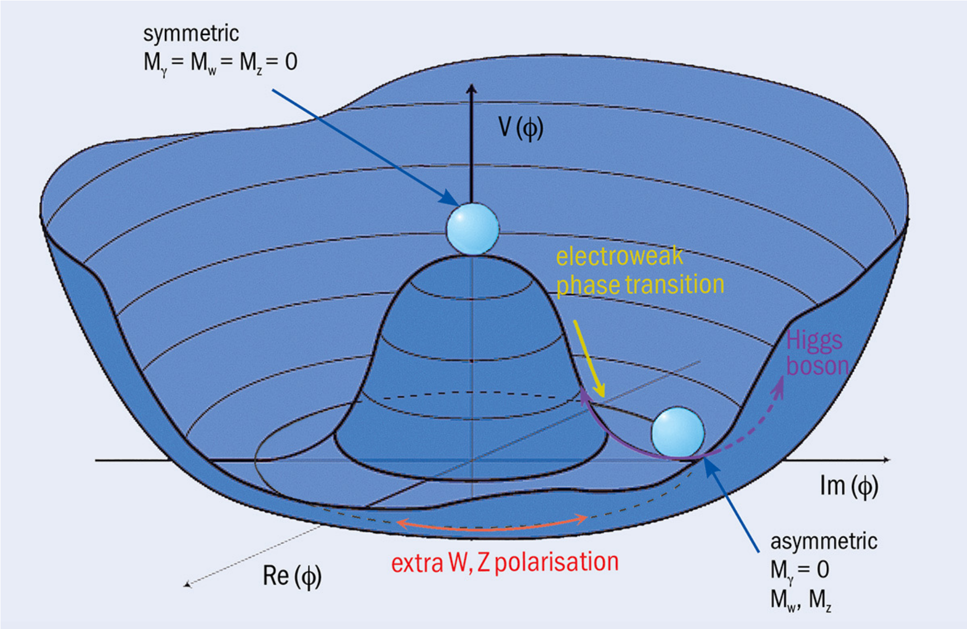
Machine Learning for Tracking with the ATLAS detector

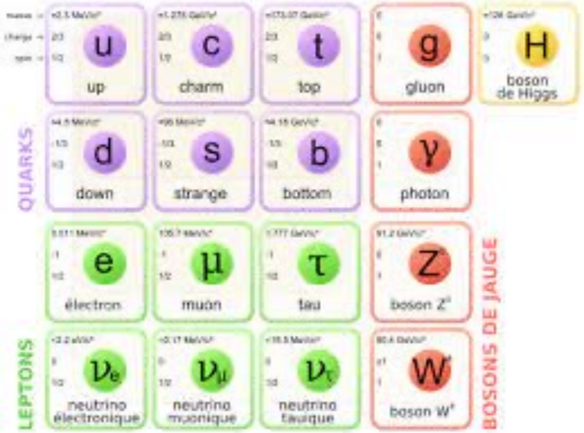
Sylvain Caillou (*IN2P3-CNRS)*

Journée Scientifique LPT/L2IT

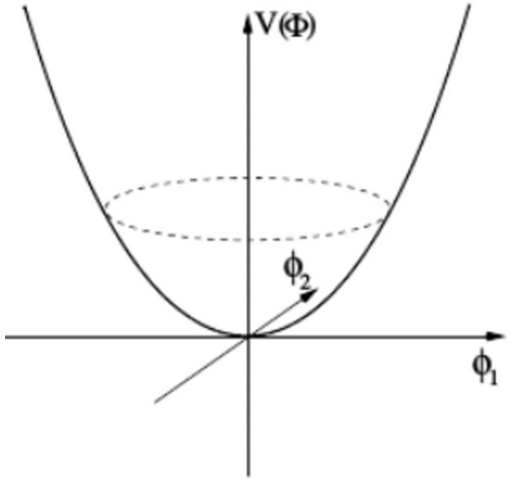
January 26th, 2023

The Higgs boson: The thrill of the chase (before 2012)





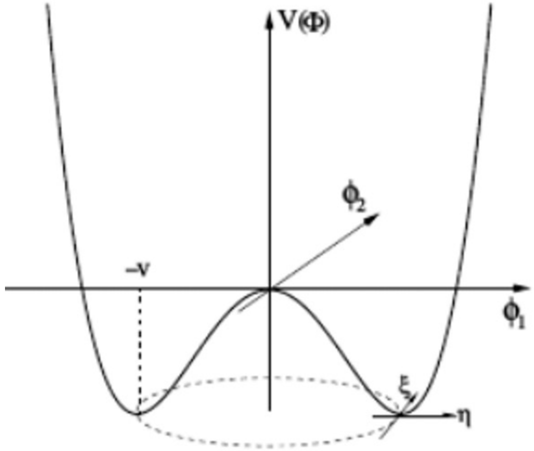
Just after Big Bang
Hot Universe



$m_H = 0\ GeV$

Violent phase transition
Symmetry breaking

Today
Cold Universe



Predict by theory :

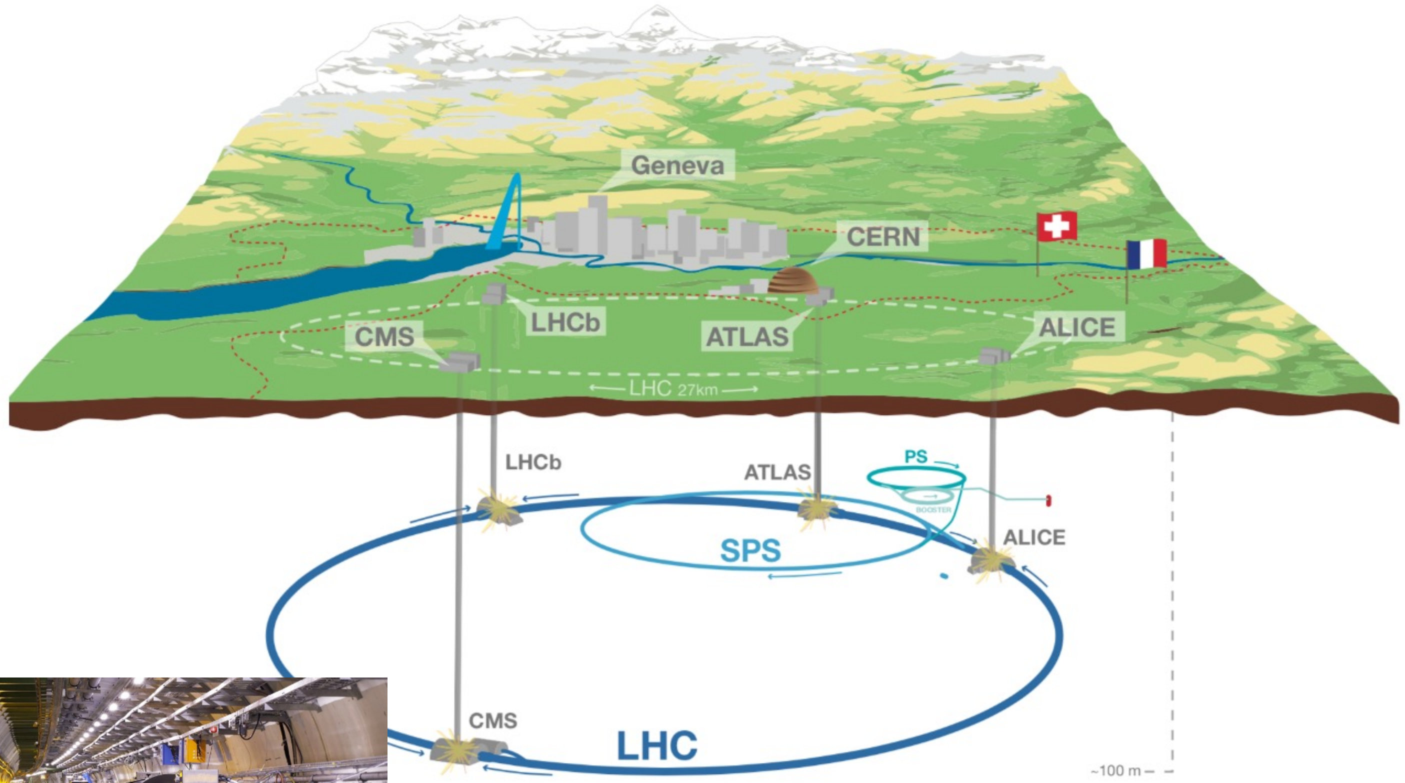
$$v = (\sqrt{2}G_F)^{-1/2} \approx 246 \text{ GeV}$$

$$m_H = \sqrt{\lambda/2}\ v$$

$$m_H \approx 125\ GeV$$

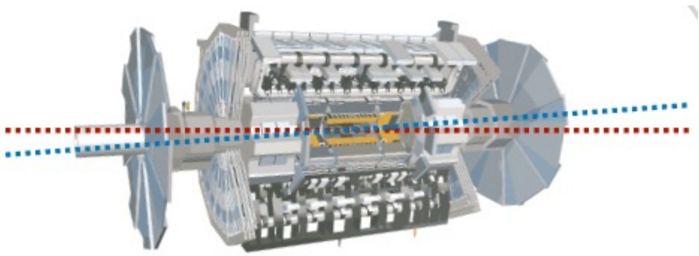
$\Rightarrow$ Construct a machine able to detect the Higgs Boson around 125 GeV

Large Hardron Collider (LHC) at CERN

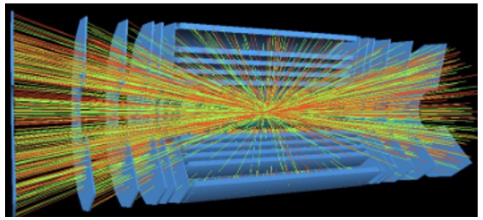


- Highest energy synchrotron with 27km circumference, 100m underground. Located at the border of France and Switzerland.
- Proton-proton collisions at 13TeV with 25ns bunch-spacing
- 2 generalist detectors ATLAS and CMS
- Design to find the Higgs Boson!

