AI & Dark Matter

A - Current situation – production use of AI/ML

NB: For this inventory we only consider 'modern large-scale AI/ML techniques' in the scope of this survey (i.e. not BDTs and/or lightweight NNs etc).

Where is the major current impact of AI in your research area? What are the physics areas of application where AI is having a major impact internationally in production use in your research area? Briefly sketch the purpose of application and what ML/AI architectures/techniques are currently used (LLM, GNNs etc…) along any with major computing resource requirements (for training / for application).

In the XENONnT dark matter detector, and similar mid-size experiments, several **neural networks are part of production pipelines** for event reconstruction and classification. Some of them are "lightweight", others use modern methods including graph convolutions and neural posterior estimation.

The field is doing **R&D towards more intense/impactful AI use in production**. For example, we see long-range time correlations in our detectors, which could be analyzed with transformers similar to language models. Similarly, there have been attempts to replace (computationally intense parts of) waveform simulators with AI models.

Finally, **large language models** have been trained on collaboration code and information to provide chatbots that can give technical support to (starting) scientists.

What is the involvement of Nikhef scientists in current efforts? Are you involved in or internationally leading in R&D* on the application of AI/ML methods in your research area? [*: AI/ML R&D here = research and development of ways to deploy AI/ML techniques within your research domain not core computer-science research of entirely new AI techniques] Who are the in-house experts? What is their expertise? Please distinguish staff vs PhD/PD expertise.

Staff expertise:

- **Jelle Aalbers** teaches a course on Deep Learning for Physics at the RUG, has developed/deployed several AI/ML models, and collaborated with astronomers and Google researchers on a deep learning project using simulation-based inference.
- **Auke Pieter Colijn** is an early adopter of AI-accelerated coding, and has used it for several significant software projects.

PhD/PD expertise:

- **James Mead** (before joining Nikhef) developed jet tagging algorithms for LHC data, both BDTs (XGBoost) and DNNs (Keras), and for a time managed the MC production for the

IceCube Upgrade used in ML model training for event reconstruction. He taught courses on analysis in python and developed lessons for the HSF on classification problems and hyperparameter tuning.
- **Marjolein van Nuland-Troost** has experience with deep learning from her earlier work, and studied applying this for event reconstruction for DUNE and XENON.
- **Maricke Flierman** has worked with an MSc student and outside researchers to deploy self-organizing maps (an unsupervised neural network technique) for event classification for the XAMS onsite R&D detector at Nikhef.
- **Kelly Weerman** is working on a Transformer Model to tag background events with long-range correlations that are difficult to distinguish with the current likelihood selection. She is also working on a benchmarking dataset.

To what extent use MSc/BSc projects in your group focus on AI/ML use? Do you have experience with Comp.Science (AI) and/or Math students (Bsc/Msc/PhD) in your group working AI/ML in physics?

Some of these projects involve deep learning; for example, a student trains a model and checks if it outperforms an existing technique.

Are you (at Nikhef) using AI-based coding assistance tools?

Yes, most of us who code regularly use either ChatGPT, Copilot, or a combination of models for coding assistance.

B – Mid-term future (2-4 years) – effects of ongoing R&D in known AI/ML

On scale of O(3) years future of ML/AI in HEP is reasonably predictable, since it is dominated by deployment of currently known AI/ML techniques and less on unpredictable emergence of new techniques. What is the expected ML/AI use in your research area in the next years? Extrapolating from current experience, where will future/improved deployment of ML/AI bring strong gains in physics performance in the next few years? What AI/ML techniques do you expect to perform strongly in the near future (LLMs, foundation models, simulation-based inference, generative models etc etc) Are there major novel ML/AI application areas in the pipeline? (i.e. areas where ML is now not used)

More of our analysis will likely be tuned by gradient rather than graduate student descent; for example, the clustering/grouping of signals, and certain event selections.

It is harder to predict whether **training very large models on "all the data"** will make a big impact. We may see AI-enabled breakthroughs in e.g. our understanding of long-range time correlations in our detector, or a data compression / anomaly detection algorithm that saves us significant time and money.

