

Update

MAX IV Strategy Report 2016–2026

May 2019

Summary

The vision of the scientific scope and impact that MAX IV is poised to deliver through 2026 as described in the 2016-2026 strategy report is still very much valid. However, our planned goals of growth to 25 financed beamlines in 2026 was too ambitious. It is much more likely that MAX IV will have 16 beamlines operational in 2023, with four to five more funded and under construction for a total of 20-21 beamlines by 2026. With this number of beamlines in 2026, the number of users performing experiments will be closer to 2 000. It is necessary to adjust our goals for the coming decade due to current operational funding coupled with existing staffing, the real-time scales for procurement, construction, and commissioning of beamlines, and past delays in beamline delivery. The time scale for bringing up new beamlines is typically five to six years from the start of funding to the arrival of first users, and key resources must be shared with beamlines in operation as well as with ones under construction. With a new focus on project management and a more reliable schedule for delivering beamlines, we believe the goals are realistic given the constraints above as well as our current understanding of opportunities for future financing of new beamlines through 2030.

The operations costs for MAX IV during 2019-2023 are principally covered by the Swedish Research Council, 14 Swedish universities¹ including host Lund University, the Knut and Alice Wallenberg Foundation (KAW), Vinnova, the Novo Nordisk Foundation in Denmark (NNF), the Tresearch consortium, and the Academy of Finland. There are currently discussions on-going with the Swedish Energy Agency and FORMAS to formalise their contribution to the operations cost for this period. However, there is currently a gap of approximately 50 MSEK per year during 2021-2023 between the budget applied for in 2016 and the committed funding, as illustrated in Figure 1.

A vision of future science

The unprecedented high brightness and stability of MAX IV enable new opportunities in a broad range of scientific research areas as well described in the 2016-2026 strategy report. In particular, the brightness and concomitant high coherent flux produced by undulator sources on the 3 GeV storage ring will enable experiments with far greater sensitivity and higher resolution in space, energy, and time.

The brighter the source, the more total light or light in a narrow spectral band, can be concentrated onto a sample under study or be used to image it. Only the coherent light from a source can be focused to a diffraction limited spot or be used to form interference fringes. Imaging techniques that depend on a nanofocused beam of X-rays or that use methods such as ptychography (at the SoftiMAX and NanoMAX beamlines), holography (SoftiMAX), and coherent diffraction (NanoMAX and FemtoMAX) directly benefit from this unparalleled coherent flux. These techniques open new possibilities for understanding the function as well as structure in biological systems such as cells and subcellular organelles, new materials and more efficient sensors and devices that exploit charge, lattice, orbital and spin degrees of freedom in electronic and magnetic materials, and nanomaterials and composites including biomaterials with entirely new properties for technology and medicine. In addition, the

¹ Chalmers University of Technology, Karlstad University, Karolinska Institutet, KTH Royal Institute of Technology, Stockholm, Linköping University, Linnaeus University, Luleå University of Technology, Lund University, Malmö University, Stockholm University, Swedish University of Agricultural Sciences, Umeå University, University of Gothenburg, Uppsala University

intense coherent beams produced by MAX IV accelerators enable study of phase transitions, response to external stimuli such as electrical fields, and dynamical evolution of complex materials, polymers and liquids including gel formation and visco-elasticity and elastic behaviour in colloidal systems using time-resolved coherent X-ray scattering methods such as X-ray photon correlation spectroscopy (at the CoSAXS beamline).

The spectral brightness of MAX IV makes it possible to perform resonant inelastic X-ray scattering measurements at the Veritas beamline with a greater degree of control over energy and momentum transfer than ever before. This means that fundamental excitations in energy and correlated materials can be studied at unparalleled sensitivity and resolution, down to the level of individual vibrational excitations in molecular systems. The resulting improvement in spectral quality will open the door to an understanding of new classes of phenomena, and it is envisioned that, for example, local ultrafast electron-phonon interactions, which determine the thermal transport properties of many materials, can be investigated in detail.

At MicroMAX, the high brightness of MAX IV will enable crystallography experiments on protein crystals as small as one micrometer and serial crystallography on difficult-to-crystallise proteins in a time regime complementary to that addressed by X-ray free-electron lasers, microseconds to milliseconds, which is ideally suited to study of membrane proteins, enzyme catalysis, and other systems.