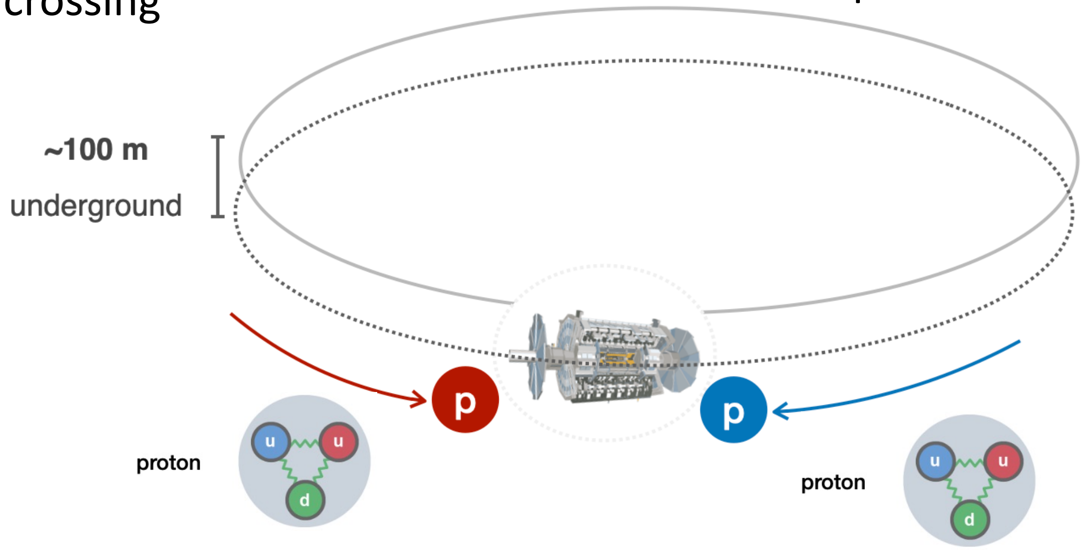
The ATLAS detector

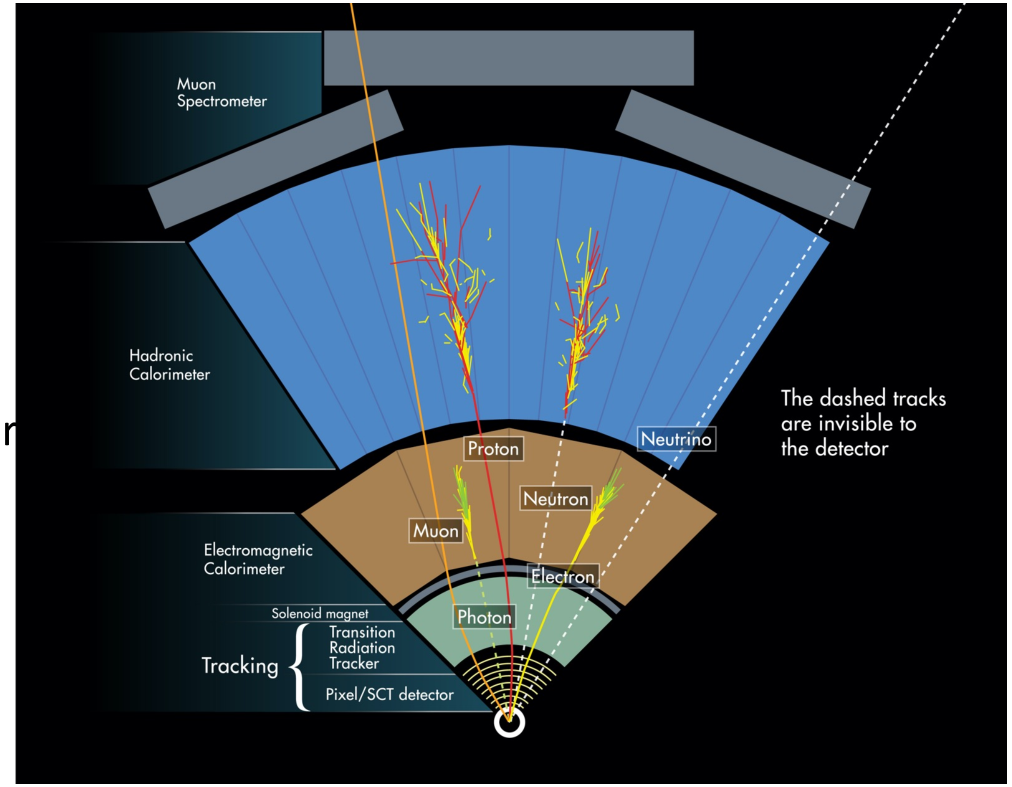


p-p collisions happen at the center of the detector where the beam lines are crossing



p-p collisions produce a flow of particles which are are coming from the Impact Point through the detector

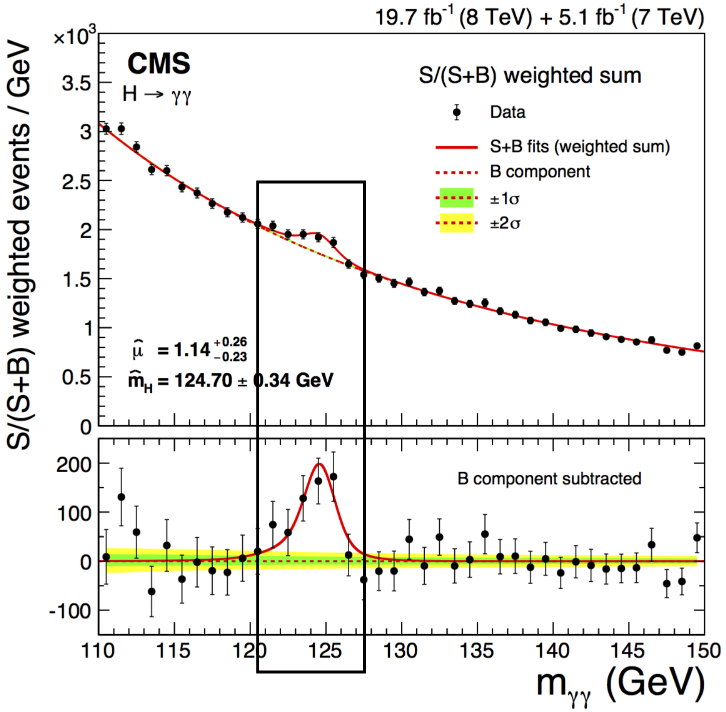


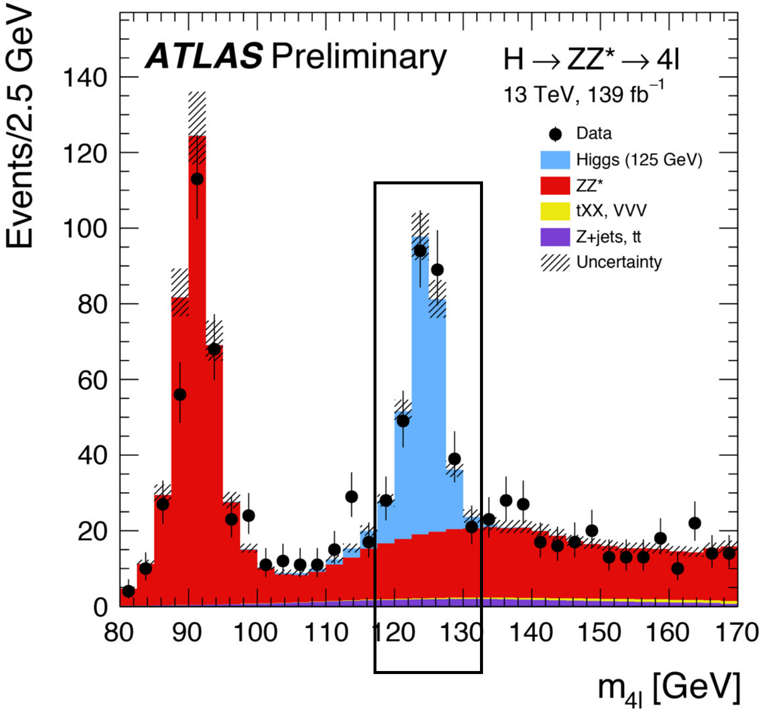


The detector is composed by sub-detectors , each of them delivering a specific type of information

Images from : “[Modèle standard : Comprendre l’univers avec l’aide des bosons]” (J.Manjares)

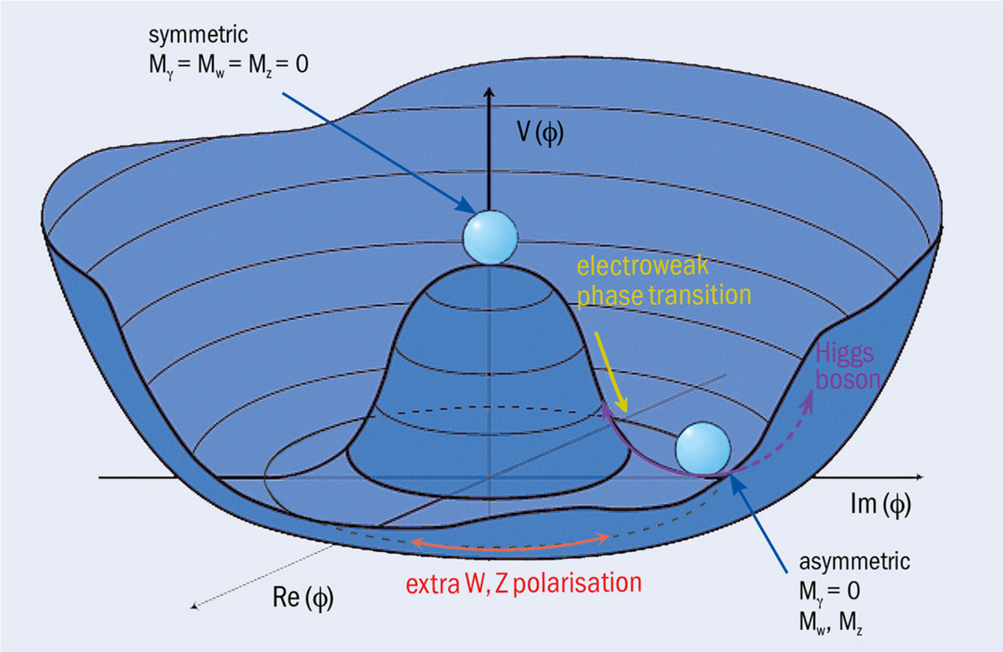
Higgs discovery (2012)





