

LINXS Annual Report 2020

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Executive Summary and reflections from the LINXS Director

2020 was a year that will be remembered for the global coronavirus pandemic, but, for LINXS, it has also been a year of significant developments in terms of how we do our work and the tools we use to achieve our mission. The pandemic has led to new ways of working and interacting online. LINXS has embraced these opportunities in the form of webinars, zoom meetings and hybrid online-physical meetings/seminars. This imposed new reality has been both challenging, since it restricted physical interaction, and beneficial, catalysing digitalisation and new developments, as well as providing new perspectives on the role and value of LINXS. We have successfully taken almost all of our events and meetings online and we are developing good online practices, digitally equipped our physical premises and increased the number of activities in total. Online activities also lend themselves to being able to better capture content on the LINXS webpages and, in many cases, we are also finding that online is a good and sustainable approach, e.g., to reduce travel. In fact, we can see that digitalisation and hybrid activities, when appropriate, will be a key part of our working practices in the future and our engagement with a wide audience across different time zones and countries. However, physical interactions are a cornerstone of the LINXS approach, and we look forward to the world opening up and allowing the return to meetings in person at LINXS.

In the autumn we welcomed a new theme, “New Materials for energy and sustainability”, and published a new call towards the 5th LINXS theme. The new theme will address a number of cutting-edge scientific questions from a fundamental perspective, but with a view towards current global challenges, as well as developing the x-ray and neutron communities in these areas. The theme is a great complement to our existing themes, with its focus on hard matter, and expands LINXS community into new areas. At the other end of the theme cycle, Imaging would have been the first theme to reach its conclusion, at the end of 2020; activities will, however, continue until the summer 2021 since many of the planned events needed to be postponed.

To further the development of the educational aspect of our mission, we launched an educational feature to our website and work on our wiki is well underway. Our two new webinar series, “Let’s Dive into the Atoms” and “CoWork”, have highlighted the interest in, on the one hand, introductory discussions for new users of x-ray and neutron techniques and, on the other hand, focused in-depth exploration of a cutting-edge field. Participation from all over the world far exceeded expectations.

During the year we were also able to observe, through the development of the working groups’ activities, that LINXS has an important role in “incubation” of initiatives and transdisciplinary research communities beyond LINXS, at local, national, and international levels. Concrete examples are the “Antibodies in Solution” research programme that has developed strong international connections, including with NIST in the USA, and national funding initiatives around the Nordic Lights on Food of the Food Science and Technology working group. Furthermore, LINXS has played a key role in the development of a project for a Swedish Beamline at ESS for GISANS. Such demonstrations of how LINXS activities can develop national/international networks and nurture long-lasting external projects and collaborations is great to see and we are considering how LINXS can best support such developments so that these initiatives can continue to grow outside LINXS.

Stephen Hall,
LINXS Director

The LINXS Mission

ESTABLISH

LINXS as a world leading advanced study institute for all scientific and technological disciplines which can benefit from the use of neutrons and x-rays.

PROMOTE

science and education focusing on use of neutrons and x-rays in research and development, and help educate potential users of ESS, MAX IV and other major research infrastructures to enable ground-breaking research.

ATTRACT

world-leading scientists for short-term focused research visits to contribute to excellent science. The goal is to further research collaboration within national and international research networks, especially for early career researchers.

CREATE

international networks and enhance the visibility of Sweden internationally in the use of neutrons and x-rays. We want to invigorate the dialogue between academia and society in all aspects of large-scale research infrastructures using neutron and x-rays. The goal is to become a nucleus for local, national and international activities in Science Village Scandinavia and a think-tank initiating new ideas and themes.

Reflections from the Scientific Advisory Board

The LINXS Scientific Advisory Board (SAB) is made up of high-level international researchers in science involving neutrons and x-rays. The SAB provides advice on the scientific direction and strategy for LINXS, including, for example, reviewing applications for new themes. The SAB provided the following summary of their impressions on the LINXS scientific activities in 2020.

“The SAB congratulates LINXS for keeping the activities up and running despite the restrictions due to the Covid-19 pandemic, which affect the operation of LINXS very significantly. Despite this adverse situation, LINXS maintains its activities on a qualitatively and quantitatively very high level and attracts many participants locally, nationally, and internationally. Furthermore, LINXS explores new virtual formats, which appear to be very successful and well-received by the community. This experience will extend the possibilities of LINXS and is likely to be very valuable also beyond the Covid-19 pandemic; for example, concerning international participants and internationally leading speakers in virtual and hybrid (physical/digital) events as well as the opportunity to offer more ‘delocalized’ events. This was only possible due to an exceptional effort and excellent new ideas by the interim director, Stephen Hall, as well as the staff and others involved in LINXS.”

LINXS scientific achievements and impact

During 2020, four LINXS themes were in operation with 19 associated working groups (WGs), which included four Research Programmes (RPs) (see Annex 1). Following an open call for theme proposals and the subsequent SAB recommendation, the fourth theme “New Materials for energy and sustainability” (New Materials) started in September 2020. This new theme fulfilled the selection criteria, including an important aspect of developing the focus area of hard matter, which has been less well represented across the existing LINXS themes. The increase in the number of LINXS working groups during the year and the breadth of science

represented by them is a testament to the growing interest in exploiting x-rays and neutrons across an increasing range of research areas. It also demonstrates LINXS's role in catalysing this interest. In the following, the scientific activity in the four themes is summarised and representative cases are presented in Annex 6.

Imaging Theme outcomes and reflections

2020 marked the final year for the Imaging theme, although the Covid-19 pandemic led to a number of challenges in completing the theme and working group objectives. Therefore, some activities will be continued in 2021. However, the effects of the pandemic also led to some positive, and unexpected, outcomes, such as the highly successful CoWork webinar series and the hybrid Northern Lights on Food Masterclass.

At the start of 2020, the Imaging theme had a strong program for the year and got off to a good start with two innovative "try-out workshops" in the GeoArCH working group. These workshops were carried out in collaboration with the Elettra Sincrotrone (Trieste, Italy) and the Heinz Maier-Leinitz Zentrum (Technische Universität München, Germany). LINXS is very grateful to both these facilities and the colleagues there who made these events possible. These events enabled researchers to get direct hands-on experience in using large-scale facilities and to also try imaging their own samples. Equally important as the imaging, were the interactions and community building around the beamtime. Ideally these events would have been followed up with further activities relating to the data analysis and developing full beamtime proposals. However, directly after the event in Germany, the world started to close down due to the pandemic.

The closure of Europe due to Covid-19 hit many events, not least the 3rd hackathon under the QUANTIM working group. This aimed to follow the previous successful hackathons with the objectives to develop and distribute competences in image analysis and visualization; specifically, this time, the focus was 3D visual annotations, plus to establish new collaborations. These events profit enormously from the direct interaction of the participants, but the pandemic and the weather worked against it this time. Only about 6 of the 30 registered participants could be present in person due to the onset of the restrictions connected to Covid-19 and the main organiser, Rajmund Mokso, was caught on the wrong side of the Öresund bridge, which was closed due to strong winds. However, at the last minute we were able to arrange that the experts gave their tutorials remotely and members of the group stepped up to coordinate, as Rajmund took the long route to Lund via Helsingor/Helsingborg. Ultimately, in addition to the online tutorials, most of the teams with data were able to interact during at least half a day with the experts over zoom or skype. The key impact of these hackathons is that they establish collaborations between teams who would otherwise very rarely come in contact with each other. Short term, scientists get their existing data explored and published, whilst imaging experts become involved in the projects and publications. Long term, the collaborations established can result in grant applications with significantly better chances for success in terms of using 3D imaging to help answer specific scientific questions.

Further hackathons have been postponed until physical meetings are possible, although the QUANTIM working group did partner with DTU on the "Large 3D and 4D image analysis workshop", which was part of a series of workshops in the framework of the "Mummering" EU ITN network.

Shortly after the hackathon, further restrictions led to the last-minute cancellation of the 2nd LINXS/SWEDNESS neutron image course. The aim was to postpone and be able to hold this in-person, but due to on-going restrictions, this is now planned to be online during 2021. The

ambitious programs of the Soil Science working group (including a hands-on workshop in x-ray spectroscopy techniques at MAX IV), as well as those of the TBS working group (including workshops around Sweden) had to be cancelled, but certain aspects will hopefully still be realised in 2021.

