

Charged particle trajectography using a novel geometric deep learning algorithm

Search for additional Higgs-boson-like particles in ATLAS Run 2 data.

8



Charline Rougier

Michel Daydé Vladimir Gligorov Frédéric Machefert Amber Boehnlein Marumi Kado Jan Stark

President of the jury Rapporteur Rapporteur Member of the jury Member of the jury Supervisor



19th September, MRV, Amphithéâtre 2

The **S**tandard **M**odel (SM) is a gauge theory describing the electromagnetic, weak and strong interactions.

The matter is described by fermions:

- quarks,
- leptons.

Interactions are mediated by **bosons**.







We know the SM is not the end of the story. Many questions remain without clear answers:





I am an experimentalist!

If there is an extended scalar sector, we can observe its effects:

• Modifications of the 125 GeV Higgs boson properties

Require precise measurements of the H properties.

• Discovery of BSM decays of the 125 GeV Higgs boson



• Direct discovery of new scalar particles



Slide 2

Tracking

Back-up-content



The most simple extension of the scalar sector introduces two new real singlets.



Two new additional scalar particles h_1 and h_2 .

What can we infer about their expected properties?

> Their properties highly depend on the specifics of the beyond the SM theory.

$$\begin{array}{c} m_{\rm H} > m_{h_2} > m_{h_1} \\ m_{h_2} > m_{\rm H} > m_{h_1} \\ m_{h_2} > m_{\rm H} > m_{h_1} \\ m_{h_2} > m_{h_1} > m_{\rm H} \end{array} \right\}$$

Two-real-scalar-singlet extension of the SM: LHC phenomenology and benchmark scenarios Tania Robens,^{1,*} Tim Stefaniak,^{2,†} and Jonas Wittbrodt^{2,‡} ¹Ruder Boskovic Institute, Bijenicka cesta 54, 10000 Zagreb, Croatia ²DESY, Notkestraße 85, 22607 Hamburg, Germany (Dated: March 20, 2020) Link Abstract

Many others BSM predict additional bosons

hig



The most simple extension of the scalar sector introduces two new real singlets.



Two new additional scalar particles X and S.

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non-exhaustive examples



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Let's hunt these new additional scalars



The Large Hadron Collider



Currently, the best tool to test the scalar sector is the Large Hadron Collider (LHC):

- Designed to produce p-p collisions at $\sqrt{s} = 14$ TeV
- Also produce heavy ions collisions





The ATLAS (**A** Toroidal LHC ApparatuS) is a 4π detector with a onion-*layers* cylindrical shape.







<u>Slide 2</u> <u>SH</u> <u>Tracking</u> <u>Back-up-content</u>

 $X \rightarrow SH \rightarrow SM$, with $m_X > m_S + m_H$

The search is done using the ATLAS Run 2 dataset, corresponding to an integrated luminosity of 140 fb⁻¹ recorded at $\sqrt{s} = 13$ TeV.



CMS already publicly released <u>results</u> on this analysis: no signal is seen.

Search for $X \rightarrow S(b\overline{b})H(\gamma\gamma)$: backgrounds

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Final state is $\overline{b}b\gamma\gamma$.

Other SM processes have the same final state: single Higgs production, di-Higgs production and continuum background.

Resonant backgrounds









Selection of the signal

Di-photon

- We select 2 photon candidates compatible with an Higgs decay:
- Apply identification criteria
- Reject photons from the decay $\pi^0 \rightarrow \gamma \gamma$
- ✓ Kinematic requirement to optimize the Higgs resonance peak: $\frac{p_T}{m_{\nu\nu}} > 0.35 \ (0.25)$
- ✓ $m_{\gamma\gamma} \in [105, 160] \text{ GeV}$





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- We reconstruct b-jet candidates:
- \checkmark Reconstruct the stream of particles from the jet using the anti- k_t algorithm with R=0.4
- ✓ $p_T > 25 \text{ GeV}$
- ✓ $N_{central jets} \in [2,5]$
- ✓ b-tagging: identify the flavor of the quarks

Selection of the signal: categories

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When $m_X \gg m_S + m_H$:







After the preselections:



Large phase space targeted by the analysis — design, train and use several Neural Networks ?