The Higgs boson implications and prospects for future discoveries

Since 2012: accumulate more statistics
Coupling Higgs with other particles: show the relation between their masses and the Higgs Field
Ultimate goal: understanding the Higgs potential today
Very important as it could give indications on the first instants of the universe

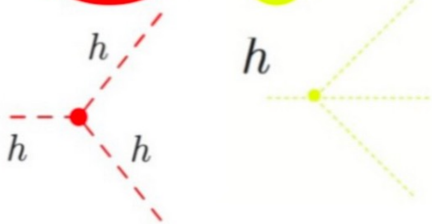


Higgs potential in the standard model:

$$V(\Phi) = \mu^2 \Phi^+ \Phi + \eta (\Phi^+ \Phi)^2$$

expansion around the minimum

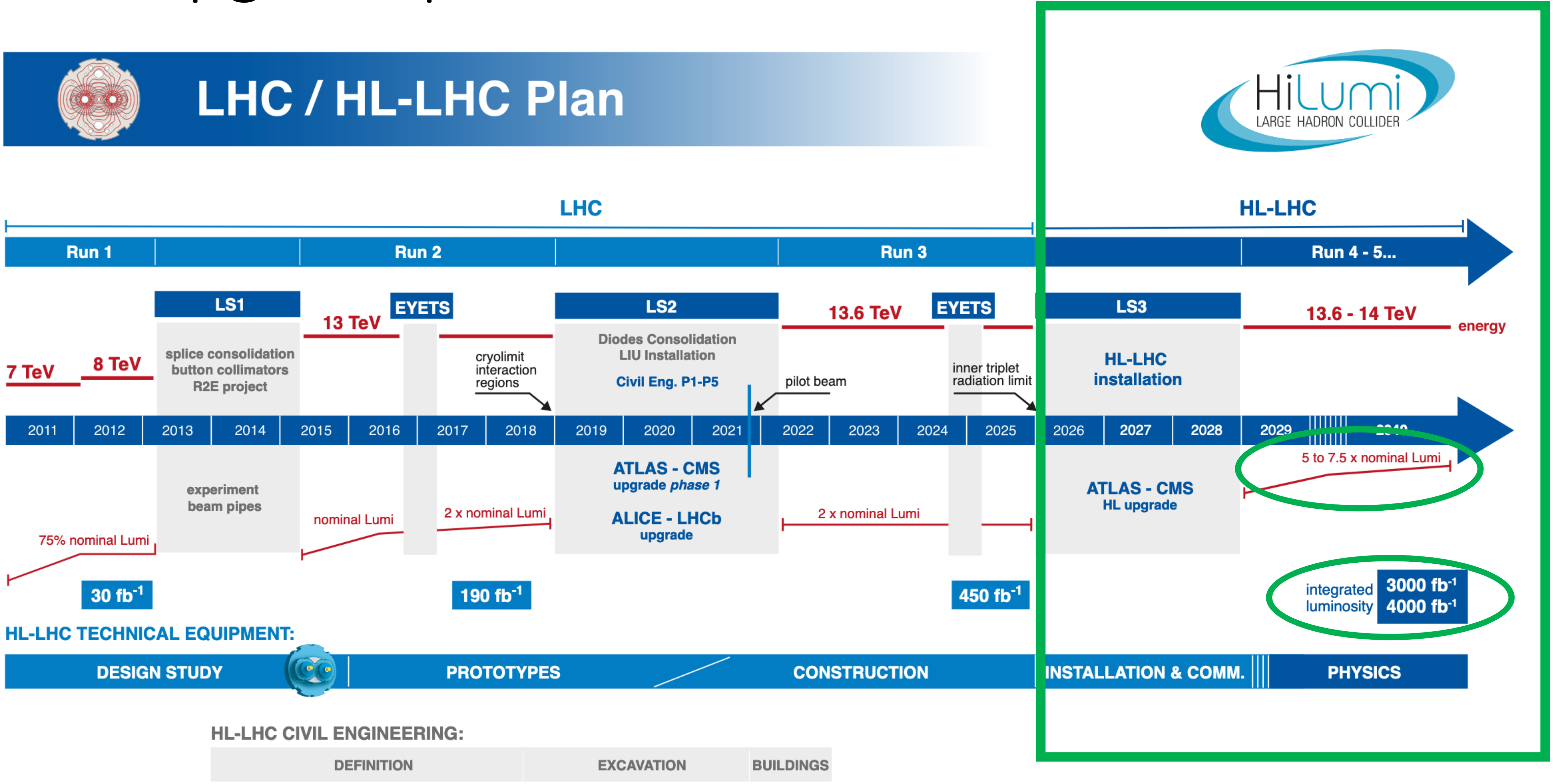
$$\frac{1}{2} m_H^2 h^2 + \sqrt{\frac{\eta}{2}} m_H h^3 + \frac{\eta}{4} h^4$$



A measurement of the Higgs self-coupling is the only way to experimentally reconstruct the Higgs potential (reconstruct its shape close to the minimum)

Problem: H->HH self-coupling is extremely rare !
⇒ Need a lot more statistics
⇒ HL-LHC

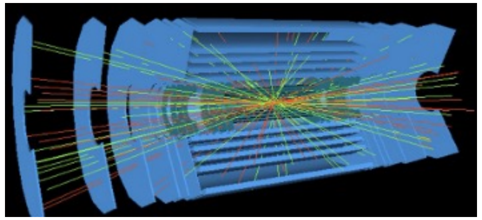
LHC upgrade plans



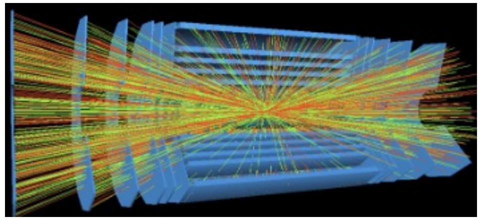
HiLumi-LHC (HL-LHC) era

$30\ fb^{-1}$	$190\ fb^{-1}$	$350\ fb^{-1}$	$3000\ fb^{-1}$
2011 -2012	2015 -2018	2022 -2024	2027 -2040
Run 1	Run 2	Run 3	Run 4-5…

LHC: 40 millions crossings of bunches of protons per second !



For HL-LHC we can not go beyond that but we can increase the density of bunches :

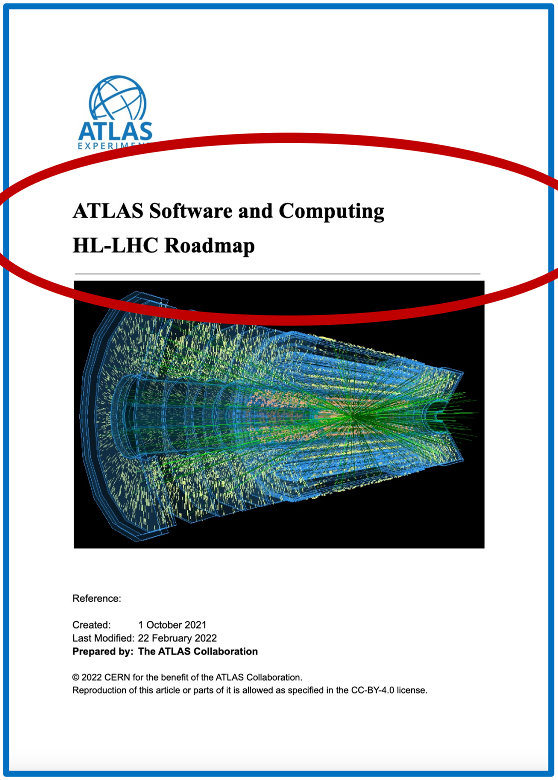


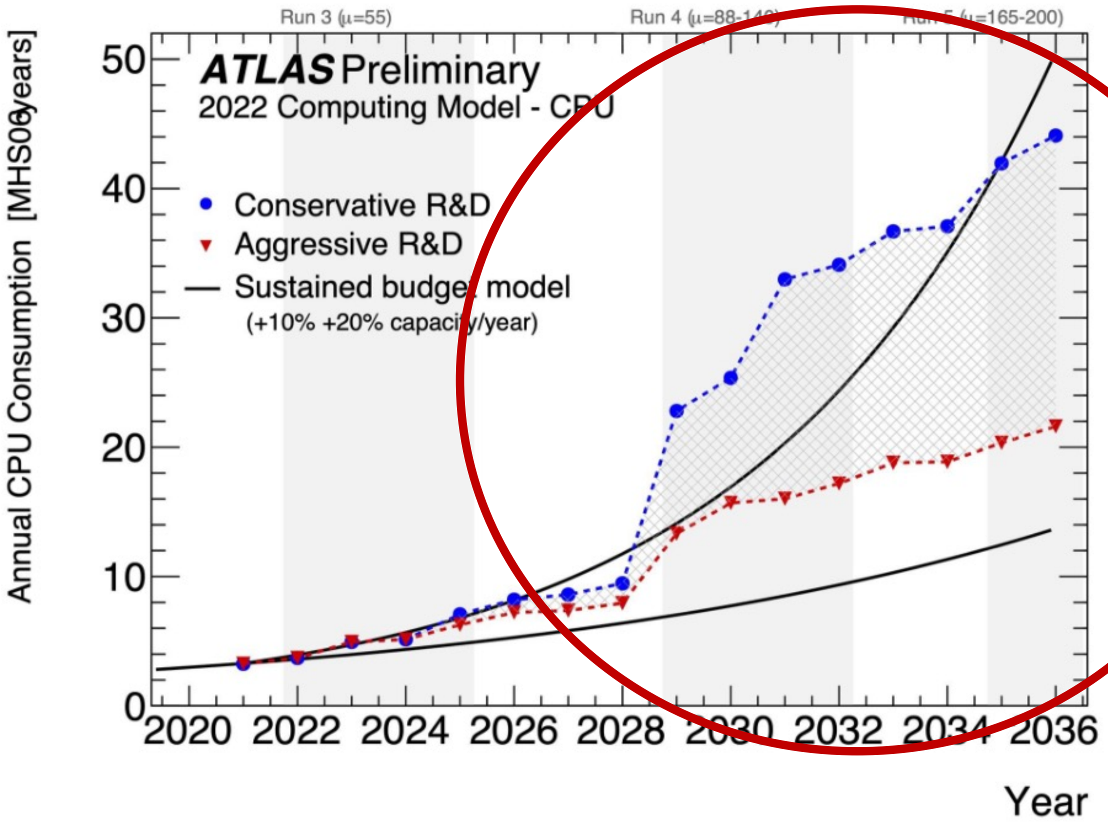
The High-Luminosity phase this is:

