SMASH
machine learning for science and humanities postdoctoral program

Jožef Stefan Institute

Simulation of Particle Physics Silicon Detectors with Transformers

1st SMASHING WORKSHOP
October 7, 2024

I FEEL SLOVENIA

Co-funded by the European Union

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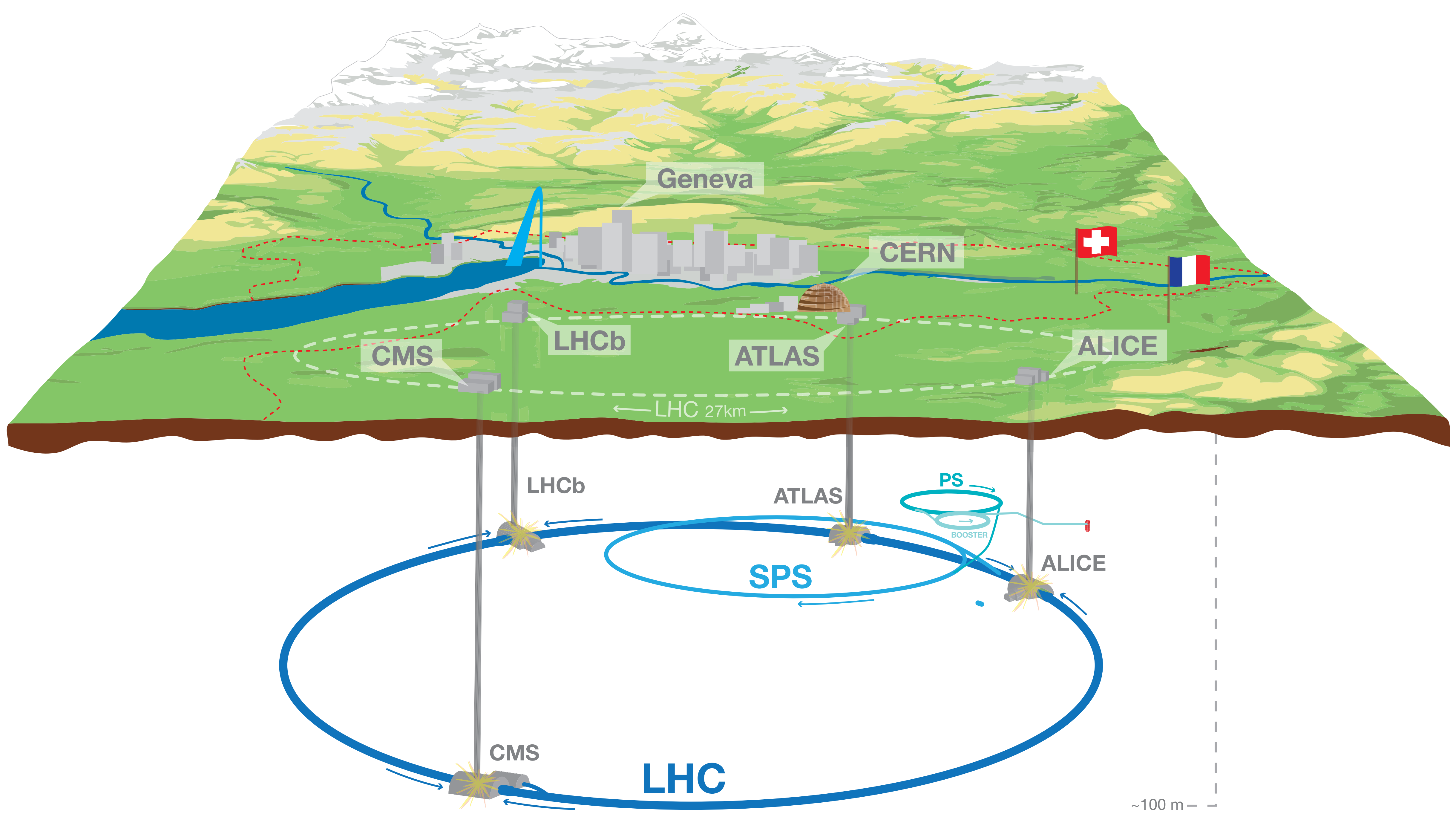
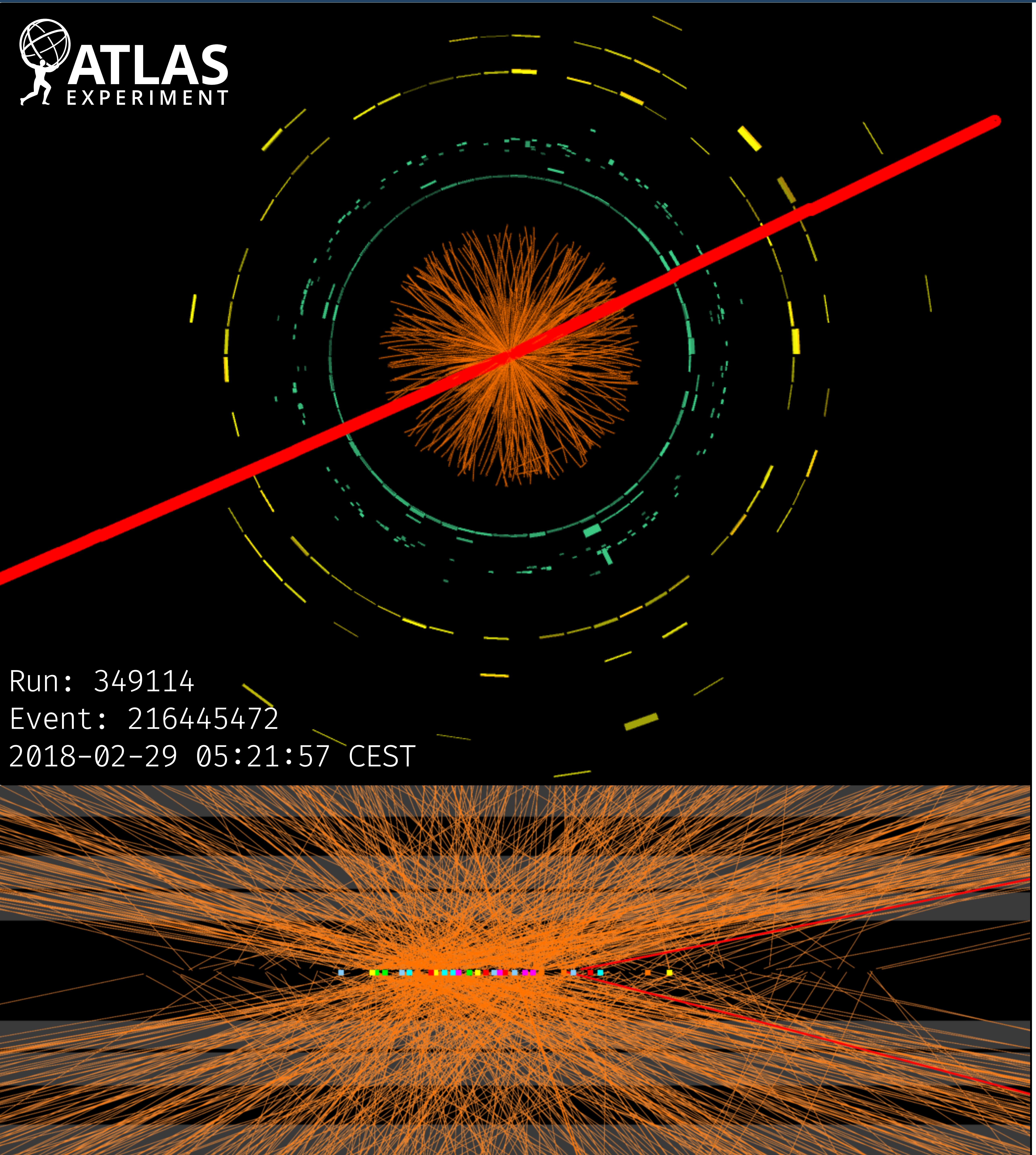
Jožef Stefan Institute



Source: CERN

- Largest particle collider — circumference of 27 km:
  - up to 40 million proton-proton collisions per second
- HL-LHC upgrade targeting 2030.
  - data rate 7-10 times greater
  - average number of collisions per bunch crossing rising to as much as 200, from 30-60 currently



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  - data rate 7-10 times greater
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- ATLAS detector a general purpose experiment.
  - Need to measure particle momentum and energy.

The Need for Monte Carlo Simulation

- A large part of the LHC physics programme relies on accurate Monte Carlo simulation of collision events.
  - every single particle needs to be simulated
  - detailed (full) detector response simulation most intensive
- Producing simulated samples → majority of experiments' CPU requirements
  - CMS used 85% CPU for Monte Carlo production during 2009-2016
  - half spent detector simulation

The Need for Monte Carlo Simulation

Source: ATLAS Software and Computing HL-LHC Roadmap

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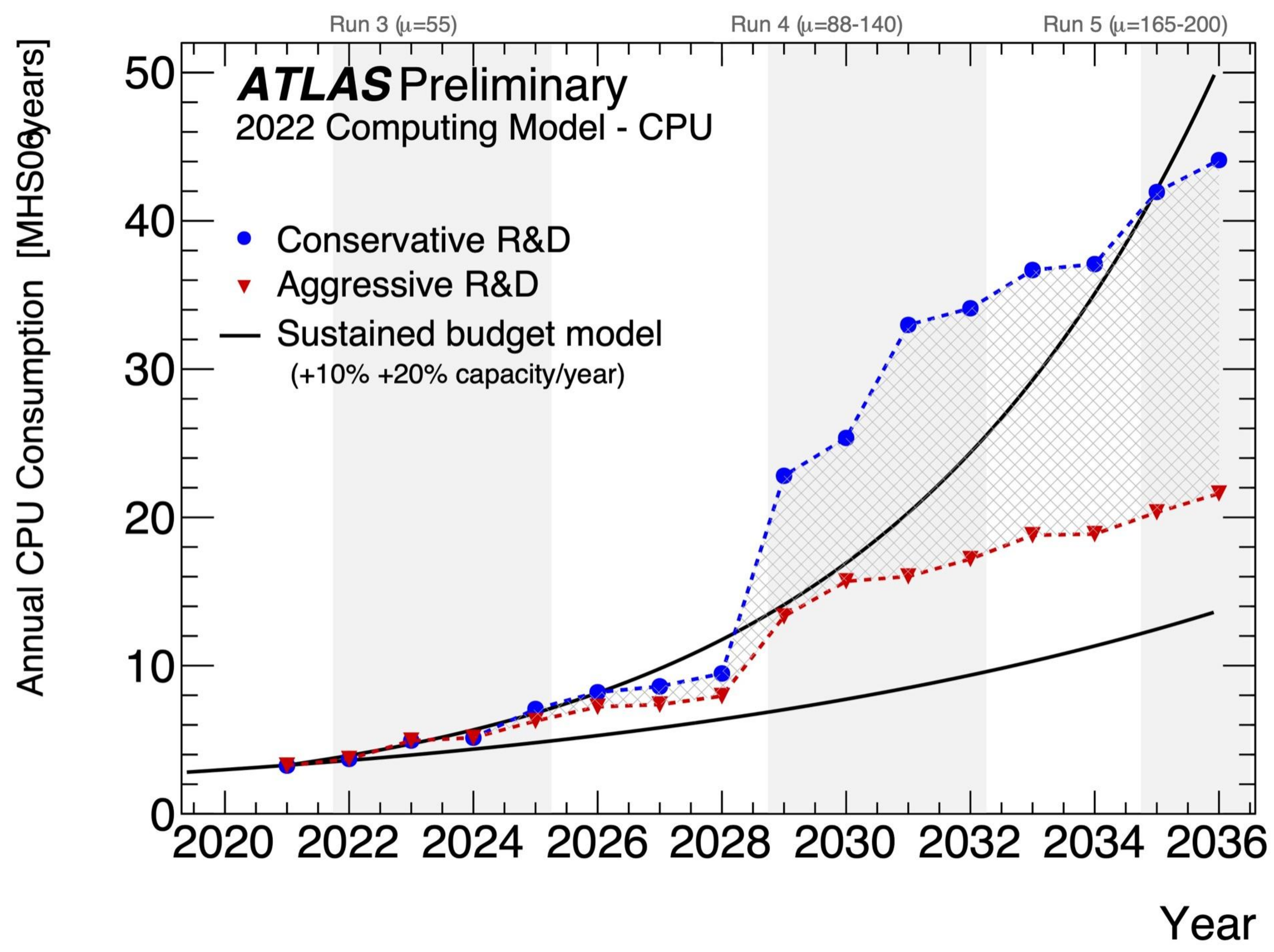
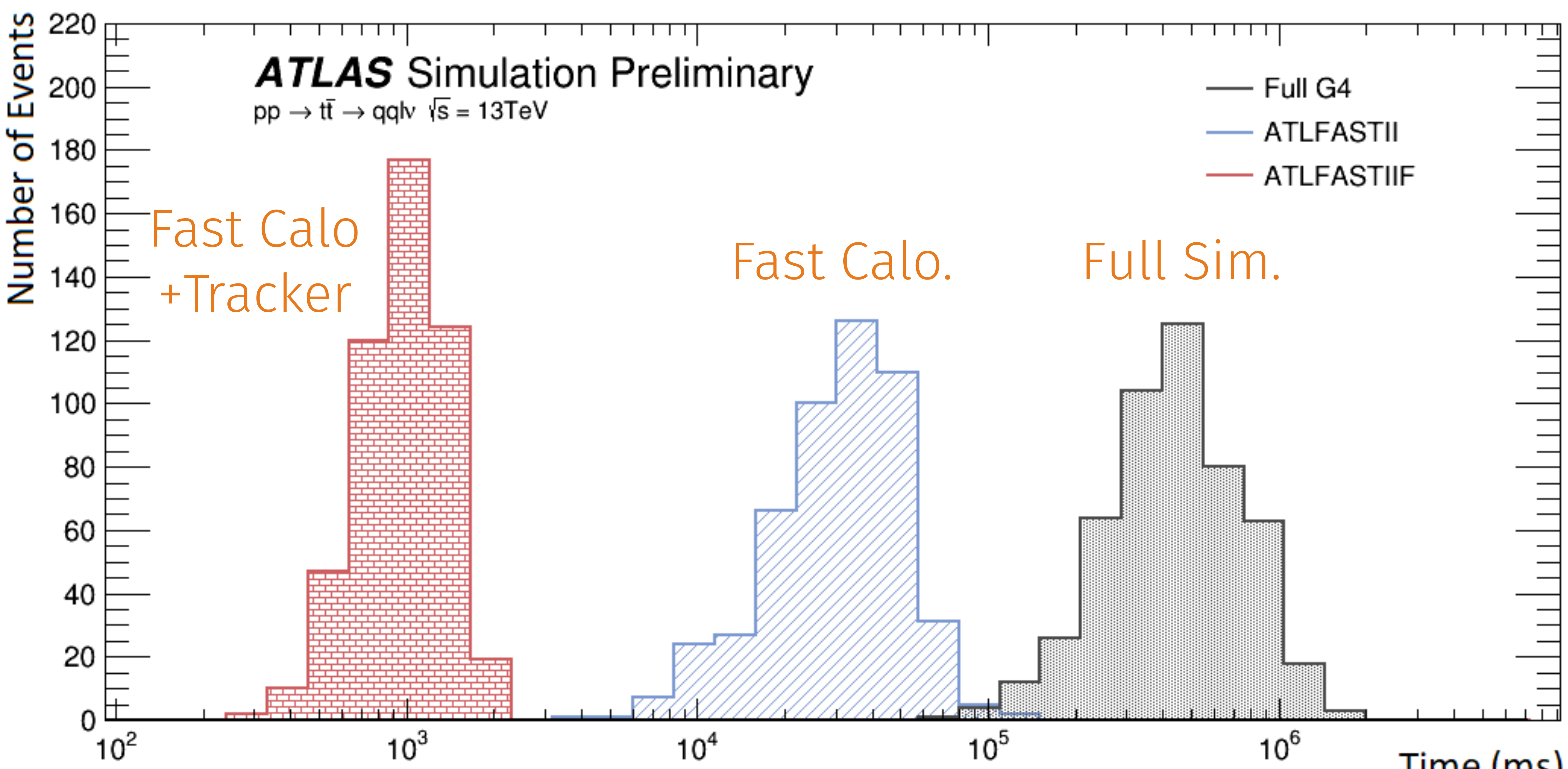