The Food Science and Technology working group quickly adjusted to the “new normal” and held a “Northern Lights on Food” Digital Workshop in June, while postponing the larger conference for June 2021 as a hybrid event. The online workshop was organised as a brainstorming session for the potential to create an advanced research centre focusing on the use of x-ray and neutron-based techniques in food research. The workshop was followed by several follow-up meetings and discussions (approx. 20 meetings) that, together with the workshop, were very successful in bringing together relevant researchers around new and interesting topics to advance food science using advanced x-ray and neutron techniques. The outcome was the gathering of national (Swedish) food science and advanced technology experts, from both academia and industry, around four different scientific topics: Structure of Food – Raw Materials, Structure of Food During Processing, Food Interactions at Interfaces, Structure of food and correlation with bioavailability and sensorial perception. The activities also led to several new collaborations at Lund University and nationally across Sweden, including through the engagement of researchers that were new to the area and connecting them with existing x-ray and neutron users.

The (temporarily) improved situation over the summer enabled the Food working group to go ahead with the planned Northern Lights on Food “Masterclass”, a first LINXS event in hybrid form, physical and online; this was a very successful event with good interactions between all (remote and local) participants via breakout rooms, presentations and direct feedback on written proposals. There were participants in-place and online from several countries, with 26 students and 14 lecturers from academia and industry with backgrounds in food and colloid science, as well as x-ray and neutron science experts. In addition to the educational and network aspects, the event triggered ideas for future working group activities and new insights into how to run such hybrid events (which have the advantage of reducing the need for participants to travel). Furthermore, the event was filmed and will form the basis of a new webinar series in 2021.

Fellows in the Food Science and Technology working group were also successful in getting funding from the Lindqvist Stiftelse for a new research project, connected to their work with LINXS. The project, entitled “Dietary regulation of Gut and Blood Brain Barrier function”, focusses on using x-ray and neutron scattering to study the structural and compositional changes of this barrier that occur during exposure to food components and gut microbiota. The aim is to provide a stronger link between researchers in medicine, food science, biophysics and neutron and x-ray techniques. Researchers from the working group also submitted to the FORMAS sustainable food system call “Research centres for sustainability and competitiveness in the food system” with the title “Northern Lights on Food – Advancing food structure, processing and function with MAX IV and ESS”. The aim was to explore the unique opportunities for Swedish food research and production presented by MAX IV and ESS. Unfortunately, the initiative was not funded, but the community created continues to expand and works on new research funding opportunities.

A clear theme highlight of the year and a positive result of the Covid-19 restrictions was the CoWork webinar series under the “New Opportunities in Imaging with X-rays and Neutrons” working group. The series is dedicated to the exploitation of the coherence properties of x-rays for advanced materials characterisation, with a special focus on inverse microscopy

techniques, such as Coherent Diffraction Imaging (CDI), Ptychography and Holography (see analytical report in Annex 5). CoWork (Coherence Workshop) was originally envisaged as a focused (physical) workshop to increase awareness towards the capabilities offered by coherence-based x-ray techniques and create the basis for a larger user community that will exploit and develop them. Covid-19 restrictions led to the original concept being adapted to a webinar series with initially modest expectations and the first set of webinars were very well received. Subsequently the program has been continually extended and there has been a steady increase of the number of participants, (from an initial 40 to 174 subscribers today), with a core of people attending most seminars and others joining for specific ones. Importantly, the activity has also attracted an international community of experts in the techniques proposed, many of whom have contributed with presentations and active participation in discussions – each seminar has had a Q&A session followed by longer, less formal, discussions in smaller groups. CoWork has clearly provided an important forum in these times of limited international scientific interactions and has demonstrated that the goals of LINXS can still be fulfilled, even when physical meetings are not possible. LINXS hopes to follow this online success with a real physical meeting where it can further build the community and enable significant advances in the area of coherence-based x-ray techniques. Reflections and insights from the CoWork series, as a representative LINXS case for 2020, are included in Annex 6.

In summary, 2020 was a challenging, but successful year for the Imaging theme. In addition to the activities outlined above, the theme members have also been involved in activities relating to the wider community, including instrument proposals for the PetraIII upgrade to PetraIV (in collaboration with the Swedish Material Science beamline at PetraIII and CeXS) and working to develop the local and national x-ray tomography communities (proposals were submitted relating, at the national level, to “Sci3D: Swedish Centre for Imaging in 3-Dimensions / Science in 3D”, and a related Lund University platform “lu.ndimage”).

The plan is to hold some of the postponed events in 2021, including, hopefully, a final symposium, before concluding a very successful theme.

Dynamics Theme outcomes and reflections

The LINXS dynamics theme progressed very well in 2020 and focus has been on the working group research activities within their research programmes (RP). The pandemic presented quite some challenges, such as the cancellation of new guest researchers’ visits, but work shifted online, which led to increased interactions, efficiency and global outreach. Below is a short summary of each working group and RP.

WG1: Dynamics and Structure of Biological Macromolecules working group

➤ ***RP: Simulation, theory, and software development for anisotropic systems***

Predicting the solution structure of complex molecular systems, such as anisotropic colloids, proteins, viruses, pose a particular challenge due to intermolecular interactions between solutes, co-solutes and solvent. Molecular simulations and approximate theory offer routes to generate configurational space from which thermally averaged scattering intensities, measured in static scattering experiments, and intermediate scattering functions, obtained in quasi-elastic scattering experiments, can be evaluated. While there exist numerous solutions for spherical particles with centrosymmetric interaction potentials, this is not the case for anisotropic shapes and interactions. This RP brings together researchers working towards the latter, to share ideas and advance the methodological toolbox for analysing, understanding and predicting experimental data.

During 2020, the RP expanded its computational toolbox for predicting scattering functions from computer simulations and used this in a comparative experimental (SAXS) and theoretical study to understand the solution behaviour of enzymes. Furthermore, two new projects involving were initiated. Firstly, a novel method was developed to include solvation water around multiple biomolecules for a more accurate theoretical prediction of, e.g., solution structure factors. This is a collaboration between LINXS fellows from Lund University and Aarhus University (Denmark). The second project has implemented methods to analyse how electrostatic anisotropy affects protein-protein interactions, which is very well aligned with identified topics from the late 2019 mini-meeting, "Scattering in Anisotropic Systems". Again, simulations and experiment go hand-in-hand and it is expected that the developed methodology will be broadly applicable in the scattering field. All developed software has been published as open source.

➤ ***RP: Antibodies in Solution***

Monoclonal antibodies are of high interest to the pharmaceutical industry due to their potential as efficient therapeutics for, e.g., cancer treatment. However, many questions on how antibodies behave in solution, particularly at the high concentrations needed for the administration of physiologically efficient doses, remain to be solved. A major obstacle, which has severely hampered systematic fundamental studies by individual research groups, has been the limited access to sufficient amounts of well-defined antibodies.

The research programme "antibodies in solution" was created to tackle the challenge outlined above, by securing sufficient amounts of well-defined antibodies and to perform a concerted research investigation that covers all relevant length and time scales needed to understand the properties of individual antibodies, as well as those of concentrated solutions. The programme has gathered 14 international experimental and theoretical/simulation experts who, together with their research groups, have committed themselves to this collective effort.

A milestone in the "antibodies in solution" program was achieved in 2020 when two sources for sufficient amounts of high-quality monoclonal antibody material - the basic prerequisite for this ambitious venture - could be identified and welcomed as partners in the programme: (i) the American National Institute of Standards and Technology (NIST); (ii) a major Pharmaceutical Company from Switzerland. Based on this breakthrough, a kick-off meeting ("Antibody Kick-off Meeting") for all the members of the programme could finally take place in December 2-4, 2020.

The first two afternoons of the kick-off workshop, (day 1 and day 2) were devoted to the scientific aspects, which was open to the group leaders, representatives of the organizations providing the mAb material and the antibody Steering Group Members, as well as the close collaborators/group members of the individual group leaders who are part of the RP. Registration (via Indico) and participation was only possible upon personal invitation. In total there were 54 registrations, and 40 - 50 participants at any time during these afternoons on Zoom. The programme comprised an introductory talk by the programme leader, 13 scientific presentations by the group leaders of the experimental and theoretical/simulation groups, plus presentations by the NIST and pharmaceutical company representatives. The third afternoon (day 3) was reserved for discussions only and was a closed meeting of the involved group leaders, the steering group plus the NIST and Pharmaceutical Company representatives, corresponding to 21 participants. The objective of these discussions was to develop a roadmap for the programme. These discussions were chaired by Prof. Dieter Richter. Part of the debate took place in breakout rooms within smaller sub-groups (three experimental and one theory/simulation group) with distributed tasks to optimise the efficiency of the process. Based

on these discussions, each of the subgroups will develop their ideas within a specific area and work on a written plan. The participants will meet again via Zoom in the beginning of 2021 to discuss the outcome and further steps.