- ➢ More data,
- ➢ 5 times more intense beams,
- ➢ ~10 times more Integrated luminosity
- ➢ More complex collisions,
- ➢ Extremely sophisticated detectors: **New Inner Tracker for ATLAS : ITk**

HL-LHC: Data computing challenges

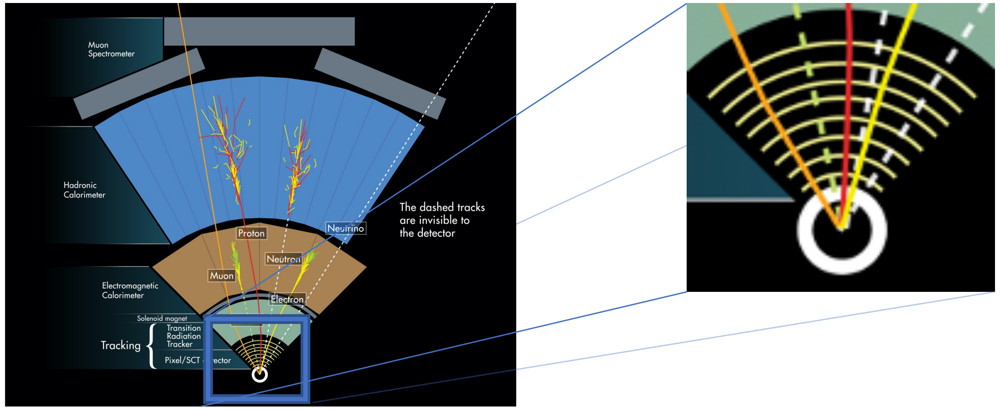
HL- HLC ⇨ Unprecedent data rates and event complexity ⇨ Unprecedent challenges for software and computing

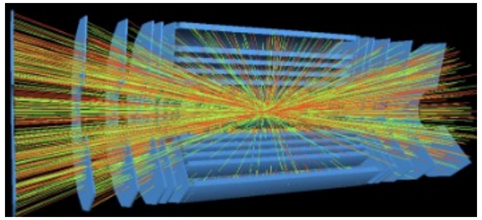


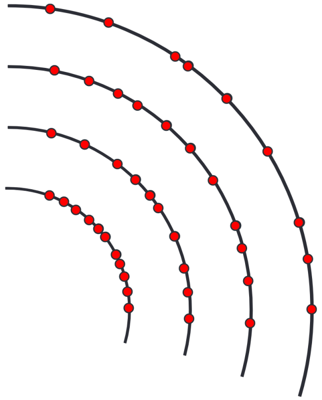


Tracking charged particle in the Inner Tracker

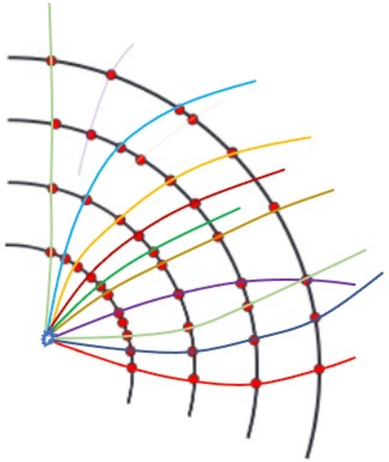
A collision of a 2 bunches will produce multiple p-p collisions and a flow of particles are coming from the Impact Point through the detector







Particles interact with the modules of the detector and produce “hits” in the detector (i.e. a cloud of 3D-geometric Euclidian Space Points) which are the data of the inner tracker



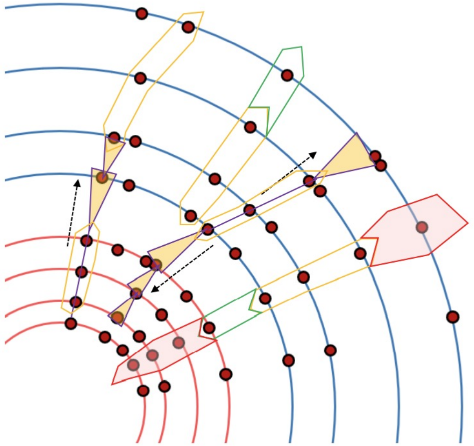
Tracking is the reconstruction of charged particles tracks in the inner detector (i.e. the sequence of hits associated to a particle)

Crucial step of the event reconstruction as a good reconstruction is required to fit correctly fundamentals parameters of the particles

Tracking charged particle in the Inner Tracker

⇒ Existing tracks reconstruction algorithms based on *Combinatorial Kalman Filter (CKF)*

⇒ *Used for Run1 to Run 3 very optimized and performant but very CPU-intensive computation*



1. propagate p_{k-1} and its covariance C_{k-1} :

$$q_{k|k-1} = f_{k|k-1}(q_{k-1|k-1})$$
$$C_{k|k-1} = F_{k|k-1} C_{k-1|k-1} F_{k|k-1}^{T} + Q_k$$

with Q_k ~ noise term (M.S.)

2. update prediction to get $q_{k|k}$ and $C_{k|k}$:

$$q_{k|k} = q_{k|k-1} + K_k [m_k - h_k(q_{k|k-1})]$$
$$C_{k|k} = (I - K_k H_k) C_{k|k-1}$$

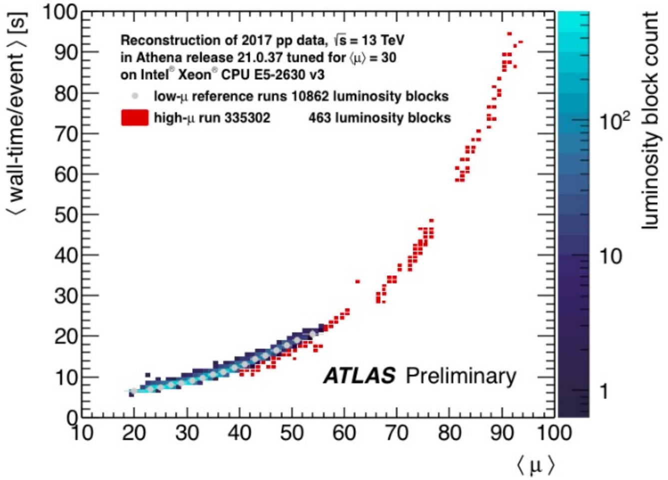
with K_k ~ gain matrix :

$$K_k = C_{k|k-1} H_k^{T} (G_k + H_k C_{k|k-1} H_k^{T})^{-1}$$

⇒ *CKF alone* won't fit the data combinatorics of HL-LHC unless unless it use an unrealistic amount of CPU resources

⇒ **The HL-LHC physics program could not be completed** (obviously not an option…)

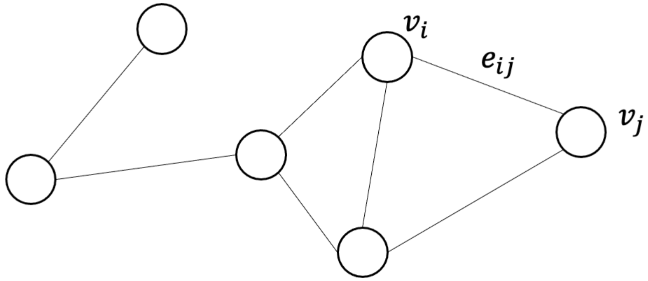
⇒ Need to investigate Machine Learning (ML) solution

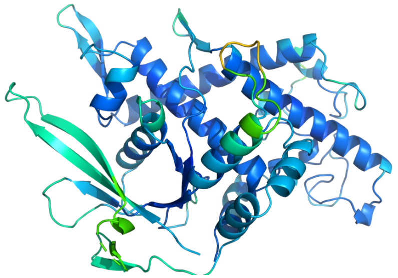


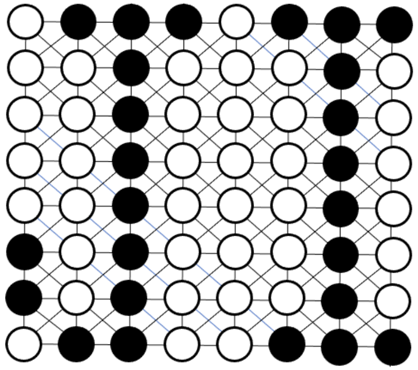
The rise of geometric ML and representation learning

⇒ Geometric and graph-based ML methods have become one of the hottest fields of AI research
⇒ Graph Neural Networks (GNNs) capture deep geometric and structural patterns in data represented as graph

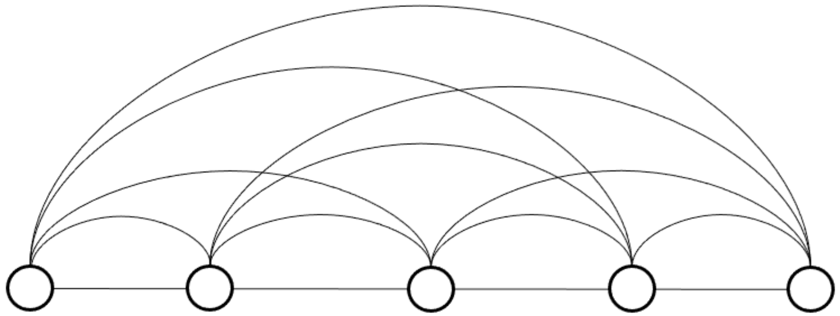
[What does 2022 hold for Geometric & Graph ML?](#)
Michael Bronstein