Roadmap for accelerator development: 2016-2030

The 2016-2026 Strategy report contains a detailed long-term plan for further developments of the MAX IV accelerators (the MAX IV Accelerator Roadmap), which covers the period 2016-2030. The fact that the accelerator part of the strategy report covers an even longer time perspective than the strategy report originally intended is a consequence of the fact that significant accelerator developments often take several decades to mature and materialise. Indeed, sketches of the MAX IV design concept were circulated as early as 2001, i.e. 15 years before its inauguration. The Accelerator Roadmap consists of a brief survey of the current international arena in both storage-ring and linear-accelerator based light sources. It realises that over the next ten years, a number of new sources will build upon the successful implementation of the multi-bend achromat concept at MAX IV to go even further in brightness and coherence. As a result of these developments, MAX IV will be increasingly challenged over the next decade and needs to act vigorously to maintain its competitive edge.

Given the extended time frames typical of major accelerator projects mentioned above, the scenario identified three years ago is still accurate today, with an even larger number of projects going into the sub-nanometre emittance regime for storage-ring based sources. At the same time, developments of various seeding techniques for linear accelerator-based free electron lasers continue to be implemented to increase pulse-to-pulse repeatability and longitudinal brightness at ever shorter wavelengths.

The accelerator roadmap defined in the 2016-2026 strategic plan is, therefore, also still valid and relevant today. In fact, a number of its foreseen development programs are already on-going, the largest being the preparation of a conceptual design report (CDR) for a soft X-ray free-electron laser, a projected co-funded by KAW, MAX IV, Lund University, Stockholm University, Uppsala University and KTH (the last three institutions joined in the Stockholm-Uppsala FEL Centre). The CDR is expected to be delivered by early 2021, later than expected in the original roadmap, as a result of the need to focus resources at MAX IV on the completion of already funded beamlines. The implementation of single-bunch mode in the 1.5 GeV ring is another example of action planned in the roadmap – single-bunch mode has been demonstrated and will be first offered to beamlines in spring 2020. Moreover, theoretical studies aiming at improvements to beam brightness in the 3 GeV storage ring have continued. Last but not least, the roadmap includes the very important goals of achieving the performance parameters defined in the MAX IV Detailed Design Report as well as implementing regular

high-reliability 24/7 accelerator operations. All of these have either been achieved or are on the way to being achieved according to plan.

Current Beamline Portfolio

The portfolio of beamlines currently funded at MAX IV includes the 14 projects listed in the 2016-2026 Strategy Report and are listed in Table 1. This includes operational as well as construction funding, except for the potential gap shown in Figure 1 and an as-yet-undetermined operations budget beyond 2023. Both construction and operational funding were secured for two additional beamlines, MicroMAX and ForMAX, since the Report was submitted in September 2016. The funding for the construction and first ten-year of operation of the MicroMAX beamline comes from NNF. Financing for the construction phase of ForMAX comes from KAW. Funding for a subsequent ten-year operations budget comes from Tresearch, a Swedish national academic and industrial platform with interest in the development of new materials from renewable resources from forestry products. Financing and development of these two beamlines are thus in line with the MAX IV strategy to secure an increase of funding from international sources as well as from industry.

Collectively, these 16 beamlines address an important strategic balance that MAX IV needs to obtain between experiments that exploit the brightness of the MAX IV sources and ones that are world-leading but also serve a large and diverse Swedish research community. This includes brightness and coherence-driven programs such as at the Veritas, NanoMAX, SoftiMAX, and CoSAXS beamlines, flux-driven programs at Balder and HIPPIE, high time-resolution at FemtoMAX, and a range of soft X-ray spectroscopic and imaging capabilities serving long-standing and active communities in the Nordic countries. Of this suite of funded beamlines, four are in operation and accepting general users, seven are in commissioning, and five more are in various stages of construction with completion dates for the last two, ForMAX and MicroMAX, planned for 2022. Figure 2 shows their locations on the Linac, 1.5 GeV and 3.0 GeV rings and their current status.

Optimising user experience

Funding from KAW for the establishment of a data storage and management system, allows MAX IV to develop a data storage system that will be able to maintain all of the data generated at MAX IV in a meaningful way. MAX IV will work with users and beamline staff to collect important metadata that will allow for significant searches and retrieval, especially when data is combined in a big data set. By storing the data in a single, secure location and by assigning metadata tags at the point of collection, we will ensure that data generated at MAX IV will be useful and accessible for decades to come. This project will also ensure that data generated at MAX IV is not randomly distributed on researcher hard drives in their home laboratory but made accessible to the research community in the spirit of the European Open Science Cloud. Collaborations with users for linking this system to platforms for data processing and analysis will further assure that this storage system will be meaningful.