The Antibodies in Solution RP is a unique effort that, if successful, will fill a research gap of broad societal interest. An advanced fundamental knowledge and understanding of antibody solution behaviour, as the prospective outcome, can, in time, revolutionize drug development and the use of antibodies in other areas. With the progress made in 2020 (acquisition of access to sufficient high-quality antibody material and kick-off meeting with all actors involved), the biggest hurdle has been overcome and the way is cleared for the dedicated research work.

Reflections and insights from the Antibodies in Solution RP, as a representative LINXS case for 2020, are included in Annex 6.

WG2: Characterizing soft matter with X-ray Photon Correlation Spectroscopy (XPCS) working group

X-ray Photon Correlation Spectroscopy (XPCS) is a technique that allows access to the dynamics of molecules and particles in a sample. It has been applied in condensed matter systems, for example glasses, but is under-exploited for biological and soft matter, where it could bridge the gap between the timescales accessible by neutron spectroscopy and light scattering. The technique is of relevance for following collective processes, such as diffusion, relaxation and reorganization. XPCS will benefit greatly from the new synchrotron x-ray sources that provide high coherent flux, such as MAX IV and the ESRF and APS upgrades.

This workgroup seeks to address some of the technical difficulties of XPCS (detector speed, signal to noise and beam damage) by bringing together key relevant research groups in Europe and the USA.

The XPCS working group at LINXS helped initial feasibility measurements in October 2020 during measurements of the coherent flux at CoSAXS and MAX IV. The LINXS support included helping to provide appropriate test samples for the measurements and analysis of data. In addition, during 2020, a proposal for an expert commissioning experiment on CoSAXS was accepted, with the aim of successful demonstration of XPCS at CoSAXS (and to provide a detailed plan of the steps required to do this). Experiments are planned to be carried out in 2021.

Following the work in the WG, a Röntgen-Ångström Cluster (RÅC) grant proposal was submitted and accepted for funding, with Peter Schurtenberger as the PI for the Swedish partners. The grant started in 2020.

“The research programs of the Lund Institute of Advanced Neutron and X-ray Science (LINXS) focusing on “Dynamics and structure of biological macromolecules” and “X-ray Photon Correlation Spectroscopy” were vital for initiating this joint RÅC proposal”, says Peter Schurtenberger.

WG3: Dynamics and Structure of Biological Macromolecules working group

➤ *RP: Structure and dynamics utilizing the GISANS technique*

The grazing incidence small-angle neutron scattering (GISANS) technique enables the structure and morphology of surfaces, films and interfaces to be investigated. The GISANS technique lies in between two well-established methods, neutron reflectometry (NR) and small angle neutron scattering (SANS). A concerted Swedish initiative to prepare for the design and construction of a GISANS instrument has been developed during the last couple of years thanks

to the close collaboration and joint efforts of all the main Swedish research institutions with neutron activities. The objective of this community is to submit a proposal for the potential instrument, SAGA, to the next call for instruments at the ESS, expected in 2023. Surface and interface science, as well as colloid science, are research areas where Swedish academic research is world leading. Research areas concerned span from surfactant and lipid self-assembly, advanced polymer coatings, nanoparticle stability and deposition, materials science and energy to hard condensed matter physics, quantum materials and magnetism. Moreover, interfaces are integral to major research fields in chemistry, physics, biology and engineering science. LINXS has in its mission to help create international networks and enhance the visibility of Sweden internationally in the use of neutrons and x-rays. In this respect the GISANS program has put Sweden and Swedish scientists at the forefront of the discussions towards building a unique instrument at ESS. These discussions have also promoted the dialogue between academia and industry with respect to industry participation in the science at ESS.

The GISANS community building intensified during 2020. A key activity has been a virtual workshop at LINXS on September 26th, with 124 registered participants (up to 95 online at a given time), with 68 registrations from Sweden, of which 48 were from major universities and research institutes, 14 from facilities, including funding agencies, and 6 from industry. There were also 54 registration from the international community spanning from Japan to USA and Argentina. Subsequently, a letter requesting funding from the Swedish Research Council (VR) to build the case for a Swedish proposal for a GISANS instrument at ESS was submitted, on the request from VR. This letter was very well received. A key strength with this initiative is that it has engaged all Swedish stakeholders, as well as scientists from ESS, with a clear commitment from all to work together. Furthermore, LINXS has been recognised by the participants in this process as an ideal and neutral platform to progress this national initiative.

With the progress made during 2020 and potential support from the Swedish Research Council, the stage has been set to start to realise the case for a Swedish initiative to build a dedicated GISANS instrument at ESS. Funding to support the initiative is expected in mid-2021 and LINXS is prepared to host postdocs to work on the proposal for a Swedish initiated GISANS instrument at ESS. The RP also hopes to be able to invite a LINXS fellow within the GISANS program during 2021.

➤ ***RP: Sample environment and data evaluation of biological membranes***

Recent years have seen strong research efforts on the lipid component of biological membranes. While many studies have been focused on membrane structure, including curvature, the dynamics aspects are crucial for the function of the membrane including those of membrane bound proteins. The relevant time scales extend from seconds to nanoseconds; therefore, a combination of techniques and modelling tools is required. The RP's mission is to promote integration between biophysics, pharmaceuticals, medical sciences and clinical sciences with a focus on sample environment and relevant model systems that mimic membrane related events and also allows detailed structural and dynamic analyses using x-ray and neutron scattering techniques.

The RP has been successful in attracting outstanding scientists for short-term focused research visits to contribute to the science of the RP, to further research collaborations and widen the national and international research networks. Two LINXS guest research fellows, Dr Christopher Garvey from ANSTO, Australia, and Professor José Campos Terán from Universidad Autónoma Metropolitana Unidad Cuajimalpa, Mexico, have been pivotal in building up the competence and network in many aspects of sample environment and science of biological membranes in very concrete terms (see also Annex 4). This involves responsive

microgels as support for lipid bilayers together with Prof. Thomas Hellweg, Bielefeld University (Germany), who was LINXS guest research fellow 2019. Several new contacts have been made, both local and national, and links to other programs have been identified; most notable the links to GISANS for using this technique to study curved membrane using nanostructured surfaces as support. Through the visiting researchers and other activities in the RP, LINXS has become a hub for the research area and has also inspired other initiatives, e.g., within SciLifeLab by colleagues at Umeå University. The RP also has strong links with early-stage career researchers within the SWEDNESS graduate school.

Several initiatives were launched during 2020 that unfortunately could not be realised as planned due to the Covid-19 situation. These included a dedicated session at the ESS/ILL user meeting that was planned for September 2020 in Lund. However, the meeting program was significantly reduced with the transfer to a virtual meeting. The session will hopefully be realised during the next user meeting in 2022. A Neutrons in Biology meeting, with focus on membranes and membrane proteins, was planned together with Professor Trevor Forsyth at ILL, but, also, due to Covid-19 could not be realised; it is hoped that this meeting can be held in 2021, eventually in digital or hybrid form. Plans are also underway to organise a SWEDNESS PhD course within life science applications of neutrons, where biomembranes will be an important part. With these events and new national connections, including with Umeå University, the RP will continue during 2021 until the conclusion of the theme.

Integrative Structural Biology (ISB) Theme outcomes and reflections

2020 was a year of many positive developments for the Integrative Structural Biology theme, despite the big showstopper of the Covid-19 pandemic. After two very successful ISB symposia in 2018 and 2019, the ISB core group had already before the pandemic decided to not have a symposium in 2020. Instead, the plan is to have a final symposium at the end of 2021 or beginning of 2022, when the theme concludes. Despite the pandemic, ISB held a number of the planned events (described below) and organised a LINXS seminar on February 27th by Professor Christine Ziegler, Regensburg University on “Membrane transport regulation by lipids”. In addition, Prof. Karin Lindkvist took over as ISB core group leader after Jens Lagerstedt.

The time-resolved working group started the year by welcoming its first guest researcher, Dr Stefano Mezzasalma, a soft matter theorist at the Ruđer Bošković Institute in Zagreb. To kick-off his Stefano’s stay in January, the working group organized a mini symposium with Stefano and three other speakers to trigger scientific collaborations. During his visit Stefano worked primarily on studying protein dynamics by exploring the protein response to radiation fields in the THz frequency domain. His work involved strong collaboration with a number of researchers, including from University of Gothenburg and Linnæus University. Stefano’s visit lasted from January to April, which was the height of the first wave of the pandemic, but, with the support of the LINXS staff, we were able to get him back home safely.