CNNs can be seen as a specific use case of GNNs on regular grid graphs (i.e. images)



« Graphs » « represents » « relations » « between » « entities »

Large Language Models (BERT, GPT3, etc) based on Transformers architectures in Natural Language Processing
operate on fully connected graph (i.e. text sequences)

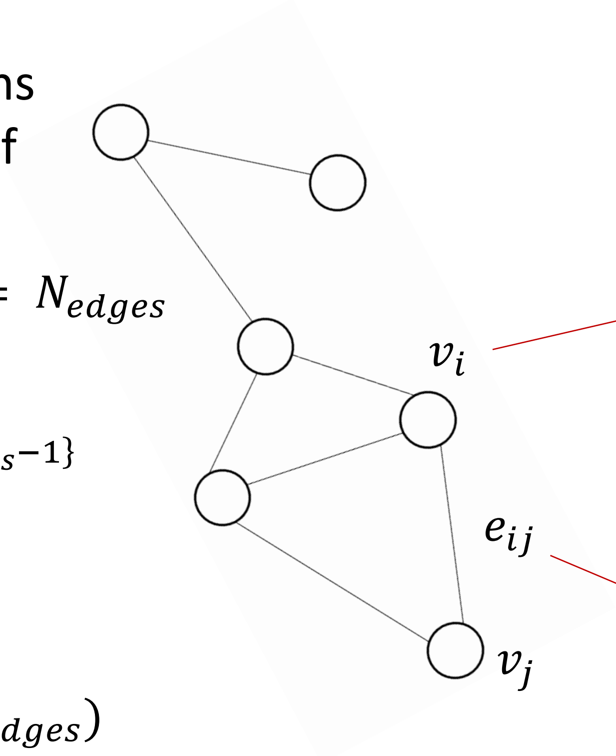
In 2021 triumph of Geometric ML and a paradigm shift in structural biology: Breakthrough in prediction of the 3D folding structure of a protein by AlphaFold 2 (deepmind)

Data representation as graph

« *In many ways, graphs are the main modality of data we receive from nature. This is due to the fact that most of the patterns we see, both in natural and artificial systems, are elegantly representable using the language of graph structures*. » P. Velickovic

A graph represents the relations (*edges*) between a collection of entities (*nodes*).

$$G = (V, E), |V| = N_{nodes}, |E| = N_{edges}$$
$$V = \{v_i\}_{i \in \{0,\ldots,N_{nodes}-1\}}$$
$$E = \{e_{ij} = (v_i, v_j)\}_{i,j \in \{0,\ldots,N_{nodes}-1\}}$$



$$nodes\ features\ (N_{nodes} \times N_{nodes\_features})$$
$$\begin{bmatrix} \alpha_0^0 & \ldots & \alpha_0^{N_{nodes\_features}-1} \\ \vdots & \ldots & \vdots \\ \boxed{\alpha_i^0} & \boxed{\ldots} & \boxed{\alpha_i^{N_{nodes\_features}-1}} \\ \vdots & \ldots & \vdots \\ \alpha_{N_{nodes}-1}^0 & \ldots & \alpha_{N_{nodes}-1}^{N_{nodes\_features}-1} \end{bmatrix}$$

$$edges\ features\ (N_{edges} \times N_{edges\_features})[optional]$$
$$\begin{bmatrix} \beta_0^0 & \ldots & \beta_0^{N_{edges\_features}-1} \\ \vdots & & \vdots \\ \boxed{\beta_k^0} & \boxed{\ldots} & \boxed{\beta_k^{N_{edges\_features}-1}} \\ \vdots & & \vdots \\ \beta_{N_{edges}-1}^0 & \ldots & \beta_{N_{edges}-1}^{N_{edges\_features}-1} \end{bmatrix}$$

$$edge\ index\ (2 \times N_{edges})$$
$$\begin{bmatrix} i_0 & \cdots & i_k & \cdots & i_{N_{edges}-1} \\ j_0 & \cdots & j_k & \cdots & j_{N_{edges}-1} \end{bmatrix} \forall e_{ij} = (v_i, v_j) \in E$$

Graph connectivity is represented as an Adjency matrix or in COO format

Graph Neural Network

- Non linear projections of nodes (eventually edges) features in High Dimensional Latent Spaces
- Capture deep structural patterns in the graphs
- Train the GNN task to project data in a final latent space where samples are linearly separable
- ML tasks can be Node Classication/ Regression , Edges classification, link prediction , graph classification…

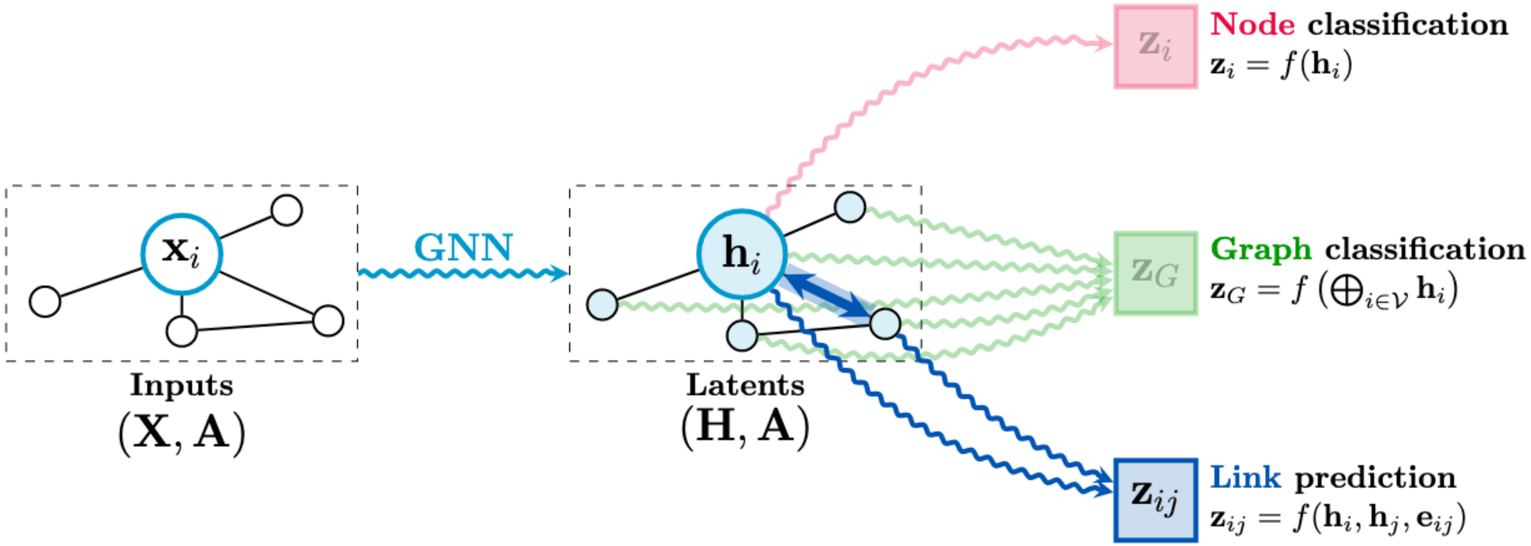
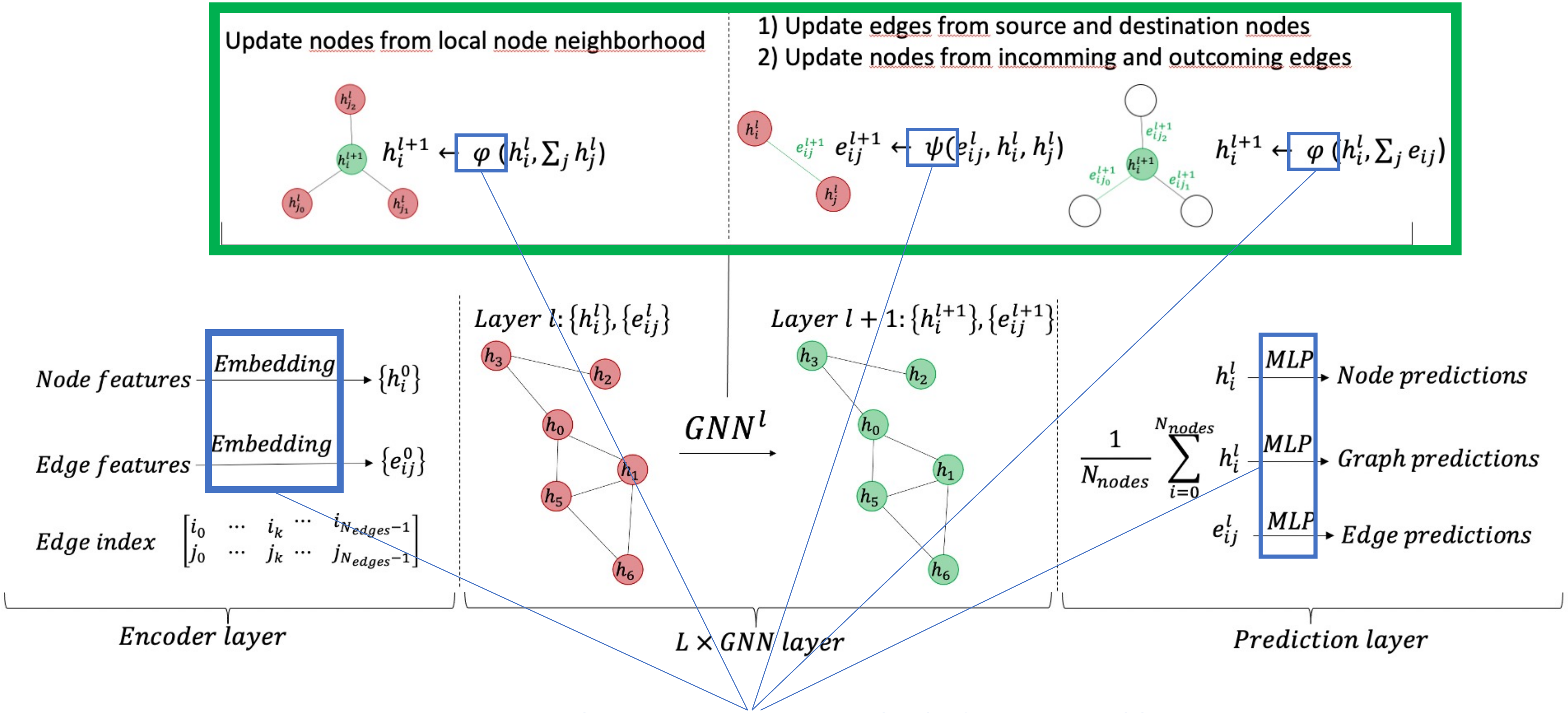