Parametrized Neural Network (PNN)



- Parametrized with m_{S} and m_{X}
- Input features $\rightarrow m_{b\bar{b}}$ and $\widetilde{m}_{b\bar{b}\gamma\gamma}$

$$\widetilde{m}_{b\bar{b}\gamma\gamma} = m_{b\bar{b}\gamma\gamma} - (m_{\gamma\gamma} - 125 \, {
m GeV})$$



- Parametrized with $\boldsymbol{m}_{\boldsymbol{X}}$
- Input features $\rightarrow p_T^b$ and $\widetilde{m}_{b\gamma\gamma}$

$$\widetilde{m}_{b\gamma\gamma} = m_{b\gamma\gamma} - (m_{\gamma\gamma} - 125 \,\mathrm{GeV})$$

The PNN shape varies depending on the $m_{\mbox{\scriptsize S}}$ and $m_{\mbox{\scriptsize X}}$ hypothesis.



Apply for each targeted mass point a dedicated requirement on the PNN classification score.

Signal and background modelling



Modeled with a Double-Sided Cristal Ball:



Include also all resonant backgrounds.

Continuum background:



Exponential with a normalization taken on the data sideband.





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Systematic uncertainties

Photon energy scale





S



 $(m_X, m_S) = (230, 90) \text{ GeV}$



Observed local significance





No significant excess is seen in ATLAS Run 2 Data for the $X \rightarrow S(b\bar{b})H(\gamma\gamma)$.



Upper limits on the cross-section

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Limits are found to be better at higher masses due to a better signal efficiency and lower background. Observed 95% exclusion limits on $\sigma(pp \rightarrow X \rightarrow SH \rightarrow b\bar{b}\gamma\gamma)$.

The red line is the border between the 1 b-tagged and 2 b-tagged category.







No $X \rightarrow S(b\bar{b})H(\gamma\gamma)$ signal using ATLAS Run 2 Data corresponding to an integrated luminosity of 140 fb⁻¹.

Does not mean that our X and S do not exist.









Upcoming upgrade of the LHC:

- Increase the luminosity of the accelerator by a factor 3
- Increase the data taking rate of the experiment

Sharp increase of the event complexity: Number of simultaneous proton-proton interactions: $40 \rightarrow 200$

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SH

Hillymi High-luminosity era

The LHC experiments are upgrading their detector to cope with the harsher environment.

In ATLAS, this includes:

- Installation of a new Inner **T**racker ITk
- Installation of a a High-Granularity Timing Detector •
- Upgrade of trigger and data acquisition system •
- Replacement of the muon small wheel





Tracking during HL-LHC: a computing challenge

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Track reconstruction is a key step in the event reconstruction, allows to estimate physics parameters of charged particles (p_T , d_0 , z_0 , φ , ...).



Sixty years before this thesis : track reconstruction with a pen and a ruler. Picture from: M. Elsing



ATLAS current inner detector Run 1 ~ 12 pile-up interactions Tracking done using digital readout and algorithms.
 Attack
 Attack<

The algorithms will become too slow to cope with the combinatorics within the CPU budget.

Can we accelerate the algorithm ?





How to deploy a Machine Learning solution for tracking?

> Ask the ML: organize a tracking challenge on the Kaggle platform:



The challenge provides an open source tracking dataset, using a detector geometry mimicking the one from the LHC general purpose experiments.

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الم ال	de	201	Top Quarks	😍 🦷	0.92182	10	2y
ader	2	_	outrunner		0.90302	9	2y
	3	—	Sergey Gorbunov	P	0.89353	6	2y
	4	-	demelian	- A	0.87079	35	2y
	5	-	Edwin Steiner	- A	0.86395	5	2y
	6	—	Komaki	Suret Sular	0.83127	22	2y
	7	_	Yuval & Trian	R	0.80414	56	2y
	8	_	bestfitting		0.80341	6	2y
	9	_	DBSCAN forever		0.80114	23	2y
	10	_	Zidmie & KhaVo	33	0.76320	26	2y



No groundbreaking solution: ML is not at the core of the best algorithms

Why is it so difficult to use ML for tracking?

