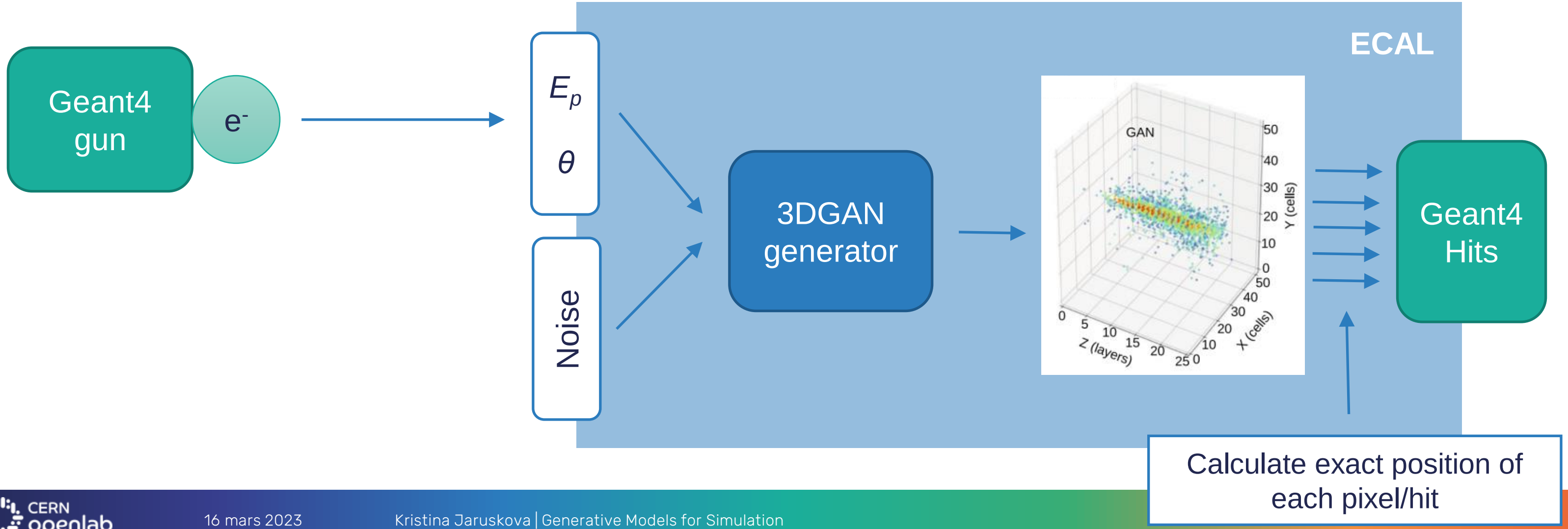
- 3DGAN model
  - Simulating ECAL region of a detector that was designed for CLIC – single electron
  - Input: initial particle energy E_p and incident angle θ + random noise.



3DGAN and Geant4 integration



- 3DGAN model
  - Simulating ECAL region of a detector that was designed for CLIC – single electron
  - Input: initial particle energy E_p and incident angle θ + random noise.
- Starting from Par04 example (Geant4) – Geant4-based framework with VAE for inference (only ECAL)
  - Manual detector definition → using GDML file with LCD ECAL description
  - Replace VAE with 3DGAN
  - Prepare input to 3DGAN and adjust post-processing of the model output