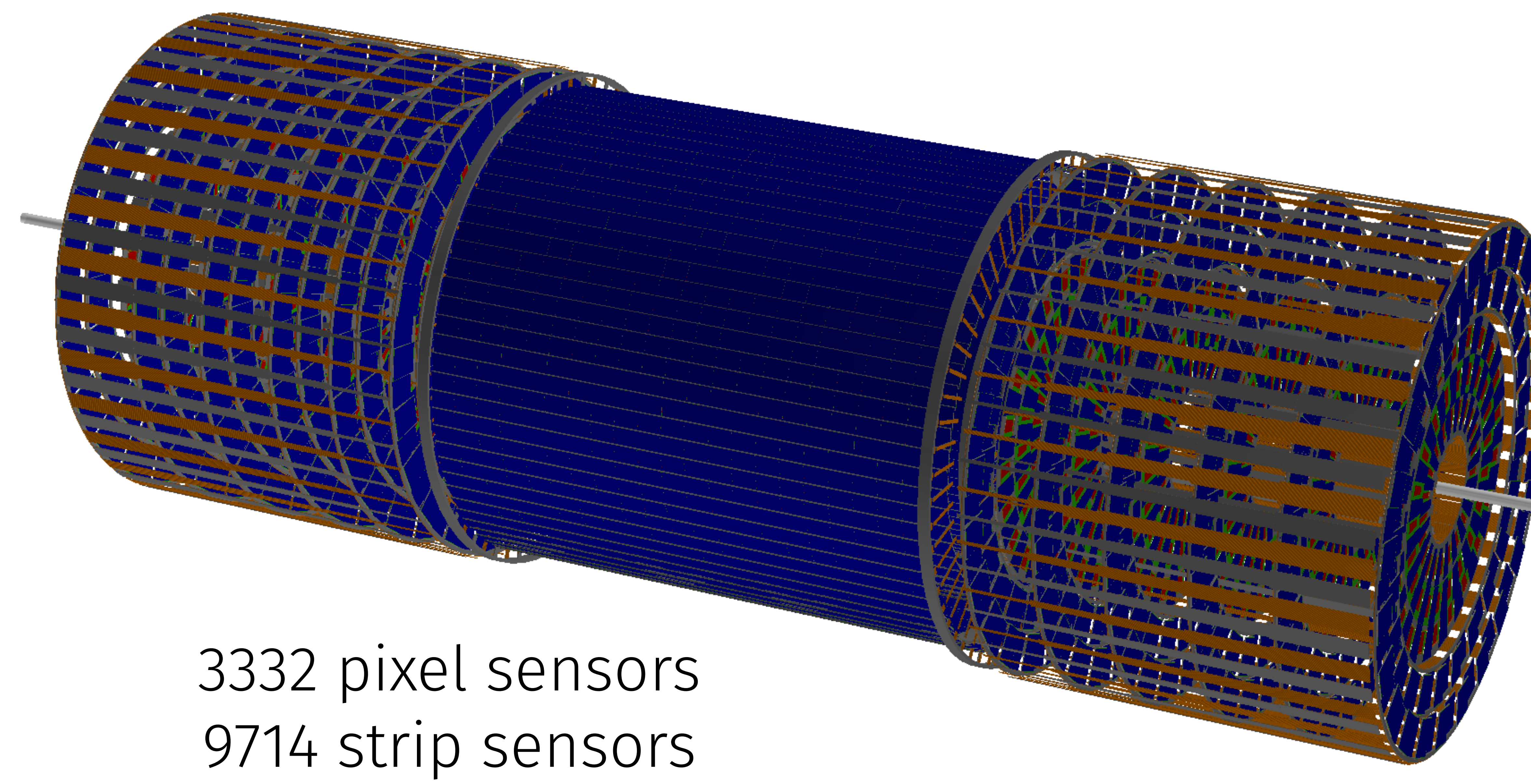
- Current methods do not scale with HL-LHC data rates and more aggressive R&D is needed.

- Large efforts to speed-up simulation — fast simulation.
  - Detector response to a particle is parameterised.
- Fast simulation for particle physics successfully applied at calorimeter level.
  - Derived for different particles at different energies and parts of calorimeter.
  - Generative neural networks also used.
  - Order of magnitude speed-up achieved.
- Tracking detectors fast simulation not production-ready yet.
  - Machine learning target of this project.



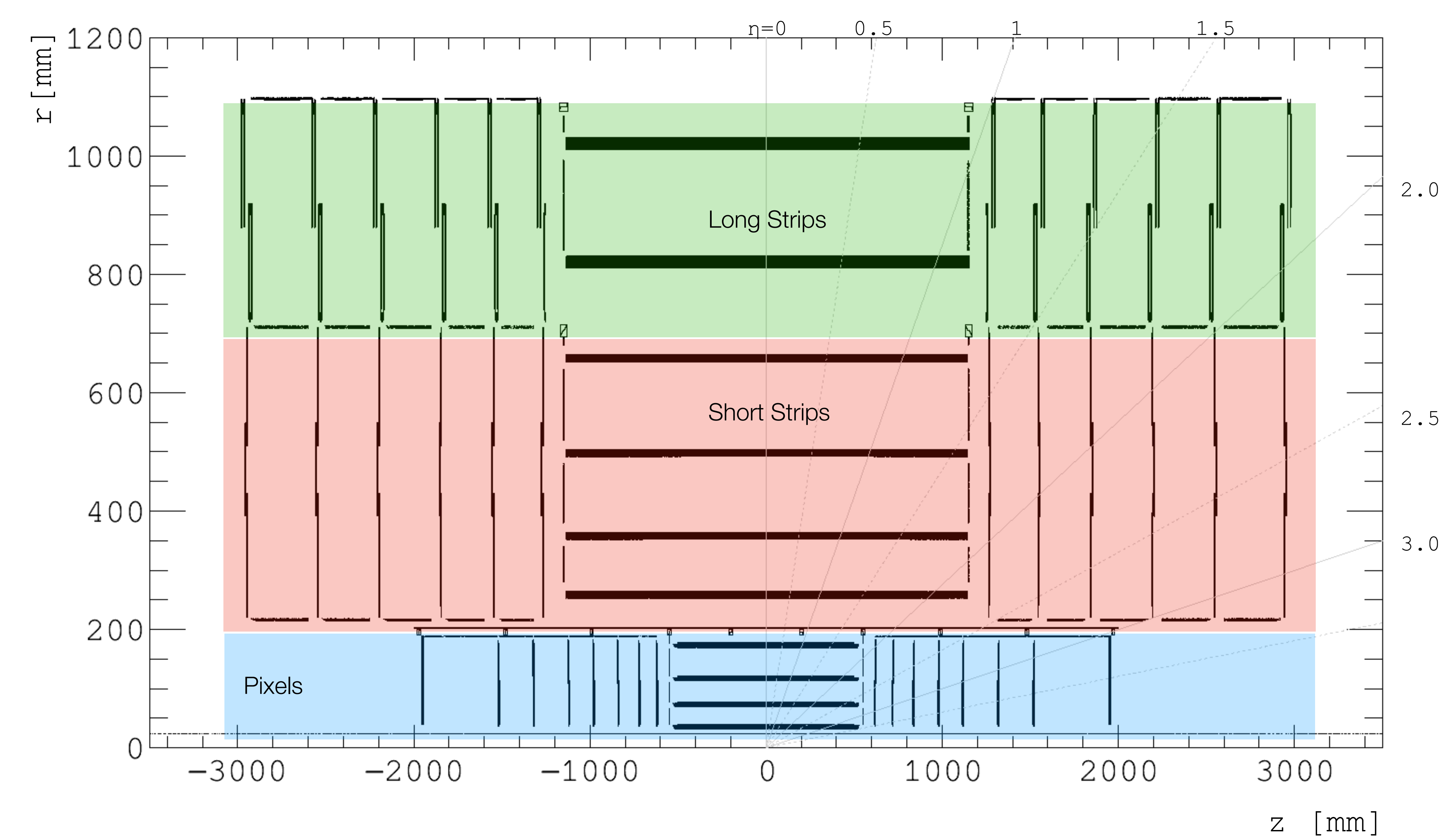
Open Data Detector

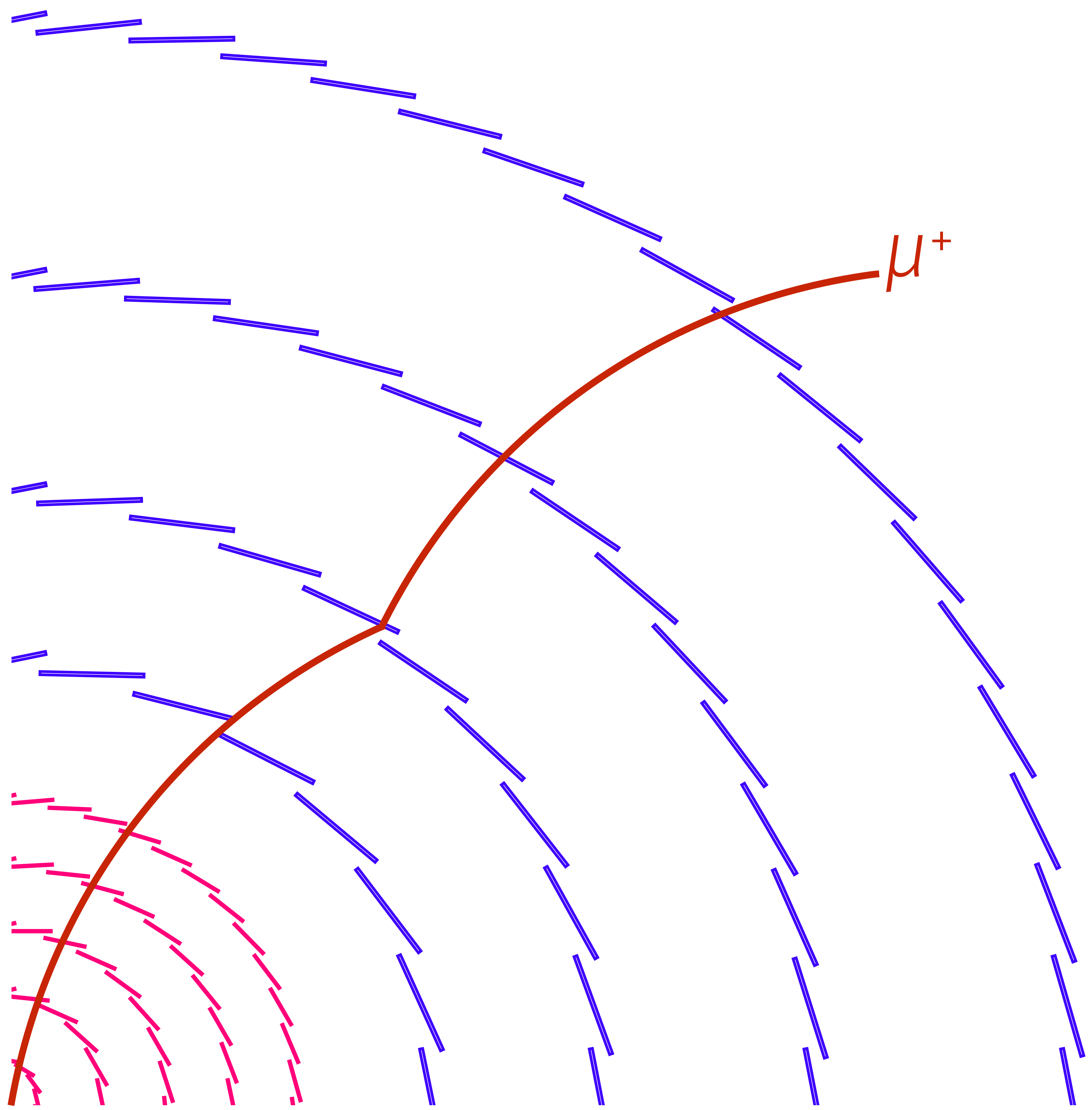
- A generic, HL-LHC style tracking detector.
- Each sensor split into multiple readout channels.
  - Can be described as a 2D surface.
- Goal to be reasonably close to a real-world detector.
  - Loosely modelled after the ATLAS ITk (58700 sensors, ~5 billion electronic channels).
- Ensures the ability to generalise R&D projects for silicon tracking detectors.