The main activity of the time-resolved working group during 2020 was to be a workshop in May. This was finally organized as a virtual event in November. The three-day workshop had 18 speakers, 6 posters, a panel discussion and around 170 registered participants. The workshop covered many aspects of time-resolved structural biology and included scientific results, as well as presentations of experimental and computational methods. The event provided a good overview of the subject and allowed the participants to learn about methods they were not familiar with. The talks included examples of scientific studies using a wide variety of techniques, including NMR, x-ray and neutron scattering, x-ray and electron

crystallography, single particle Cryo-EM, Raman- UV/vis and IR spectroscopy, as well as several different computational methods. Interactions between the participants worked surprisingly well online, although this cannot be compared to what is possible at a physical meeting. Reflections and insights from the Time Resolved Structural Biology workshop, as a representative LINXS case for 2020, are included in Annex 6.

The membrane protein working group was formed towards the end of 2019 after a couple of brainstorming meetings with both local and international participants interested in the research area. The outcomes of these meetings were the successful, official formation of the working group, identification of key topics that will be addressed and suggestions for activities. The working group had planned activities for 2020 but decided to postpone them for 2021. During 2021, the group is planning to have two workshops, the first one focusing on protein expression and sample quality control and the second with a focus on sample preparation for structural biology and structure determination by different methods, including x-ray crystallography, neutron crystallography and single-particle cryo-EM.

The strong program of the amyloid working group was, obviously, curtailed, but the group was determined to progress and organised a very successful online workshop in May focused on "User-friendly analysis of spectroscopy data with Quasar - multivariate statistics and machine learning". This event was followed by a second workshop 13-15 January 2021. The workshops resulted in a new collaboration between the French Soleil light source and the Lund University Physics department. A planned meeting entitled "Heart and Mind", focusing on the cardiomyopathy and neuropathy in relation to amyloidogenesis, will be held on the 5th of March 2021. A further meeting building on the successful "Mind the Gap in Amyloid Structure" workshop, (focusing on the interdisciplinarity and multi-technique approaches needed to relate biophysical analyses of amyloid system to real clinical relevance) held in 2019 has also been postponed and will be held in December 2021. A meeting aiming to highlight and promote the application of SAXS and SANS for the characterization of amyloid systems is planned for November 2021.

Members of the amyloid group have also been involved in outreach activities, delivering seminars and teaching. For example, Dr Oxana Klementieva, a senior lecturer at Lund University Medical faculty and LINXS Assistant Director, delivered a lecture at SciLifeLab entitled "How to become a Life Science researcher that uses synchrotron light and neutron applications" in September, and has also been involved in a PhD course on "MAX IV/ESS-based imaging for medical and biomedical research".

During 2020, the "Biocompute and Artificial Intelligence" working group set up a collaboration with AI Lund and the COMPUTE Research School to promote connections between the x-ray/neutron community and the machine learning community. These organisations have around 1800 and 600 members, respectively, and play a central role for hosting machine learning-related activities at Lund University. AI Lund is also an outreach organization with many members from other academic institutions, industry and the public sector. Several joint activities were initiated, including a joint online seminar series. The two seminars held so far were attended by members from both communities, including participants from outside Sweden, and resulted in lively discussions. This series will be continued in 2021. Another joint activity involved two local Covid-19 hackathons in connection with the national and EU hackathons, respectively. A third hackathon developing machine-learning solutions for x-ray/neutron research was planned but had to be postponed to 2021 due to the pandemic. In addition, LINXS-related topics were introduced in the curriculum of "AI for Medicine and Life Sciences" courses of the COMPUTE PhD school, which will run again in 2021. Finally, the

working group leader Sonja Aits, presented the LINXS “Biocompute and Artificial Intelligence” working group and other artificial intelligence activities at Lund University at an event hosted by the digital innovation cluster Mobile Heights.

During 2020, ISB started a new working group, “Lund Integrative Structural Biology Centre Initiative”. The aim of this working group is to investigate the interest and potential in placing an integrative structural biology centre at Brunshög, between MAXIV and ESS, and to help catalyse the discussion and development of these ideas. The first workshop will be held on February 18th, 2021, with three invited speakers from integrative structural biology centres in Europe. For this first meeting, PIs that are directly working with structural biology in the Lund area have been invited, and, if the workshop has a positive outcome, open workshops with a wider audience will be organized by the working group during 2021.

New Materials Theme outcomes and reflections

The New Materials for Energy and Sustainability theme started in September 2020 and will run until the end of 2023. The theme aims to push forward the development and characterization of new materials with potential future applications in the fields of energy and sustainability, bringing together x-ray and neutron experts with material development experts.

The new theme is a great complement to the existing themes with its focus on hard matter and will expand LINXS community into new areas. It is both scientifically interesting and extremely relevant to current global challenges. Global demand for energy is rapidly increasing, and the need for more efficient and reliable sustainable energy sources remains one of our greatest challenges.

– With our theme, we want to explore how new hard materials may help to contribute to a sustainable transition, especially in terms of characterisation of materials and sampling. We will focus on bringing together our various areas of expertise, and explore both neutrons and x-ray techniques, says Elizabeth Blackburn.

The theme divides its work into five working groups: “Functional magnetic materials”, “Charge transfer materials”, “Light harvesting processes”, “Catalysis”, and “Nanostructures and interfaces”. Each group has identified a set of questions that will guide their work by identifying scientific questions where a network approach can be helpful. This set-up is both in spirit of LINXS’s work practices, and a way to create collaborations between different experts. By the end of the theme operations, the working groups hope to have answered some of the questions identified as key, as well as developed tools and guidelines for how to use some of the tools and techniques available to help other researchers.

Examples of the questions that the new theme will address include: what are the structural and chemical process that occur during the operation of electrochemical devices such as batteries? How does the combination of viscosity and polarizability influence the structural re-orientation of light sensitizers/polymers, and how can this influence be used to extend the charge separation lifetime? Other key goals include achieving a fundamental understanding of the function of catalysts for the development of sustainable industrial processes, and developing magnetic imaging through optimised experimental, data reduction and analysis protocols.

Whilst the initial structure and goals of the theme have been well defined in the proposal, there is also scope for new initiatives and working groups, as the theme wants to capture new ideas as people get interested and engaged in the work.

– Overall, the theme is a great opportunity to explore different research areas, with researchers who are all interested in finding answers to some common problems. You cannot work in isolation, research moves forward by collaboration: across groups, fields, and countries. That is what really excites me: to work together to find out things that could be of benefit to many, says Elizabeth Blackburn.

The theme will also work to advance transdisciplinary collaboration with the aim that to succeed in bringing people together from the different areas and to show that one can work on something new! A secondary goal is to make people more aware of the different available techniques and provide guidance on how to pick the right technique for the job.

A digital kick-off symposium was held on 2 November 2020 with three plenary talks, covering topics from reflectometry to catalysis, followed by initial discussion groups for the five initial working groups. The symposium was well attended, with 10-15 people participating in each working group discussion meeting. Subsequently, each working group has started developing their activity programmes, detailed individually below.

WG 1 - Functional Magnetic Materials working group

The first network meeting was held in December and will continue on a monthly basis. The first activity will be a workshop on micromagnetic simulations and their use in analysing scattering data planned for late March/early April 2021.

WG 2 - Charge Transfer Materials working group

Together with Light Harvesting Processes, this group has set up a weekly open LINXS meeting, running since early December. So far, joint beamtime proposals have been discussed.

WG 3 - Light Harvesting Processes working group

An EXAFS workshop is being prepared for summer 2021, ideally in conjunction with a long-term visitor. This will cover 25-30 participants and last one week. A MAX IV beamtime proposal to contribute to the programme is being prepared.

WG 4 - Catalysis working group

A kick-off meeting was held in December to introduce the members of the working group to each other. So far, two LINXS seminars have been planned for spring 2021. Reflections and insights from the Catalysis working group, as a representative LINXS case for 2020, are included in Annex 6.

WG 5 - Nanostructures and Interfaces working group

The activities of this group will develop with further input from the other working groups. At the moment, a potential ESS-NanoLund workshop is being discussed for the second quarter of 2021.

LINXS Strategic & Operational Achievements

LINXS defined a specific strategic and operational plan for 2020 to guide and streamline efforts in consolidating LINXS as an institute, in realising the LINXS mission, in developing and running activities, and in establishing the conditions for future growth. The Covid-19 pandemic in spring drastically altered plans for the year, but, at the same time, provided new opportunities to invest in aspects of the LINXS mission that were not yet prioritised. Strategies, such as digitalisation, increased online activities and world outreach, as well as the

development and online availability of educational material, brought new value. The following summarises the development of LINXS in 2020 with respect to its strategic and operational plan.

Science Strategy

At the beginning of 2020, the LINXS leadership worked on clarifying the scientific mission of LINXS and its role. While the science strategy is conditioned by the yearly development plan of its operational themes, there are concepts and overall principles that needed clarification. Work resulted in the following conceptualisation.

