Novel Applications of Artificial Intelligence in Physical Sciences and Engineering Research (AIPSE)
Academy Programme
Final Evaluation

ACADEMY OF FINLAND

Contents

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Executive summary

This report documents a panel evaluation of the Academy of Finland's Academy Programme Novel Applications of Artificial Intelligence in Physical Sciences and Engineering Research (AIPSE). The evaluation was initiated by the Academy of Finland.

Nine projects were funded under the AIPSE programme. The projects' average size was less than 800,000 euros, and the duration was four years (with an initial funding period of 2018–2021). At the time of the evaluation, seven projects had been completed, and two projects had been granted an extension due to Covid-19.

Overall, the projects have achieved results of a very high quality. A number of projects were hampered by Covid-19 and recruitment issues and were delayed. The Academy of Finland extended their funding periods; the projects were yet to be completed at the time of writing.

We observed a slight tendency that projects excelled either in their contribution to breakthroughs in the domain science or in AI. For an effort of this size and duration, impressive results were achieved. It is the opinion of the panel that excellence in both domain and AI sciences can only be expected for projects of a larger investment and especially of a longer duration.

While all projects had, at the end of their period, had a noticeable impact on both the domain science and AI research, the panel did observe considerable heterogeneity at the entry level, where some domain scientists already used AI methods and some AI researchers already were engaged in the domain science. However, this was not the case in all projects, and some thereby had a longer journey towards success, partly explaining the duration of the extensions granted.

Some heterogeneity in data types was also observed. Some projects used synthetic data, some lab data, whereas others utilised real-world data only (e.g. based on in-situ environmental or remote sensing data). In general, the panel observed a trend that projects employing more controlled data had a higher degree of excellence and a higher impact on the domain science. This may also be related to the limited size and duration of the projects.

In domain sciences where lab or synthetic data cannot be obtained, it is the recommendation of the panel that larger efforts in person-years be made if these projects are selected for funding.

The journey of domain science researchers to embrace AI sciences and use them for breakthroughs travels through different levels of maturity: (i) having digital data (ii) using AI tools, (iii) influencing AI tools, and finally (iv) developing AI tools for the domain science (see also Fig. 1 later in Subsection 3.1.1). The AIPSE programme was designed to bring the domain sciences to level ii. Instruments of a longer duration, like AI-focused research centres, are expected to be necessary to bring domain scientists to level iii.

While the research domains and AI methods were diverse, there was a male dominance among the PIs (nearly 90%) both in AI and domain sciences. The panel encourages the Academy of Finland to design instruments to accelerate gender diversity.

1 Introduction

The Board of the Academy of Finland made the decision to launch the AIPSE programme in 2016. A workshop for discussing the more specific contents of the programme was organised soon after in 2016. The steering group prepared the programme memorandum in 2016–2017. The memorandum is available at www.aka.fi/aipse.

1.1. Scope and objectives of the programme

The objectives of the programme were divided into primary and other objectives.

The primary objective of the programme was to:

- produce scientific breakthroughs in projects that combine high-level AI research with high-level physical sciences or engineering research and in which AI plays a central role in facilitating breakthroughs either in AI research or in physical sciences or engineering research.

The other objectives of the programme were to:

- identify new areas of application and opportunities for research collaboration in physical sciences and engineering
- promote new kinds of research collaboration and so to regenerate research
- harness data for productive use and actively utilise open data in the projects funded.

The scope and objectives of the programme are described in the programme memorandum (www.aka.fi/aipse).

1.2. Calls for applications

The programme organised one call for applications. The total funding budget of the programme was 7 million euros. In total, nine projects were funded, most of them consortium projects. The funded projects are listed in Appendix A.

As mentioned earlier in this report, the Academy of Finland funded AI-related projects in the ICT 2023 programme in parallel with the AIPSE programme in 2018–2019. These AI-related ICT 2023 projects were taken under the coordination of the AIPSE programme, but left outside this final evaluation of the programme.

2 Evaluation

2.1. Premises of the evaluation

The nomination letter of the steering group for the AIPSE programme stated that the decision on the final evaluation will be made by the steering group.

In 2021, the steering group decided that the final evaluation of the programme will focus on analysing the results of the programme against all stated objectives of the programme.

The Academy of Finland decided on the evaluation process and collected material to support it. The evaluation panel was recruited to carry out the evaluation in late 2021 and early 2022.

2.1.1. Panel members

The panel was assembled in 2021, and it included the following members: Professor Mads Nielsen (panel chair), University of Copenhagen, Denmark, Professor Anne Verhoef, University of Reading, United Kingdom, Professor Mykola Pechenizkiy, Eindhoven University of Technology, the Netherlands, and Professor Dr Stefan Blügel, Forschungszentrum Jülich, Germany.

2.1.2. Terms of reference

The goals of the panel were to provide a programme-level synthesis of the results of the programme against the stated objectives, and, based on the findings, to provide recommendations for the Academy of Finland.

First, the panel was asked to evaluate the nine research projects of the programme individually, project by project, and separately against the evaluation questions 1–4 (see Appendix B for the evaluation questions). Second, the panel was to form a programme-level synthesis of the results of the programme based on these individual evaluations.