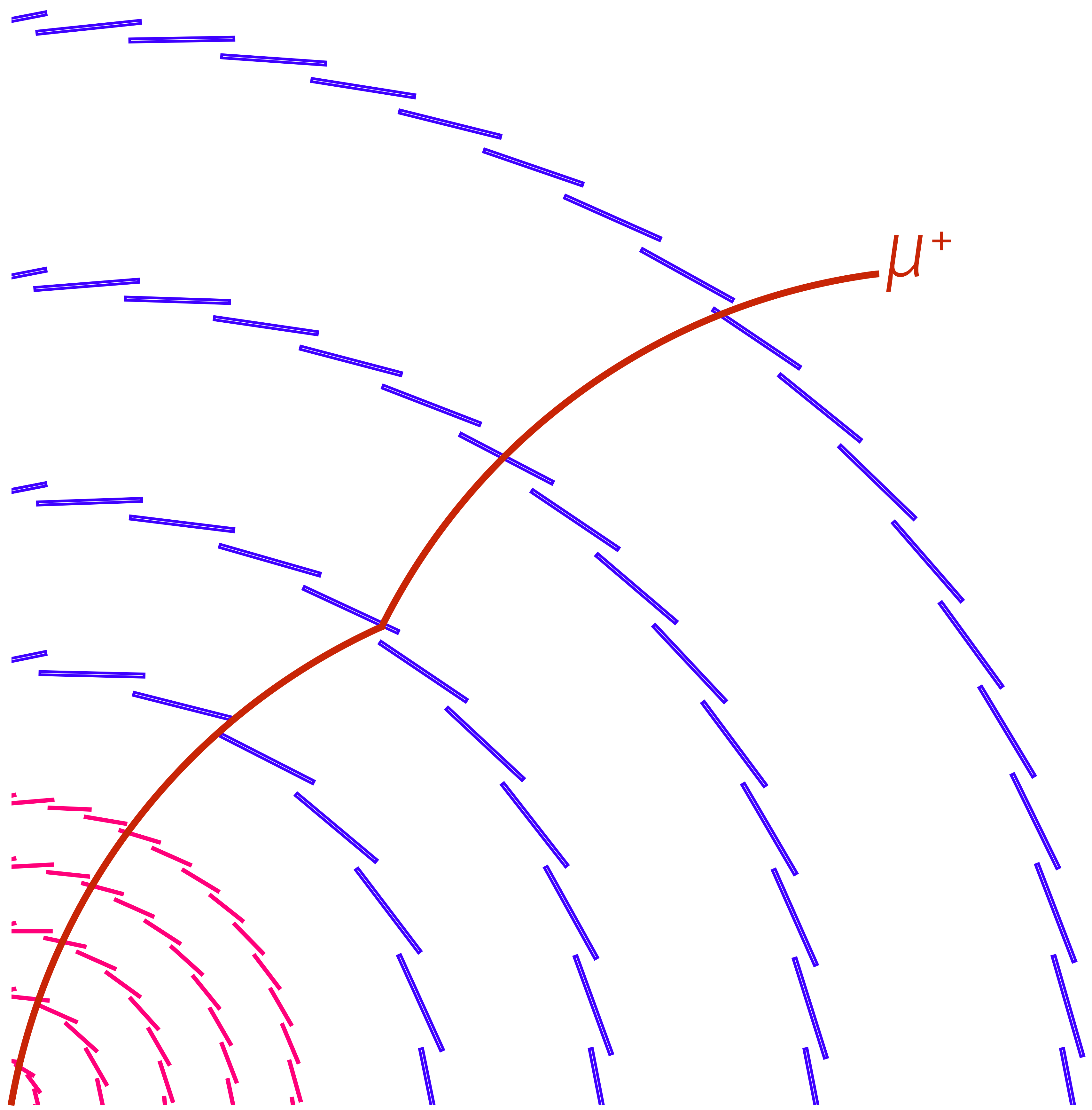
3332 pixel sensors
9714 strip sensors

Source: The Open Data Detector Tracking System

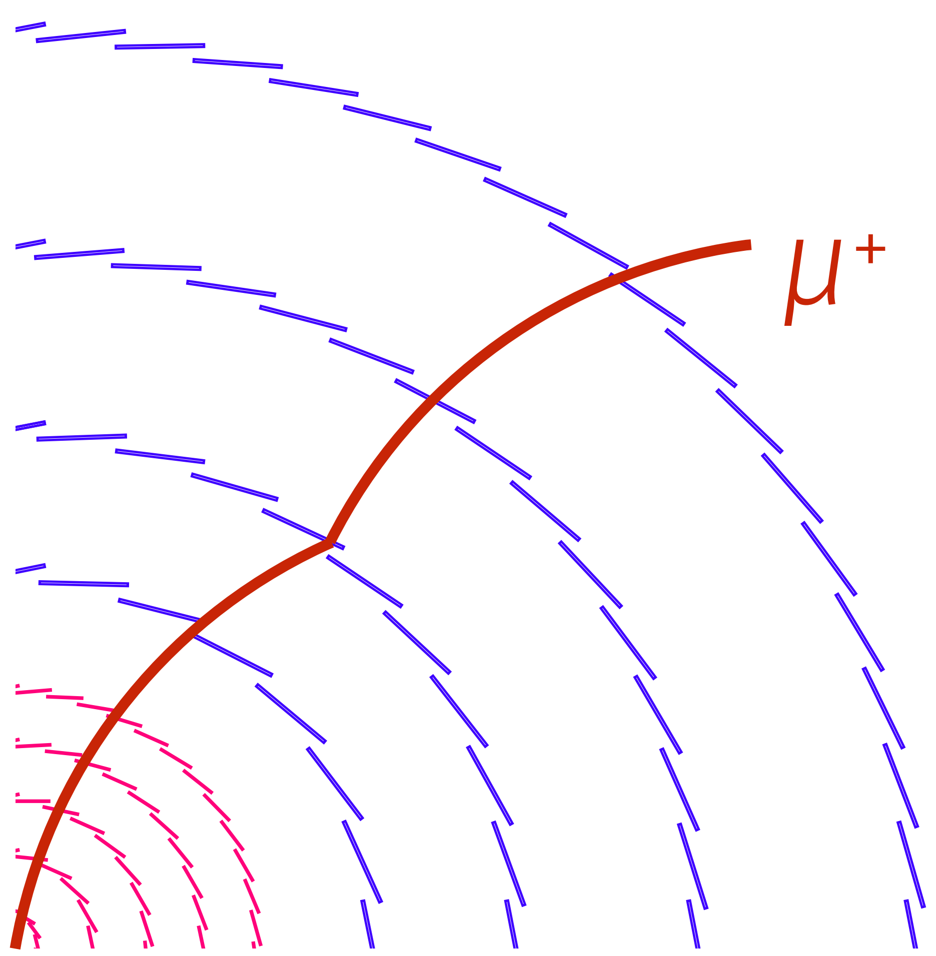


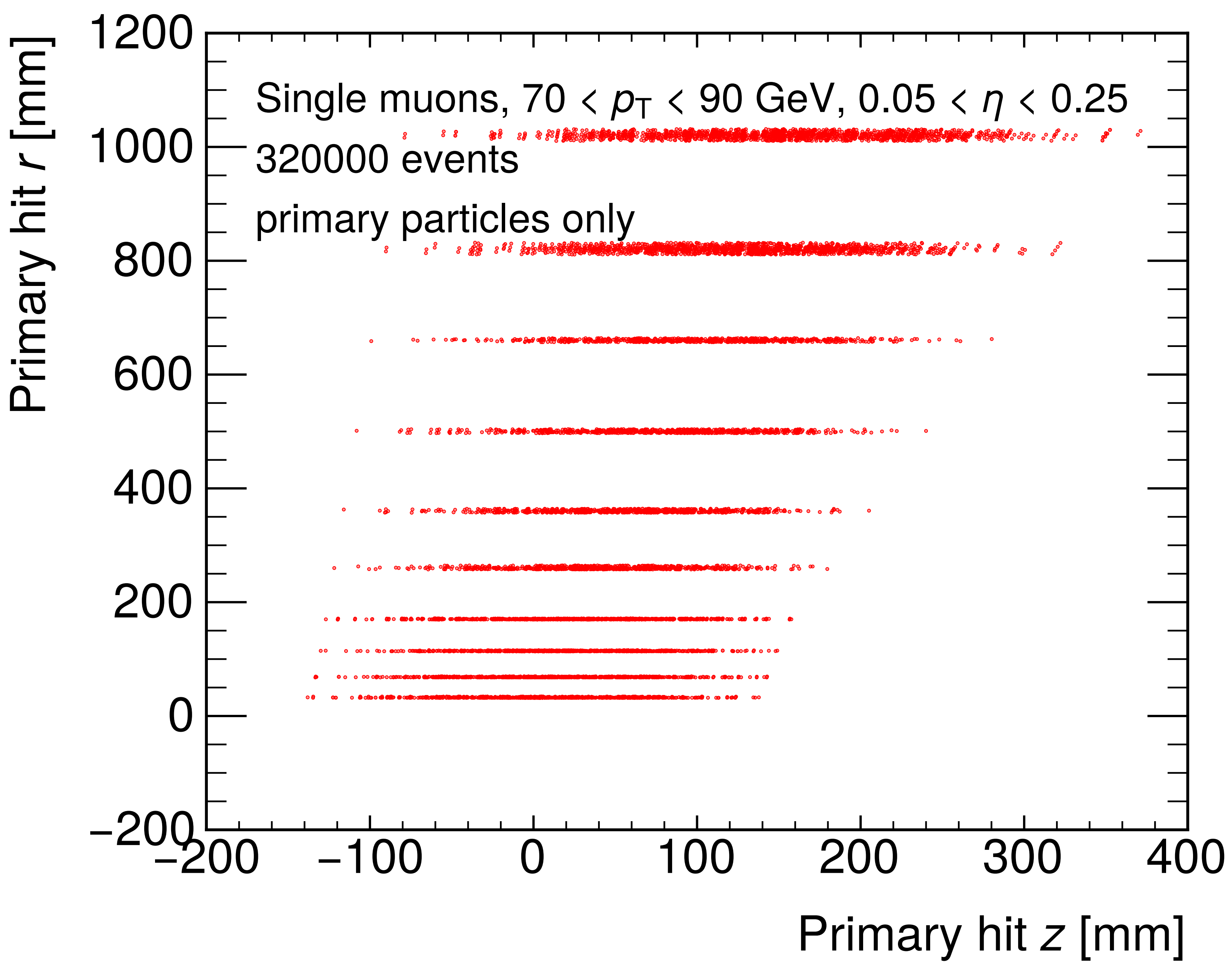


- Sensitive to charged particles (electrons, muons, charged hadrons).
  - curved track (helix) due to magnetic field
  - simulating induced electric charge in sensitive detector elements

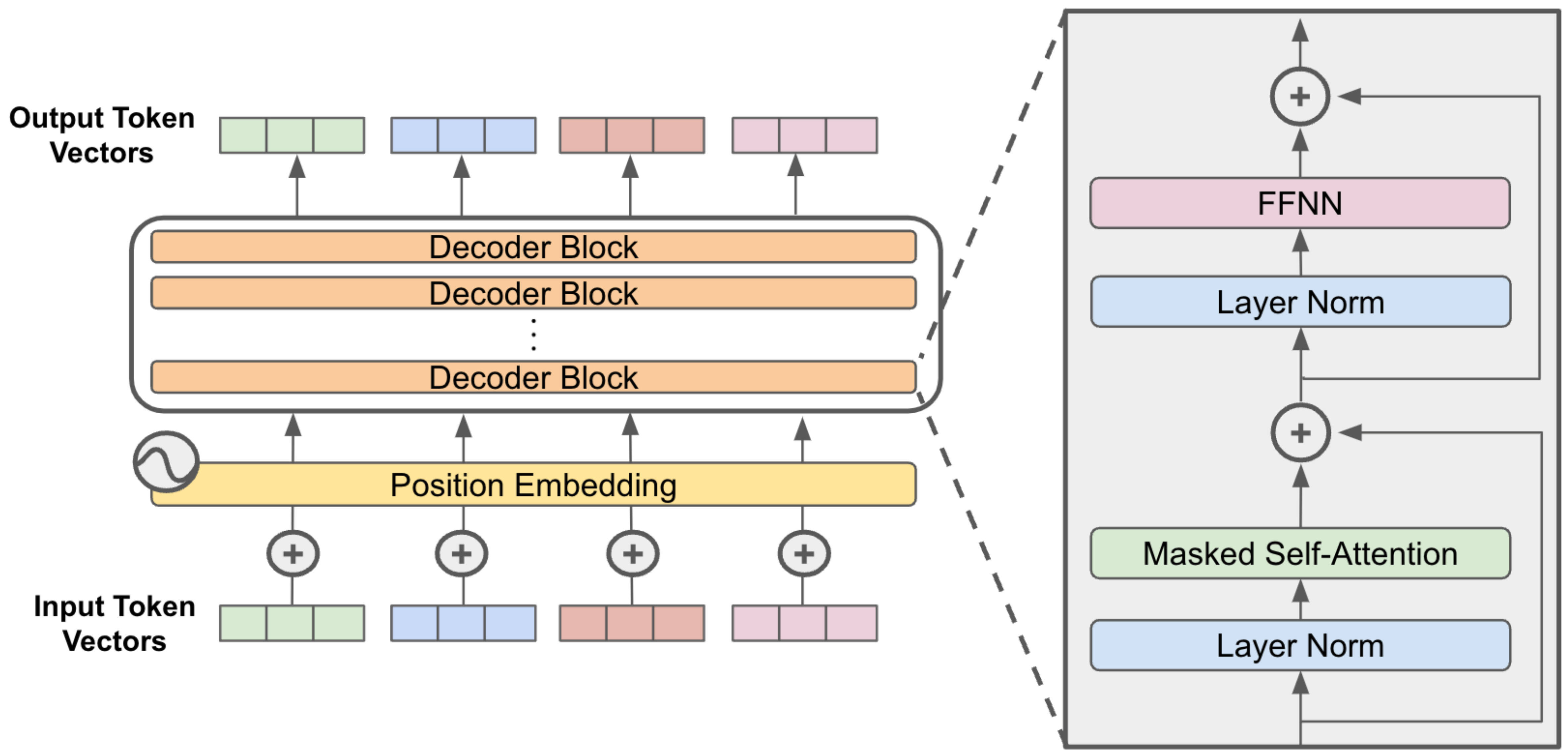


- Sensitive to charged particles (electrons, muons, charged hadrons).
  - curved track (helix) due to magnetic field
  - simulating induced electric charge in sensitive detector elements
- Multiple processes need to be simulated but for now limited to:
  - single muon events
  - multiple-scattering





- A sequence of detector hits.
  - With additional start and end "virtual hit" to describe input and output state with the same data structure.
- 7 features per hit:
  - particle ID + geometry ID
  - particle momentum (after the hit)
  - hit position on the sensitive detector (local)
- Each hit is an element of a sequence, each particle has its own sequence.
- Local coordinates taken to constrain hits on the sensitive parts and prevent them happening in the vacuum.



Source: Cameron R. Wolfe

- Transformers popular nowadays to deal with sequential data (most commonly LLMs), see 1706.03762.
- Using decoder-only architecture.
  - Input/output data are the same.
  - Target to predict the next element of the sequence.
  - The famous example are the GPT family of models.
- Specialised on discrete sequences which are tokenised (sequential integers).
  - Can be anything e.g. words, detector modules, ...
- For this application all continuous data is discretised (rounded to two decimal points) and each feature is tokenised separately.