LINXS is an advanced studies institute for x-ray and neutron related science with a broad perspective with respect to research topics. Above all, LINXS aims to promote excellent research by excellent researchers, wherever they come from in terms of topic area, research approach, geographical location and affiliation. At the core of LINXS concept is what constitutes an "advanced studies institute". The archetype is the Princeton Institute for Advanced Study (IAS), which is best known for hosting Albert Einstein. IAS was founded in 1930 and still brings leading scientists together and gives them the resources, time and space to do science that advances the limits of human knowledge. There are now a number of similar institutes worldwide based on different funding models and operating principles. The KITP, in Santa Barbara (USA), and the Pufendorf institute, in Lund, are specific inspirations for the working principles of LINXS. In the context of LINXS, it is recognised that "advanced" is relative; the forefront of science that can be done with the help of light sources and neutrons can be found at different levels and manifestations depending on which community is involved. For LINXS, "advanced" refers to:

- advancing science and understanding through new interdisciplinary connections;
- bringing different scientific communities together, especially experimentalists, theoreticians and modellers;
- advancing the scientific possibilities, capabilities and limits of knowledge for as many different disciplines, areas and communities as possible.

LINXS views research as a continuum across subject areas involving experimentalists, method developers, theoreticians and modellers. The working practices should, therefore, encourage interdisciplinary, intersectorial and inter-methodological engagement to exploit diversity and complementarity. The research at LINXS should be cutting-edge for the respective research area and should be community and research driven; i.e., the drive should be from the bottom up with the Scientific Advisory Board (SAB) as a quality control mechanism.

To achieve its scientific mission, LINXS should:

- maintain a broad perspective across LINXS themes, promote interdisciplinary research and develop networks and interactions;
- attract excellent researchers from all related science areas to interact with and help develop the community and create future world-leading research, researchers and research networks;
- maintain a flexible approach to encourage the possibility for new ideas to develop - LINXS should be an incubator for new science and can be a launch-pad to bigger projects, which might continue beyond LINXS;
- foster internationalisation of the research community;
- encourage the involvement of young researchers with a vision towards a LINXS Young Academy.

Strategic objectives

- *Advance LINXS as a nucleus for x-ray and neutron based research*

LINXS is becoming established as a centre for x-ray and neutron based research at local, national and international levels. In 2020, LINXS worked on building upon its established platform and expanding this online, widening the awareness and international outreach, as well as strengthening its scientific profile with new working groups and a new theme on hard matter.

New working groups were established during 2020. In the ISB theme, the “Membrane Proteins - Structural resolution and homology modelling” formally started in January 2020 and the “Lund Integrative Structural Biology Centre Initiative” in the fall. The new theme on “New Materials” started with its 5 working groups and aims to advance the development and characterization of new materials with potential future applications in the fields of energy and sustainability (see under “LINXS scientific achievements and impact” above).

The Covid-19 pandemic in spring stopped or postponed LINXS activities, but also hastened the move to fully digital and hybrid (digital and physical) events, which attracted much wider participation from all over the world. Despite or, actually, just because of the pandemic and the online development, LINXS increased the number of activities in 2020 to 39; 31 organised by LINXS and 8 in partnership with other organisations (see Annex 2). A significant number of these events were webinars in the two webinar series initiated during the year. Most activities were run online through the year, but there were 7 that were “in real life” (IRL) or hybrid.

In all its activities, LINXS strives for gender balance and diversity, encouraging working groups and collaborators to consider, as much as possible, gender balance in invited speakers, members of panels, guest researchers and other factors that can be influenced directly in activity organisation. Gender balance is a long-term effort, as there is a traditionally skewed institutional set-up in the main scientific communities that relate to LINXS.

The strategic goal to increase digital participation in the LINXS activities was met with great success. The activities attracted more than 1900 participants from all over the world. The 526 participants registered for events through the LINXS Indico system with complete data, provide a good statistical base for the LINXS indicators (see “LINXS in Numbers” below). This clearly shows that LINXS has been very successful in developing online activities and a solid online presence. There have also been many benefits from the shift to “online”, which should be built on to strengthen LINXS as an international institute. Furthermore, digitalisation did not only result in widened international participation, it also contributed to fulfilling sustainability goals. LINXS will continue this progress and, when advantageous, have hybrid or online activities to complement the essential physical interactions and encourage wider online participation.

Towards establishing LINXS as a “go to” for information around x-ray and neutron-based research, apart from the new webinar series, LINXS also initiated the development of a Wiki on techniques and relevant facilities/infrastructures. The aim is to have an integrated knowledge-base and associated tools assembled in a single Wiki as an open resource to attract and help new (and existing) users to x-ray and neutron facilities. The LINXS Wiki is under development based on the same backend as Wikipedia for interoperability (Mediawiki engine) The wiki will also include a semantic plugin, with amongst other features, that will help to provide a tool that is not just for cataloguing information, but also for structuring the available information in interactive ways, depending on users’ needs.

Another important digitalisation activity during the year was making recordings of webinars in an “educational materials” section of the LINXS website to contributing to the LINXS mission to help educate potential users and expand the facilities’ user base. This platform has been further expanded to promote relevant education material from other initiatives and collaborating organisations. LINXS has also worked to identify, disseminate and publicise the output and outcomes from LINXS activities (see under “Focus on capturing the outputs and added value”).

The usage of LINXS affiliation and acknowledgement in scientific publications and presentations has increased in the past year (see list of scientific publications in Annex 3). Even if LINXS does not make the usage of its affiliation mandatory and the number of publications with a LINXS affiliation is not seen as a central evaluation criterion, this is, nevertheless, good to see. Further effort is needed to promote usage of the affiliation by LINXS fellows to contribute in the aim to grow a “quality stamp” reputation and to highlight the role played by LINXS in advancing science.

A growing number of researchers from other parts of Sweden have been involved in both working groups and activities. Furthermore, international involvement outgrew expectations, increasing the LINXS visibility. Based on feedback received by the end of the year and in various research and strategic meetings, LINXS is becoming a recognisable name, known as a centre for x-ray and neutron-based research at local, national and international levels.

Increased external networking and collaboration opportunities is also visible in LINXS’s involvement in funding applications such as the “Northern Lights on Food” network with funding from FORMAS and a grant through Lindqvist Stiftelse (see under Imaging above). The Imaging theme has also been active in supporting funding proposals where LINXS can play a role in supporting the scientific or community building goals (see Imaging above).

LINXS’s “Networking Initiative”, towards increased utilisation of photon- and neutron-based technologies by researchers from throughout Sweden and to support other Swedish universities to increase their user base, was inevitably halted by the pandemic. In this context, LINXS did not receive any formal decision on the associated application to Vinnova/VR for funding of a series of workshops at other universities in Sweden. The same fate awaited the “Visiting Programme” application to Crafoord, as the pandemic froze the aim to increase the number of guest researchers visiting Lund.

LINXS also formally supported applications for funding including to the VR infrastructure accessibility call and, in particular, the “Metals and manufacturing @ next generation sources” that was awarded funding (Dnr 2020-06159) from the Swedish Research council. LINXS will closely collaborate with the project in the coming years, not least for joining forces in the development of the LINXS Wiki.

In summary, LINXS is showing its important role in incubating and supporting research projects as an initiator (through working groups), as partner or as the inspirator. Even if funding proposals are not funded, the involvement of LINXS in such activities is an important component in the development of transdisciplinary scientific communities.

Examples of collaborative project developments include:

- Initiation of collaboration behind funded RÅC project on protein dynamics
- Northern lights on Food FORMAS project partner
- Partner in FORMAS Food centre project proposal
- Implicated in at least 2 VR accessibility to infrastructure projects
- Mentioned in at least 3 LU/NMT infrastructure projects

- Mentioned in EUGloH infrastructure project

In 2020, LINXS was approached in a number of contexts to participate in applications that boost networking and competence building on the European level, such as MSCA, ITNs, COFUND and others. LINXS will keep working actively to involve itself in appropriate applications (networking and educational actions) on the European level going into the next year. LINXS continues to participate to the Helmholtz-Lund International School (HELIOS) – Intelligent instrumentation for exploring matter at different time and length scales.

- **Post-doctoral programme**

LINXS postdoctoral fellow Dr Anurag Kawde works with Prof. Tõnu Pullerits at the Chemical Physics division of the chemistry department at Lund University and in close collaboration with the NanoLund Facilities. As a LINXS postdoctoral fellow, Dr Kawde develops scientific activities relating to the LINXS mission as well as contributing to the LINXS community building and outreach activities.