Through funding from Vinnova, we have recruited a temporary second industrial relations officer (IRO, previously industry liaison office, ILO) has been recruited. The IROs are working in defining branch specific obstacles, needs and appropriate routes of entrance to the MAX IV facility. The strategy to engage the Swedish industry through strategic and thematic industry-focused initiatives as for example through workshops, meetings with branch representatives (from, e.g. forestry, food, metals, energy sectors) and similar has proven to be successful and which we continue to develop.

Strategic plan through the next decade

The brightness and stability of MAX IV are its most outstanding features. The world recognises this and looks to MAX IV for technical leadership in these respects as well as eagerly for the latest scientific developments. The founding vision for MAX IV that led to the initial suite of beamlines capitalised on this leadership. However, MAX IV is now at a key point in time as it completes this beamline suite and

transitions to operating it. Given the long time scales for developing the science cases for funding and building new beamlines and the rare opportunities these instruments provide, it is imperative that we begin the long-range planning now for the next suite of beamlines needed by the community.

This planning should incorporate the extensive thinking that has already gone into beamline concepts such as iMAX (nano to micro-scale full-field 3D imaging), MIRARI (infrared chemical imaging and spectroscopy at the micrometer scale), DiffMAX (structural characterisation of energy, catalytic, soft, and metallurgical materials by diffraction and scattering) and MedMAX (multi-scale 3D imaging for medical, biological and soft matter samples), in addition to new concepts. However, rather than carry out this planning piecemeal, it makes sense to formulate a coherent strategy that exploits both the unique features of MAX IV and serves its current and future communities.

For example, interest in tools for high-resolution X-ray microscopy, which can exploit coherent X-rays, is growing rapidly in fields relatively new to synchrotron radiation such as cultural heritage and environmental science as well as in more traditional fields such as condensed matter and the life sciences. Due to its broad range of applications, X-ray microscopy and imaging utilize a wide range of X-ray energies however most of the applications demand photon energies which MAX IV excels in delivering, the tender to hard X-ray (1-12 KeV) region. Strong microscopy capabilities exist elsewhere in Europe, but no one facility currently leads in this area. In particular, development of coherent X-ray imaging methods such as ptychography, including Bragg, fast (fly-scan) and 3D variants is in an early stage worldwide. Much like "high definition" has come to dominate the video world, three-dimensional X-ray imaging is not just viewed as desirable but essential to advance scientific understanding. Similarly, provision of in-situ and operando environments for imaging the structure and evolution of real materials and systems under real conditions is not just niche but are essential for the advancement of many branches of science and technology. In addition to combining imaging and time-resolved methods in novel ways such as pump-probe microscopy and coherent diffractive imaging, MAX IV is also uniquely able to host entirely new capabilities such as inelastic X-ray microscopy which would combine its strengths in inelastic scattering with X-ray nanofocusing, opening the door to chemical imaging of, for example, lithium shuttling within the electrodes of working battery cells with exquisite specificity.

Similarly, continued development of beamlines for macromolecular crystallography will be crucial to stay competitive. For example, applications that are the basis for MicroMAX are rapidly developing and progressing. Progress in methods such as CryoEM also are impacting the field both competitively and complementarily, and need to be addressed.

Looking further out, the unique capabilities of MAX IV are ideally positioned to contribute to the rapidly developing fields of quantum materials, quantum optics, and quantum sensing with unprecedented capabilities. While application of X-rays to these areas is still in its infancy, it appears likely they can exploit the coherence (both first and higher-order) properties of the beams produced by MAX IV to probe single defects, quantum states, and switching at the quantum scale as well as emergent behaviour and phase transitions involving quantum phenomena.

MAX IV, together with world-leading strengths at Swedish universities, is in an ideal position to take a leading role in developing these methods and making them available to the user community. Now is the right time to consider strategically how together we develop MAX IV as a regional centre for capabilities such as these, bringing new and compelling opportunities for Sweden as well as to international researchers.

The European and global context also matters as we formulate a coherent science strategy. New fourth-generation machines such as SIRIUS, ESRF-EBS, and APS-U are under construction, and others are in the planning stages. These developments notwithstanding, MAX IV, has and will maintain a competitive advantage in two key respects: One, as the first multi-bend-achromat synchrotron light source to turn on, it has a three to five year lead over the next facilities (ESRF-EBS and SIRIUS) slated to come online. Both upgraded and new facilities require focused effort and time to advance from the

