

# **AI task force – 3<sup>nd</sup> meeting**

Wouter Verkerke

# Agenda

1. Review summary of AI use and future plans in the various groups
2. Next steps & agenda items for meetings

# Current AI - production use

(1.1)	Object reco	Object ID	Calibration	Sig/Bkg discrimination	Anomaly/ Glitch detection	Stat. analysis/ param est
<b>Alice</b>	Tracking ITS & MFT (cellular automaton)	Flavor tagging with DNN	Jet energy with DNN	Simple models	Unsupervised, reinforcement learning	
<b>ATLAS</b>	Boosted objects with GNN	Flavor tagging with GNN	Mass regression of heavy objects	Wide range, including DNNs,	Variety of methods	LR of MVA score NSBI methods high-dim NN (SUSY)
<b>LHCb</b>	Small/fast track reco models	Simple classifiers	Simple classifiers			
<b>GW</b>					DeepExtractor	FlowMC, JIM, Jester (JAX), Flex. <b>WW:</b> <b>NSBI used?</b>
<b>DM</b>	NN event reco (lightweight to GNN)	NN classification (lightweight to GNN)				Neural posterior estimation
<b>Pierre Auger</b>	DL shower reco (RNN/GNN)	-	-	-	-	-
<b>Neutrino</b>	-	-	-	-	-	
<b>eEDM</b>	-	-	-	-	-	-
<b>Theory</b>	Jet substructure	Jet tagging				SMEFT, WEFT, PDFs etc with (G)NN

# Current AI – Nikhef in AI application R&D

	Nikhef involvement in current AI application R&D (2.1)
<b>Alice</b>	Combining tools (transformer + OneClass SVDD) – WV: incomplete answer
<b>ATLAS</b>	Track reconstruction, jet flavor tagging, boosted object mass regression, NSBI, foundation models, anomaly detection, physics language models
<b>LHCb</b>	ML ops in trigger, topics in IRIS-HEP, PINNs for track extrapolation, anomaly detection (with Maastricht)
<b>GW</b>	Parameter estimation and glitch characterization
<b>DM</b>	Event classification mostly WV: inferred answer, probably incomplete
<b>Pierre Auger</b>	- (end user only)
<b>Neutrino</b>	MSc projects on shower/particle ID
<b>eEDM</b>	-
<b>Theory</b>	SMEFT/WEFT/PDF fits, jet substructure

# Current AI – Nikhef experts

	Staff (2.2)	PhD/PD (2.2)
<b>Alice</b>	A. Grelli (DNN on FPGA), M. Verweij (LSTM... transformers)	"Plenty"
<b>ATLAS</b>	S. Caron (broad), C. Nellist (selection) S. Rettie (in tracking) (W. Verkerke / L. Brenner – interface stats & ML), applications: F. Filthaut, T. du Pree, M. Vreeswijk	Z. Wolfs, P. Moskvitina, M. Silva, K. de Vries, O. Karkout, A. Sidley, W. Leinonen, L. Franco(PD)
<b>LHCb</b>	To some extent: R. Aaij, M. van Veghel, J. de Vries	X. Chiotopoulos
<b>GW</b>	A. Samajdar	M. Lopez (PD), P. Pang (PD), T. Dooney, L. Negri, T. Wouters, H. Narola
<b>DM</b>	J. Aalberts (DL/SBI). A. Colijn (AI-accelerated coding)	J. Mead (PD), M. v Nuland, M. Flierman, K. Weerman
<b>Pierre Auger</b>	-	T. Bister (PD)
<b>Neutrino</b>	R. Bruin (somewhat)	
<b>eEDM</b>	-	-
<b>Theory</b>	J. Rojo	

