



BESLUT

Datum för beslut:
2025-01-17

Diarienummer:
KTH-RPROJ-0276016

Beslut om ett strategiskt initiativ, KTH GAIN – Generative AI for Next-Generation Science

Detta beslut har undertecknats elektroniskt.

Beslutet

KTH:s vicerektor för forskning beslutar att:

- Finansiera *KTH GAIN – Generative AI for Next-Generation Science* med 1 mnkr centrala medel under 2025.
- Utse Dan Henningsson, SCI-skolan, som ansvarig forskningsledare för satsningen.
- KTH GAIN – Generative AI for Next-Generation Science bör förhålla sig till det andra beviljade Strategiska initiativet KTH Centre for AI, såväl i innehåll som kommunikation.
- Återrapportering enligt utvärderingskriterier, för dialog om fortsatt bidrag ska vara Forskningsberedningen tillhanda 15 januari 2026.

Ärendet

KTH:s initiativ för forskningssatsningar inrättades enligt förslag från Översyn av KTH:s särskilda forskningssatsningar (Dnr: KTH-RPROJ-0276016). Förslaget innebär att centrala medel ska kunna användas till direkt finansiering av tre- till femåriga forskningsinitiativ med det huvudsakliga målet att dra in externa forskningsanslag.

Under föregående år har Forskningsberedningen arbetat vidare med att konkretisera förslaget, och kommit fram till ett antal kriterier för ett KTH Strategiskt initiativ samt kriterier för utvärdering (Protokoll 10/2024):

Kriterier för KTH Strategiskt initiativ:

- Strategiska forskningsinitiativ är ett sätt för KTH att kraftsamla inom områden där det krävs nya samarbeten som är viktiga utifrån KTH:s vision och mål. Det kan dels vara att förstärka ett område som redan finns eller utveckla ett nytt.
- Strategiska forskningsinitiativ ska kunna initieras av både forskare, KTH:s ledning och forskningsberedningen.

- Strategiska forskningsinitiativ är satsningar med central finansiering på 0,5 - 3 mnkr per år i max fem år.
- Målsättningen för en beviljad satsning är att generera betydande externa bidrag till KTH om totalt minst 100 mnkr. Det kan vara externa bidrag från flera olika finansiärer som tillsammans stärker området för forskningsinitiativet. Utväxlingen blir den viktigaste indikatorn som följs upp årligen.

Kriterier för utvärdering av beviljat KTH Strategiskt initiativ ska ske efter ett år enligt nedan:

- Projektansökan – En eller flera projektansökningar.
- Kraftsamling - Vilka PI' s är med i projektansökan/ansökningar?
- Förberedelsearbete inför utlysningar.
- Exempel på nya forskningssamarbeten.

Till Forskningsberedningens möte den 18 december inkom förslaget KTH GAIN - Generative AI for Next-Generation Science, med professor Dan Henningsson, SCI-skolan, som ansvarig forskningsledare, se bilaga 1.

Baserat på Forskningsberedningens diskussion rekommenderas Vicerektor för forskning att stödja att förslaget beviljas sökt budget, 1 mnkr för år 2025 samt att KTH GAIN bör förhålla sig till KTH Centre for AI såväl i innehåll som kommunikation. En utvärdering ska ligga till grund för diskussion om fortsatt finansiering och i vilken omfattning. (KTH-RPROJ-0276016 Protokoll 10/2024).

Detta beslut har fattats av vicerektor för forskning Annika Borgenstam efter föredragning av forskningsrådgivare Johan Schuber.

Kungl. Tekniska högskolan



Annika Borgenstam, vicerektor för forskning KTH



Johan Schuber, forskningsrådgivare, avdelningen för forskningsstöd inom Verksamhetsstödet

Bilaga 1: projektförslag

Sändlista

För åtgärd:

Dan Henningsson, SCI-skolan

Kopia till:

Skolchef SCI-skolan

Controllergruppen, controller@kth.se

Chefen för avdelningen för forskningsstöd Maria Gustafson

Tf Kommunikationschef Gunilla Iverfelt

Anna Aminoff

Sanna Pehrson, avdelningen för forskningsstöd

Expeditionsdatum:

2025-01-17

KTH Strategic Research Initiative proposal

Project idea: Develop an AI for Science platform at KTH to leverage large infrastructure investments, EU-funded Centers-of-Excellence, KAW and SFO funding that are foreseen in the near future.