Deep machine learning applied to tracking

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Why is it so difficult to use ML for tracking?

All the problem lies in the data representation: raw data from tracking detectors are **sparse** data.

Data fed to Neural Networks are frequently represented as an image.

Unsuitable for our tracking detector data.

More natural representation:



Deep machine learning applied to tracking

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Why is it so difficult to use ML for tracking ?

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Unsuitable for our tracking detector data.

More natural representation:

Proof of principle by Exa.TrkX project





Tracking with a Graph Neural Network





The interaction Network model







The interaction Network model















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<u>SH</u> Tracking





The interaction Network model


Simulated sample

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ATLAS simulated sample: $t\bar{t}$ with $\langle \mu \rangle = 200$ at $\sqrt{s} = 14$ TeV

- About 10k charged particles per event
- About 300k space-points per event

Define target particles

- $p_T > 1 \text{ GeV}$
- No secondaries
- No electrons
- At least 3 space-points in the detector

Select $t\bar{t}$ and pile-up interactions



Graph creation: the module map

The path of a target particle is followed through ITk to record all possible **connections** between triplets of silicon **modules**:

- > Built using 90 000 tt events with $\langle \mu \rangle = 200$
- It comprises 1 242 665 connections
- Direction "*inside-out*" is given to edges.

On average, the graphs have O(270k) nodes and O(1.3 million) edges.





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Training the GNN

A technical challenge

Simple GNN architecture configuration

Require 200 GB of GPU memory to train the model

Use of memory management technique.



Configuration of the GNN architecture

- 2 layers in each MLP
- 128-dimensional space parameters
- 8 message-passing iterations

$$L_{BCE}(W,b) = -\frac{1}{N} \sum_{i=1}^{N} \left[y_i \log(p_{w,b}(x_i)) + (1-y_i) \log(1-p_{w,b}(x_i)) \right] \times w_i$$
$$w_i = \begin{cases} 1 \text{ for true edges} \\ 0.1 \text{ for fake edges} \\ 0 \text{ for non-target edges} \end{cases}$$

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<u>SH</u> Tracking

Edge classification performance

Cut at s = 0.5 on the edge classification score



Efficiency and purity degradation in the central region.

What is the source of the inefficiency ?



Investigation of the GNN edge-performance

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GNN track reconstruction efficiency















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THÈSE In vas de l'obtention da DOCTORAT DE L'UNIVERSITÉ DE TOU Délinet par l'Université Tradouse 3 - Parl 5 A Ph.D. in 3 years



















Thank you for your attention





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Content back-up

Analysis PNN architecture PNN score cuts signal cutflows Yields and signal efficiency Summary of systematics Impact of systematics CMS results Likelihood fit

GNN Tracking

Misc FCC LHCb Tracking Timing SPs vs clusters resol QT: seeder validation TrackML-like GNN results Origin fake edges More GNN edge perf plots Track selection Comparison with CKF Inference benchmark Graph topo MM vs ML GSF

Analysis: PNN architectures

2 b-tagged category



				_		
den	se_2		input:	(None, 49)	
Dense	relu		output:		None, 45)	
			L			
drop	out_2	iı	iput:	(N	lone, 45)	
Dro	pout	οι	itput:	(N	Jone, 45)	
den	se_3		▼ input:	((None, 45)	
Dense relu		1	output:		(None, 81)	
drop	out 3	iı	▼ nput:	(1)	Jone, 81)	
Dro	pout	t output		(N	lone, 81)	
dense_4			input:		(None, 81)	
Dense sigmoid			output:		ar 1)	

Number of hidden layers	4
Layer 1 dropout rate	0.05
Layer 2 droport rate	0.1
Layer 3 dropout rate	0.2
Layer 4 dropout rate	0.1
Learning rate	0.009137
Optimizer	Adam
Loss function	Binary Loss
Initial bias	0.118
Signal class weight	0.945
Background class weight	1.062
Batch size	212613
Number of batches	2
Number of epochs	2000

In both category, final activation function = sigmoid Automatically tuned with Keras Tuner (maximize AUC) Similar for 1 b-tagged category