The exact evaluation questions were drafted by the Academy of Finland, reflecting the objectives of the programme. The programme PIs were made aware of these evaluations questions, such that they could write the summary reports by adequately answering the questions in their summaries. The list of evaluation questions is given in Appendix B.

The panel was asked to write the present evaluation report based on the its work and findings. The panel was given a time frame from January 2022 to May 2022 to perform the actual evaluation work. The final report was completed in September 2022.

It should be noted that the evaluation covers the nine projects of the AIPSE funding call solely. There were a number of projects from the ICT 2023 programme of the Academy of Finland (www.aka.fi/ict2023) that were taken under the coordination of the AIPSE programme during 2018–2019, but the steering group decided to leave these outside this evaluation.

2.1.3. Materials for the panel

The key materials delivered to the panel in order to carry out the evaluation were:

- the programme memorandum
- the summary reports by the nine projects of the programme.

It should be further noted that another important source of information for the panellists was the final seminar of the programme. At the seminar, eight project PIs gave presentations, and the panellists could ask them questions.

2.1.4. Process

The panel's assignment started with a kick-off meeting in March 2022. The final AIPSE seminar, attended by all panellists, was organised on 30 March 2022, and the closed panel meeting to discuss the results of the programme was held on 31 March 2022. Starting from the kick-off, the panel first worked individually with studying the summary reports. The panel held several video meetings. During, between and after the online meetings the panel produced the essential findings documented in this document and finalised the report.

3 The panel evaluation

3.1. Introduction, summary and general impressions

3.1.1. Introduction

Nine projects were funded under the AIPSE programme. The projects' average size was less than 800,000 euros, and the duration was four years. At the time of the evaluation, seven projects had been completed, and two projects had been granted an extension due to Covid-19.

Before proceeding to the description of the successes and challenges of the AIPSE programme, we wish to clarify some taxonomy regarding the development of research by AI, and in AI (see below, "Research by AI"), and the types of data used (see below, "Research data types). These will be used in our analysis of and recommendations to the AIPSE programme.

Research by AI

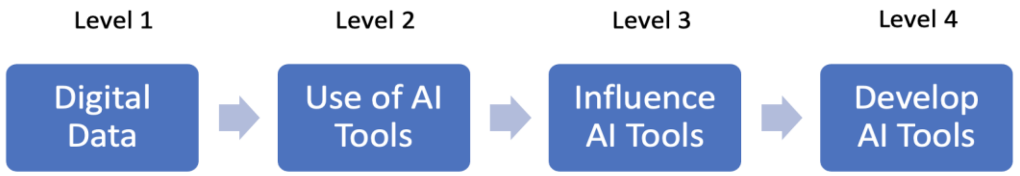

Figure 1. *Maturity of research by use of AI tools to further other sciences. At maturity level 1, researchers are not using AI, but they are ready for it in terms of having data in digital form. At level 2, they are furthering their research area by using publicly available AI tools others have developed and validated for a particular science domain. At level 3, researchers influence the tools in their science area by collaborating with those that develop the tools; they are potentially part of the scientific validation cycle. At maturity level 4, the researchers themselves develop the AI tools needed to progress their research area. An example here is bioinformatics where developing new tools is an integrated part of the research.*

The AIPSE programme, bringing researchers from AI and physical and engineering sciences (S&E) together, had an ambition for the domain researchers to reach at least level 3. The programme did not define at which maturity level the projects would start, and some heterogeneity was observed.

Similar maturity or complexity scales may be created for other relevant aspects of the AIPSE programme, but as they underpin the analysis below to a lesser degree, we only hint at some of these here. Firstly, the maturity of AI/S&E interdisciplinary collaboration ranging from pure data analysis by AI; AI researchers involved in experimental design; AI researchers involved in generating research hypotheses. Secondly, the profoundness of the AI research in an interdisciplinary project ranging from (i) replication of AI experiments with same data and method, (ii) using known methods on new data, (iii) adjusting known methods to subserve given analysis targets, and finally (iv) to create new methods and/or AI paradigms.

Research data types

The projects in the AIPSE programme used and created various sources of data spanning the spectrum displayed in Figure 2. Of the nine projects, five primarily used synthetic data, two used lab data (one of which also used synthetic data), and three used real-world data only.

Figure 2. *Complexity of data used for analysis. Synthetic simulated data are, all other things equal, simplest to analyse as all data variations and noise sources are artificially induced and thereby well known. Laboratory data are more complex as real noise and real variations are present, but the whole idea behind lab experiments is to design the lowest possible level of unwanted variations and noise sources. Real-world data are beyond the control of the scientist and comes with natural variation and noises, as well as errors in induced by the monitoring and classification methods, for example.*

For the quantitative assessment of projects, the panel adopted a grading scale of 1 (Fair), 2 (Good) and 3 (Excellent) to allow for some simple quantitative analysis. Each project was consensus-graded on six aspects:

1. Important breakthroughs/progresses in research
    a. within the domain science of physics or engineering by AI
    b. within the AI sciences
    c. of application of existing AI technologies in the domain science
2. How successful has the project been in identifying new areas of application and opportunities for collaboration (of AI in research)?
3. How successfully has the project promoted new kinds of research collaboration or generated new research avenues?
4. How successfully has data been harnessed for productive use and how actively has open data been utilised in the project?