# Current AI – BSc/Msc project | coding tools

	Master and Bachelor student projects with AI? (2.3)	Use of AI coding tools? (2.4)
<b>Alice</b>	About 70% of student projects have AI use, collaboration with UU math	Some members using it
<b>ATLAS</b>	Many (probably almost all), also have few CS AI MSc students in group	Limited (mostly Sascha)
<b>LHCb</b>	Very positive experience. Multiple CS AI students as well	Sparse use of co-pilot, various levels of ChatGPT
<b>GW</b>	So far about 10 MSc/Bsc theses with AI use	Co-pilot and ChatGPT used
<b>DM</b>	Some Msc projects with NL	Co-pilot and ChatGPT used by most
<b>Pierre Auger</b>	Sporadic use	Co-pilot and ChatGPT used
<b>Neutrino</b>	Three Msc projects	n/a
<b>eEDM</b>	-	WV: answer missing
<b>Theory</b>	A handful of BSc/MSc exploring ML applications	Co-pilot and ChatGpt use starting, want support and data protection

# Near future AI –use, applications, resources

	Expected future AI use (3.1)	Novel AI applications (3.2)	Resource requirements (3.3)
<b>Alice</b>	Inference and explainability, generally much more broad use	Use in FPGA trigger, transformers in tracking, generative AI simulation	No clear, biggest reqs likely for AI tracking of PbPb collisions
<b>ATLAS</b>	Increased use in all areas, move to larger AI models (foundation models), strong increase of use in stat analysis NSBI & unfolding,	Already used almost everywhere ML on FPGA in TDAQ/trigger	Large GPUs(H100 etc) for tracking & foundation models, otherwise mostly modest use of inference models (L40S etc)
<b>LHCb</b>	Inclusive ftag with transformers, Generative models for simulation, more extensive use in online and trigger	Anomaly detection, reco of complex signatures, full event interpretation	GPU in trigger farms and datacenters
<b>GW</b>	Replace classical parameter estimation and glitch detection tools with AI-based tools,		GPUs recently acquired as part of grant (L40S), access to Snellius
<b>DM</b>	Possibly training on 'all data' (but gains hard to predict now)		GPUs for student model training, large models may require investments?
<b>Pierre Auger</b>	Improved classification & reco with GNNs and LLMs (gains unclear now)	Possibly in radio trigger and arrival detection interpretation	unclear
<b>Neutrino</b>	Improve classification & reco (in particular hadronic FS in Orca),	determine composition of CRs, use mixed LL/AI models (WV: this is really NSBI)	Not yet known
<b>eEDM</b>	AI(NN) for experimental design optimization	stabilizing feedback using FPGA	-
<b>Theory</b>	Simulation based inference (but generally unsure)		-

# Near future AI – Nikhef involvement in R&D

	Ambitions (4.1)	Leading institutes intl (4.2)	Comparison with Nikhef (4.3)
<b>Alice</b>	Be part of new developments in analysis and tracking	Scattered over many institutes worldwide	We lack computer scientists, could profit more from collab with math & AI. Lack of PhDs. So far compute cluster was sufficient
<b>ATLAS</b>	Sascha: AL/ML leader in HEP worldwide. ATLAS group: strong AI/ML involvement in all areas in diHiggs (selection, calibration, regression, inference). Tracking: strong involvement in HL-LHC AI tracking (Sebastien, Sascha), R&D on statistical properties of ML methods (Wouter & Lydia)	Paris (Rousseau), Germany (Heinrich, Plehn), Geneva (Golling), US (Cranmer, Whiteson, Nachman, Brehmer). With exception of Cranmer, mostly 1-person efforts	Staff size & expertise comparable to world leaders, but much more limited in PhD volume and in computing resources
<b>LHCb</b>	Jet reconstruction / substructure, isolation at high PU, ftag with transformer models, AI tracking, online use of AI/ML	MIT (multiple areas), Coruna (ftag), soon Spain with supercomputers and funds	A bit behind, but expecting to catch up. Less dedicated focus on AI, but excellent infrastructure. Leading online
<b>GW</b>	Replace classical parameter estimation and glitch detection tools with AI-based tools (VV – replicated from 3.1)	Cambridge, Glasgow, Johns Hopkins	We are among leading institutes
<b>DM</b>	Possibly training on ‘all data’ (but gains hard to predict now) (VV – replicated from 3.1)	-	-
<b>Pierre Auger</b>	Still in exploratory phase. Likely more involvement in data analysis and reconstruction	KIT, Aachen, Erlangen	Nikhef has little expertise and person power. Not enough info on infrastructure.
<b>Neutrino</b>	Should get into business, but first need to educate selves	Ecap, Erlangen	n/a
<b>eEDM</b>	Optimize experimental design and use feedback loops with AI/ML (VV - replicated from 3.1)	-	-
<b>Theory</b>	-	-	-