In 2020, Dr Kawde initiated a collaboration with Prof. Serena DeBeer from the Max Planck Institute of Chemical Energy Conversion in Germany. This project is on the investigation of the solar-assisted process for N₂ conversion to ammonia. At the national level, Dr Kawde collaborated with the Department of Physics of the Umea University in relation to studies of solid-state electrode systems and their theoretical prediction towards solar-assisted chemical processes. Locally, Dr Kawde has also developed a successful collaboration with Prof. Rajni Hatti Kaul from the Biotechnology department to study kinetic reaction mechanism for biomass derivatives conversion, as an alternative to polyethylene. The project has yielded some exciting results with a manuscript ready to be submitted for publication. Dr Kawde also has a strong collaboration within the chemical physics division at Lund University (Dr Jens Uhlig and Prof. Arkady Yartsev) to study excited charge carrier mobility at various timescales.

With the ongoing Covid-19, physical science meetings were practically impossible during much of 2020. In this context Dr Kawde initiated, with PhD Candidate Veronica Lattanzi, the successful LINXS webinar series “Let’s drive into the atoms!” dedicated to the educational aspect of the large-scale facilities such as synchrotron and neutron sources. The first six webinars were arranged in the summer of 2020. Experts in the field discussed various natural science experiments that one could perform at such facilities. The second group of webinars in the fall was focused on complimenting lab experiments with experiments at large-scale facilities. The experts also guided the audiences on how to write compelling beamtime proposals (see Annex 5).

- ***Build LINXS as a vibrant, active and attractive interdisciplinary community with a physical interaction hub in Lund in close proximity to MAX IV and ESS***

MAX IV and ESS are LINXS “core partners” and collaboration further developed in 2020. More generally, the “LINXS community”, of collaborating organisations in working groups and activities, grew significantly. The list of collaborating organisations, along with the affiliations of the LINXS fellows, are listed and continuously updated under the specific “LINXS Community” section of the website.

At a local level, LINXS worked with Lund University's Research Quality Evaluation Project 2020 (RQ20) as part of Lund University External Engagement effort. This enabled LINXS to demonstrate its role in contributing to research quality through its mission and operations.

Due to the Covid-19 pandemic in spring, physical meetings at LINXS were limited or not possible. Theme core group, working group, management, operational board and SAB

meetings swiftly moved online as LINXS eagerly explored the advantages that the digital reality had to offer for progress and outreach. This resulted in increased international participation in the LINXS communities and in the pool of researchers interested in spending time at LINXS after the pandemic. Moreover, this online activity strengthened links to international networks in particular. New working groups emerged during the year to create new scientific communities, stimulating discussions and development of ideas at LINXS. Online work proved to be time efficient and increased participation somewhat, but did inevitably, restrict spontaneous discussions that occur around the LINXS lounge with a cup of coffee. The loss of such physical interactions, which often lead to exciting new scientific perspectives and tacit knowledge transfer, was the main blow from the pandemic.

LINXS reacted quickly to the new restrictions due to the pandemic, investing in equipment and developing solutions for digital events and data capturing. The digitally equipped LINXS premises were also made available to collaborating organisations and to Lund University faculties to help in the urgent need for hybrid events. Consequently, the LINXS premises were used by other groups from Lund University, mainly for PhD defence events.

In general, the usage of the LINXS premises by working groups and other hosted groups (such as two ESS internal strategy days, LU@SVS project group, Diabetes LUDC and the Lund Tomography community) was good until the outbreak of the pandemic and after the summer until the second wave in November (see Annex 2). Nevertheless, work is still needed to develop the premises as a place where there is constant scientific activity and interaction, which is essential to the goal of facilitating interactions and developing new scientific synapses. This work needs to intensify after the pandemic and requires developments within the structure of LINXS, in the working practices of the themes and working groups, in how the guest researcher program is run and the communication across the LINXS community.

An aim of LINXS is to move its physical location at the heart of Science Village Scandinavia (SVS). However, development of SVS has been delayed and the first building is now expected to be ready towards the end of 2024. Consequently, LINXS was obliged to renew the rental contact on its current premises at IDEON for another 3 years until the fall of 2024. However, LINXS is active in the SVS development discussions, within (included in LU@SVS work) and outside Lund University. LINXS is also constantly investigating possible emerging solutions for the long-term establishment at SVS. In this context, LINXS has good contact with the new SVS director and management team.

- **LINXS Visiting researcher programme**

LINXS is founded on the idea of bringing researchers together and promoting interactions within and across disciplines to fertilise research. To this end, LINXS continued its visiting researcher programme in 2020, as part of its work to attract world-leading scientists. The programme brings international researchers to LINXS for short-term research visits. During their time at LINXS, these researchers share their expertise and knowledge with the LINXS network and support the development of international and regional networks and scientific collaborations. Whilst the visiting researcher program was a success in 2019-2020 and a good continuing program was planned for 2020, the pandemic stopped all visits for most of the past year. Nevertheless, LINXS hosted three international guest researchers in 2020, one prior to the onset of the pandemic and two that were already at LINXS since 2019.

Dr Stefano Mezzasalma, a soft matter theorist at the Ruđer Bošković Institute in Zagreb, was a guest researcher with the “Time-Resolved Structural Biology” working group in the ISB theme between January and April 2020.

Within the Dynamics theme, Prof. José Campos Terán from Universidad Autónoma Metropolitana Unidad Cuajimalpa, Mexico, and Dr Chris Garvey from the Australian Nuclear Science and Technology Organization, Australia, continued as guest researchers until August and December 2020, respectively.

The guest researcher's hosts took on the responsibility of ensuring the guests were well integrated into LINXS activities and the wider community. This involved activities with the guest and host, plus other events at LINXS to develop the working environment and interactions across LINXS. These activities include the Mini-symposium by the Time-Resolved Structural Biology working group, (January 24, 2020) and the webinar of Dr Chris Garvey (also captured in the LINXS educational material). The guest researchers also participated in the LINXS Science Days and presented their research and ideas around advancing LINXS.

The results of the visiting researcher program are already reflected in a number of publications (see Annex 3) and seminars, plus, most importantly, in new research collaborations. LINXS also publicised and highlighted the value of the visiting researcher program and its outputs in a series of news articles on its website. A video interview with the Stefano A. Mezzasalma, where he talks about his experience of being based at LINXS and his views on scientific collaboration and progress, was developed in the end of 2020 and can be viewed on the website.

Naturally, the pandemic put a halt to the visiting researcher program as several foreseen guest researchers were not able to come to Lund. The pandemic also hampered activities to attract researchers in visiting Lund and spending time at LINXS as physical activities were postponed. On the other hand, the increased international participation in online events increased the interest of researchers to get involved and visit LINXS post-pandemic. An analytic report of the Visiting researcher programme is in Annex 4.

- ***Solidify and extend LINXS's scientific portfolio within and between the existing themes***

LINXS has been successful in developing more long-term research activities, and its portfolio of activities expanded to include webinars and online solutions for workshops and hackathons were developed. With the start of the new theme in the fall, the LINXS community grew significantly and contributed to an increase of interactions within and across themes.

LINXS Science days were developed as a forum to bring researchers from across LINXS together to facilitate cross-theme discussions and the development of new "scientific synapses". LINXS organised a physical Winter Science Day at the beginning of the year, a virtual Town-Hall and Discussion Meeting in the fall and a larger, virtual LINXS Science Day in December open for international participation and with a concrete focus on science. LINXS fellows and guest researchers presented their work and raised international interest in getting involved, as indicated by relevant communications.

– The Winter Science Day was a great moment to get a snapshot of what is going in our working groups. We hope that such LINXS-wide events can generate new ideas, (cross-theme) collaborations and fruitful discussions around x-ray and neutron related research. It is clear that we now have a great breadth of research taking place at LINXS and we hope everyone can profit from being a part of this strong and diverse community, says Stephen Hall, Director of LINXS.

As LINXS grew, there were two theme leaders who were not formally members of the LINXS management group, which previously had not been the case. As a result, a monthly "Science Management Meeting" was initiated to facilitate cross-theme communication and science strategy implementation across themes. In general, the core groups were encouraged to

quickly develop activities such as mini-symposiums and workshops into more focussed research activities. It was also recommended that the theme leaders and associated core groups should have regular updates from the working groups to aid their development.

- ***Establish a new theme and develop towards further calls for themes***

In 2020, LINXS fulfilled the aim of having 3-4 concurrently running themes with different ending dates by concluding a call for themes to enable a dynamic renewal of the community.

Imaging was the first theme scheduled to complete its three-year course in the end of 2020. Due to the pandemic the theme activities were prolonged with events moved to spring 2021 and the final conference scheduled for the summer. The process of concluding a theme was established during 2020 for the conclusion of Imaging and includes a final report on results and output, as well as future emerging opportunities spurring from its work.