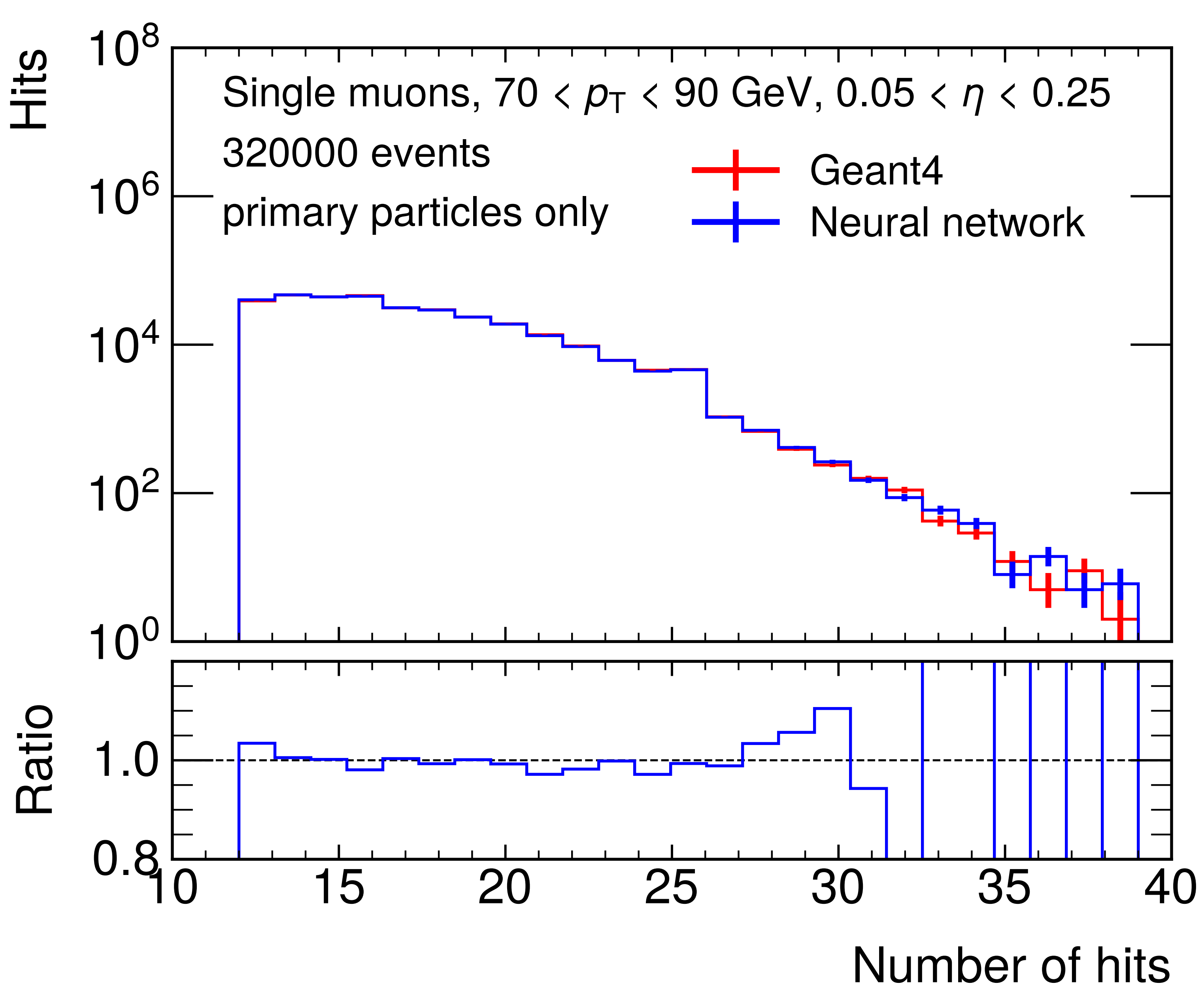
Training & Inference Setup

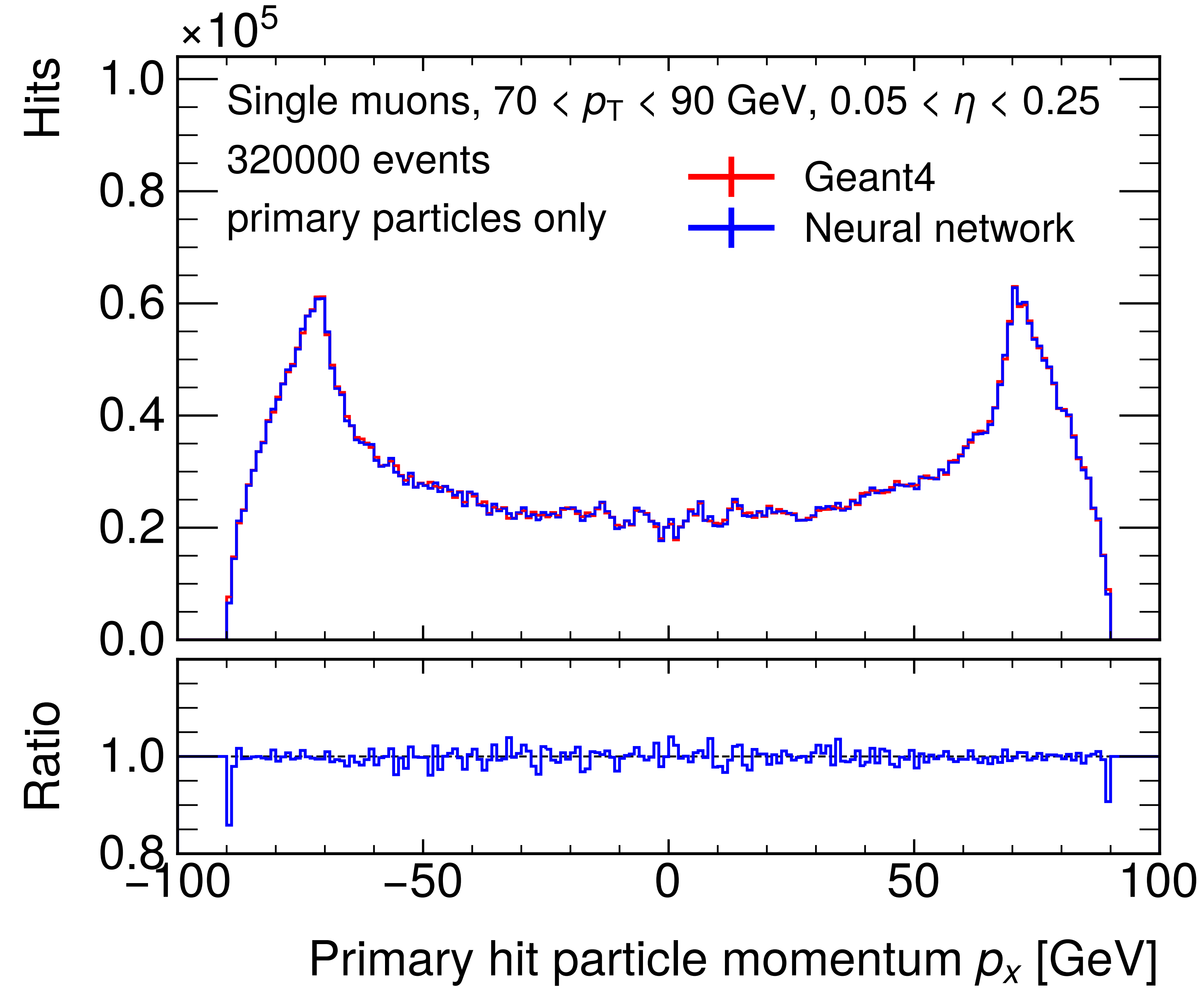
- Sample details:
  - single muons, $70 < p_T < 90$ GeV, $0.05 < \eta < 0.25$
  - 320000 events
  - training : validation : test = 2 : 1 : 1
  - augmented with random numbers between 1 and 10000
- Training performed on a workstation with a NVIDIA GeForce RTX 4090 GPU.
  - Duration ~1 week.
  - Vega also used but not for these specific results.
- Learning rate variation using cosine annealing with warm restarts with a period of one epoch and fixed amplitude.
- Inference: most probable next sequence element

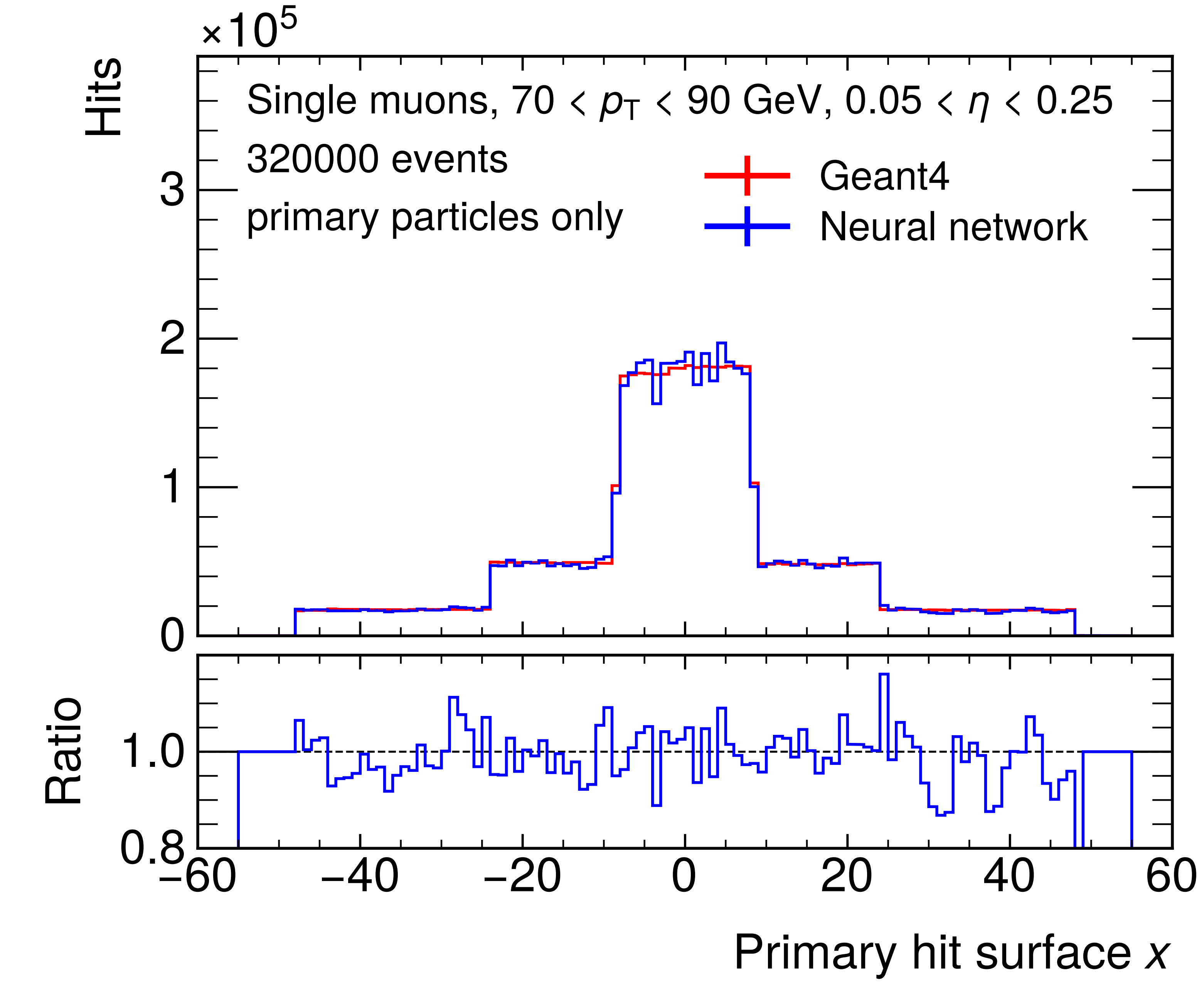
Model Parameter	Value
input dimension	128
layers	3
heads	4
feedforward dim.	512
activation	GELU
dropout	0.1

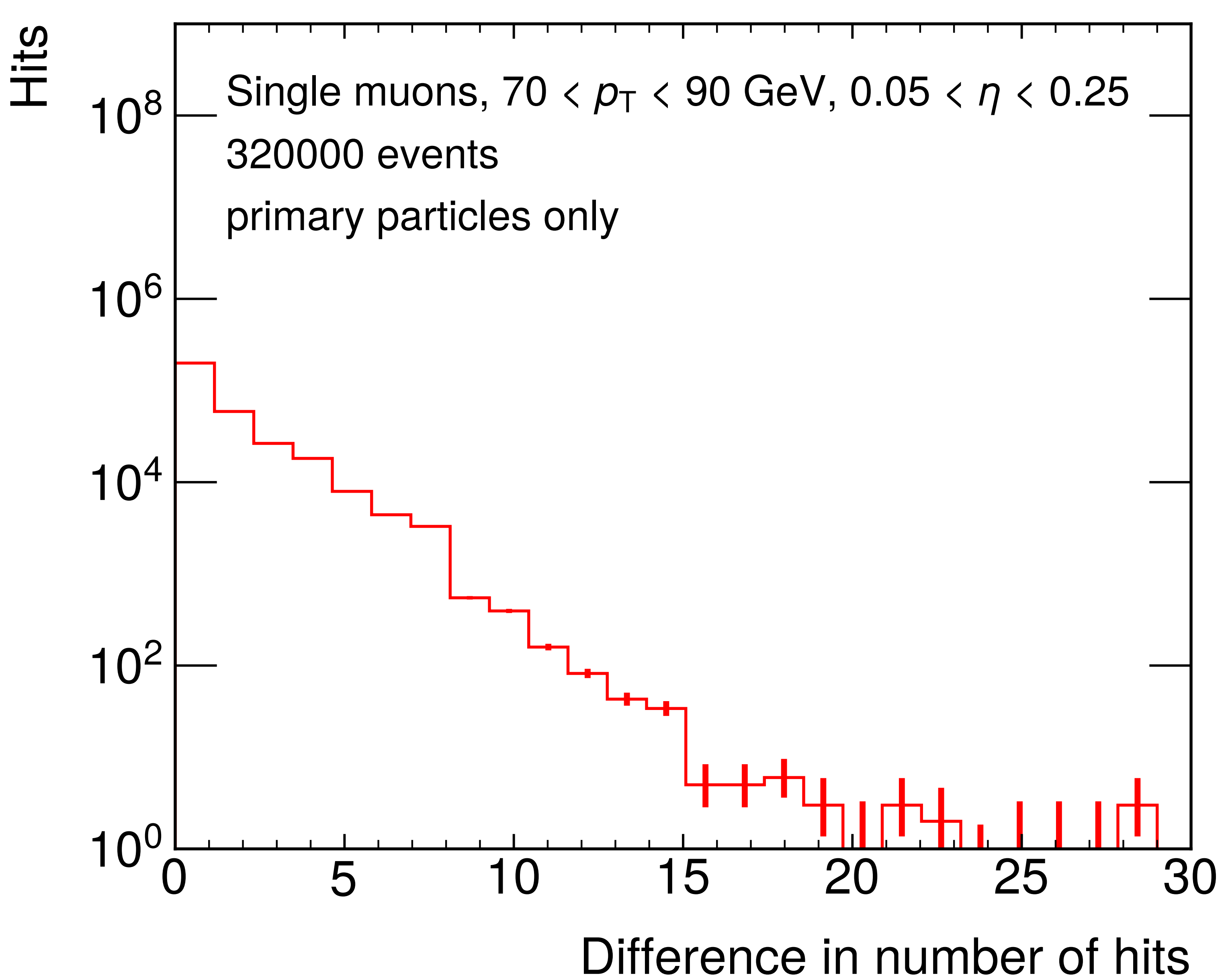
Training Parameter	Value
epochs	6000
optimizer	AdamW
learning rate	0.001
weight decay	0.01
gradient clipping	5.0
batch size	512

Results: Simulation (1)