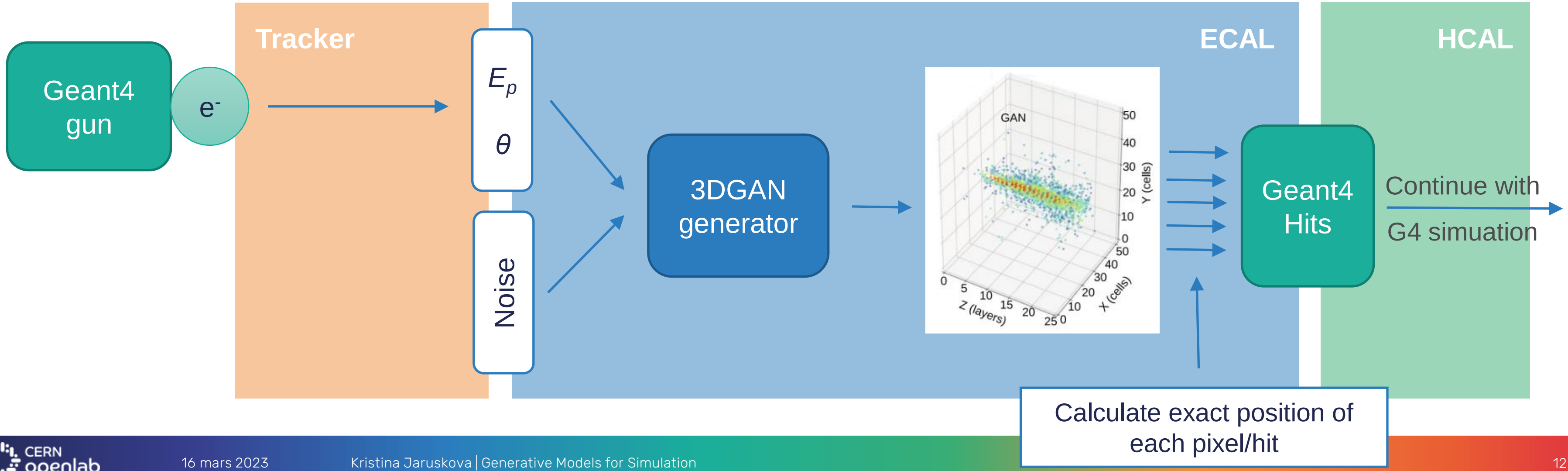


3DGAN and Geant4 integration

- 3DGAN model
  - Simulating ECAL region of a detector that was designed for CLIC – single electron
  - Input: initial particle energy E_p and incident angle θ + random noise.
- Starting from Par04 example (Geant4) – Geant4-based framework with VAE for inference (only ECAL)
  - Manual detector definition → using GDML file with full LCD detector description
  - Replace VAE with 3DGAN
  - Prepare input to 3DGAN and adjust post-processing of the model output

Work in Progress

- Include the full detector description and simulate the whole passage.
- Compare full and fast simulation performance (speed up).



Next talk…

- Drawback of 3DGAN and other fastsim models - one model per specific MC dataset.
- Change in detector material, size, thickness of layers → generate new training data and train a new DL model

- Idea – one large model that can adapt to some changes in the detector design

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- Idea – one large model that can adapt to some changes in the detector design

→ Foundation Models

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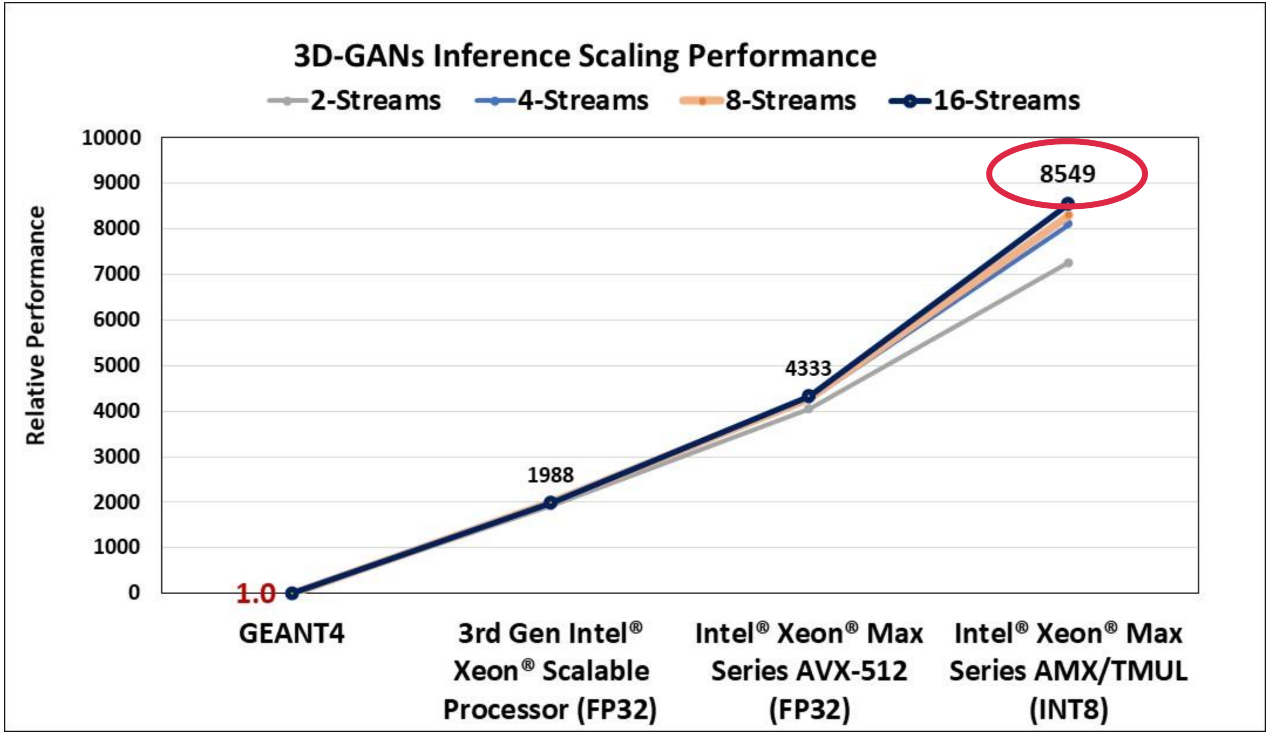
Configuration Details