The call for a new theme process, which started in autumn 2019, was concluded before the summer and a new theme, "New Materials", started in September 2020. The new theme followed a rigorous and transparent two-step application process and developed a clear scientific development plan. The selection process was based on external expert evaluation by the LINXS SAB, with the remit to ensure scientific excellence and complementarity within LINXS.

The new theme considered the lessons learnt from the previous theme developments and established active core group and working group interaction and presence at LINXS and online. Moreover, early activities towards identifying goals and objectives for focussed research efforts were identified in the November kick-off.

To continue its renewal process, LINXS launched a second theme call in September (Reg.nr F 2020/1138). The SAB was closely involved in the process and recommended a more "applied science" focus relating to the application of x-ray and neutron based science to socioeconomic, environmental, health, cultural or industrial challenges where they can implicitly make a difference. The call was open to applicants from partner organisations (currently Lund University) and was widely communicated through the LINXS website and contact list, as well as relevant Lund University faculty newsletters and official communications. The LINXS call process, documentation and evaluation criteria have been further refined and include explicit requirements to demonstrate international ambition for the research area, have the potential for significant impact at an international level and describe a clear strategy for how the proposers will engage with the international community. The internationalisation of the core and working groups of the LINXS themes is important to the mission of becoming a world leading advanced study institute for all scientific and technological disciplines that can benefit from the use of neutrons and x-rays.

Two complete proposals were received prior to the stage 1 deadline of October 30th. Following the SAB's recommendation, one theme proposal was accepted to proceed in the second stage evaluation in spring 2021 when a final decision will be reached.

- ***Expand and improve the visitors program integrated into the LINXS mission***

The successful visiting researcher program had a good plan of visits for 2020 that took into account the lessons learnt in 2019 to strengthen the program and to maximise the benefits for LINXS, the visiting scientists and the LINXS community. As previously mentioned (see section on Visiting researcher programme above), one guest researcher was able to visit LINXS from January to April 2020, just prior to the outbreak of the pandemic, and two others already at LINXS concluded their visits during the year.

The pandemic did not allow for more guest researchers at LINXS but did provide time for better coordination between LINXS and the working groups. In preparation for the post-pandemic period, guidelines for the visiting researcher program were discussed with the working groups to encourage wider participation of guest researchers in LINXS activities and within the LINXS community, as well as bigger diversity. A lesson learned from 2019 was that the most beneficial visits are short-term, from a few weeks to a maximum of 3 months, and having a concrete work and hosting plan within the working group. The procedure to apply for a guest researcher was clarified and made more open and transparent. This could, in the future, lead to a general call for guest researchers.

In the fall, LINXS worked together with the working groups on their planning of guest researchers' visits in 2021. The uncertainty around the time when the pandemic will subside puts a strain on any planning, but an effort to increase flexibility and review plans is constant.

LINXS also investigated funding opportunities to support the visiting researcher program, as this is clearly an attractive and visible activity for potential funders to support. However, partly due to the pandemic, the relevant application to the Crafoord foundation was not successful.

- ***Promote and facilitate education of both new and advanced users of x-ray and neutron methods***

A key part of the LINXS mission is to educate both new and advanced users. However, ESS and MAX IV, as well as other large-scale research facilities and organisations also have this in their remit. Therefore, LINXS has worked to coordinated efforts with the facilities, e.g., relating to webinars, joint workshops, and participation in user meetings, in order to avoid duplication of efforts, to clarify target groups and to maximise the benefits to all concerned. It is important for LINXS to have education and training activities aimed at different levels and not just at the basic/introduction level. Moreover, the aim is to provide a forum for promoting external educational activities through the LINXS communication channels (e.g., the events page on the LINXS website).

The LINXS premises have proven to be ideal for doctoral schools and courses and LINXS encouraged external groups to run educational activities at the premises, either as partner or hosted events. Even if physical events were restricted in 2020, the "Masterclass on Food", which was run as a hybrid event both at LINXS and online, was very successful. The event introduced researchers to the possibilities of using neutrons and x-rays in food research. The aim was to highlight how the techniques offered at MAX IV and ESS can give knowledge and insights on food structure, properties and behaviours in relation to storage qualities, uptake and nutritional value, as well as texture, perception and packaging.

As a major development step, LINXS developed two webinar series (see below) with different foci, levels and target groups. The "Let's dive into the atoms!" webinar series was an introduction to x-ray and neutron methods at a basic/introductory level. The level of "CoWork" LINXS webinar Series was more advanced/expert (see Imaging theme section above). Both webinar series were extremely successful and greatly contributed to the fulfilment of the LINXS "educational" mission, increased digital participation and international outreach, as well as the visibility of LINXS.

Recorded webinars from different activities have been made widely available in the new "educational material" section of the website, which was developed during the year and also provides links to external resources of relevant material from other organisations such as ASP (The African School of Physics) Lecture series. More generally, LINXS has been working to expand the educational material content on its website, including webinar videos,

presentations from LINXS and LINXS-hosted events, links to external resources and developing material. The content is continuously developed.

An analytic report of the LINXS Webinar Series is in Annex 5.

Operational objectives

In August 2020 there were changes in the LINXS Management group. Jens Lagerstedt left academia for a new position in industry but remains involved in the Amyloid working group and continues to be a valuable collaborator. LINXS is extremely grateful for Jens's work to the development of LINXS from its early formation in 2018. Marie Skepö became LINXS Vice-Director and Oxana Klementieva, associate senior lecturer and head of the Medical Microspectroscopy research group at the Medical faculty at Lund University, entered the management group as the new LINXS Co-Director. Furthermore, Karin Lindkvist, Professor in Medical Structural Biology at Lund University, took over the role of core group theme leader of the Integrative Structural Biology theme. Elizabeth Blackburn, from Synchrotron Physics in the Science faculty of Lund University, heads the new "New Materials" theme.

- ***Appoint and integrate a new director***

The formal evaluation process of the 24 applicants for the new LINXS Director role started in January 2020. The evaluation committee included representatives from Lund University and the LINXS SAB, while work was facilitated by LINXS. 10, mostly senior, high-level international scientists with very impressive records of scientific accomplishments and experience, were called for a preliminary interview in spring and a final list of five candidates was decided in the summer. The whole process was delayed due to the pandemic, as the candidates were unable to travel to Lund. One candidate withdrew his candidacy due to personal reasons and four candidates were called for a second, deeper interview. These interviews were carried out online in the fall, as were the candidates' scientific presentations to the wider Lund and international research community. The evaluation committee concluded its final evaluation in the beginning of December 2020.

Negotiations are expected to progress in the beginning of 2021 and the ambition is to install the new director in the summer, depending on negotiations and practicalities (not least pandemic restrictions). Due to the long recruitment process, the NMT faculties decided to extend the management group membership until the end of 2021 for the Vice- and Co-Directors and until June 2021 for the current interim director, assuming that the new Director would be able to start around this time.

One important result of the recruitment process has been the realisation of the importance of the new Director's vision for the future of LINXS. The process also helped key leaders at Lund University to discuss the vision and mission of LINXS across faculty borders and come to a clearer understanding of the LINXS role and potential at local, national and international levels. It is noteworthy that the recruitment process and final offer is made through a unique collaboration between the Lund University faculties of Science, Medicine and Engineering, demonstrating the strategic importance of this recruitment, not only for LU, but also for Swedish research and potential LINXS stakeholder organisations at a national and international level.

- ***Secure medium and long-term funding***

During 2020, LINXS has consistently worked towards securing long-term funding, and to plot a sustainable path forward. There has been a consolidation and clarification of the support from the Lund University faculties of Science, Medicine and Engineering (NMT faculties) and a

formal decision to jointly provide LINXS with basic funding for 2021-2025. LINXS is extremely grateful for the NMT support, which demonstrates the commitment of the faculties to the role of LINXS as a tool in realising the Lund University strategic priority of being a driving force in developing and utilising the full potential of MAX IV and ESS.

Contact has been ongoing with the new VR/VINNOVA office to communicate the LINXS mission and role in the Swedish ecosystem around the MAX IV and ESS facilities. This role has been more established and communicated to national stakeholders and a specific effort to engage other Swedish universities continued, but progress was slowed due to the pandemic and due to the focus on recruiting a new Director at LINXS.

As already mentioned, a funding application was made to support the visiting researcher programme in 2020 (unsuccessful) and its national "Networking Initiative" effort (halted). Going forward, LINXS will increase its efforts to receive external funding from foundations, specifically to boost and realise its visiting researcher programme and a potential postdoc programme. Such specific programs could be branded with the contributing foundation name. To this end, LINXS solicited and is receiving help from the LU Development Office in approaching Swedish foundations. Approaching international foundations will be revisited in conjunction with the appointment of a new Director.