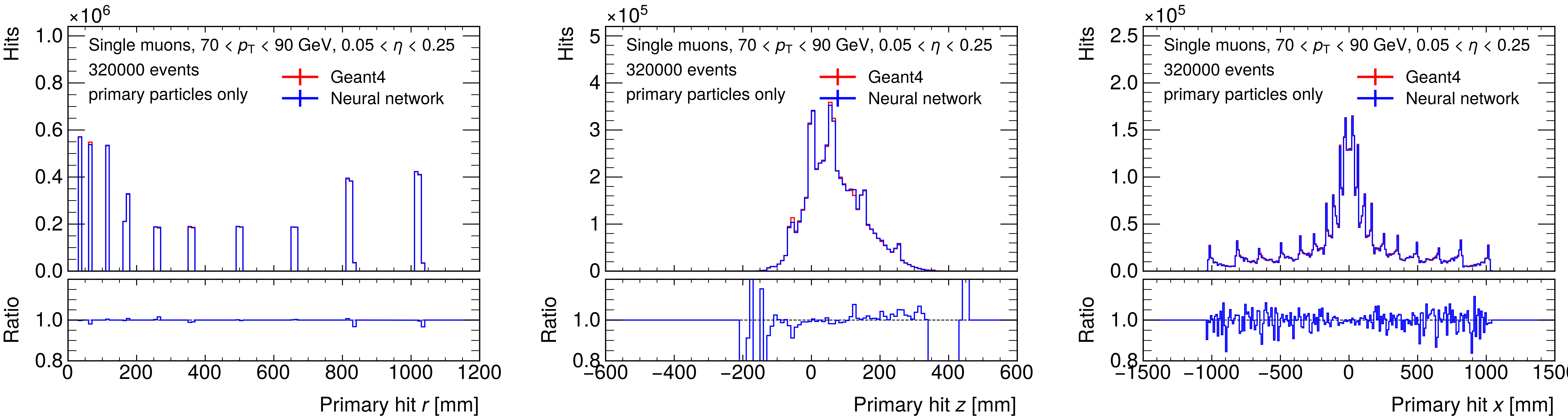




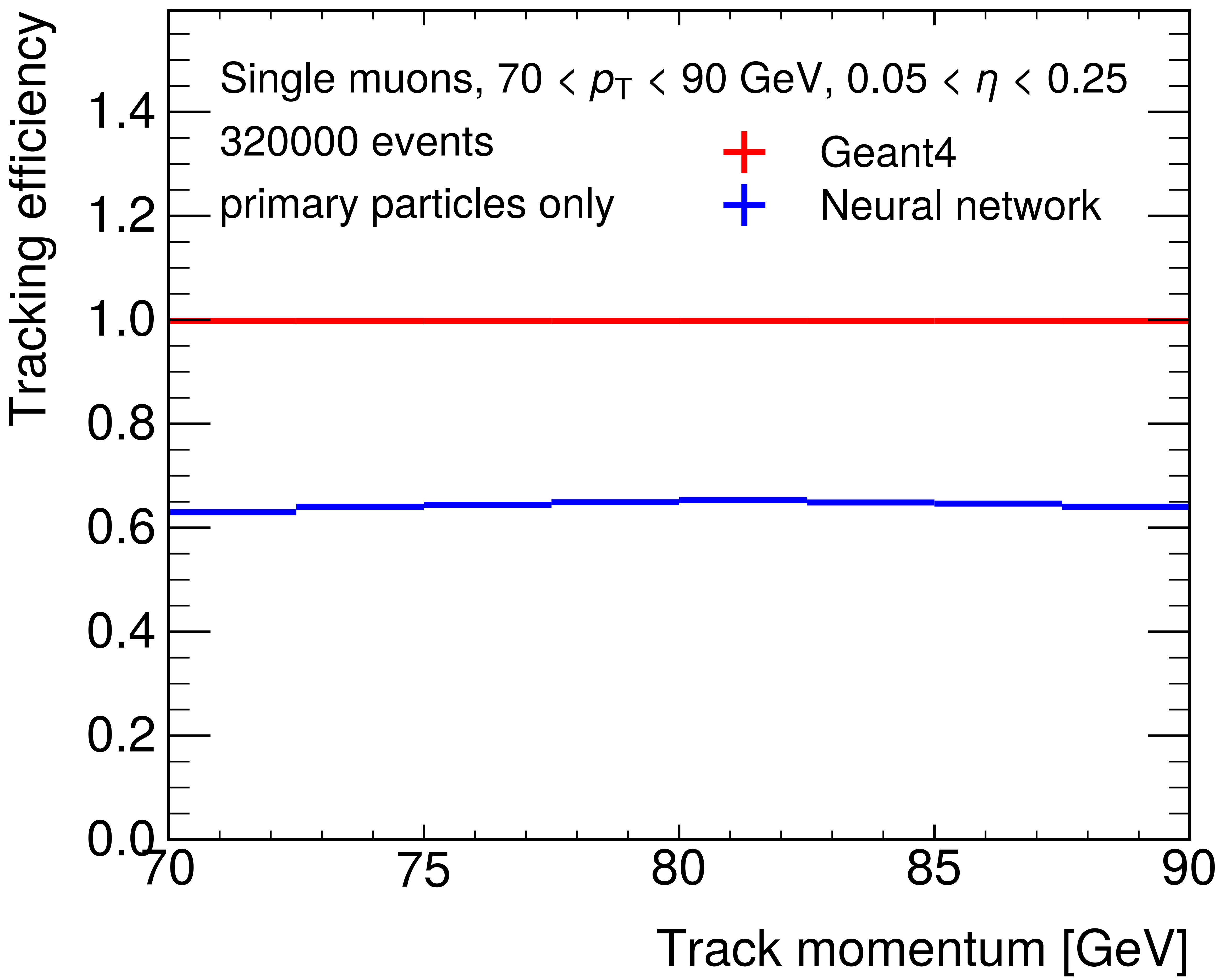


- Good agreement with full simulation.
  - Coordinates fluctuating a bit up to ±10 %.
- Number of hits accurately reproduced.
  - Some difference seen but random numbers included in inference.

Results: Simulation (2)



- Global coordinates show good agreement describing complex detector structure.
- Larger deviations in tails of the *z*-coordinate due to lower statistics.
- Inference also performed on the same GPU: ~4 s / 10k particles



- Evaluating performance using the ACTS (A Common Tracking Software) framework.
  - Default test setup for the Open Data Detector.
- Seeding efficiency only ~65 % compared to 99 % for full simulation.
  - Hit displacement from the estimated helix is too large.
  - Rounding has no significant effect on the reference sample.
  - Detailed investigations ongoing.

- Transformers can describe a sequence of physics data very well.
    - Physics performance not sufficient yet, needs optimisation.
- Training relatively long, but inference is fast.
- Future plans:
    - Optimise the current setup for better tracking performance.
    - Describe continuous features with floating point numbers.
    - Try proper generative sampling of a transformer.
- I want to thank for ideas and tips from my ATLAS collaboration colleagues and the Visual Cognitive Systems Laboratory at Faculty of Computer and Information Science.

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Co-funded by the European Union

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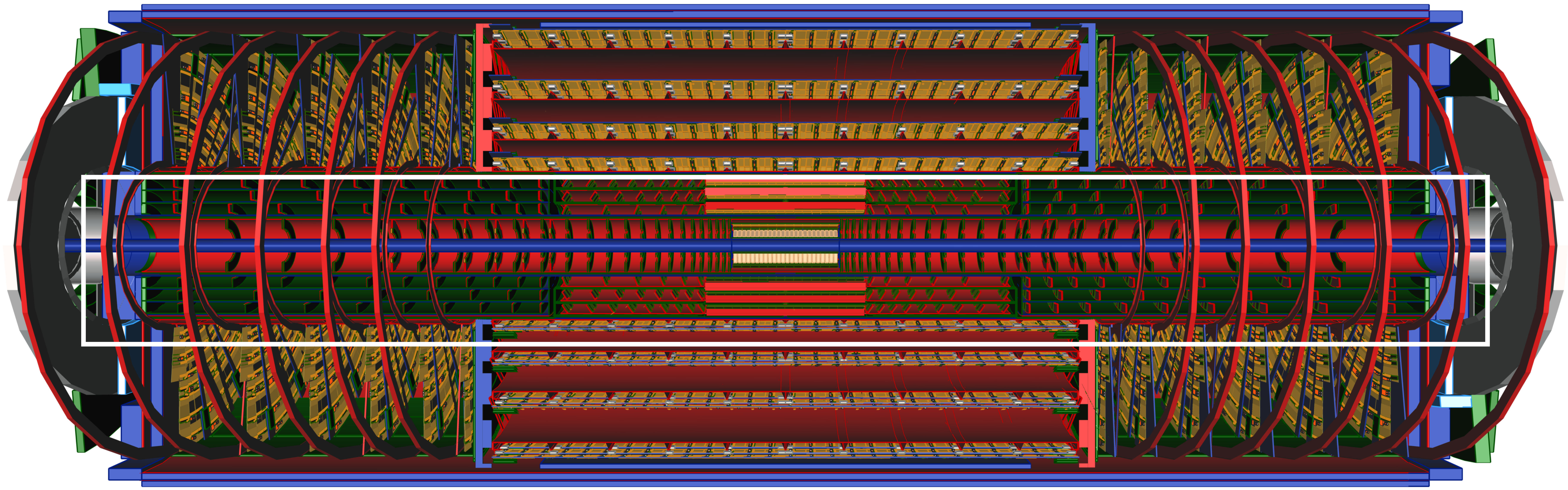
The operation (SMASH project) is co-funded by the Republic of Slovenia and the European Union from the European Regional Development Fund.



Source: ATL-PHYS-PUB-2021-024

Pixel detectors

- 2D silicon detectors
- 5 barrel, 9 endcap layers
- 9164 modules
- up to 614400 readout channels per module

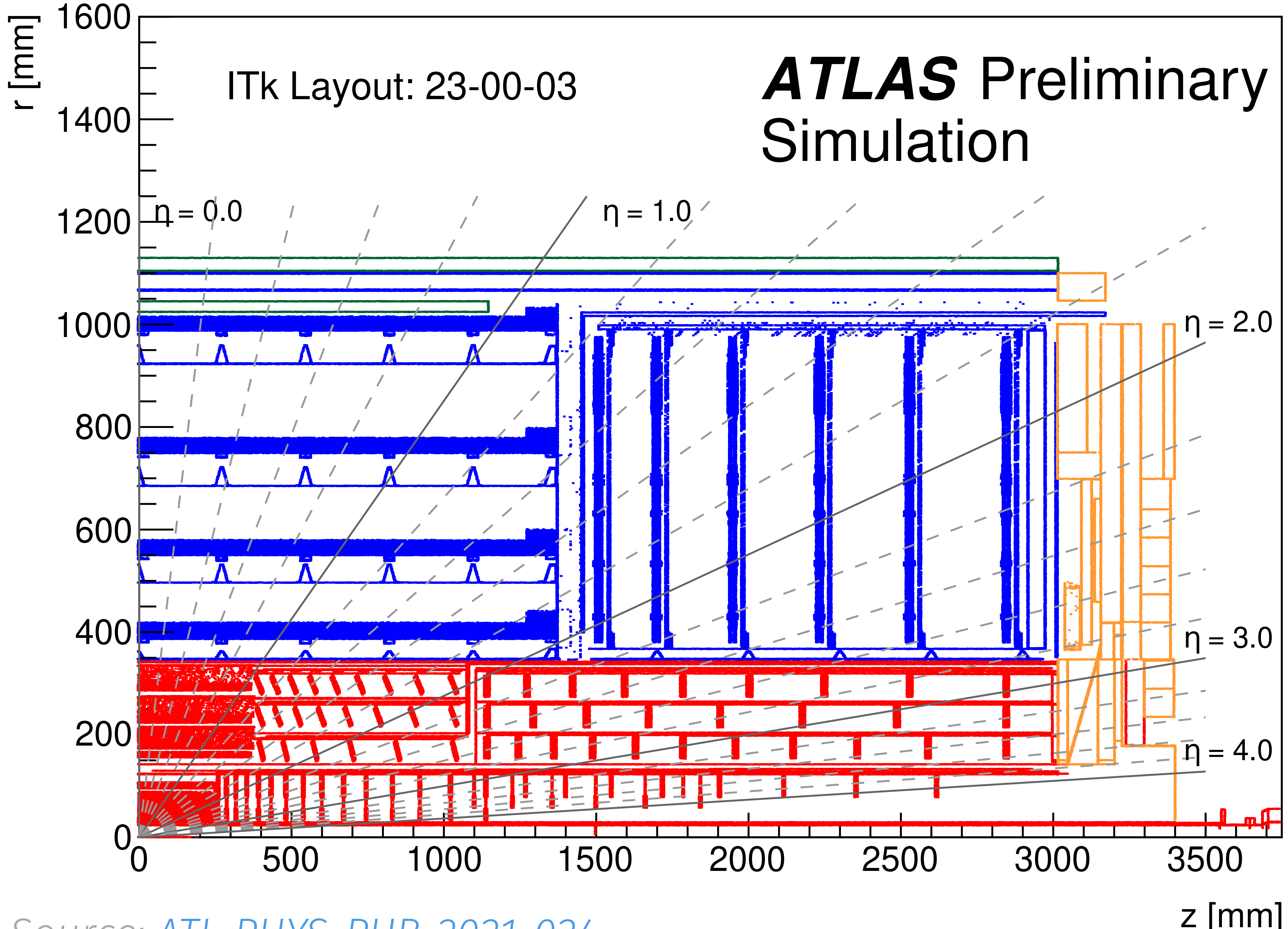
Strip detectors

- 1D silicon detectors
  - double-modules with 90° rotation to gain 2D detection
- 4 barrel, 6 endcap layers
- 49536 modules
- up to 1536 readout channels per module