Optimization of the PNN classification cuts

Slide 2 SH <u>Tracking</u> Back-up-content

We know from previous analysis, that we will be able to use the asymptotic approximation if we guarantee to have at least 9 event in the $m_{\gamma\gamma}$ data side-band. We want to maximize the significance:



$$Z_A = \sqrt{2} \left[(S+B) \ln(1+S/B) - S \right]$$

$[\mathbf{m}_{\mathbf{X}}, \mathbf{m}_{\mathbf{S}})$ [GeV]	PNN cut value	$\begin{array}{c} (\mathbf{m_X},\mathbf{m_S}) \\ [\text{GeV}] \end{array}$	PNN cut value	$[\mathbf{GeV}] \tag{Markov} \label{eq:markov} \begin{bmatrix} \mathbf{m_X}, \mathbf{m_S} \end{bmatrix}$	PNN cut value
(170, 30)	0.56	(245, 50)	0.92	(500, 300)	0.91
(180, 50)	0.81	(245, 70)	0.92	(600, 70)	0.86
(185, 30)	0.80	(245, 90)	0.91	(600, 170)	0.88
(190, 15)	0.70	(250, 15)	0.78	(600, 200)	0.87
(190, 50)	0.90	(250, 100)	0.91	(600, 300)	0.88
(200, 70)	0.92	(250, 110)	0.91	(600, 400)	0.91
(205, 30)	0.91	(300, 30)	0.92	(750, 70)	0.97
(205, 50)	0.91	(300, 70)	0.90	(750, 110)	0.93
(210, 15)	0.75	(300, 110)	0.92	(750, 170)	0.84
(210, 70)	0.92	(300, 170)	0.92	(750, 200)	0.81
(220, 90)	0.91	(400, 30)	0.88	(750, 300)	0.88
(225, 30)	0.92	(400, 70)	0.90	(750, 400)	0.81
(225, 50)	0.92	(400, 110)	0.89	(750, 500)	0.82
(225, 70)	0.92	(400, 170)	0.88	(1000, 70)	0.98
(230, 15)	0.74	(400, 200)	0.89	(1000, 110)	0.61
(230, 90)	0.91	(500, 30)	0.92	(1000, 170)	0.82
(230, 100)	0.91	(500, 70)	0.91	(1000, 200)	0.76
(240, 100)	0.91	(500, 110)	0.89	(1000, 300)	0.73
(240, 110)	0.90	(500, 170)	0.90	(1000, 400)	0.55
(245, 30)	0.92	(500, 200)	0.87	(1000, 500)	0.67

Blue cell = 1 b-tagged category

S Analysis: cutflows before PNN cuts

Selection	(190,15)		(250,110)		(600, 170)		(1000, 300)	
	Yield	Efficiency	Yield	Efficiency	Yield	Efficiency	Yield	Efficiency
All events	148.18	100.0%	148.78	100.0%	144.19	100.0 %	143.64	100.0 %
Pass trigger	93.41	63.0%	97.40	65.5%	126.71	87.9%	133.82	93.2 %
Has primary vertex	93.41	63.0%	97.40	65.5%	126.71	87.9%	133.82	93.2%
2 loose photons	73.44	49.6%	77.38	52.0%	86.76	60.2%	95.58	66.5%
$e - \gamma$ ambiguity	73.40	49.5%	77.35	52.0%	86.72	60.1%	95.55	66.5%
Trigger match	66.94	45.2%	70.35	47.3%	84.48	58.6%	94.85	66.0%
Photon tight ID cut	57.19	38.6%	59.72	40.1%	71.82	49.8%	80.21	55.8 %
Photon isolation cut	49.60	33.5%	49.80	33.5%	65.62	45.5%	74.99	52.2%
Rel. $p_{\rm T}$ cuts	45.59	30.8%	46.01	30.9%	60.46	41.9%	71.61	49.9%
$m_{\gamma\gamma} \in [105, 160] \text{ GeV}$	45.56	30.7%	45.96	30.9%	60.37	41.9%	71.48	49.8%
$N_{lepton} == 0$	45.53	30.7%	45.9	30.9%	60.30	41.8%	71.34	49.7%
$N_{centraljets} \in [2, 5]$	17.03	11.5%	30.42	20.4%	54.53	37.8%	68.62	47.8%
1 b-tagged selection	10.71	7.2%	14.67	9.9%	21.95	15.2%	24.31	16.9%
2 b-tagged selection	0.59	0.4%	9.94	6.7%	23.60	16.4%	30.83	21.5 %

Table 6: Cutflows for some generated MC signal sample. A signal cross-section of 1 fb is considered.