What are the expected future computing resource requirements (for training / inference)? What is the involvement of Nikhef scientists in ML/AI deployment R&D for next years? What is the ambition of your Nikhef research program for AI/ML use and deployment R&D?

Many students/researchers will need GPUs for model training. If larger machine learning models (transformers etc.) become part of our regular analysis pipeline, some **investments in GPUs at processing sites** (online and offline) might be needed.

Are there clear leading institutes/consortia in the international field in these R&D efforts? How do Nikhef efforts compare to these in a) expertise, b) person-power, c) infrastructure?

Who are your partners nationally and internationally in your efforts & ambitions? What expertise, person-power, infrastructure are you missing to compete effectively and/or realize your ambitions?

- **Christopher Tunnell's group at Rice University**, which works at the intersection of computer science and physics and is also in the XENON collaboration. For example, the self-organizing maps mentioned above were initially deployed on this problem by a Rice PhD student (Luis Sanchez) and then later on XAMS data in collaboration with Maricke Flierman and an MSc student (Tobias den Hollander).
- **Aobo Li's group at UC San Diego**. Aobi Li is an expert in ML and is currently helping KamLAND with AI benchmarking efforts. Kelly Weerman spent a month at UCSD to work together with Aobo.

What are your expectations and/or plans related to AI-driven coding assistance and/or ChatGPT-style AI (physics) knowledge services?

As capable and feasible open-source models become available, a reasonably likely scenario is a **research and coding assistant LLM** trained on a large quantity of private data (e.g. the collaboration's wiki and analysis source code). Early attempts towards this have already been made in the collaboration.

C – Long-term future (5-10 years) – future directions

Given the pace of developments in AI/ML, predicting the evolution of its future possibilities on a 5–10y scale is rather speculative. Instead, here we focus on future application areas where disruptive improvements in AI/ML can make a difference. Thinking 'Disruptively Big': what research applications are a good target for future AI methods? What are problems 'of interest' that are currently unsolvable (from practical computational point of view) but could be solvable with disruptive AI methods? In other words, are there paradigm-changing way of thinking about solving physics problems if 'unlimited computational' abilities were to be available?

On this timescale we are considering next-generation dark matter experiments such as XLZD, and entirely new experimental efforts. There is an opportunity to redesign our analysis and computing pipelines here, possibly with a larger role for AI/ML.

D – Other

Is there any other information regarding the use and potential of ML/AI in your research area that is relevant to be discussed in the task force?

We are wondering if it is possible to create a one day (and recorded) **AI/ML bootcamp**. Many people come into the group having never seen the basics but also feeling overwhelmed at the amount of introductory resources to choose from.

AI & EDM

B – Mid-term future (2-4 years) – effects of ongoing R&D in known AI/ML

On scale of O(3) years future of ML/AI in HEP is reasonably predictable, since it is dominated by deployment of currently known AI/ML techniques and less on unpredictable emergence of new techniques. What is the expected ML/AI use in your research area in the next years? Extrapolating from current experience, where will future/improved deployment of ML/AI bring strong gains in physics performance in the next few years? What AI/ML techniques do you expect to perform strongly in the near future (LLMs, foundation models, simulation-based inference, generative models etc etc) Are there major novel ML/AI application areas in the pipeline? (i.e. areas where ML is now not used)

The EDM group is interested in using neural networks to optimize experimental design and feedback loops. We are using an FPGA (Liquid Instruments Moku Pro) capable of running neural networks, and are concretely exploring using this for giving stabilizing feedback to a molecular decelerator.

What are the expected future computing resource requirements (for training / inference)? What is the involvement of Nikhef scientists in ML/AI deployment R&D for next years? What is the ambition of your Nikhef research program for AI/ML use and deployment R&D?

In terms of resources, we would likely benefit from expertise / information exchange, e.g. with others who do similar projects, or have experience with model compression / quantization. At this point the computational requirements are hard for us to predict.

Given the small scale of the EDM, we offer an opportunity to experiment with neural net feedback loops with a quick turnaround time.