Image from « Everything is Connected: Graph Neural Network » P. Velickovic

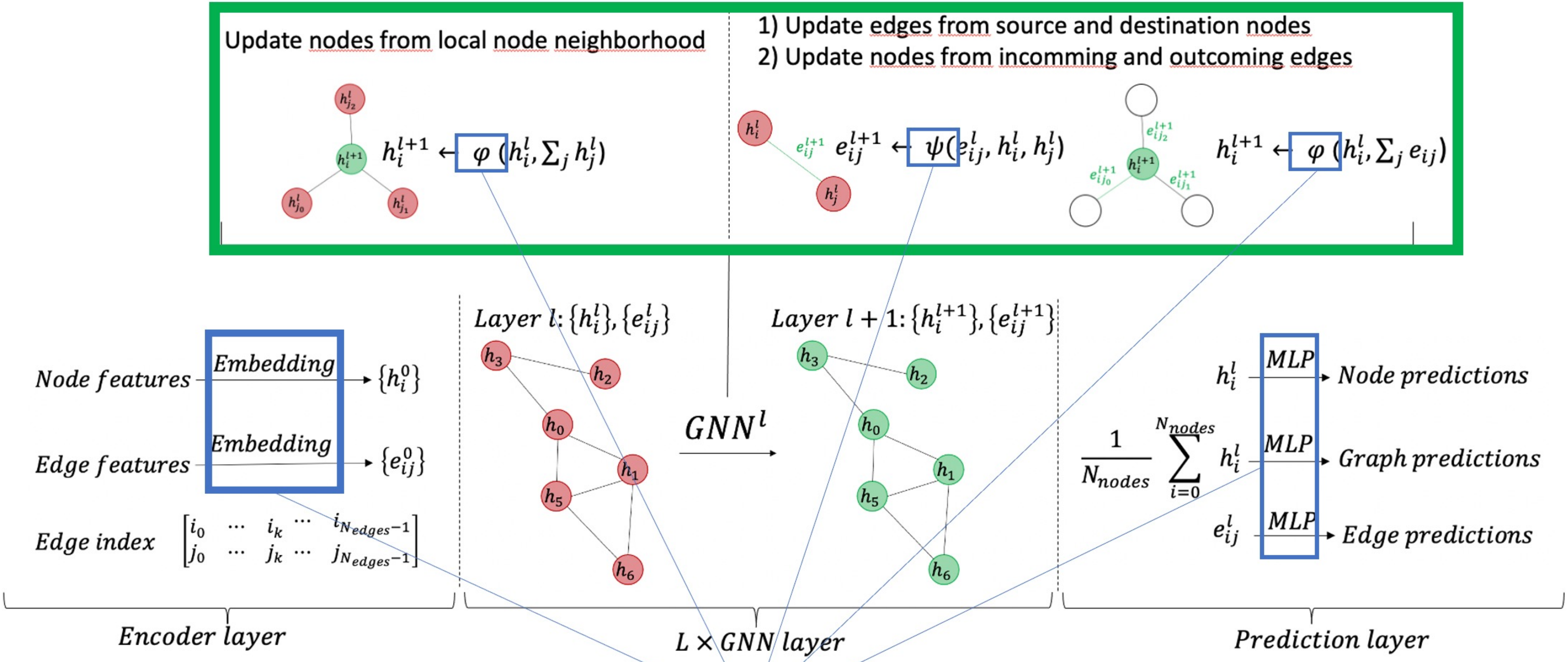
Graph Neural Networks

Message Passing allow the capture of deep structural patterns



MLPs compute non linear projections in high dimensional latent spaces

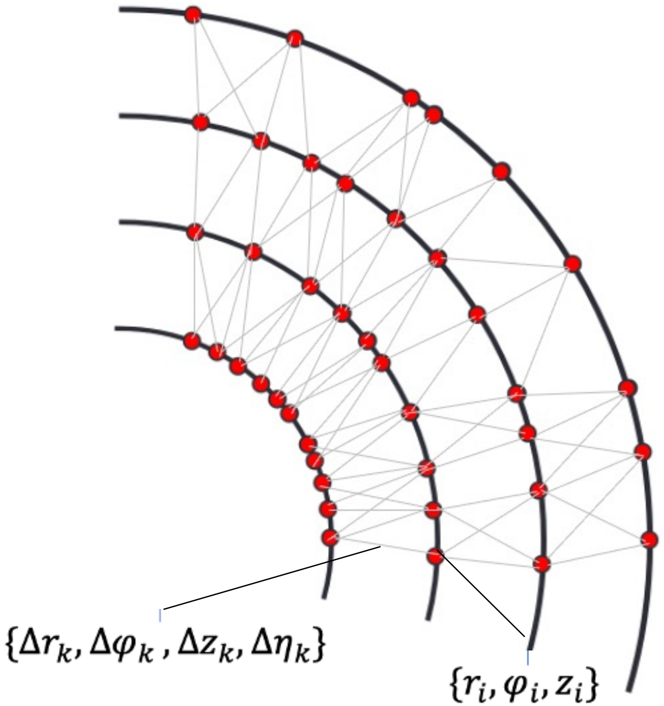
Message Passing allow the capture of deep structural patterns

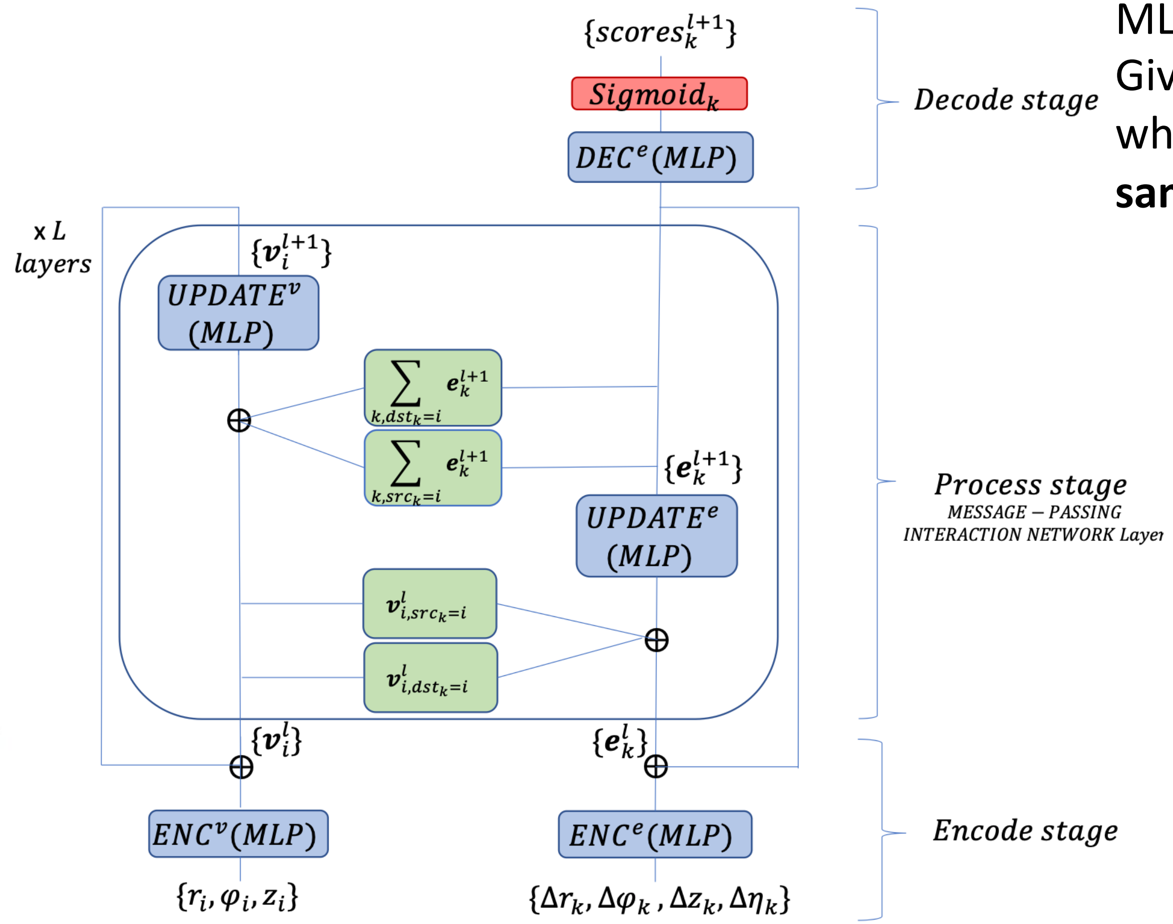


MLPs compute non linear projections in high dimensional latent spaces

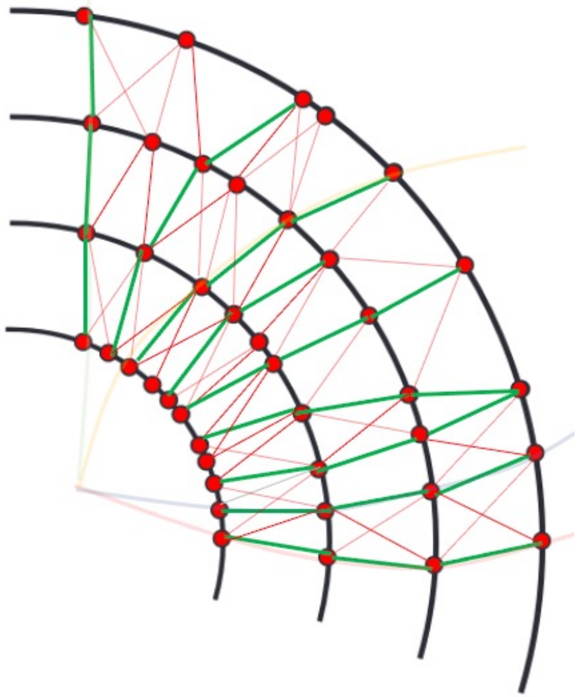
Geometric ML for tacking

Represent detector data as graph





ML Task : **Classify the edges**
Give a high scores to edges which connect **2 hits of the same particle**