# Near future AI – Nikhef involvement in R&D

	National and int'l partners (4.4)	What is missing to realize ambition (4.5)	Expectations coding assistance(4.6)
<b>Alice</b>	Changes per project	PhDs & PDs, computer scientist	Importance will grow in time
<b>ATLAS</b>	Sascha: Uva(C. Weniger), RU( AI dept), SURF, eScience Center, Lydia: groups in Heidelberg, Munich, US. Ftag/reco: largely through ATLAS collaboration	GPU infrastructure, broader/visible AI/ML group at Nikhef, in-house AI expertise. Own inference machine at Nikhef / participation in European effort	In-house coding/knowledge tools that are safe for use.
<b>LHCb</b>	SURF, DACS (Maastricht) ; Coruna, LHCb collaboration	Person power to the work (PhD+PD), ML + statistics expertise with focus on math	Experiment-specific and/or private ChatGPT (concern about review code of AI generated code)
<b>GW</b>	UC Louvain, Potsdam	In-house AI experts	Importance will grow in time. (Our in-house expertise is not sufficient to match ambitions.)
<b>DM</b>	Rice U (C. Tunnel) & UCSD (A. Li)	(VV - answer missing)	Research and coding assistant (LLM) trained on private data (pilots in Xenon)
<b>Pierre Auger</b>	KIT and Aachen	Education, training, documentation, acces to GPUs	Requires institutional support for optimal use
<b>Neutrino</b>	n/a	Self-education	No formal plans, but expect that importance increases
<b>eEDM</b>	-	Expertise & expertise and information, opportunities for joint projects	-
<b>Theory</b>	-	Support in form of joint PHD to explore options	-

# Long-term future – AI potential

	‘Disruptively big’ ideas for future AI applications (5.1)
<b>Alice</b>	Lead-Lead track reconstruction (WW ??), detector simulation and design, extract physics from the tails
<b>ATLAS</b>	Large Physics models as natural end point of LLMs and foundation models. AI-assisted optimal detector/sensor design
<b>LHCb</b>	Pat. rec in high pileup, Lattice QCD, generic model-independent anomaly detection, optimal detector design, global reoptimization of software
<b>GW</b>	Tools for the Einstein telescope – current methods don’t work (partly funded in awarded XL)
<b>DM</b>	Redesign of analysis and computing pipelines of next-gen experiments (XLZD etc)
<b>Pierre Auger</b>	Full 3D reco of galactic magnetic field. AI-assisted optimal layout of observatory. Unthinned simulations (w/o energy cutoff)
<b>Neutrino</b>	Signal detection in acoustic neutrino detectors
<b>eEDM</b>	-
<b>Theory</b>	Lattice QCD

# AI – Other comments

	Other comments (6.1)
<b>Alice</b>	Alice has a stats & ML forum where we try to steer the various efforts
<b>ATLAS</b>	Happy to help (Sascha) / Need to invest in both hardware and person power
<b>LHCb</b>	Structured training of people beyond superficial use
<b>GW</b>	
<b>DM</b>	Can we have an AI/ML bootcamp – for new people to get started
<b>Pierre Auger</b>	-
<b>Neutrino</b>	Basic knowledge and education is missing, propose education of Nikhef staff
<b>eEDM</b>	
<b>Theory</b>	