ITk Pixel Modules Detail

ITk Strip Modules Detail

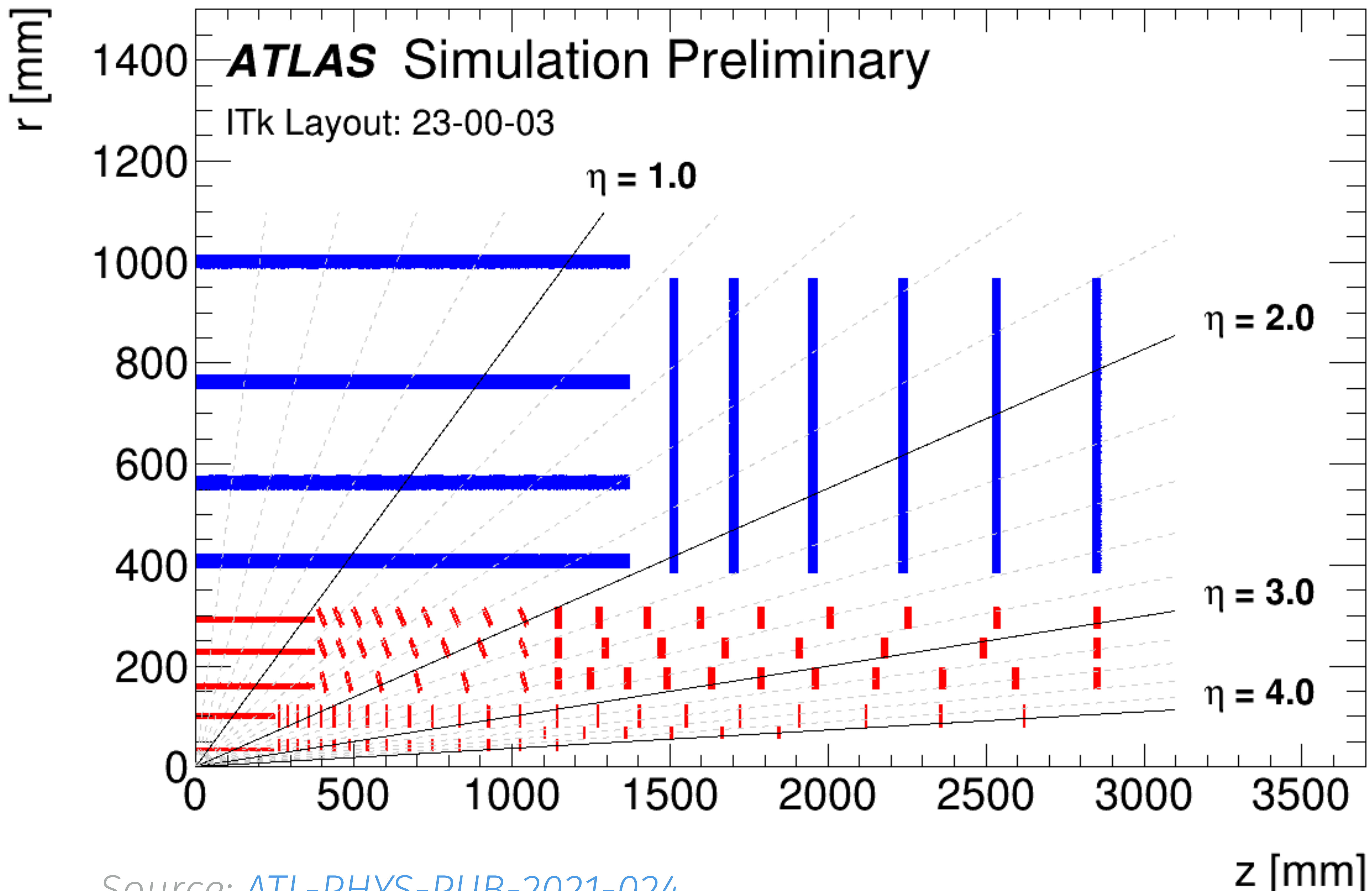
red: ITk Pixel System, blue: ITk Strip System



Source: ATL-PHYS-PUB-2021-024

- Particles interact with all the material of the detector.

red: ITk Pixel System, blue: ITk Strip System



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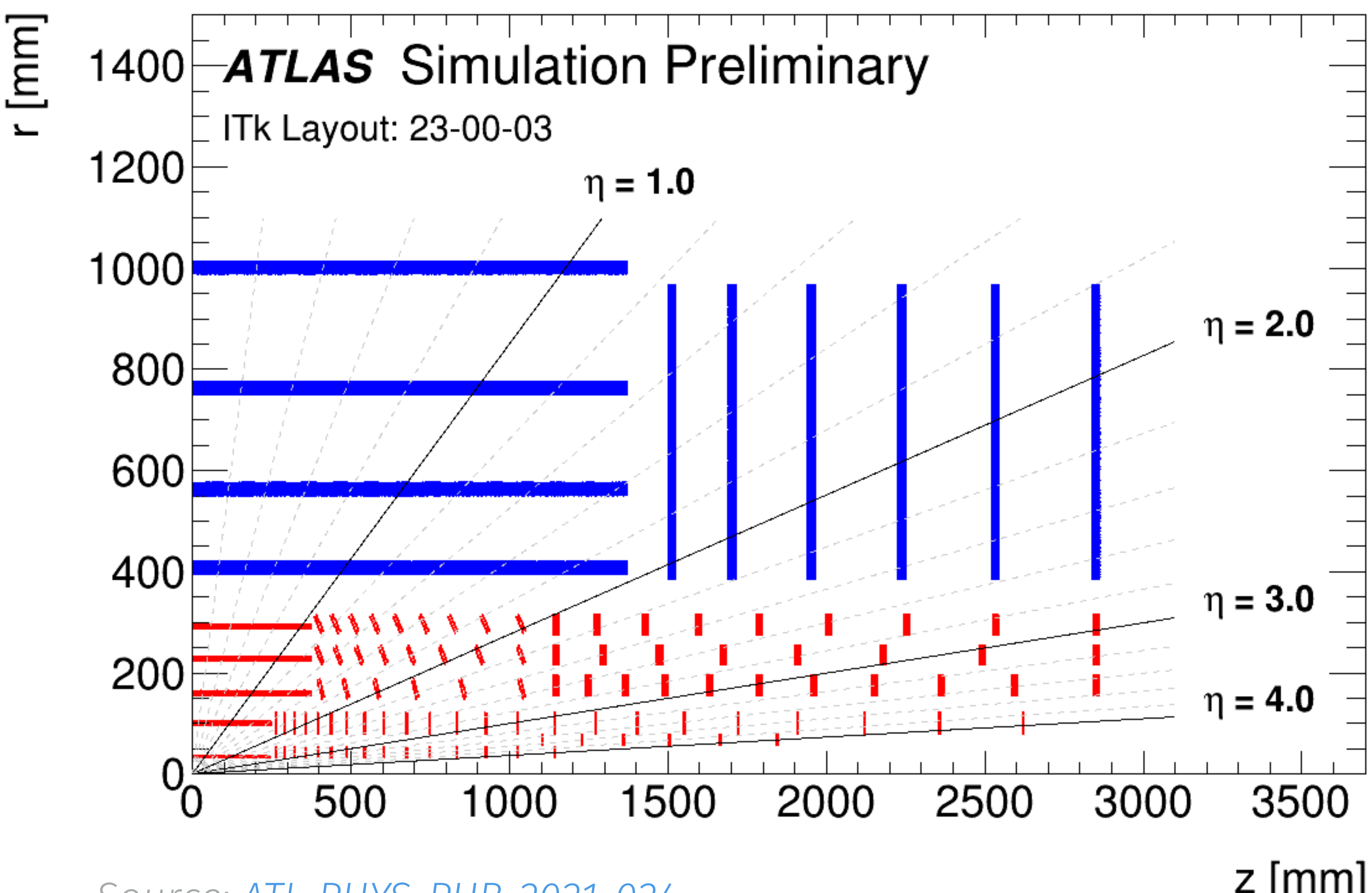
- Particles interact with all the material of the detector.
- Only the sensitive detector part can actually detect charged particles.
  - Measuring the energy loss via induced electric charge.

Simulation of Silicon Tracking Detectors

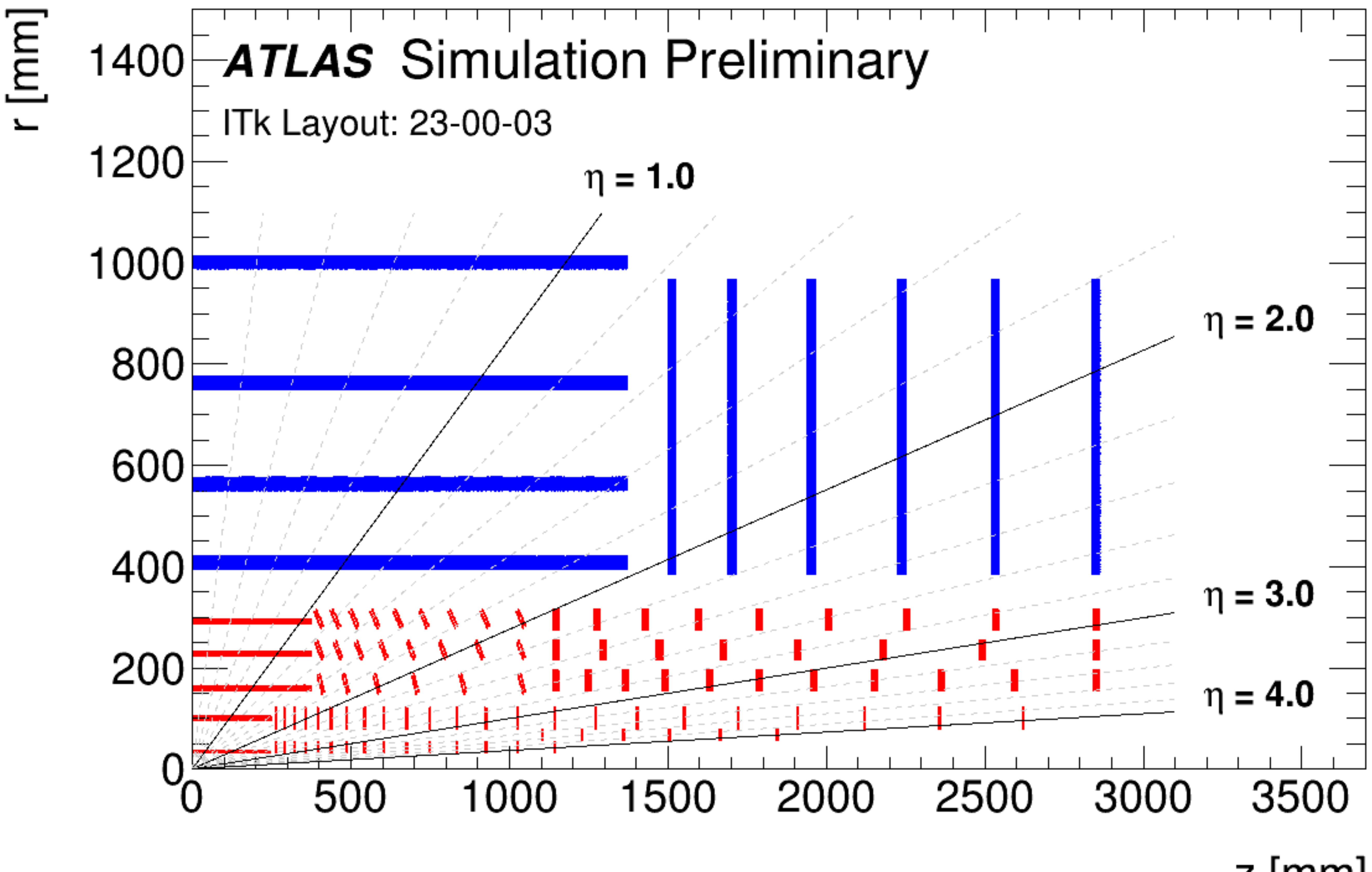
red: ITk Pixel System, blue: ITk Strip System



Source: ATL-PHYS-PUB-2021-024

- Particles interact with all the material of the detector.
- Only the sensitive detector part can actually detect charged particles.
  - Measuring the energy loss via induced electric charge.
- Energy loss independent of the readout — simulation performed per-module.
  - Much lower number of elements to simulate.
- Each particle makes a “hit”:
  - coordinates
  - particle energy lost

red: ITk Pixel System, blue: ITk Strip System



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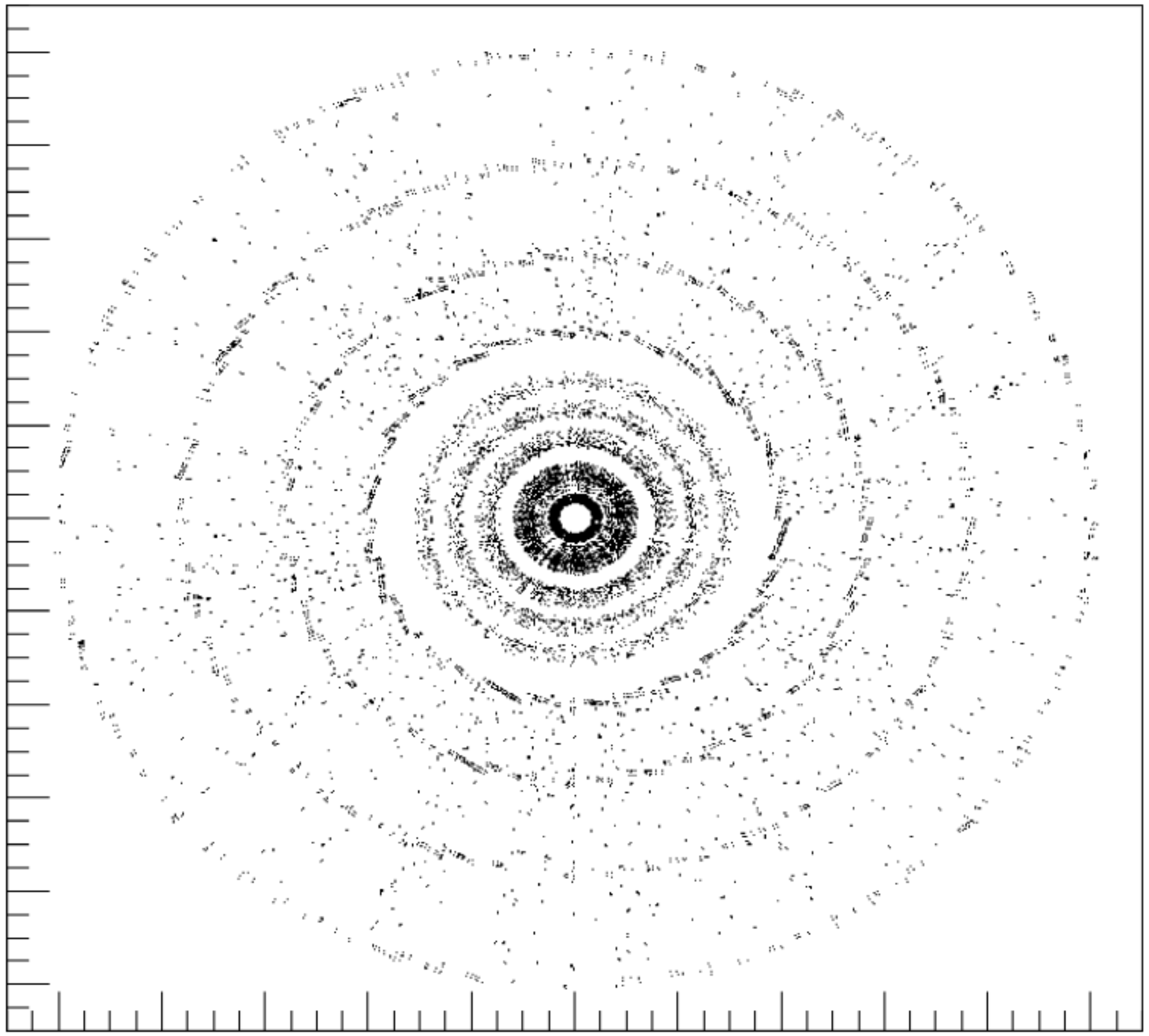

The Need for Monte Carlo Simulation

- A large part of the LHC physics programme relies on accurate Monte Carlo simulation of collision events.
  - generation of physics events and their immediate decays
  - simulation of the detector and physics interactions
  - digitisation of the detector response (readout)
  - (simulated events are reconstructed the same way as collected data)
- Producing simulated samples → majority of experiments' CPU requirements (CMS used 85% CPU for sim. during 2009-2016, half was spent detector simulation).