Title: KTH GAIN – Generative AI for Next-Generation Science

Dan Henningson (interim) PI, SCI

Ricardo Vinuesa Co-PI, SCI

Erik Lindahl Co-PI, SCI

Anna-Karin Tornberg, Co-PI, SCI

Wei Ouyang, Co-PI, BIO

Patrick Norman Co-PI, BIO, PDC

Hedvig Kjellström Co-PI, EECS

Hossein Azizpour Co-PI, EECS

Direct funding requested (1 mnkr first year, subsequently 1-3 mnkr/year specified below and subject to documented need)

Purpose

What will be achieved with the project? What is the vision?

One of the strongest trends in AI research is the move towards *generative networks* that are able to produce complex models (e.g. a folded protein or chat interaction) instead of mere classifiers. These models require extreme-scale training both in terms of data and computational resources, and as we run out of natural training data the field is increasingly relying on adding physics-aware components to models as well as generating new synthetic training data computationally. KTH hosts some of the world's most cited researchers in scientific computing who also lead international collaborations e.g. with RIKEN, we have been the driving force of establishing the new Swedish computational infrastructure with significantly stronger AI focus, and we have been able to create leading KTH environments that span both computing and applications, e.g. as part of Science for Life Laboratory.

The purpose of the GAIN platform is to build on KTH's strengths in scientific computing to establish broad leadership in the application of generative AI methods in high-performance computing environments with particular focus on achieving impact in high profile scientific/societal challenges,

Our vision is to make KTH leading in development and training of large foundation models in collaboration with international partners (e.g. RIKEN, MPG, Argonne, ETHZ) that are then fine-tuned for specific applications, and combined with interactive data analytics to integrate how scientists generate, interact with and draw scientific conclusions from data.

How will the proposed initiative strengthen KTH and how will it contribute to fulfill KTH:s vision and goals?

Several of KTH's most cited researchers are active in this area, a couple of them rank among the top-100 researchers in the world in their subjects, and the numerous other researchers worldwide that rely on and cite algorithms, software and tools developed by KTH strongly contributes to KTH's international impact, ranking and reputation.

In particular with expected new strategic research areas in AI, quantum computing and biotechnology (as singled out by the government), we believe KTH should consolidate its efforts in these areas and in particular combine our strengths in computing, fundamental research/method development, and applications. This should ideally be in collaboration with Linköping University that we see as the other obvious national leader; together these two universities host *all three* long-term national research programs from the Knut and Alice Wallenberg foundation (WASP, DDLS, WISE), the national computational infrastructure, and all EuroHPC Centers-of-Excellence in Sweden. By joining forces we would be in an extremely favorable position to also secure leadership of a new government-funded broad AI strategic research area.

Locally, the GAIN initiative will strengthen KTH both by investing more in large language model (LLM) and foundation model research, and by helping existing groups who are internationally leading in applications and/or traditional computational methods to (1) incorporate these methods in their work, and (2) developing physics-aware AI-based modeling methods. The KTH goals of developing excellent research environments, interfacing them with industry and applications, and contributing to a sustainable future will be a guide to the development of the Generative AI for Next-Generation Science platform.

In addition, the refocusing of PDC into a center for the development of advanced software, rather than primarily being a center running local HPC clusters, will be an important part of the AI for Science platform GAIN. Advanced Research Software Engineers will be an integral part of the collaboration programs envisaged in the new platform.

How is it related to identified skills needed in society / industry and how is it connected to development of educational offerings?

