Recent Advances in the GAN-Based Fast Calorimeter Simulation of the ATLAS Experiment

LHCC Student Poster Session
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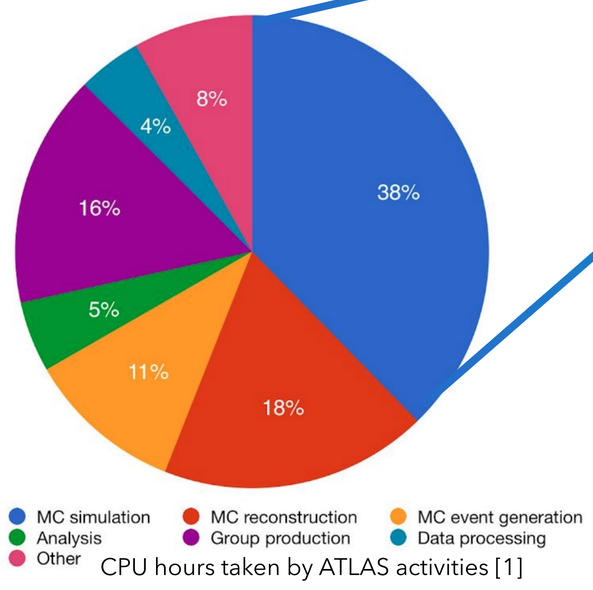
As shown at CHEP 2024 — indico.cern.ch/event/1338689/contributions/6016136

Detector simulation takes the **largest part** of ATLAS computing resources [1], of which **~80%** is just taken by **calorimeter simulation** [2]

Expected to increase with HL-LHC!

We need **solutions to ease this burden**!



CPU hours taken by ATLAS activities [1]

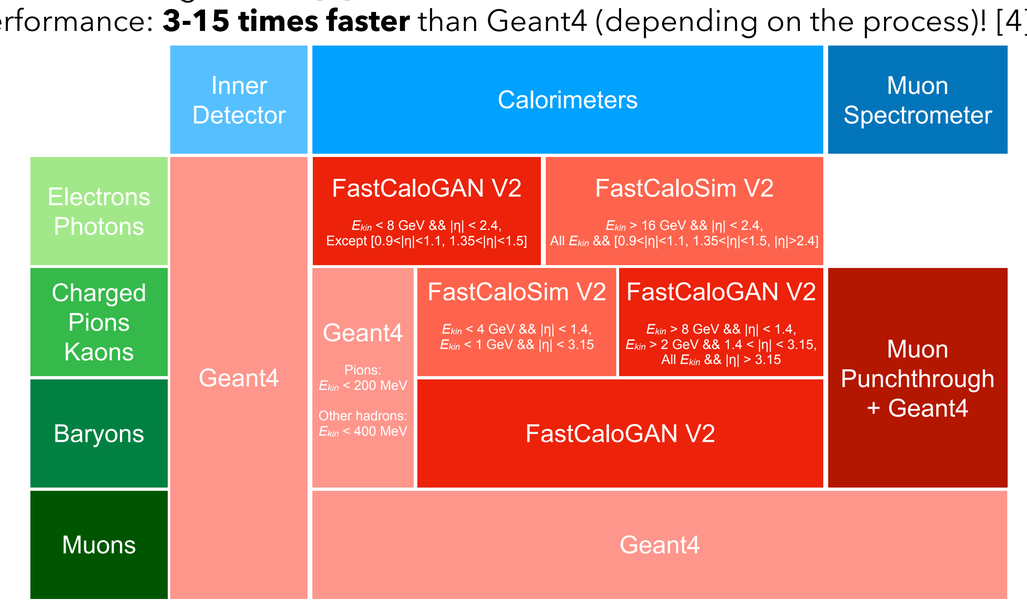
1 **Simulators** to simulate calorimeter response **fast and precisely**. Also based on Machine Learning (ML).

ML systems need large resources for training!

2 **Distribute** the heaviest part **to additional resources**.