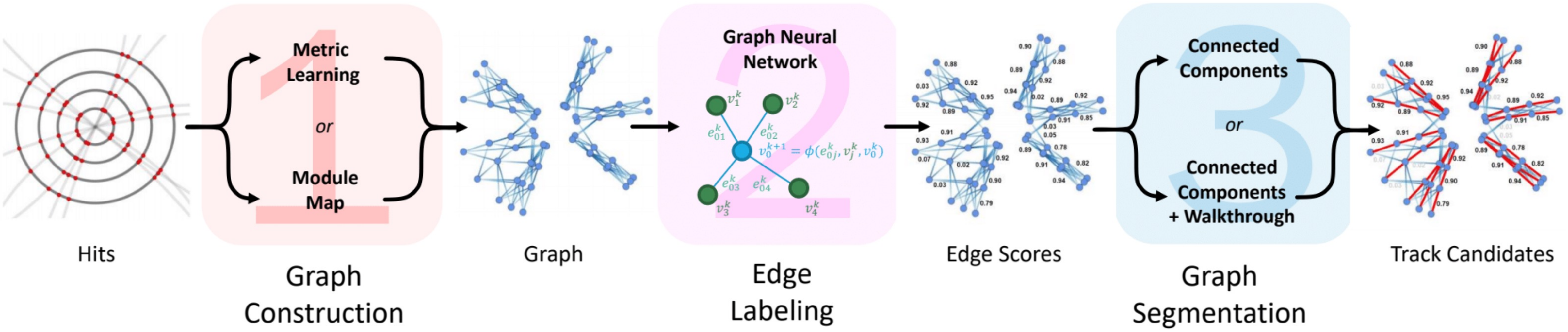


GNN project raw geometric features of the hits and of the edges in high dimentional spaces
Capture deep geometric pattern of the particle tracks

A new tracking algorithm based on GNN

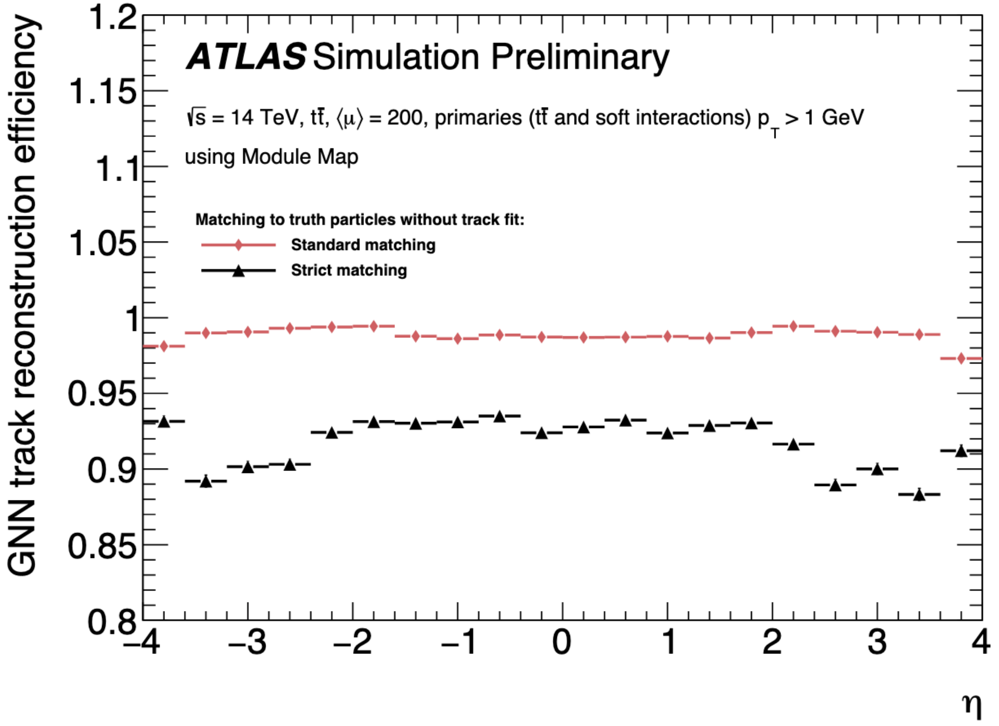
⇒ Close collaboration between L2IT & Exa.TrkX project (US DOE) started in 2021

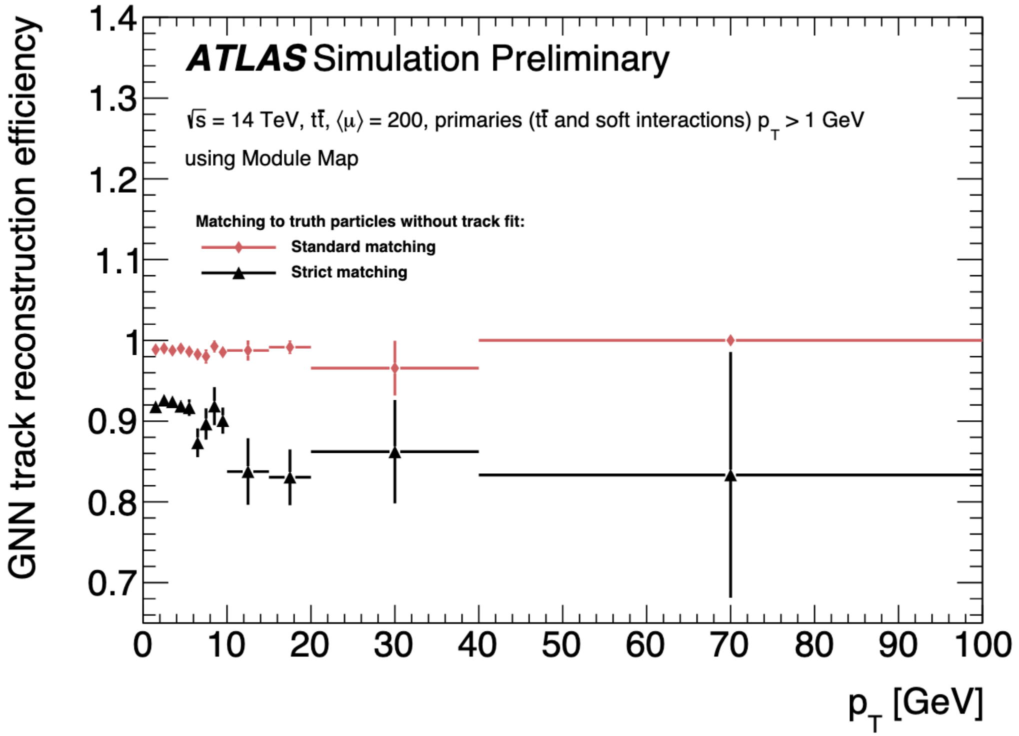
⇒ Goal: construct a Graph Neural Network (GNN) based track reconstruction algorithm for ATLAS ITk



First results with HL-LHC simulated data on ATLAS ITk

First results on ITk were approved by ATLAS collaboration in spring 2022
Presented at Connecting The Dots (C.Rougier) and published in CTD proceedings in summer 2022
More than encouraging:

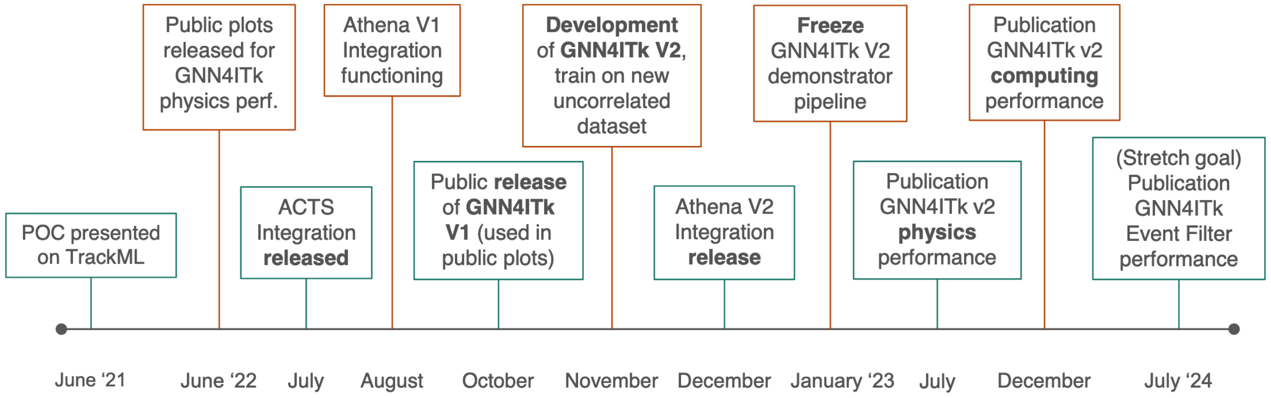




[ATLAS ITk Track Reconstruction with a GNN-based pipeline, C.Rougier et al., CTD 2022](#)
[Graph Neural Network track reconstruction for ATLAS ITk , D. Murnane et al., IML 2022](#)