The entire chapter 3.2 in Mario Draghi's recent report on "The future of European competitiveness"¹ is focused on "Computing and AI", which points of how EuroHPC

¹ https://commission.europa.eu/topics/strengthening-european-competitiveness/eu-competitiveness-looking-ahead_en

(including initiatives where KTH is already involved) is the one exception where EU has leadership as well as the immense needs of new STEM degrees as well as upskilling.

KTH researchers were responsible for writing the application that secured Sweden's first-ever EuroHPC infrastructure resource (the largest computational infrastructure investment ever made in Sweden) and are in the process of establishing the Swedish national "AI Factory" initiative that is aiming to specifically serve SMEs and industry, but also provide the national training and support.

AI models replacing traditional computational methods are already having major impact in industry since they enable interactive and cheaper prediction rather than waiting weeks for results. Foundation models in particular also have the interesting property that it is possible to perform very expensive and slow initial training of a few models, which can then be fine-tuned for a number of different applications at much lower cost – and the final prediction step (inference) is almost free compared to traditional simulations. Diffusion models are dominating applications in imaging, biotechnology, and chemistry, deep reinforcement learning (DRL) is a powerful framework for dynamic optimization, and explainable AI (XAI) is essential to identify causality in large data sets.

Why at KTH

What strengths are already in place at KTH in the form of established environments, strong collaborations and research infrastructure - synergies?

Strengths at KTH include SeRC, Science for Life Laboratory, PDC, numerous WASP, DDLS & WISE-affiliated groups, EuroHPC Centers-of-Excellence, and our strong engagement in the NAISS national computational infrastructure.

Describe and relate to the competition in the field (local/regional, national, international).

KTH has an interesting synergy and friendly competition between sectorial strengths in Computing, AI, modeling and infrastructure performed in the environments above (described by section 1 of the Draghi report), and the horizontal policies centered around DigitalFutures (covered in section 2 of the Draghi report).

In our opinion, if KTH finds a way to combine these strengths – ideally with Linköping University as a collaborator – we will not only secure instant national leadership and a key advantage to securing an upcoming national AI Strategic Research Area, but there is a possibility to establish KTH as a leading European AI environment that would both result in additional major funding on EU level as well as societal and industrial impact.

Research team

Describe the quality of the research team.

The PIs represent some of the strongest research environments at KTH, and have been leading e.g. in the establishment and leadership of Science for Life Laboratory, the KAW Data-Driven Life Science Initiative, the National computational infrastructure, all Swedish EuroHPC centers-of-excellence, and in particular the Swedish e-Science Research Center (SeRC) with its Data Science collaboration program, an initiative that can be seen as a precursor to the proposed AI for Science platform GAIN. A number of researchers in the scientific environment, Henningson, Lindahl, Vinuesa, Hess, Azizpour and Tammisola are all ERC grantees, where the research topics span from mathematics and computer science to fluid dynamics and life science, and includes the leadership of KTH's computational infrastructure. These and other excellent KTH researchers not currently listed among the PIs have worked closely with the PIs in related areas, and will be excellent complements in this Strategic Research Initiative.

Strategy for funding

Describe how the target will be achieved: > 100 mnkr in external grants to KTH.

The PIs are already attracting substantial funding to KTH through existing EuroHPC Centers-of-Excellence, and additional resources through the NAISS organization. Our aim is to increase the direct EuroHPC and Horizon Europe project funding to KTH computational projects to >30mnkr/year, and the platform will be critical for KTH to justify continued funding from the national NAISS infrastructure for people once KTH's hardware is retired – we expect this to be in the region of 10mnkr/year. In addition, we are leading the efforts to secure new EuroHPC computing infrastructure and an “AI factory” to Sweden, where the total investments are expected to be in excess of 1000mnkr, out of which a substantial part will be funding for AI experts, where a strong KTH platform would be highly competitive. Finally, we are leading the new national AI4SCIENCE seed project under the WASP umbrella (10mnkr/year), which we believe has potential to expand into a new large AI-focused KAW program after WASP.

What is the goal for external funding achieved in the short term 1-2 years, 3-5 years and 6- 10 years?