Question 1c was introduced by the panel as an additional aspect to evaluate (compared to the initial terms of reference set by the Academy of Finland), as it was observed that some projects had not generated excellent influence back on the AI sciences by publications in traditional AI peer-reviewed outlets. Notwithstanding, they still made excellent contributions by utilising and adapting state-of-the-art AI methodologies. These results were however never communicated back to the AI community.

3.1.2. Summary and general impressions

Overall, the projects have obtained results of a very high quality. A number of projects were hampered by Covid-19 and recruitment issues and were delayed. The Academy of Finland extended their funding periods; the projects were yet to be completed at the time of writing.

We observed a slight tendency that projects excelled either in their contribution to breakthroughs in the domain science or in AI. For an effort of this size and duration, impressive results have been obtained. It is the opinion of the panel that excellence in both domain and AI sciences can only be expected from projects of a larger investment and especially of a longer duration.

While all projects had, at the end of their period, had a noticeable impact on both the domain science and AI research, the panel did observe considerable heterogeneity at the entry level, where some domain scientists already used AI methods and some AI researchers already were engaged in the domain science. However, this was not the case in all projects, and some thereby had a longer journey towards success.

Heterogeneity was also observed in data types. Some projects used synthetic data, some used lab data, whereas others used real-world data only (e.g. based on in-situ environmental or remote sensing data). In general, the panel observed a trend that projects employing more controlled data had a higher degree of excellence and a higher impact on the domain science. This may also be related to the limited size and duration of the projects.

The journey of domain science scientists to embrace the AI sciences and use them for breakthroughs travels through different levels of maturity: (i) having digital data (ii) using AI tools, (iii) influencing AI tools, and finally (iv) developing AI tools for the domain science (see also Fig. 1). The AIPSE programme was designed to bring the domain sciences to level ii. Instruments of a longer duration, like AI-focused research centres, are expected to be necessary to bring domain scientists to level iii.

While the research domains and AI methods were diverse, there was a male dominance among the PIs (nearly 90%) both in AI and domain sciences. The panel encourages the Academy of Finland to design instruments to accelerate gender diversity.

3.2. Important breakthroughs and progress

The following section provides an analysis of the individual questions on breakthroughs and progress, before the panel pinpoints a couple of overall observations. The panel was asked to evaluate to important breakthroughs and progresses “in the application area” and “in AI”, but it also decided to include the question on “in application of AI”. The interplay between AI and application areas is rarely a straightforward process, and the research area of how to apply AI in other (science and engineering) research areas deserves a focus on its own, as it is often the bottleneck of progress.

3.2.1. Important breakthroughs and progress in the application area (Evaluation question 1A)

All projects reported that they had made important breakthroughs and progress in the application area. For the majority of projects (7 out of 9), we therefore graded them as good or excellent in this category (see Figure 3). Two projects were graded fair, largely because they were granted project extensions of considerable duration, and hence their project outputs had not yet been finalised. Overall, in this category higher marks were awarded for the projects (5 out of 9) that focused on the use of AI in combination with small laboratory set-ups, often combined with in silico (computer-generated/simulated) data. This is most likely due to the fact that these kinds of studies are generally easier to control, and therefore the data are easier to obtain. Here, breakthroughs included novel tools that predicted physico-chemical structures and properties at the molecular level, facilitated the development of new materials, sometimes involving novel ways of imaging, or novel findings that are important from a fundamental physics perspective. We felt that this research was pushing the frontiers in their respective research areas. In these cases, the emphasis was more on ‘stock-taking’ or mapping exercises, and on confirming our current understanding. Such findings are of course also important in research, but the outputs of these projects had a more incremental, rather than paradigm-shifting flavour, in the panel’s opinion.

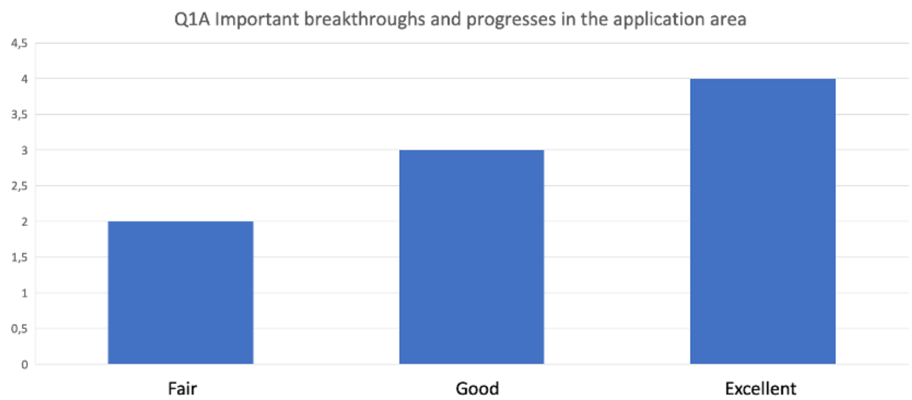

Figure 3. *Histogram of assessment of important breakthroughs and progress in the application area.*

3.2.2. Important breakthroughs and progress in AI (Evaluation question 1B)

All projects but one provided important contributions to the development and advancing of AI.