SI Analysis: signal efficiency















Analysis: single Higgs





m_s [GeV]





m_s [GeV]

Tracking: timing

Timing consideration

- The target is to run the full pipeline in < 1 second.
- Need to be fully run on GPU.

TrackML timing (Similar graph size as for ITk):

Pipeline step	V100 GPU		
Graph construction (metric learning)	~ 500 ms		
Graph construction (module map)	In progress target ~ 100 ms		
GNN	~170 ms		
Connecting component	~100 ms		
(See this paper)			

How to improve: GPU kernels have dedicated operation for NN. But the GNN model is much complex with its 8 message-passing operations and the way the memory is therefore handle.

Using dedicated GNN kernels could only improve the timing, the memory consumption and the energy cost.



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<u>SH</u> Tracking

Tracking: resolution of clusters and SPs in strip

<u>SH</u> <u>Tracking</u> <u>Back-up-content</u>

Slide 2



(c) Cluster and space-point resolution vs z.

(d) Cluster and space-point resolution vs r.

Figure 12.4: Cluster and space-point resolution in the ITk strip subdetector. The resolution is defined as the difference in z or r between the simulated Geant4 hit positions and the reconstructed cluster and space-point ones.

Motivation

Porting and validation of the new ITk seed maker algorithm of r22 to r21.9. This back-porting allows us to study the new seed maker with well-understood simulated samples produced using r21.9.

Jira ticket <u>here</u>



Two seed makers: validation of the release 22 seeder is now possible by comparing to the default ITk seeder of release 21.9.



• Comparison of the new ITk seeder with the default one

Using the 400 $t\bar{t}$ events with $\langle \mu \rangle$ =200 :

	Default seeder	New seeder	Ratio new / default
Total number of seeds	12 419 289	9 866 806	79.4%
PPP seeds	10 234 093	7 702 037	62.0%
SSS seeds	2 185 196	2 164 769	99.0%
Total number of seeds giving a track	1 383 446	1 336 765	96.6%
PPP seeds giving a track	932 797	888 978	95.3%
SSS seeds giving a track	450 649	447 787	99.4%
Tracking efficiency	90.396%	90.282%	99.99%
Fake tracks rate for 9 clusters	6.68×10 ⁻³	6.51×10 ⁻³	97.5%

The New ITk seeder find less seeds than the default one, especially in the pixel. The tracking efficiency is slightly degraded as well.

21.9



- \odot The New ITk seeder produces no seeds for d_0 > 0.7
- \circ η distribution is buggy, but it is only use in the validation Ntuple.

Let's hunt bugs

	Default seeder	New seeder	Ratio new / default
Total number of seeds	12 419 289	12 563 203	101.2%
PPP seeds	10 234 093	10 378 008	101.4%
SSS seeds	2 185 196	2 185 195	100.0%
Total number of seeds giving a track	1 383 446	1 389 585	100.4%
PPP seeds giving a track	932 797	938 936	100.6%
SSS seeds giving a track	450 649	450 649	100.0%
Tracking efficiency	90.396%	90.398%	100.0%
Fake tracks rate for 9 clusters	6.68×10 ⁻³	6.69×10 ⁻³	100.0%

This does not degrade the tracking efficiency. More seeds are produced, so the tracking efficiency is slightly improved.




https://arxiv.org/abs/2103.00916



SI Summary of included systematics

		Signal	ttH	ggH	ZH	Others single Higgs	Di-Higgs	Continuum
Theory	Yield	Parton shower	QCD scale PDF+ α_s					
Experimental	Yield	Luminosity Photon trigger efficiency Pile-up scale factors Photon energy resolution and scale Photon identification efficiency Photon isolation efficiency Jet energy resolution and scale Jet η calibration Flavor tagging efficiencies Jet Vertex tagger Jet pile-up offset			Negligeable	Negligeable	Spurious signal	
ShapePhoton energy resolution and scalePhoton identification efficiencyPhoton isolation efficiencyPhoton trigger efficiency			Negligeable	Negligeable				

S Analysis: impact systematics





Investigation of the GNN edge-performance

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Non-fiducial particles = particles with $|\eta| > 4$ or $r_{vertex} > 26$ cm





CMS already released <u>public</u> results on this analysis.