first operation of the new machine to delivering science from the beamlines. Work at MAX IV in areas such as hard X-ray Bragg coherent diffraction and nanoimaging that exploit the high coherent flux currently uniquely available are already underway at MAX IV and are attracting top international user groups working in these areas. Work at MAX IV that builds on the strong Swedish scientific legacy in high-resolution soft X-ray spectroscopy in areas such as inelastic scattering, ambient pressure photoemission, and time-resolved measurements will also continue to lead the world. Second, as a green-field facility with its wise investment in an agile accelerator system, a 3 GeV storage ring, and emphasis on stability of the entire facility, MAX IV is well positioned to compete strategically in these areas, i.e. cutting-edge brightness and stability driven experiments that enable measurements at the highest sensitivity and resolution with soft to moderately hard X-rays, while also serving a vibrant Nordic community with a longstanding user base. Other facilities will certainly compete too, but have complementary strengths such as access to higher X-ray energies and serve complementary user communities.

As was stated in 2016, the Strategy Report should be viewed as a living document. With this in mind, our strategic thrust must now shift to considering the future needs of the academic and industrial communities. Their input is essential as we together plan the scientific scope and technical capabilities going forward. We, therefore, propose a two-year time frame to request community input and formulate the science strategy needed to develop the next ten or so beamlines to build out MAX IV. Beginning with workshops already planned for the 2019 User Meeting, we propose to hold a series of workshops focusing on community needs and new beamline concepts through spring 2020, culminating in the autumn 2020 User Meeting dedicated to crystallizing the future science strategy and roadmap outlining the beamline portfolio planned for 2020-2030.

In this context, the closing lines of the Executive Summary in the 2016 Strategy Report are still very much on-point three years later: "We are committed to a continuous dialogue with the community to maximise the benefit for the users. While we focus on the national academic community, we are open to international and industrial users and welcome their contributions to development and operation of the facility. With the support of our funders we will make MAX IV a hub of Swedish science and innovation and through continuous development maintain a world-leading position for the future."

Figures & Tables

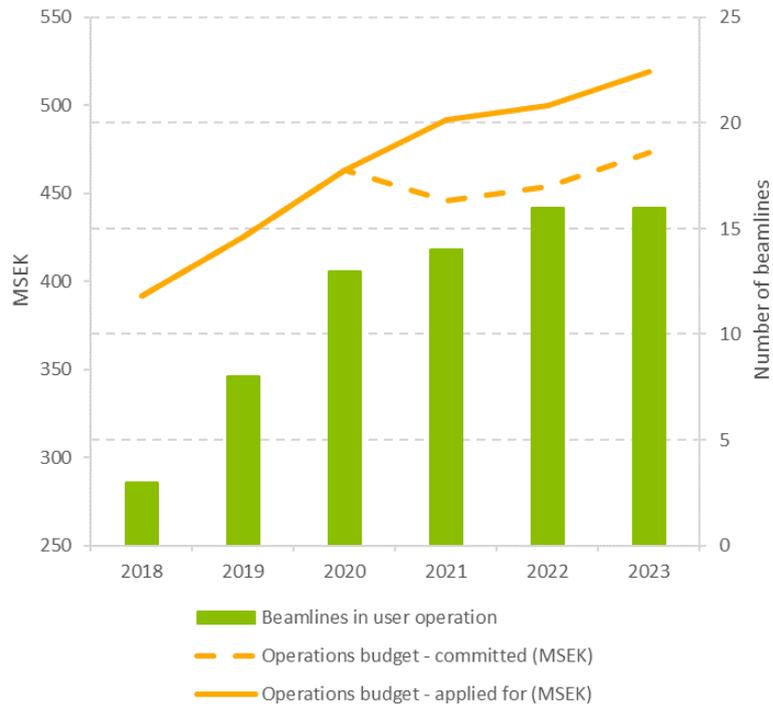


Figure 1. The number of beamlines in user operation and operations budget for 2019-2023. The solid line shows budget applied for in 2016. This figure is an updated version of Figure 3 in the Strategy Report 2016-2026 to show the current situation.