Two highlights:

- Minimal Learning Machine
- Pattern detection in large temporal graphs using algebraic fingerprints

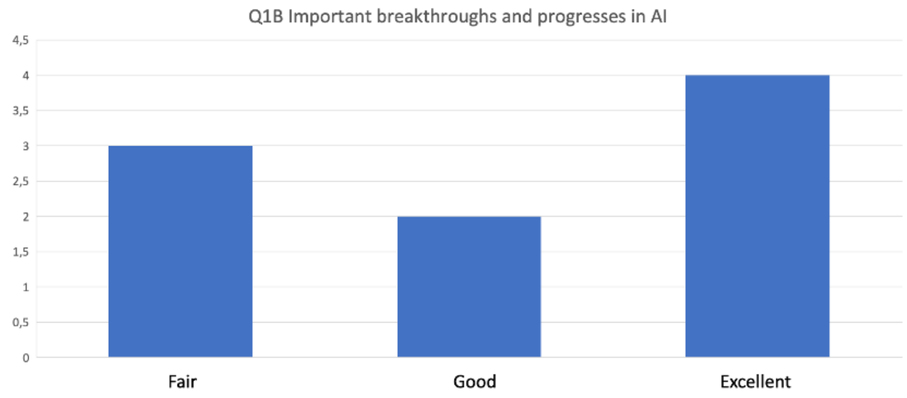

Figure 4. *Histogram of assessment of important breakthrough and progress in AI.*

3.2.3. Important breakthroughs and progress in application of AI (Evaluation question 1C)

We identified four projects with excellent progress in the application of AI.

We witnessed that they had an excellent understanding of what can be expected from the known computational tools and concepts in AI and how to turn their use and their adaptation into an abruptive advantage for the scientific domain. Accordingly, they targeted domain-oriented problems or applications, respectively, to make maximal impact or use.

To give a highlight and to illustrate what we mean by this type of research, we here focus our assessment on an individual excellent project.

This included an image recognition problem, which led to a tool to determine the type of molecule based on atomic force microscopic images, or a tool to determine the metastable configurations of a molecule on a substrate by modelling the unknown energy landscape, or the replacement of a computing-time intensive solver of a generalised nonlinear time-dependent Schrödinger equation by a significantly faster and memory-efficient neural network, which led to the development of a device for an on-demand supercontinuum spectrum for molecular spectroscopy, to name just a few.

The projects recognised that training data are a key part of their model, and this is one they can control. Most data were synthetic, or in silico, which they generated themselves or took from a computational data basis. They also acknowledged that the inclusion of additional experimental data would be an important challenge. It was also impressive to see that they tested the efficiency of available algorithms, that they modified and adopted existing algorithms to their advantage (e.g. distance-based atom configuration models to speed up atomistic simulations). In some cases, they included AI software in bigger software toolboxes (e.g. BOSS, Bayesian Optimisation Structure Search, or the Auto-Co-AFM automated solution for carbon monoxide functionalisation), which they made available to the wider scientific domain.

In general, we saw the largest progress in projects that took the exercise of bringing AI to an application domain seriously as to identifying the bottlenecks in this process, often limited by data availability or computational resources. Some projects excellently demonstrated the understanding of these bottlenecks and developed methodologies for handling these using, for instance, synthetic or augmented data.

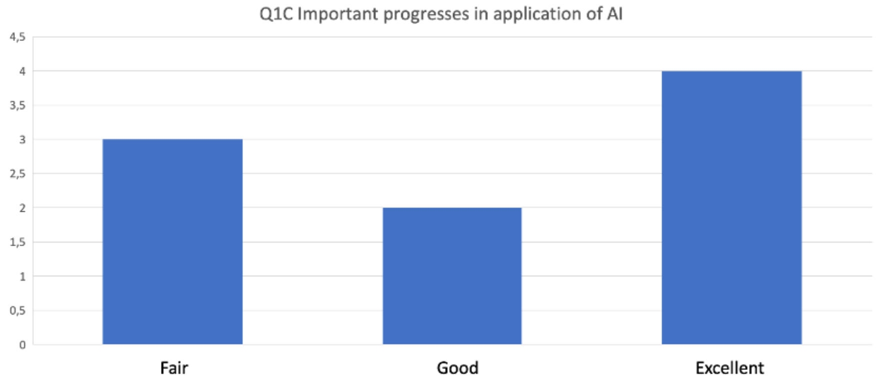

Figure 5. *Histogram of assessment of important breakthroughs and progress in application of AI.*

3.2.4. Analysis of important breakthroughs and progress

In this section we look at some cross-cutting trends of contributions to AI and the application area. Furthermore, as projects differed in their use of data, we also assessed the relation between data types and contributions to breakthroughs.