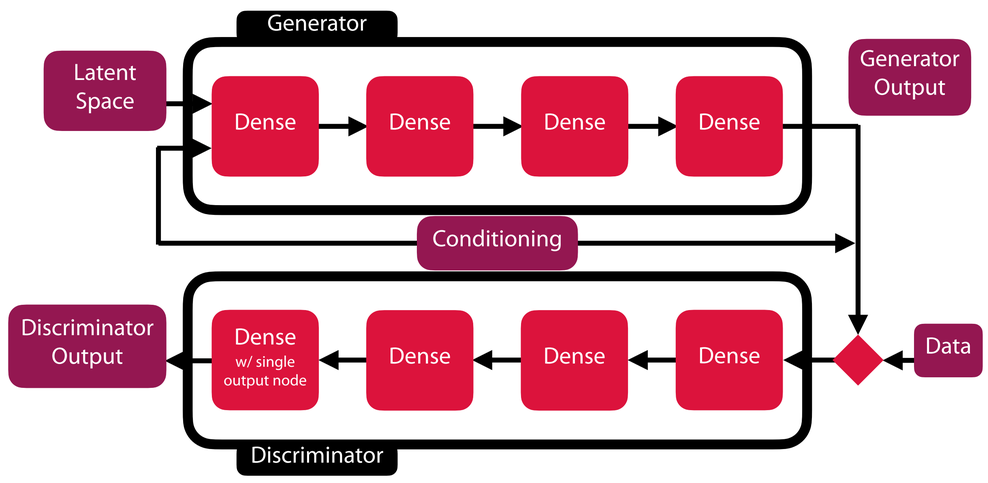
AtlFast3

- AtlFast3 is the ATLAS fast simulation tool, already in production for Run 3 [2]. It combines two fast simulation systems:
  - **FastCaloSim**, based on parametrisations;
  - **FastCaloGAN**, based on **GANs** (*Generative Adversarial Networks*).
- The **reference** for performance evaluation is the "traditional" simulation system ***Geant4*** (*full simulation*). Depending on particle type and energy, AtlFast3 employs **the fast simulation system returning the most accurate simulation** with respect to Geant4 (image below [3]).
- Performance: **3-15 times faster** than Geant4 (depending on the process)! [4]



FastCaloGAN

- Fast simulation system based on **Wasserstein GANs** [5].
- **Simultaneous training of two neural networks**:
  - **Generator**: aims to generate Geant4-like showers;
  - **Discriminator**: aims to distinguish between generated and Geant4 showers;
  - Once equilibrium between the two is reached, FastCaloGAN is ready to simulate calorimeter response, which it does **much faster than Geant4 with good accuracy.**



- **Work in progress** for final part of Run 3/Run 4:
  - **Improved** and finer voxelisation that reduces bias due to calorimeter geometry (fineness actually not that easy to handle!)
  - **Good GAN results** (good χ^2 vs Geant4): **GANs can be further improved!**
  - Research **diffusion** models and Invertible Neural Networks (**INNs**), to be added if results are good.

FastCaloGANtainer

- Usage of FastCaloGAN requires its GANs to be trained, which requires **large resources**!
- FastCaloGANtainer makes it possible to **train** FastCaloGAN **on unpledged resources outside CERN** (thus without using e.g. the CERN batch system *LXBATCH*).
  - **Resource saving + further performance improvement!**
- Based on an Apptainer **container** with the standard ATLAS software environment and CentOS 7 operating system.
  - Requires libraries CUDA-11 and CuDNN for GPU usage.
  - Additional software required for running is installed in the container, making it **independent** of the system where it runs.

Performance

- Training runs **3-4x faster** on Leonardo (**A100** GPUs) and 2-3x faster on CNAF-HPC with respect to LXBATCH at CERN. **Supercomputers give a great performance boost!**
- **To do**: run on other resources (also cloud), architectures (ARM) and for more particle types, code optimisation (both general and to take even more advantage of multi-CPU/GPU nodes).

The Leonardo supercomputer at CINECA in Bologna [6]

ATLAS Work in Progress

Resource	**Type and Owner**	**Hardware and Software**	**Pion Results** One GAN for all energies	**Photon Results** Two GANs, one for energies ≤ 4 GeV, one for greater energies
LXBATCH	CERN batch system. Reference cluster	CentOS 7 (for used nodes), CVMFS, HTCondor, V100 GPUs	Runtime: 12 h χ^2/NDF ~ 2	Runtime: 30-31 h χ^2/NDF ~ 5
Leonardo	The 7th most powerful cluster in the TOP500 ranking [7], at CINECA	RHEL 8.7, no CVMFS, SLURM, A100 GPUs, isolated nodes	Runtime: 3.5 h χ^2/NDF ~ 2	Runtime: 6.5-7.5 h χ^2/NDF ~ 5
CNAF-HPC	INFN-CNAF HPC cluster (close to WLCG INFN-T1)	CentOS 7, no CVMFS, SLURM, V100 GPUs	Runtime: 6 h χ^2/NDF ~ 2	Runtime: 9-10 h χ^2/NDF ~ 5

References

[1] The ATLAS Coll., *ATLAS HL-LHC Computing Conceptual Design Report*, CERN-LHCC-2020-015 (2020)
[2] The ATLAS Coll., *AtlFast3: The Next Generation of Fast Simulation in ATLAS*, *Comput Softw Big Sci* **6**, 7 (2022)
[3] Public plots: atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PLOTS/SIM-2024-004
[4] Public plots: atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PLOTS/SIM-2023-005
[5] The ATLAS Coll., *Fast simulation of the ATLAS calorimeter system with Generative Adversarial Networks*, ATL-SOFT-PUB-2020-006
[6] leonardo-supercomputer.cineca.eu
[7] TOP500 Ranking - June 2024, top500.org/lists/top500/2024/06

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