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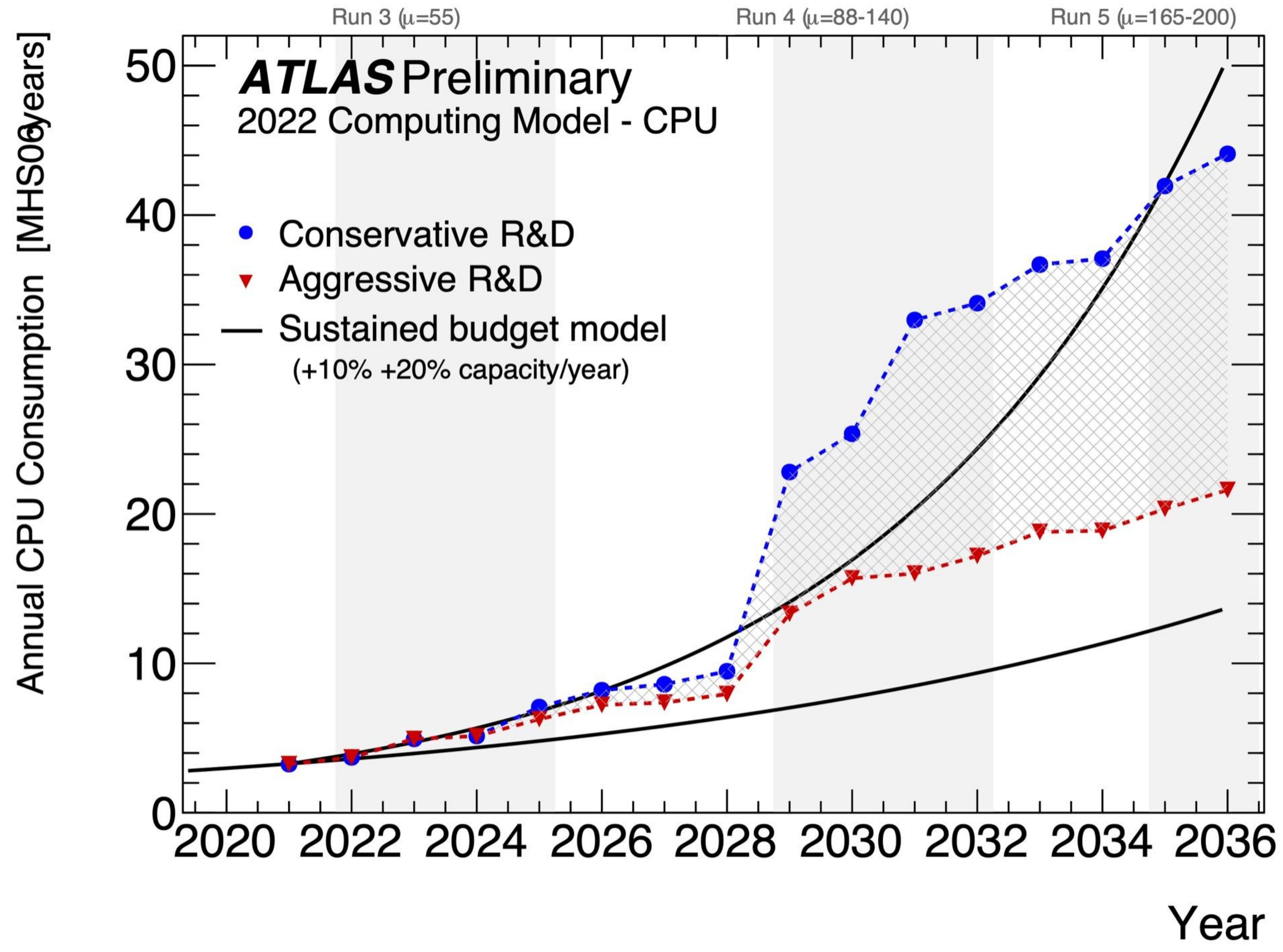

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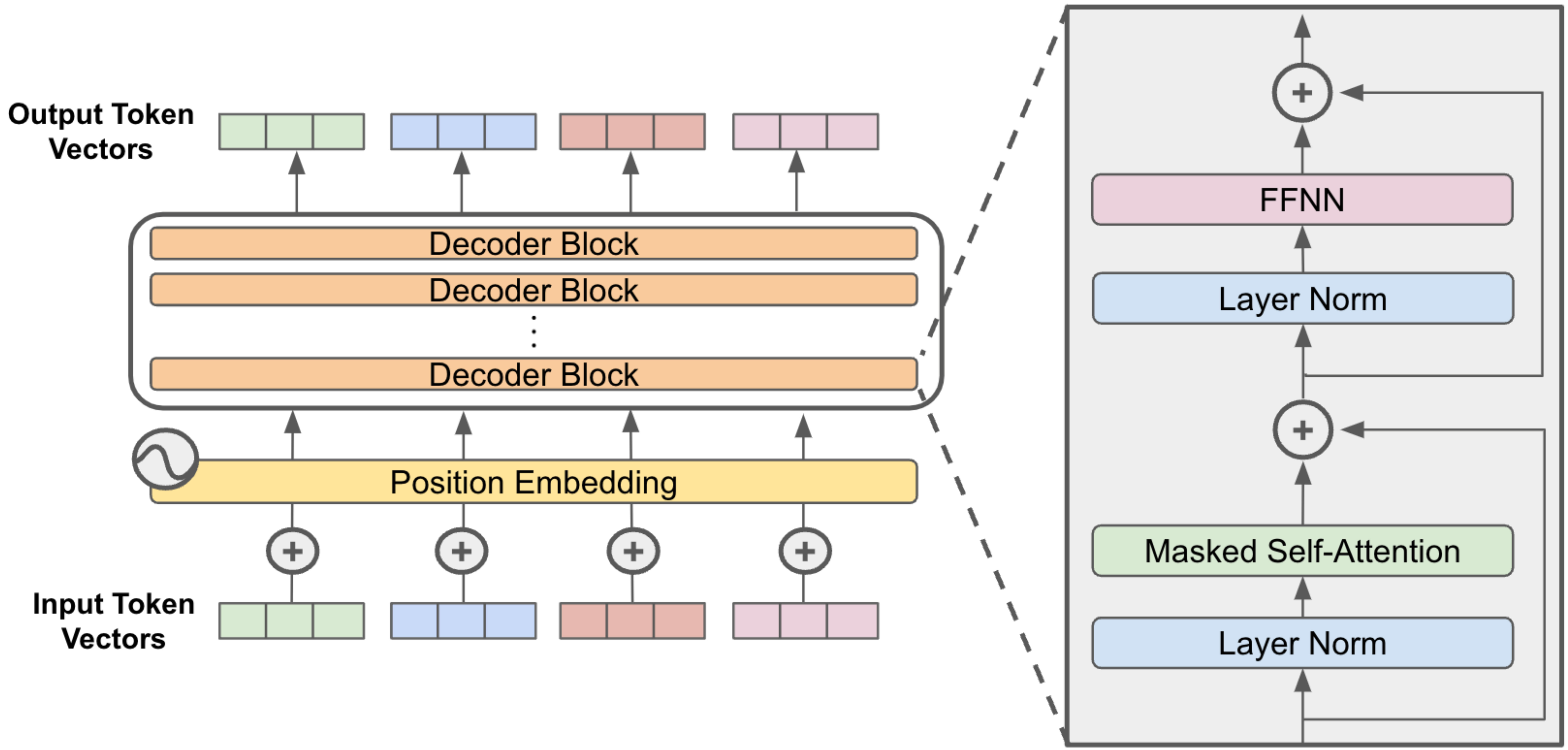
Decoder-only Transformer

Source: Cameron R. Wolfe



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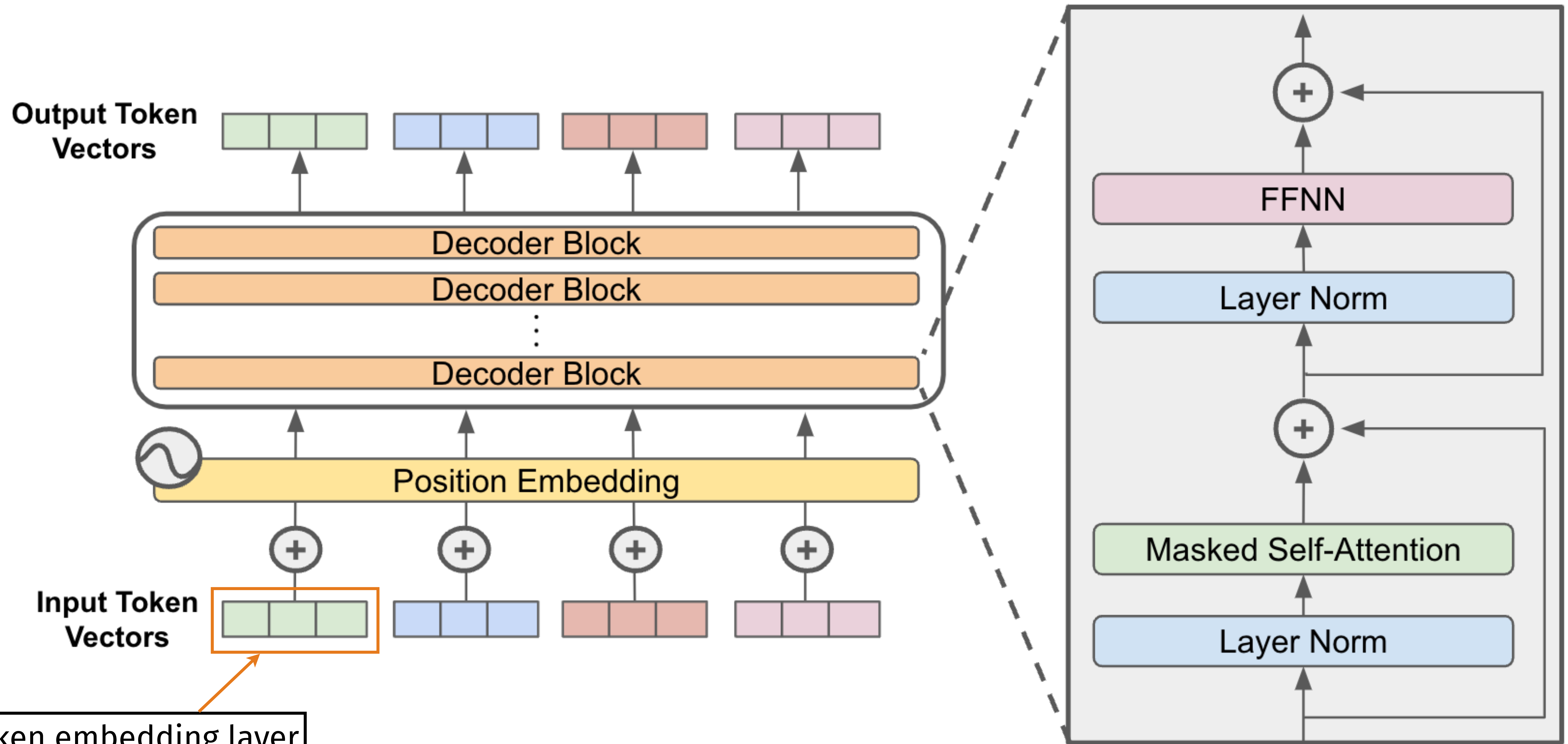

token embedding layer
d = 128
(model dim)

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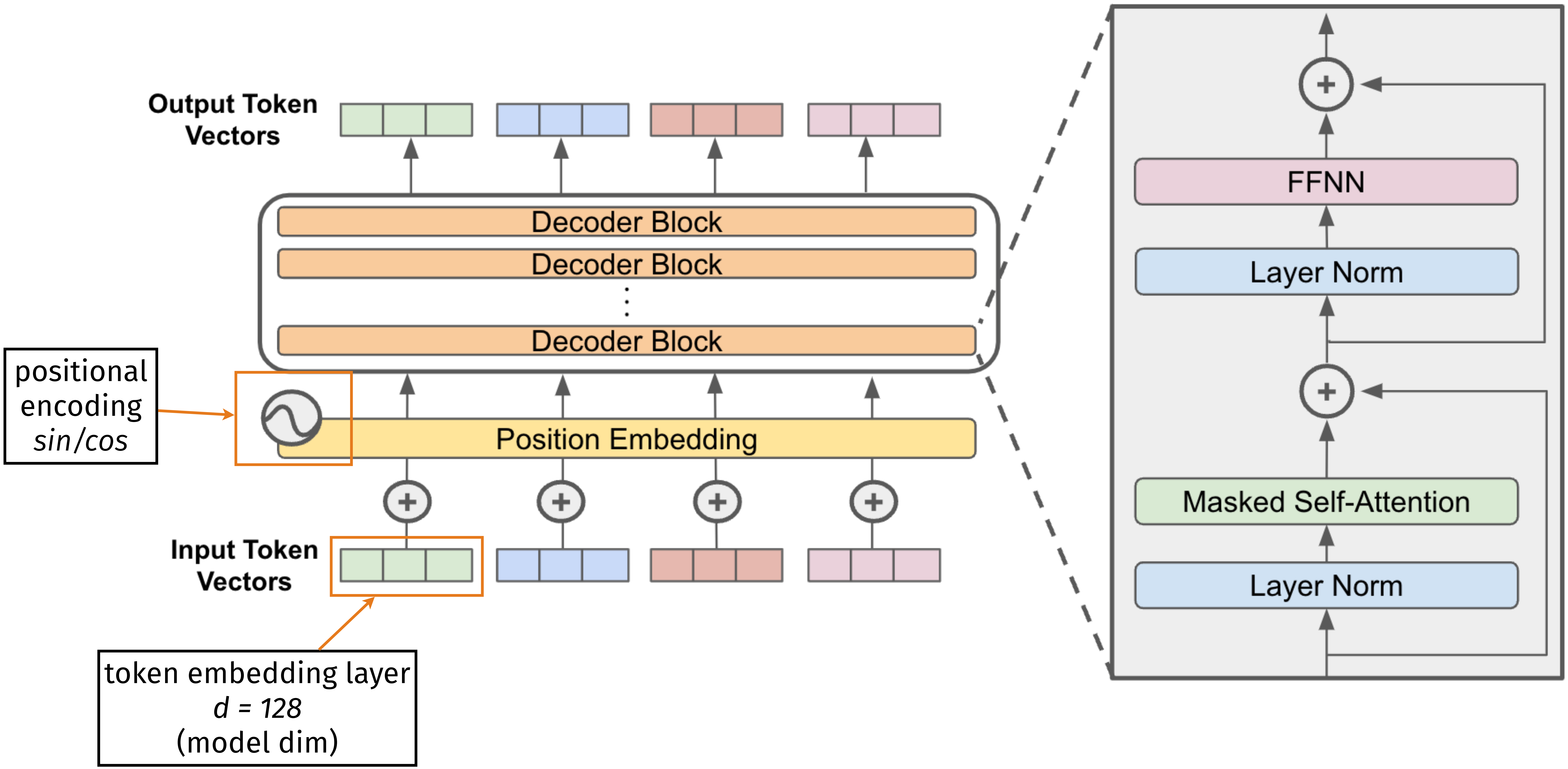