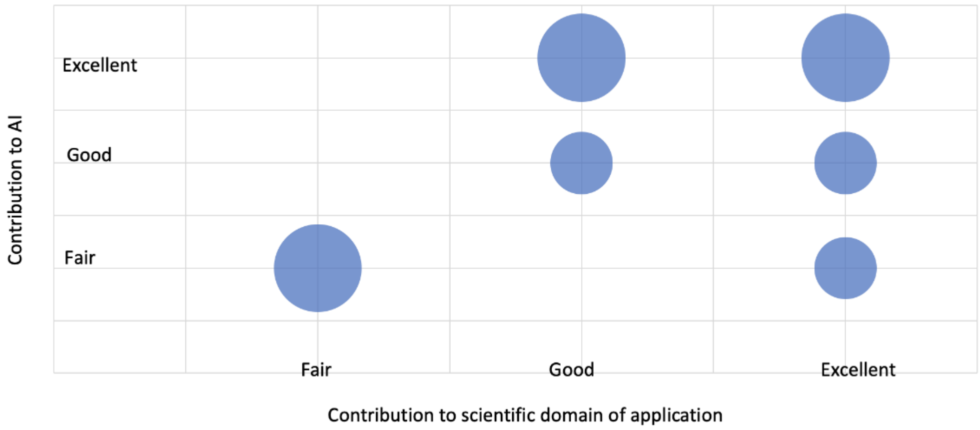

Figure 6. *Scatterplot of assessment of important breakthroughs and progress in the scientific domain versus AI. The area of the dots corresponds to the percentage of projects.*

Looking at the scatterplot of contribution to domain of application versus contribution to AI (Figure 6), we see, disregarding the lower left corner that represents projects that have not yet been finalised, no obvious correlation or anti-correlation patterns. In both categories, four out of seven finalised projects were assessed as excellent.

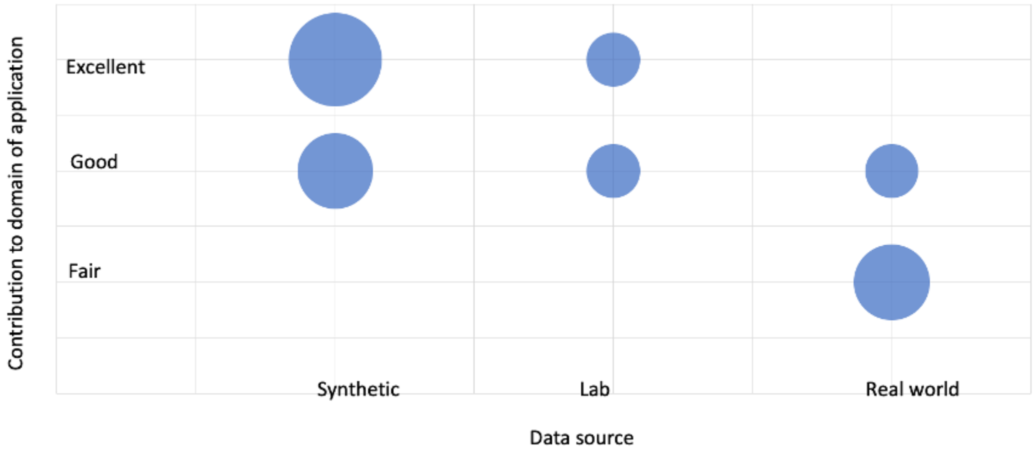

Figure 7. *Scatterplot of assessment of important breakthroughs and progress in the scientific domain versus data source.*

Looking at the scatterplot of data source versus contribution to the domain of application (Figure 7), the panel observed a clear pattern: projects with an emphasis on less controlled data had a reduced opportunity to make breakthroughs in domain science. However, this has to be assessed keeping in mind the constraints of the AIPSE programme, including the limited duration and resources.

It is the assessment of the panel that using real-world data will not necessarily lead to fewer breakthroughs, on the contrary, but it will in general require a larger effort than what could be accomplished in a project under the AIPSE programme using laboratory or synthetic data.

3.2.5. Observations on important breakthroughs and progress

All finalised projects contributed well or excellently to domain science and all but one to progress in AI research. The panel introduced a third assessment question regarding excellence to demonstrate breakthroughs in AI by utilising AI methods at a new scale or application, but without contributing to the field of AI methodology development itself. This was also illustrated by the fact that several projects had no publications in the core AI literature.

For projects of this limited duration and budget, the panel observed a tendency that projects utilising synthetic or lab data had a higher chance of making an excellent contribution to the domain science compared to projects utilising real world data only. In domain sciences where lab and/or synthetic data cannot be obtained, it is the recommendation of the panel that larger efforts in person-years are necessary if these projects are selected for funding.

3.3. Successful identification of new areas of application and opportunities for collaboration of AI

In general, the AIPSE programme provided an excellent and very timely opportunity to bring the domain sciences and the field of AI closer together or to make them interact. The areas of application presented in the nine projects are in line with the new opportunities the broader science community finds in AI worldwide. In the physical sciences funded in this call, these application projects have been in image analysis, force field models, structure optimisation, surrogate models or in general predictive modelling and parameter estimation.

One perhaps somewhat misrepresented area was materials informatics, although project 4 had some thoughts in this direction (an AI-guided property map or design map for new materials). This is not a criticism, but with funding for a limited number of projects, not all opportunities can be leveraged; that is simply a fact.

We thought that the projects were in line with what is going on worldwide: eight out of nine projects did extremely well in interacting with AI or incorporating AI principles (maybe by the more obvious methodologies from the viewpoint of AI, such as neural networks and deep learning). Four projects were considered excellent because they have a worldwide impact on AI sciences, either through the software they provide to the community or through the principles in the combination with the software that can be applied or modified or extended to related communities. To name an example, the training of AFM (atomic force microscopy) images and the subsequent analysis of unknown molecules by AFM in project 1 can be extended to other types of microscopies.