No significant excesses are seen.

Although, local (global) significance of 3.8 (2.8) standard deviations is observed for $(m_X, m_{S(Y)}) = (650, 90)$ GeV.





Testing for discovery

Background only hypothesis H_0



Exclusion limits



We set upper limits on the signal cross-section $\sigma(pp \to X \to SH \to b\bar{b}\gamma\gamma)$.



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Back-up-content

SH Tracking

Track selection and CKF perf

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Requirements	$ \eta < 2.0$	$2.0 < \eta < 2.6$	$2.6 < \eta < 4.0$
Number of pixel $+$ strip hits	≥ 9	≥ 8	≥ 7
Number of pixel hits	≥ 1	≥ 1	≥ 1
Number of holes	< 2	< 2	< 2
Number of double holes	≤ 1	≤ 1	≤ 1
Number of pixel holes	< 2	< 2	< 2
Number of strip holes	< 2	< 2	< 2
$p_{\mathrm{T}} \; [\mathrm{MeV}]$	> 900	> 400	> 400
$d_0 \; [m mm]$	≤ 2	≤ 2	≤ 10
$z_0 [{ m cm}]$	≤ 20	≤ 20	≤ 20







SI Comparison with CKF

Slide 2 SH <u>Tracking</u> Back-up-content



Average number of strip hits on a track as a function of the true pseudorapidity η_{true} for hard scattering primary particles from $t\bar{t}$ decays at $\langle \mu \rangle = 200$. The tracks, i.e. sets of hits, from the two track finding methods are fit using the method that is part of the standard reconstruction (<u>ATL-PHYS-PUB-2019-014</u>). Tracks found by the CKF and the subsequent ambiguity solution (<u>ATLAS-TDR-025</u>) are selected using the standard quality requirements (cf. Table 7 of <u>ATL-PHYS-PUB-2019-014</u>) and are required to satisfy $p_T > 1$ GeV. Tracks found by the GNN are required to satisfy criteria that are slightly less strict: at least 6 silicon hits, transverse impact parameter $|d_0| < 20$ mm, longitudinal impact parameter $|z_0| < 25$ cm and $p_T > 1$ GeV. The simulated particles matched to reconstructed tracks are required to satisfy $p_T > 2$ GeV to avoid turn-on effects. The ratio is defined as the number of hits for the GNN track finding divided by the number of hits for the CKF track finding. The same set of 100 simulated events is used to evaluate the track hit content obtained for tracks from CKF and from GNN track finding. The differences in the number of strip hits per track from the two track finding methods is largely due to the use of space points (built from hits on both sides of a given strip module) in the GNN track finding and the use of individual hits in the CKF track finding.

S Edge classification performance





Prediction sample

- 100 events from TrackML
- Graphs have similar size as those obtained with ITK

	Quadro RTX 8000	GeForce RTX 2080 Ti Gaming GPU	
GPU memory capacity (GB)	48	11	
Runtime mixed precision (16/32)	350 ms / event		
Memory peak consumption	5.4 GB		

Study on TrackML sample, without optimization.

No memory issue during prediction

Will also benefit from dedicated kernel => large factor of improvement expected from dedicated CUDA kernel



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Back-up-content

<u>SH</u> Tracking



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-1000

1400₁

1200

1000

800

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400

200

-3000

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r [mm]



r [mm]

per node

edges I

Number of outgoing

25

20

15

10

5

0

3000

z [mm]

2000



z [mm]





-3

-2

0

η

4

2

3





- ~ 91 km ring-shaped underground tunnel
- Start of construction = 2030
- Proto-collaboration are being formed
- at least 4 detectors

	Start	Operation	
e-e	~2040 After HL-LHC	15 years	Energies from 80 to 400 GeV
р-р	~2080	25 years	100 TeV





Single electron: event display