# Some first observations – AI use & user base

- **Current AI use in production**

- **Clear ‘front-runner’ group: ATLAS+Alice+LHCb+GW+DM** where AI is pervasively in use
- Second group Auger+eEDM+Neutrino+Theory\*, with more limited AI use at the moment (but all with interest to catch up)
- Most AI use currently in object-level reconstruction/identification and event-level discrimination tasks.
- Limited use of AI in inference (limited use in GW ATLAS at present) and in simulated data generation

- **Level of AI involvement in Nikhef programs divides along same groups**

- Strong multi-front involvement in front runner group
- Limited (end-user) use in second group

- **We have a quite sizeable group of scientists involved across programs!**

- About **15 staff** – with expertise ranging from top-tier (Sascha) to ‘limited, but with strong interest’
- Another **20 PhD/PD** closely involved with AI application, plus a few more on AI method development

- **AI is commonly used in MSc/BSc projects in ‘front runner group’ (50-70%?)**

- **Generally (very) positive experiences for those participating**
- Also embedding of CS/AI students in several programs

- **Use of coding tools (co-pilot, ChatGPT) still quite limited**

- A handful of users in each program (including groups that otherwise don’t use much AI)

# Some first observations – AI in near future

- **Expected future use to increase all experiments**

- Overall use expected to become more pervasive.
- General move to **larger models** with more **ambitious goals** (transformer models directly using all data) in experiments already deploying AI (→ foundation models)
- Use of AI for **highly complex data** (HL-LHC tracking, ET GW signals)
- Production deployment of AI methods in statistical **inference**/parameter estimation (NBSI), and fast event **simulation** (GANs etc), **anomaly detection**
- Use of AI in low-latency online environment (trigger) → **FPGA** implementation (Alice, ATLAS, eEDM)
- Interest in AI-assisted experimental **design optimization**

- **Required infrastructure/resources**

- Most ambitious R&D projects (ATLAS/Alice tracking) require state-of-the-art GPUS (nVidia H100/H200), available in Snellius, not locally. LHCb needs GPU in trigger/online farms
- GW purchased already nVidia L40S for medium-term needs
- All other Nikhef applications likely (much) less demanding, but not always clear

# Some first observations – AI ambitions

- **AI ambitions of Nikhef groups**

- ‘front runner’ experiments: to have leading involvement AI application development in many areas (tracking, object identification, regression of object properties, statistical inference, anomaly detection, physics-inspired models)
- ‘second group’ experiments: deployment in reconstruction and data analysis

- **Leading institutes in AI in HEP world-wide**

- Many relatively small groups (1 staff + PhD/PD) at universities in US and Europe.
- Little overlap between leading institutes per experiment → few seem to on multiple experiments?
- Main exception – UW Data Science center / Kyle Cranmer – 20 FTE. (KC is also former supervisor many of the current strong senior scientists with groups in ATLAS)

- **Comparison of leading institutes with Nikhef**

- Often  $O(1)$  staff – thus comparable in size and expertise with Nikhef groups (with a bit of spread)
- Several groups have better connection to non-HEP AI/CS/Math experts
- Often have more sizeable PhD/PD groups working on AI projects
- In certain countries access to vastly larger computing resources (notably US, Spain in future?)

# Some first observations – AI ambitions

- **Inter(national) partners in AI development**

- national entities: SURF, eScience center
- non-HEP groups at NL universities: Grappa@Uva, AI@Radboud, DACS@Maastricht
- *But mostly through personal contacts of a few individuals or locations (Sascha, Maastricht)*
- International universities: handful of universities in Europe and US, O(1-2) per group

- **What are we missing to realize our ambitions?**

- Education/training/expertise (mostly in the '2<sup>nd</sup> group')
- Close connections to domain experts in CS/AI, math/statistics
- Sufficient in-house GPU compute power, access to large-scale NL and EU AI centers
- PhD/PD person power

- **Expectations on future of coding assistance**

- Expected to generally grow and importance and use
- Emphasis/concerns on secure (in-house) services for use on private data and/or information
- Institutional support