AI departments worldwide develop AI concepts and methods out of intrinsic motivation or application stimulus. However, the number of application domains overwhelms AI departments. Rather, it is important that AI competence is integrated into domain science via teaching, for example in the context of a master’s course, and thus AI competence and AI fluency are built up in domain science, which then drives AI development in the domains and also enables higher-quality collaboration with the AI departments in the future, which then also challenges AI science. One project reported on the cooperation of such a course in the master curriculum.

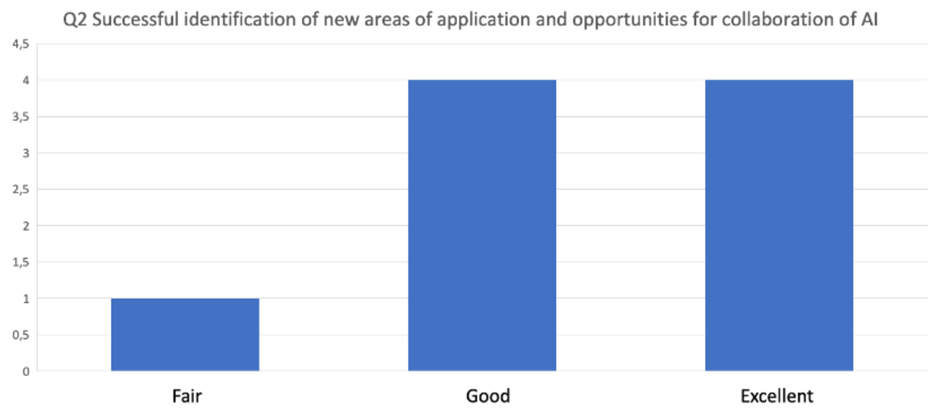

Figure 8. *Histogram of assessment of successful identification of new areas of application and opportunities for collaboration of AI.*

3.4. Successful promotion of new kinds of collaboration and generation of research

The project leads were asked to 1) describe any new (and new kinds of) research collaborations and 2) to consider whether any new research (projects) had been generated during the project.

All projects were deemed to have performed at either good (33%) or excellent (67%) levels with regards to new collaborations and generation of research, with those projects using 'real-world data' generally scoring in the good rather than excellent category (Figure 9).

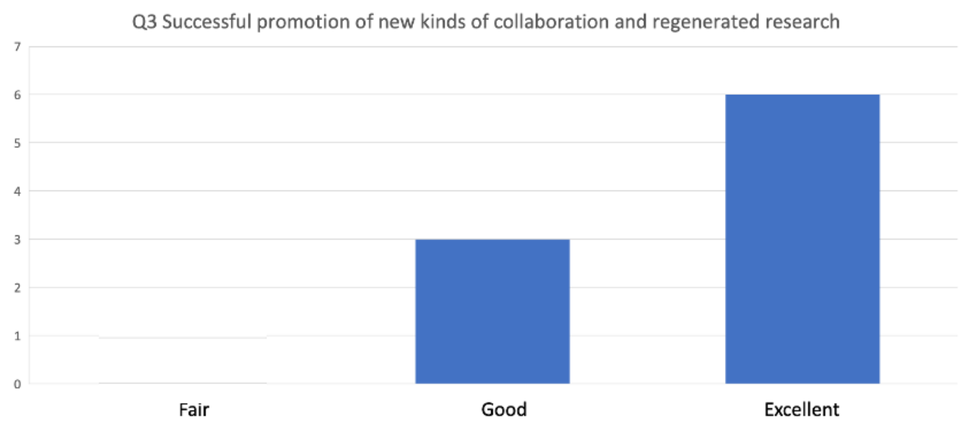

Figure 9. *Histogram of assessment of Successful promotion of new kinds of collaboration and regenerated research.*

With regards to 1), most projects rapidly established productive research collaborations between the groups in their consortium, thereby acquiring new tools from each other's fields, as well as exploring new methodologies together. In some cases, this also led to the introduction of new research problems or totally new kinds of data, differing from the normal datasets used in the AI/ML field. Some projects mentioned that the AIPSE funding had been instrumental in fostering and consolidating entirely new within-project research collaborations between physical research areas and several areas of AI, which would likely not have been feasible without the dedicated project resources.

Most projects indicated that they had successfully forged new and in some cases new *kinds* of collaborations with individuals or groups external to their own project. In some cases, the collaborations included AIPSE project researchers leaving the project to take up new positions elsewhere, while remaining active collaborators. We suppose that this facilitated new links with their institutions, although this was not elaborated upon in the report.

Also, some projects became part of Academy of Finland Flagships, such as those in artificial intelligence (Finnish Center for Artificial Intelligence (FCAI)) or those related to the application areas, or used these programmes to enhance their projects if they were already involved in them. Joining these Flagships created strong new sources of collaboration, where ideas and novel approaches are explored.

Moreover, it was also mentioned that participation in the events of the AIPSE programme introduced certain project teams to an entirely new research community; in some cases, this resulted in several new research collaborations and research project developments with other participants in the programme. In other cases, existing external collaboration networks were strengthened by making connections to new subject areas funded outside Finland, for instance in relation to Digital Twin Earth, which is being implemented via the Destination Earth (DestinE) initiative as part of the European Green Deal. Others partnered up with international universities.