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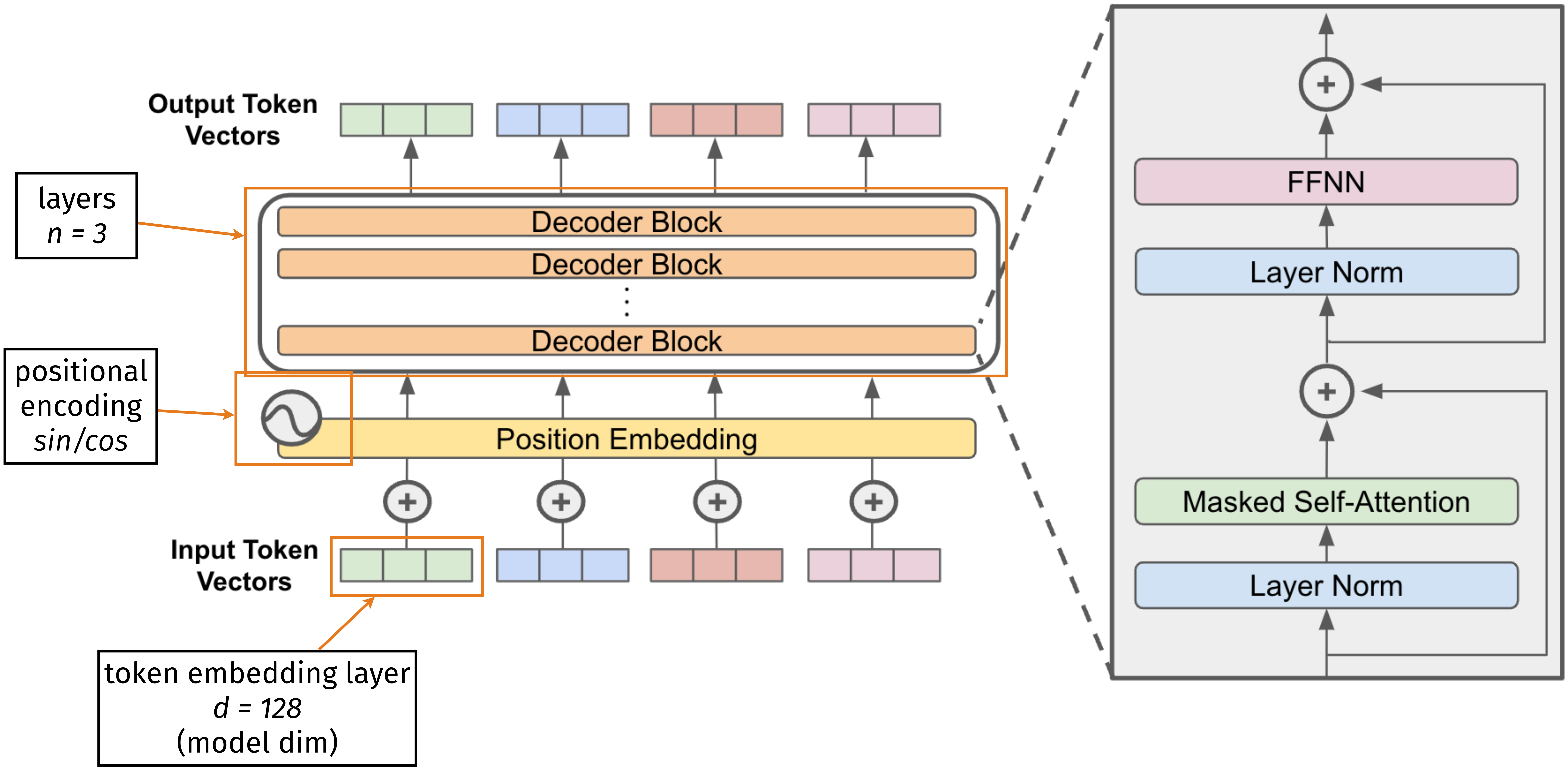

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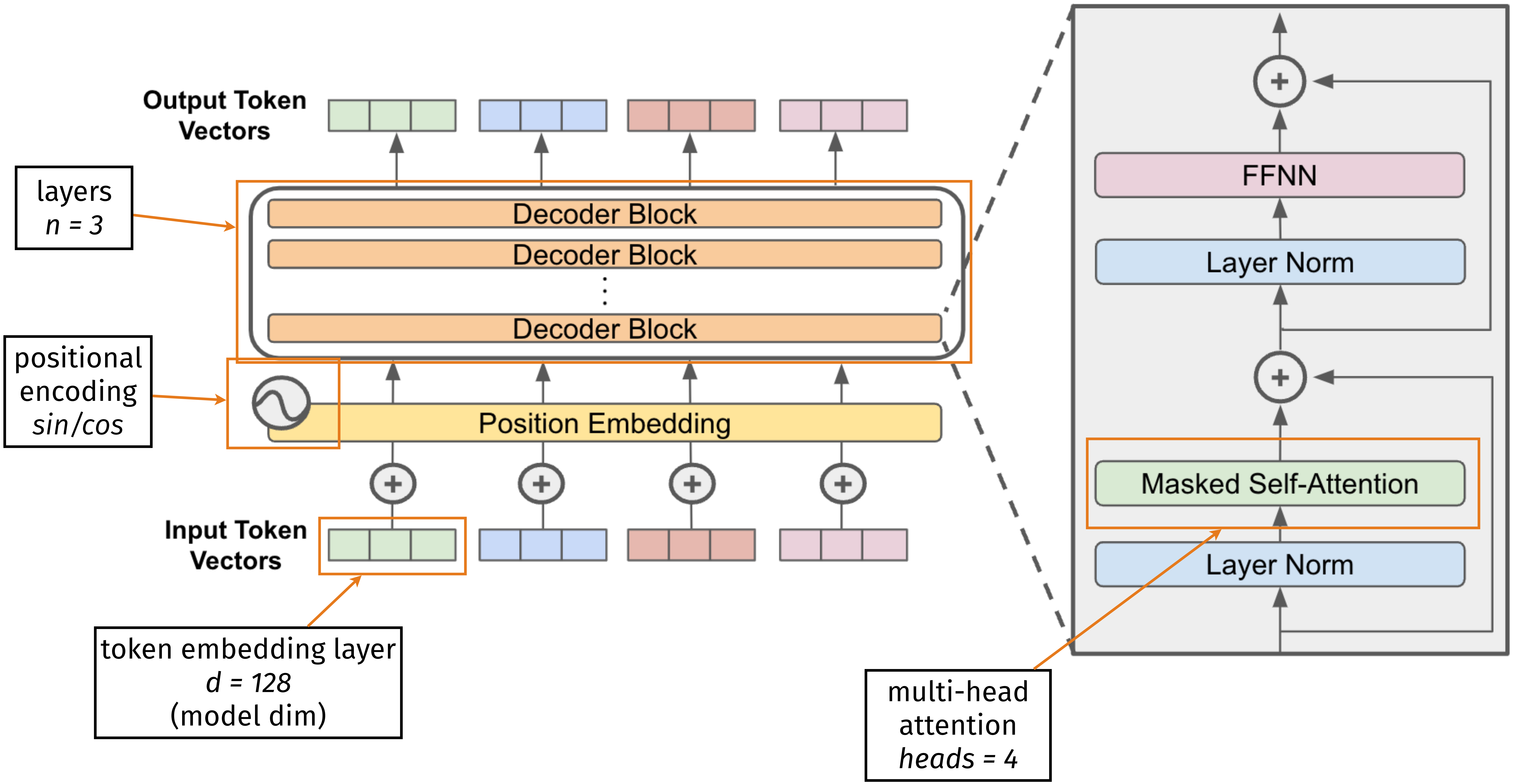

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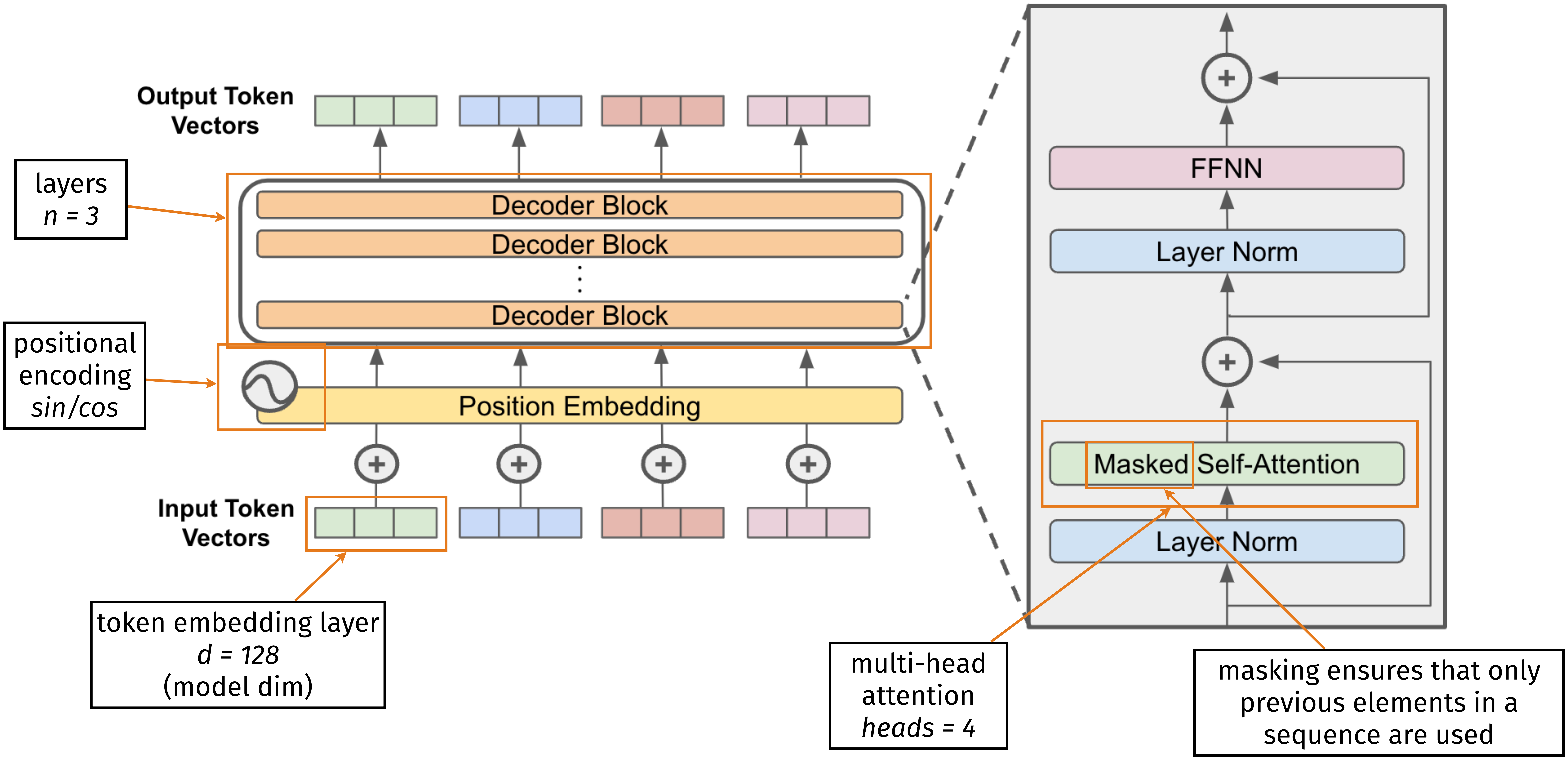

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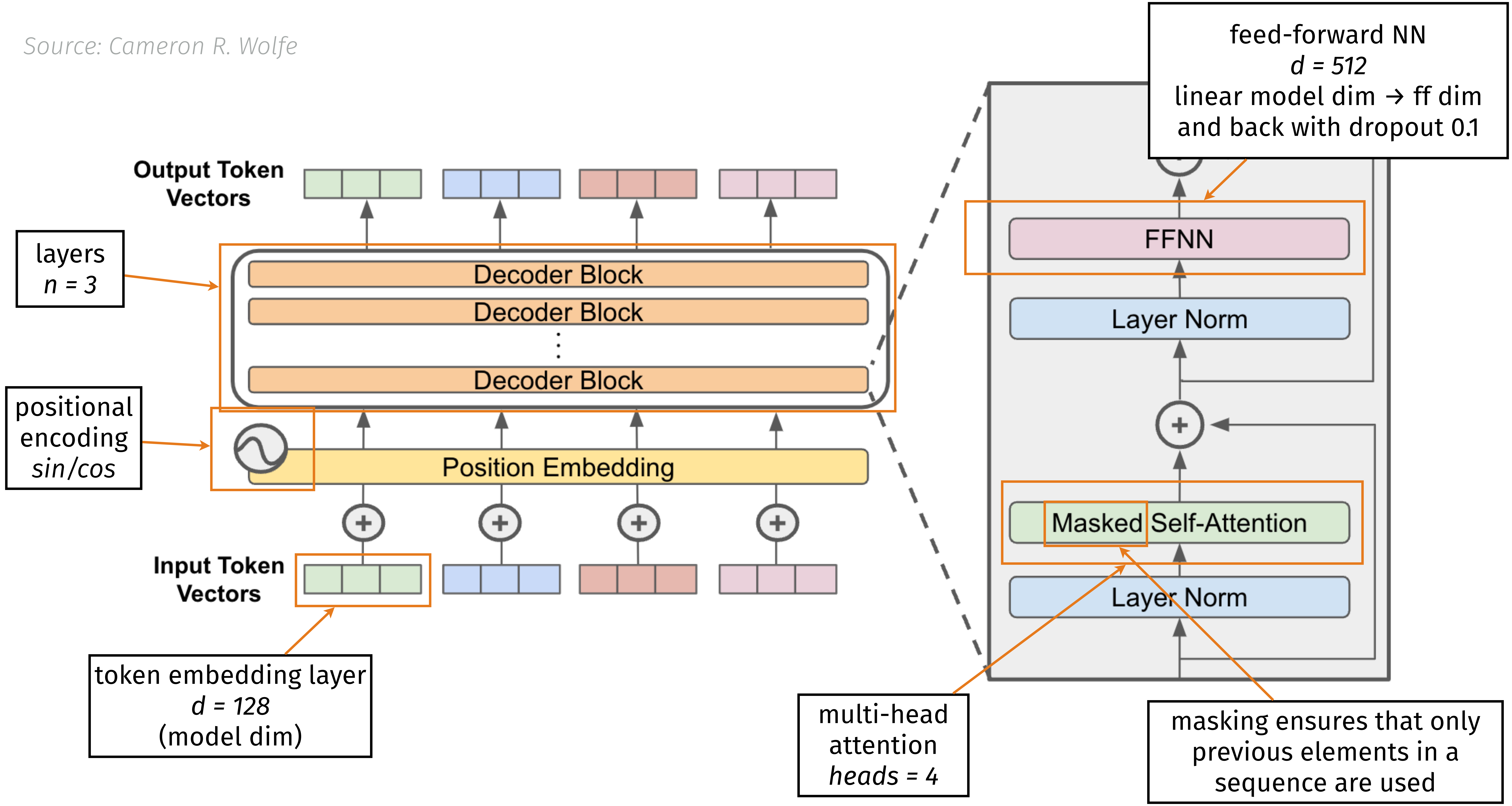

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