# Some first observations – AI long-term ambitions

- **Long-term goals that may be realizable with AI**
  - Large-scale data reconstruction from low-level data (HI PbPb tracking)
  - AI-assisted (re)design of software structure and analysis pipelines ('end-to-end optimization')
  - AI-assisted design – from sensors to entire detectors / observatories
  - Large Physics Models as evolution of foundation models (trained on low-level data, allows for high-level physics queries)
  - AI Lattice QCD



# Many areas of cross-group interest

- **AI classification strategies**
  - Pretty much every group
- **AI track/pattern reconstruction**
  - ATLAS+LHCb+Alice (+Neutrino?)
- **AI anomaly detection**
  - Known background, unknown signal
  - GW, ATLAS, Neutrino, PierreAuger, DM
- **AI physics-inspired model architectures**
  - LHCb, ATLAS, + ??
- **AI statistical inference / param estimation (NSBI etc) / stat properties of ML methods**
  - GW, ATLAS, LHCb, Neutrino, Theory + ??
  - Mostly powerful for physics problems with  $\gg 1$  parameter of interest
- **AI deployment in FPGAs for trigger, or feedback loops**
  - ATLAS, Alice, eEDM
- **AI assisted optimization of data analysis pipelines and software ('end-to-end optimization')**
  - ATLAS, LHCb, DM + ??
- **AI foundation models / full event interpretation**
  - ATLAS, LHCb, Alice, + ??
- **AI assisted detector/observatory optimization**
  - ATLAS, PierreAuger, eEDM, Alice

# Next steps

- **Driving the agenda in the short term is the submission of a grant proposal to the NWO-I 'Strategische Vernieuwingsfonds' by July 8<sup>th</sup>**
  - Along the lines of abstract submitted earlier: focus on expert person power (staff + 2 PD) + limited amount of state-of-the art HW
  - About 4 pages + figures. To be written by WV (with your input), to be submitted by JDH.
  - Durable result (beyond funding period) in align with Nikhef strategic goals
  - As 'kick starter' to setup a strong cross-program AI organization within Nikhef.
- **Important open questions to answer next (in this order)**
  1. What **goals/activities** should this new 'cross-program organization' deliver?
  2. How to best **structure/organize** this?

# Future AI organization – goals & activities

- **What goals/activities should this new ‘cross-program organization’ deliver?**
  - Organize AI education/training programs for PhD/PD as well as staff (lectures series?, schools? interactive-handson?). Education on coding assistance?
  - Involvement in setting up local LLM knowledge services (ChatGPT/DeepSeek)?
  - Organize access to AI infrastructure facilities (at Nikhef and outside [ Snellius etc ], at EU level?)?
  - Maintain in-house expertise on AI techniques that are of crucial importance for group in the Nikhef portfolio (which ones)?
  - Do R&D on development of AI techniques on HEP applications of importance to Nikhef (which ones)?
  - Community building role (meetings, workshops, etc)?
  - Become central point of contact for AI/CS and AI/Math departments for universities all over NL?
  - Become attractive partner for participation in large-scale AI funding proposals (at national or international level) [ nlaic.com ]
  - Role in (inter)national strategy discussion on roadmaps for AI?

# Next meetings

- **4<sup>th</sup> Task force meeting – Monday June 2<sup>nd</sup> 10-11**
  - Discuss goals and proposed structure of 'cross-program AI organization'
- **5<sup>th</sup> Task force meeting – Thu June 19<sup>th</sup> 14-15.30**
  - Discuss outline of the proposal text for the 'Strategische Vernieuwings fonds'
- Not sure if we need another meeting before the proposal submission
  - Will circulate draft for comments well in time
- **After summer break – more meetings (to be scheduled)**
  - Inventorize AI landscape at CS/Math departments at Dutch universities, existing connections with Nikhef, opportunities for new connections. [ Theory connections ]
  - Finalize task force report before October (decision SV fund)