Some projects mentioned new collaborative opportunities resulting from their dissemination efforts, both at AI and application fora, and in particular by sharing their tools and findings through lectures, hands-on exercises and workshops. Especially the latter revealed new application areas for their tools generated during the AIPSE project. Other projects mentioned the creation of new research lines across new disciplines, for example green technologies, active learning (e.g. to create smart dataset curation strategies or high-throughput workflows), or how to solicit human knowledge and expertise and integrate this into the machine-learning process. Finally, one collaboration grew into a new Academy of Finland Centre of Excellence, combining the strengths of machine learners and atmospheric scientists.

With regards to 2) (new research (projects) that had been generated during the duration of the project), various project teams managed to secure new spin-off projects funded by the Academy of Finland or private companies, again on the synergy between AI/ML and dedicated applications. Some postdoctoral researchers involved in certain projects left after obtaining funding from the EU on related topics (Marie Skłodowska-Curie Action).

3.5. Successful harnessing of data for productive use and use of open data

Nearly all projects made an effort and successfully have contributed to open data to ensure the reuse of data. Where this was not the case, it was mainly related to the overall less advancement of projects due to delays.

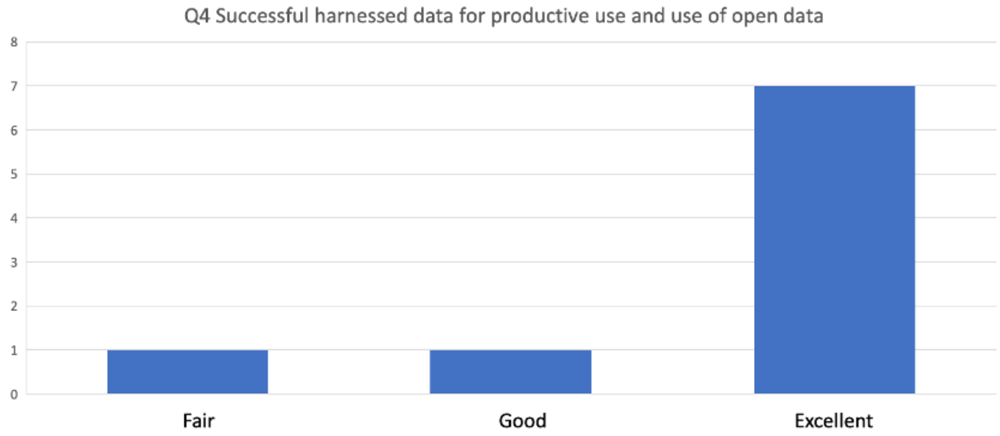

Figure 10. *Histogram of assessment of successful harnessed data for productive use and use of open data.*

3.6. Summary of observations on collaboration and open data

We deem most projects to have displayed good levels of collaboration, all of a suitable and in some cases innovative nature, both within and outside the projects, and with other domain or AI scientists. The majority of projects have made use of existing open data ranging from environmental to socio-economic data, for example. One project solely relied on publicly available data and said they did not generate any new data within the project. A number of projects used freely available AI tools (e.g. those available in Python or PyTorch). Most projects made the data, and in some cases codes and scripts they generated (e.g. via Github), available to the wider community (and others will once the project is finished). For some projects, the data sharing involved bespoke project-specific websites hosted by one of the partners, and in other cases the data or code were uploaded to widely used domain science sites that already existed. One project did not report on this.

3.7. Suggestions for potential areas where AI could foster research and vice versa

There is no question that in the coming decade AI will capture all levels of our society, for example as assistance systems. For this reason, it is very important that a society has well-educated and well-trained actors who drive and accompany this progress and also moderate and integrate it on a societal level (keyword: the power of algorithms). Such applications thus become part of the consumer mass market that finances novel, very low-energy consuming beyond John von Neumann, which will be developed as a consequence of the intensive physical, materials and electrical engineering research and development today.

Thus, the AI operation of the future will connect all the way down to the hardware level and will be an integrated part of cyberphysical systems. The mapping of AI algorithms onto the novel hardware will become an issue and the hardware realisation may have an influence on the choice or preference of the AI algorithms.

In the physical sciences, we observe a tremendous increase in the spatial and temporal resolution of lab-based as well as nationwide operated characterisation infrastructures (using neutrons, electrons, X-ray, light, atomic design) towards high-definition metrology. Only through a real-time analysis and evaluation of the acquired data via AI-based tools, for example by a digital twin, and subsequent rules on how to steer the experiments, can the potentials of such experiments be fully exploited. This motivates the development of fast AI algorithms for huge datasets (e.g., in the order of petabytes).

The exponential growth of available CPU time allows for the high-throughput computation of increasingly wider parameter spaces of ever more complex and accurate physical models (e.g., think of the chemical space of materials combined with quantum mechanical models describing novel properties or functionalities). These *in silico* data, together with experimental data used to validate the models, provide a powerful data basis for the development of rule-based design and processing principles using AI-based techniques to establish novel technologies.