- BASELINE: 3rd Gen Intel® Xeon® Scalable Processor 8360Y (AVX512, FP32 and INT8)**:** Test by Intel as of 08/21/2022. 2x Intel® Xeon® Scalable Processor 8360Y, HT On, Turbo On, Total Memory 512 GB (16 slots/ 32 GB/ 3200 MHz, DDR4), BIOS WLYDCRB1.SYS.0021.P21.2106280839, ucode 0x8d9522d4, CentOS Linux 8, kernel 4.18.0-240.22.1.el8_3.x86_64, https://github.com/svalleco/3Dgan/, Intel TensorFlow 2.10.0, Keras 2.10.0, GCC 11.20, Intel Neural Compressor: https://www.intel.com/content/www/us/en/developer/tools/oneapi/neural-compressor.html, TF Wheel intel_tensorflow_avx512-2.10.0.202230-cp38-cp38-manylinux_2_17_x86_64.manylinux2014_x86_64.whl, Python 3.8.13
- Intel® Xeon® Max Series (AVX-512 FP32): Test by Intel as of 10/18/2022. 1 node, 2x Intel® Xeon® Processors codenamed Sapphire Rapids with HBM, HT On, Turbo On, Total Memory 128 HBM, BIOS SE5C7411.86B.8424.D03.2208100444, ucode 0x2c000020, CentOS Stream 8, kernel 5.19.0-rc6.0712.intel_next.1.x86_64+server https://github.com/svalleco/3Dgan/, Intel TensorFlow 2.10.0, Keras 2.10.0, GCC 11.20, Intel Neural Compressor: https://www.intel.com/content/www/us/en/developer/tools/oneapi/neural-compressor.html, TF Wheel intel_tensorflow_avx512-2.10.0.202230-cp38-cp38-manylinux_2_17_x86_64.manylinux2014_x86_64.whl, Python 3.8.13
- Intel® Xeon® Max Series (AMX/INT8): Test by Intel as of 10/18/2022. 1 node, 2x Intel® Xeon® Processors codenamed Sapphire Rapids with HBM, HT On, Turbo On, Total Memory 128 HBM, BIOS SE5C7411.86B.8424.D03.2208100444, ucode 0x2c000020, CentOS Stream 8, kernel 5.19.0-rc6.0712.intel_next.1.x86_64+server, https://github.com/svalleco/3Dgan/, Intel TensorFlow 2.10.0, Keras 2.10.0, GCC 11.20, Intel Neural Compressor: https://www.intel.com/content/www/us/en/developer/tools/oneapi/neural-compressor.html, TF Wheel intel_tensorflow_avx512-2.10.0.202230-cp38-cp38-manylinux_2_17_x86_64.manylinux2014_x86_64.whl, Python 3.8.13