Over the next 1-2 years we expect a funding level of about 30 mnkr per year to KTH from the funding opportunities described above, in 3-5 years we expect that could increase to 60 mnkr per year from the three of them. Thus, in the next 5 years we expect the funding to KTH to be around 200 mnkr or more. If KTH is successful in the attracting a new SFO in the AI area or an AI center of the type described in the AI commission report, the funding could be substantially higher. By coordinating the two strong computing/digital environments at KTH and joining forces with Linköping University there is potential to secure new external KTH funding in excess of 100mnkr/year.

Specified funding and relationship to another similar initiative at KTH

The first year 1 mnkr is requested to be able to allow PI's to spend time working to create the envisaged excellent research environment in the area of AI for Science, and to arrange workshops and other activities furthering the plans for the GAIN platform. The subsequent few years an amount of 1-3 mnkr/year is requested, based on documented needs and an evaluation of the results to solicit funding during the first year.

In addition to the GAIN initiative we understand that there is an initiative within the area of AI, centered around the Digital Futures SFO. The funding opportunities announced over the next year within the AI area will determine if it is better to continue with two initiatives or to join forces and go ahead as one initiative for a larger AI center. The main difference between the initiatives is that GAIN has strong links with the providers of the new infrastructure needed for AI computations and related high-performance computing. It thus aligns very well with Linköping university and provides support for the needed reorientation of PDC into a software center. In this respect GAIN also has a much wider scope than the existing SFO SeRC, which does not directly involve PDC.


KTH internt beslut med e-signatur: KTH-RPR OJ-0276016_Beslut om ett strategiskt initiativ, KTH GAIN – Generative AI for Next-Generation Science

Slutgiltig revideringsrapport

2025-01-17

Skapad:	2025-01-16 (Centraleuropeisk tid)
Av:	Johan Schuber (jschuber@kth.se)
Status:	Signerat
Transaktions-ID:	CBJCHBCAABAAzR7k6DS4dzhliLw16eaL3ndte8O9UzZh


”KTH internt beslut med e-signatur: KTH-RPROJ-0276016_Beslut om ett strategiskt initiativ, KTH GAIN – Generative AI for Next-Generation Science” – historik

-  Dokumentet skapades av Johan Schuber (jschuber@kth.se)
2025-01-16 - 12:50:21 GMT+1– IP-adress: 83.249.235.114
-  Dokumentet skickades med e-post till Johan Schuber (jschuber@kth.se) för signering
2025-01-16 - 12:50:30 GMT+1
-  Dokumentet har e-signerats av Johan Schuber (jschuber@kth.se)
Signaturdatum: 2025-01-16 - 12:51:08 GMT+1 – Tidskälla: server– IP-adress: 83.249.235.114
-  Dokumentet skickades med e-post till Annika Borgenstam (annbor@kth.se) för signering
2025-01-16 - 12:51:09 GMT+1
-  E-postmeddelandet har visats av Annika Borgenstam (annbor@kth.se)
2025-01-17 - 00:25:10 GMT+1– IP-adress: 146.75.181.83
-  Dokumentet har e-signerats av Annika Borgenstam (annbor@kth.se)
Signaturdatum: 2025-01-17 - 12:11:46 GMT+1 – Tidskälla: server– IP-adress: 217.213.112.18
-  Dokumentet skickades med e-post till Johan Schuber (jschuber@kth.se) för ifyllnad
2025-01-17 - 12:11:48 GMT+1
-  E-postmeddelandet har visats av Johan Schuber (jschuber@kth.se)
2025-01-17 - 14:38:26 GMT+1– IP-adress: 83.249.235.114




KTH Sign

Powered by
Adobe
Acrobat Sign

 Formuläret har fyllts i av Johan Schuber (jschuber@kth.se)

Datum för ifyllnad av formulär: 2025-01-17 - 14:38:37 GMT+1 - Tidskälla: server- IP-adress: 83.249.235.114

 Avtal har slutförts.

2025-01-17 - 14:38:37 GMT+1



KTH Sign

Powered by
Adobe
Acrobat Sign