GNN tracking pipeline towards production deployment

Roadmap

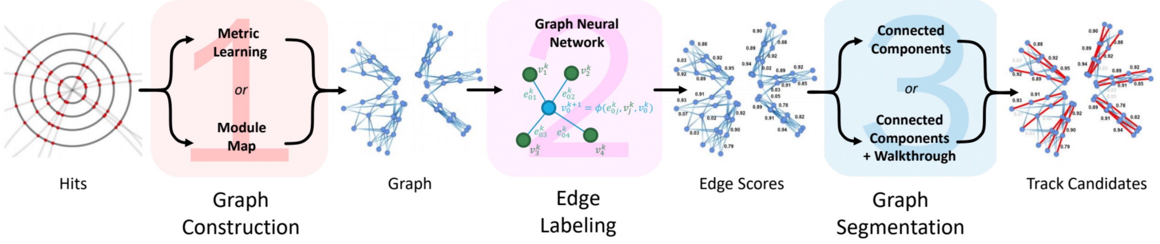


Further comprehensive study on new simulated samples

- Publication of an ATLAS collaboration paper with physic performance study, comparison with CKF
- Publication of computing performance

Software integration

[Very important effort has been done]

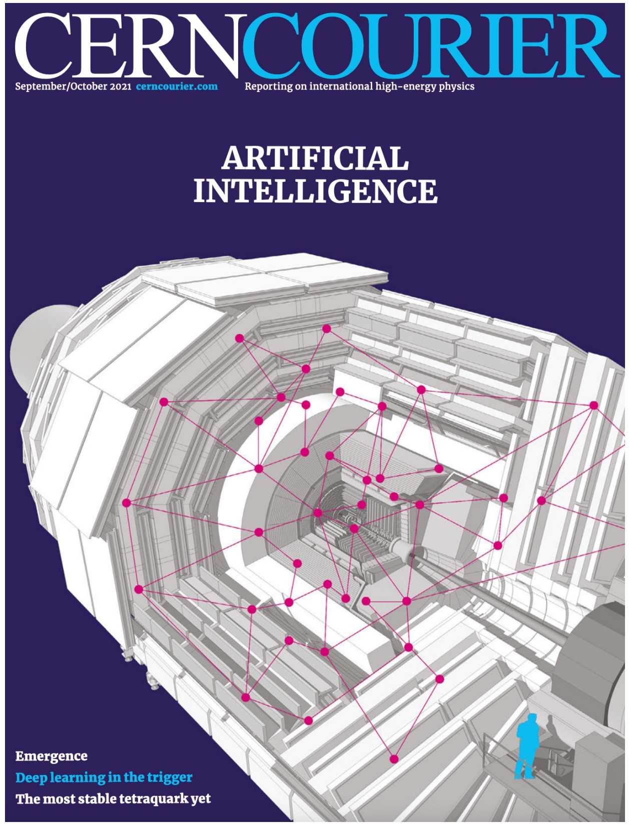


First working version of the pipeline are now integrated to ACTS & Athena

Graph-based ML in ATLAS (and particle physic)

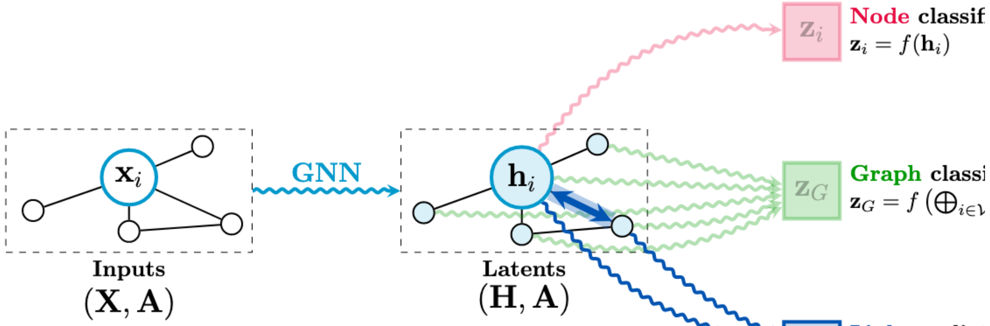
Since 2020 ML algorithms are becoming increasingly popular for a large number of LHC physics tasks, including:

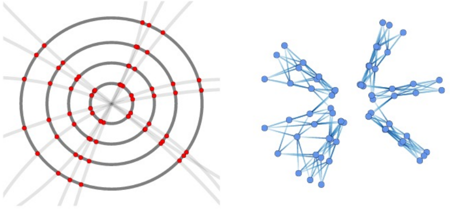
- Track Reconstruction
- Vertex Reconstruction
- Calorimeter Clustering
- Jet Clustering
- Event Reconstruction (Pileup Rejection, Particle Flow, Jet Assignment)



Frontpage of CERN COURRIER September/October 2021

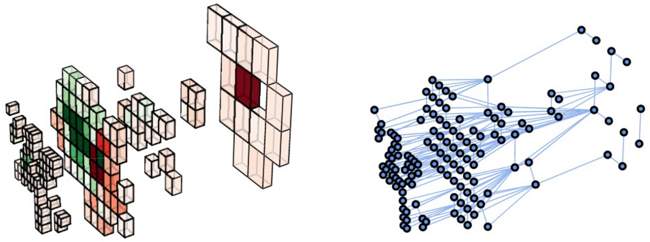
Graph-based ML in ATLAS (and particle physic)





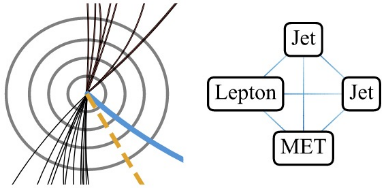
(a)

Tracking
Nodes are hits
Edges classification

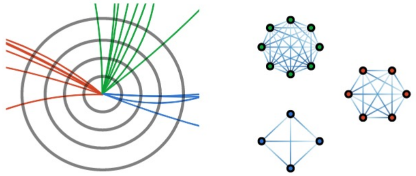


(b)

Segmenting calorimeter cells
Nodes are cells
Nodes classification



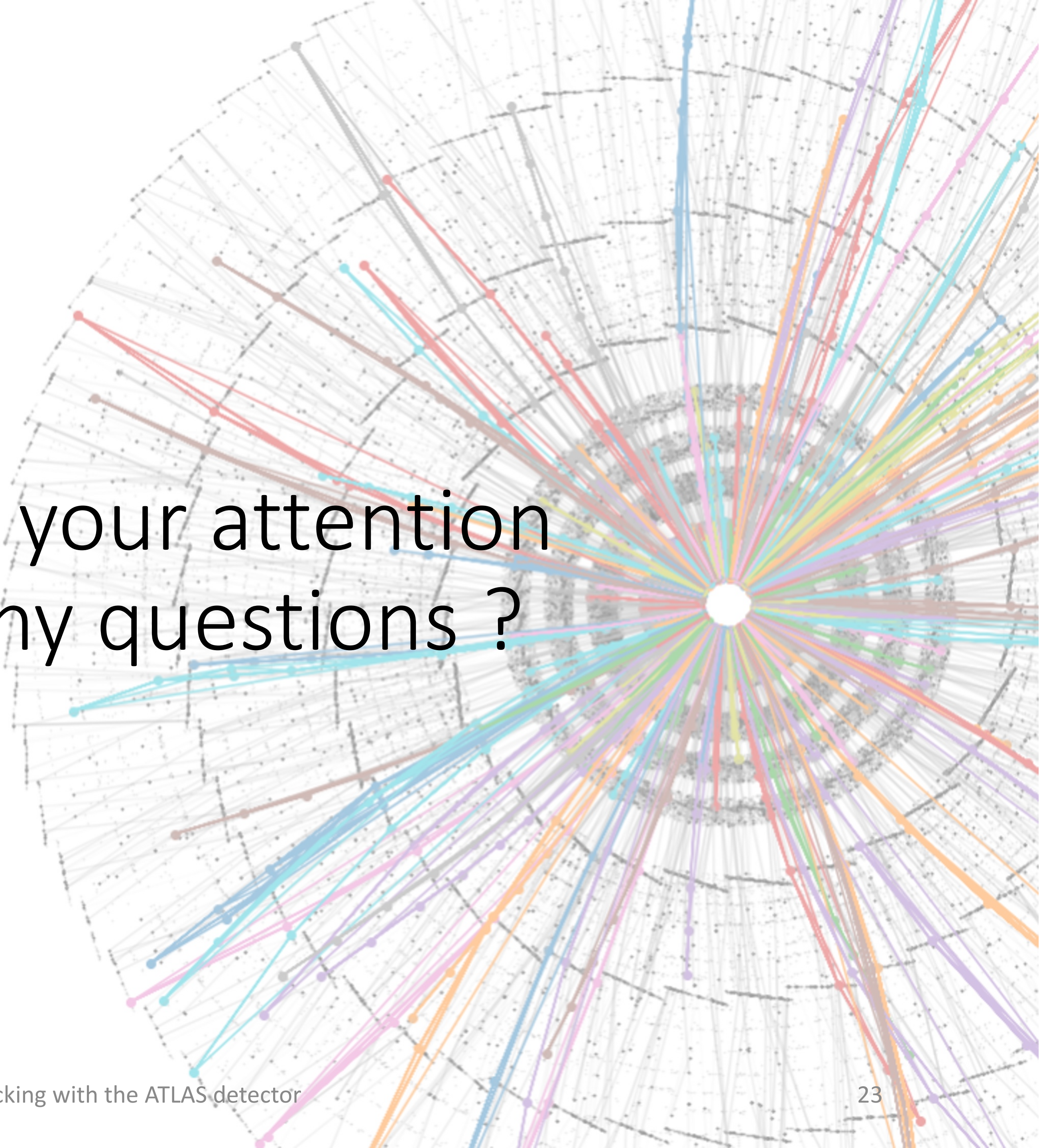
(c)



(d)

Jet tagging
Nodes are particle tracks
Graph classification

Events classification
Nodes are physics object
Graph classification



Thank you for your attention
If you have any questions ?