Quantization: Inference Throughput Performance



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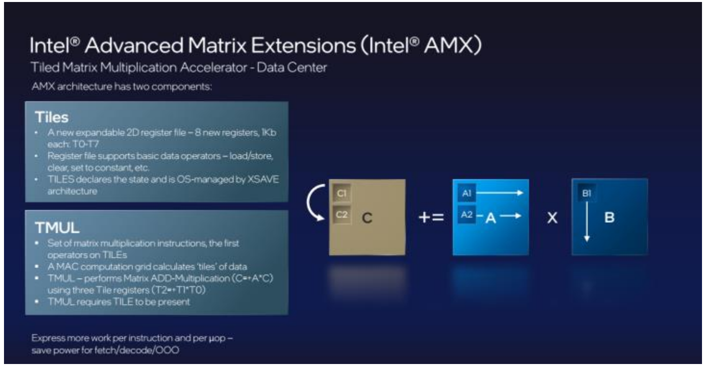
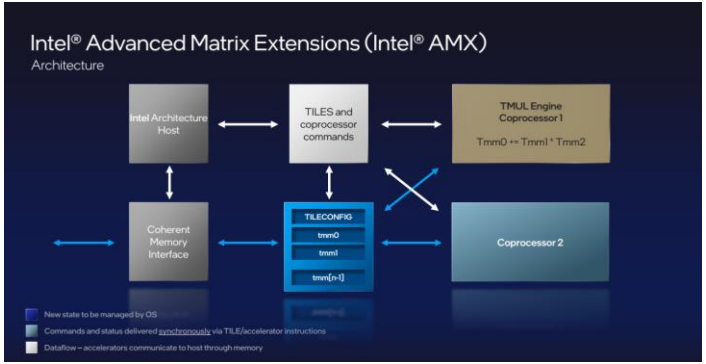
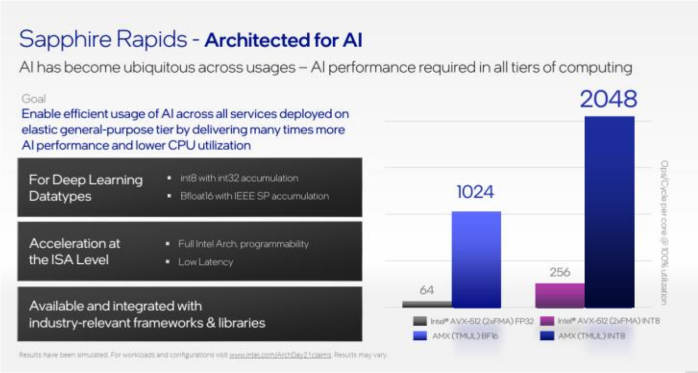
Intel® Xeon® Max Series: AMX and TMUL



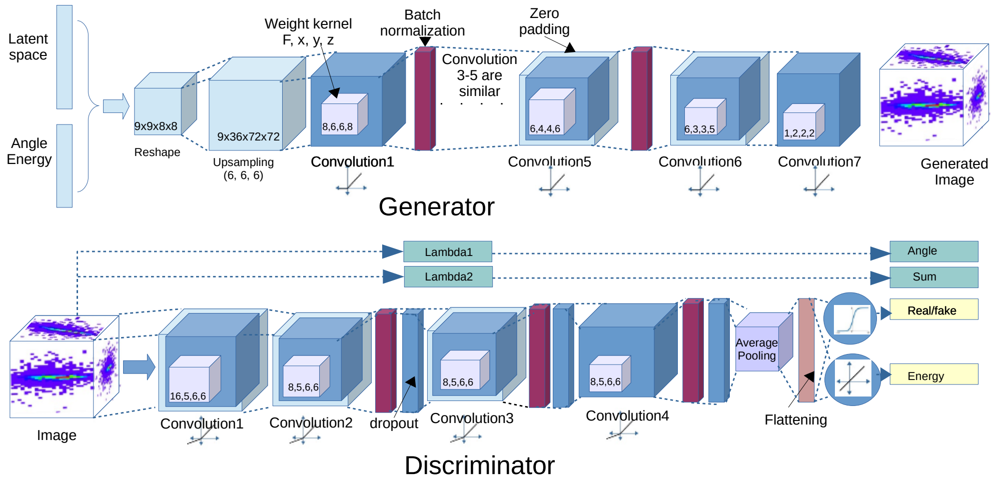




https://download.intel.com/newsroom/2021/client-computing/intel-architecture-day-2021-presentation.pdf

More about 3DGAN

- Training in 2 steps (use of transfer learning)
  1) Dataset with E_p = 100 - 200 GeV – 137k samples, 130 epochs
  2) Dataset with E_p = 2 - 500 GeV – 400k samples, 30 epochs



- Discriminator
  - Real/fake probability
  - E_p estimation
  - Angle calculation
  - Total energy calculation

  Auxiliary tasks

- Loss:

$$L_{3DGAN} = W_G L_G + W_P L_P + W_\theta L_\theta + W_E L_E$$