High-performance computing is increasingly enabled by GPUs (graphical processing units) on which many AI applications are very performant. Therefore, we will see that algorithms evaluating physical models will incorporate AI-based surrogate models that speed up the time to solution in general and additionally are very performant on GPU architectures.

After the foundation of the Quantum Technology Flagship by the European Commission, considering the societal and economic impact of AI, the establishment of a European AI Flagship seems appropriate.

3.8. Other suggestions or recommendations

Finally, the panel wishes to emphasise a few suggestions for the Academy of Finland, relating to:

- diversity
- data infrastructures and ecosystems
- emerging areas.

It is clear that the S&E and AI communities are in general male-dominated, and we also see this in the AIPSE programme. We encourage the Academy of Finland to focus on this issue. We especially encourage the Academy to focus on the next generation of research leaders and early-stage researchers.

Whereas the Academy has an admirable focus on open data, we encourage the Academy to focus on the whole scientific data ecosystem and the necessary infrastructures. One example of the interplay between sciences and AI lies in biodiversity research, where the Global Biodiversity Information Facility plays a role of curating but also linking to data so that data contributors can be accredited when data are used for science or AI, like in the iNaturalist apps.

A number of areas are emerging, such as quantum AI, use of foundation models, etc. We do not wish to emphasise one over the other, as choosing is merely a strategic decision. However, we do encourage the Academy to make the proper strategic analysis to place Finland in the forefront where it is most fruitful, taking into account current strengths in S&E and AI and future opportunities.

Appendix A: List of AIPSE projects

AIPSE call

Funding : €7 million
Funding period: 1 January 2018–31 December 2021

1: Computational tomographic atomic force microscopy (CATAFM)

- Adam Foster, Aalto University
- Juho Kannala, Aalto University
- Peter Liljeroth, Aalto University

2: Smart autonomous broadband laser light (SMALL)

- Goery Genty, Tampere University
- Alessandro Foi, Tampere University

3: Adaptive and intelligent data (AIDA)

- Aristides Gionis, Aalto University
- Jussi Kangasharju, University of Helsinki

4: Structure prediction of hybrid nanoparticles via artificial intelligence (HNP-AI)

- Hannu Häkkinen, University of Jyväskylä
- Tommi Kärkkäinen, University of Jyväskylä

5: Intelligent Crop Production: Data-integrative, Multi-task Learning Meets Crop Simulator (AI-CropPro)

- Hiroshi Mamitsuka, Aalto University
- Pirjo Peltonen-Sainio, Natural Resources Institute Finland (LUKE)

6: Artificial Intelligence for Retrieval of Forest Biomass & Structure (AIROBEST)

- Matti Mõttus, VTT Technical Research Centre of Finland Ltd
- Jorma Laaksonen, Aalto University

7: Replacing geo-engineering with robust social incentives: a first quantification of complex anthropogenic impact on air quality modeling and interaction with regulations, using agent-based simulations (ANTHRO-IMPACT)

- Nønne Prisle, University of Oulu

8: Artificial Intelligence for Microscopic Structure Search (AIMSS)

- Patrick Rinke, Aalto University
- Jukka Corander, University of Helsinki

9: AI spider silk threading (ASSET)

- Quan Zhou, Aalto University
- Markus Linder, Aalto University
- Ville Kyrki, Aalto University

Appendix B: Evaluation questions and material for the panel

1: Questions related to programme objective 1 (see [Programme Memorandum (PDF)])

Evaluation question 1A: How important breakthroughs/progresses in physical sciences and/or engineering research by means of AI has the programme generated?
Instruction for the PIs for answering this question: Describe the breakthroughs (if any) and the most significant progresses in physical sciences and/or engineering research by means of AI that you have been able to achieve in your project? Also describe the potential for future breakthroughs in your research?

Evaluation question 1B: How important breakthroughs/progresses in AI research has the programme generated?
Instruction for the PIs for answering this question: Describe the breakthroughs (if any) and the most significant progress in AI research that you have been able to achieve in your project? Also describe the potential for future breakthroughs in your research?

2: Questions related to other programme objectives (see Programme Memorandum (PDF))

Evaluation question 2: How successful has the programme been in identifying new areas of application and opportunities for collaboration (of AI in research)?
Instruction for the PIs for answering this question: Describe what kinds of new areas of application and opportunities for research collaboration have been identified in your project? What is the potential and rationality of these? You may also include research fields other than physical sciences and engineering.

Evaluation question 3: How successfully has the programme promoted new kinds of research collaboration and so regenerated research?
Instruction for the PIs for answering this question: Describe any new (and new kinds of) research collaborations and new research your project has generated.

Evaluation question 4: How successfully has data been harnessed for productive use and how actively has open data been utilised in the programme?
Instruction for the PIs for answering this question: Describe how data has been harnessed for productive use (if any) or how you have utilised open data in your project (if any utilization)?

3: Other requests for the panel
Provide suggestions for potential areas in which AI could foster research and vice versa. Provide any other suggestions.

4: Materials for the panel and closing seminar
The panel will study the projects' summaries and attend the interactive closing seminar, and this forms the key material for the panel for performing the evaluation (for answering evaluation questions 1–4). In addition to this key material, the panel will also use its own expertise and experiences for providing suggestions for potential areas in which AI could foster research and vice versa.