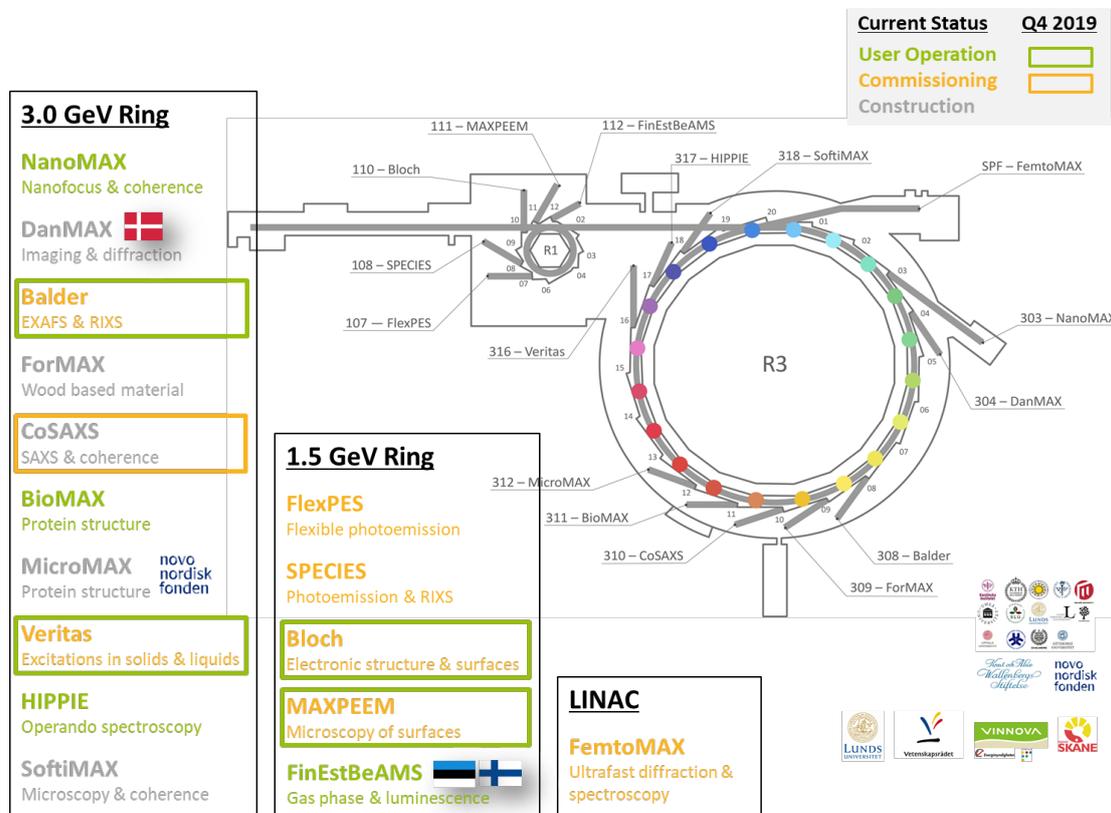


Figure 2. Current status of MAX IV 16 funded beamlines and their locations on the Linac, 1.5 GeV and 3.0 GeV rings.

Table 1. Currently funded beamlines at MAX IV.

Beamline	Accelerator	Technique
FemtoMAX	Linac	Time-resolved hard X-ray scattering and spectroscopy methods for studies of ultrafast processes
Bloch	1.5 GeV	Angle-resolved photoelectron spectroscopy (ARPES) including spin resolution (SPIN-ARPES) for detailed studies of the electronic structure of solids.
FinEstBeaMS	1.5 GeV	Electron spectroscopies and luminescence methods for studies of low-density matter and solids.
FlexPES	1.5 GeV	Soft X-ray spectroscopies for studies of low-density matter and solids.
MAXPEEM	1.5 GeV	Aberration-corrected photoelectron microscopy for investigation of surfaces and interfaces.
SPECIES	1.5 GeV	Resonant inelastic X-ray scattering (RIXS) with high resolving power and near ambient pressure photoemission.
Balder	3.0 GeV	Hard X-ray absorption and emission spectroscopy (XAS, XES) and X-ray diffraction (XRD) with emphasis on <i>in-situ</i> and time-resolved studies.
BioMAX	3.0 GeV	Macromolecular crystallography with a high degree of automation and remote access.
CoSAXS	3.0 GeV	Small and wide angle X-ray scattering (SAXS, WAXS) and coherent techniques for soft matter and biomaterials.
DanMAX	3.0 GeV	Powder diffraction and tomographic imaging of hard (energy) materials.
ForMAX	3.0 GeV	Full-field tomography, SAXS/WAXS, and scanning SAXS/WAXS imaging.
HIPPIE	3.0 GeV	Near-ambient pressure photoelectron spectroscopy on solids and liquids.
MicroMAX	3.0 GeV	Macromolecular Serial Crystallography with a wide range of sample delivery systems, time-resolved studies
NanoMAX	3.0 GeV	Imaging with spectroscopic and structural contrast techniques and nanometre resolution.
SoftiMAX	3.0 GeV	Scanning transmission X-ray microscopy and coherent imaging methods.
VERITAS	3.0 GeV	Resonant inelastic X-ray scattering (RIXS) with unique resolving power and high spatial resolution.