LINXS will also seek to expand the number of national and international partners and members. However, it has been realised that it is most important to establish a solid foundation to LINXS and, from there, build strong scientific collaborations with national and international groups before pushing further for partnerships and memberships. This is discussed further in the following.

- ***Extend LINXS's community including partnerships and memberships***

LINXS has the objective to grow from the solid foundation provided by Lund University to an institute supported by a number of national and international partner organisations and foundations. Thus, LINXS needs to consolidate and develop its community both nationally and internationally. To this end, LINXS has been increasing outreach activities and the move to more online activities and content has boosted wider participation. However, even if LINXS has been successful in growing a community of collaborating organisations, it needs to develop the member and partner base beyond Lund University. The offering model approved by the LINXS board was a first step in this effort, but it needs to be revisited in order to clarify the value proposition to potential partners. Identifying the benefits of LINXS for potential members and partners is key. The design of the operational process related to the membership and partnership model is also part of this work, as it is important to secure a transparent decision-making process.

A major milestone was reached in 2020 when LINXS welcomed the RISE Large Scale Research Infrastructure (LSRI) team as the first LINXS research group member. The LSRI team of technical experts located near or working closely with the new facilities in Lund has joined the institute's membership programme and is involved in its activities.

– While we have worked closely with LINXS before, we see the membership as an opportunity to strengthen our collaboration around engaging researchers from different parts of the country. . . Especially, competence building through education and training are important areas for us since we work towards opening up synchrotron and neutron techniques to industry and industry related research. Collaboration with LINXS enables us to reach out to academia as well as industry through strategic, and exciting scientific events and workshops. LINXS is also a platform to build important technical and scientific networks which can also help to attract new

users to the facilities, says Tomas Lundqvist, Senior Area Coordinator at RISE LSRI, and former Science Director at MAX IV.

The pandemic disrupted work with the LINXS work towards partnerships and memberships, including associated outreach activities, such as stands and presentations at selected national and international events (e.g., TechConnect Europe Innovation Conference postponed for 2021). Work with other Swedish universities in the aim to revise the LINXS membership and partnership offering to accommodate their specific needs mostly halted due to the urgent needs of universities to tackle the effects of the pandemic.

Nevertheless, significant progress has been made in the national and international visibility of LINXS through activities and strategic outreach, such as LINXS participation in the MAX IV and ESS user meetings, as well as work by LINXS working groups, such as the GISANS initiative. In the latter case, LINXS was explicitly considered as a “neutral platform” to gather national stakeholders around a specific effort and potential post-doc work.

In general, the LINXS themes end working groups encourage the involvement of non-LU researchers in their work and this is reflected in the large number of different organisations of the LINXS fellows.

Concerning interactions with industry, LINXS is open to non-academic researchers and organisations, but a specific industrial focus is not part of the current remit. On the other hand, an increasing participation of researchers from industry in the LINXS events and contact list has been observed.

It is important to note that with the recruitment process of the LINXS directorship it became apparent that the membership and partnership model will depend on the new Director’s vision for the future of LINXS. Revisiting the offering model will be a strategic priority of the new Director.

- ***Engage board and management group members for 2020-2023***

The current board mandate was officially due to finish mid-2020 but, in view of the recruitment of the new Director, it was extended until mid-2021.

In 2020 LINXS worked to engage the board members more in its decision-making and strategic priorities, as well as in its activities. Many members were also members of the evaluation committee for the recruitment of the new Director giving much time and dedication to the task. Of particular note is the significant engagement of Veronica Lattanzi, PhD student representative (NDR) to the LINXS board, who has been, and continues to be, instrumental to the development, coordination and implementation of the first LINXS webinar series “Let’s Dive into the Atoms!”. Her ambition in joining the board was to bring PhD students, and young researchers closer to x-ray and neutron methods, as well as to educate the future user community of MAX IV, ESS and other large-scale facilities. LINXS is grateful to Veronica for her enthusiastic contribution to the LINXS operations and accomplishment of educational mission.

- ***Establish a “Theme development plan”***

The processes for planning of the themes and their activities became more established in 2020. In the autumn, the themes were asked to provide LINXS with their activity planning for the next year and the level of ambition of their development plans. These plans are adjusted and negotiated in order to be included in the budget work of next year.

- ***Focus on capturing the outputs and added value***

LINXS worked to identify, disseminate and publicise the output and outcomes from LINXS activities, mainly through outreach, the development of reporting tools, expansion of the website, targeted news articles, wide distribution of the newsletter and connections to websites of collaborating organisations.

The reporting process of the themes and working groups has been standardised, and documentation of activity “output” commenced through feedback forms, which also help capture impact potential, as well as define next steps and ways forward based on the outcomes. Reporting templates for both activity reporting and for annual reporting purposes were developed and implemented.

LINXS tries to capture publications and research output using the LINXS affiliation. This is achieved using theme and working group reporting and the LUCRIS database, as well as individual reporting from the authors. Use of the LINXS affiliation is encouraged, but not obligatory, and, even if publications are significant and reported upon, they should not be considered as the main output value of LINXS.

- **Communications as a pathway to impact**

LINXS continued its efforts to use communications and outreach strategically towards realising the overall mission for LINXS, with a key success in 2020 being the increased online content including webinars and educational material. As described in response to earlier points, LINXS has become better at capturing and giving value to its outputs. This is an on-going effort, and a concrete communication plan is followed every year as a strategic pathway to achieve long lasting scientific and societal impact in the short, medium and long term.

Strategic outreach activities (see Annex 2) served to promote the LINXS science and strengthen the LINXS identity in both local, national and international contexts. A strong indicator of the latter is in the success of the Science Day in December 2020, which welcomed a number of researchers from outside the LINXS community.

Publication of the LINXS newsletter continued and the subscription list increased to 1111, increasing from 800 in the past year and with very few unsubscriptions. The main aim of the newsletter is to showcase LINXS work, activities and themes to internal and external target groups – with a view to stimulate interest and excitement, both in LINXS and in x-ray and neutron science. It also aims to attract interest for scientific collaborations and to entice other organisations towards joining the LINXS initiative through membership/partnership. The newsletter serves to strengthen and establish the LINXS identity in local, national and international contexts. In total, LINXS issued 6 newsletters in 2020. On average, 414 people opened every newsletter – ranging from 395 to 477, i.e., an average 48% opening rate, an impressive result, considering the large increase of subscriptions, and a testament to the perceived relevance of the newsletter to the LINXS community and beyond.

LINXS communicated activity results also through a series of popular science articles about LINXS themes and working group work, capturing output, value and impact potential. These articles were included in the newsletters and the website. In total, 33 news articles were produced (including announcements, theme calls, LINXS webinar series, LINXS newsletter and popular science articles). The aim of such articles is to contribute towards increasing awareness about LINXS work, showcase ongoing x-ray and neutron science and maintain the interest of researchers already invested in LINXS. Key points include highlighting the science at LINXS and the community building, plus demonstrating the value-added, scientific relevance and quality. In addition, LINXS produced some targeted articles and events directed at a wider, Swedish audience to highlight the work supported by LINXS. Two articles in Swedish about

LINXS's working groups were published on LU.se and another highlighting the Northern Lights on Food featured in the Lund University Magazine (LUM).

LINXS also produced two short films that were posted on the website: an introductory film about LINXS and a film on a guest researcher's views on the value of the visiting researcher programme.

The LINXS website is a key tool for communication and transparency. It has been significantly updated and expanded during the year, with a focus on supporting current and potential researchers at LINXS. The "Educational material" section has been developed, and the "Resources" section largely expanded to contain a document library with newsletters, annual reports, LINXS templates, instructions and publicity material. A "LINXS Community" page has also been developed to highlight the breadth of organisations involved in and collaborating with LINXS. The LINXS handbook is also regularly updated to better provide information on how to organise, communicate and report on activities, plus other information relating to working with LINXS. As already mentioned, the "Going on" section has been expanded with a news section featuring regular and timely articles on working group activities to highlight the research activities. The "Webinars" section has been added and the "Related events" section now includes outreach activities of LINXS fellows plus promotion of events relevant to, but not organised by, LINXS.

RSS feeds have been developed so that other organisations can incorporate links to their own website. MAX IV included a "happening at LINXS" section in its website and SVS included a feed to their rolling first page in order to promote LINXS at SVS.

The launch of the educational material page on the LINXS website was a significant development. The resource, featuring recorded LINXS webinars and other lectures, materials and presentations, is a repository to collect and share educational, instructive and informative material related to x-rays and neutrons. Since the launch, the initiative has been very successful – the educational page is one of the most visited on the website. The initiative serves to realise LINXS mission to promote science and education focusing on use of neutrons and x-rays and help educate potential users of ESS, MAX IV and other major research infrastructures.

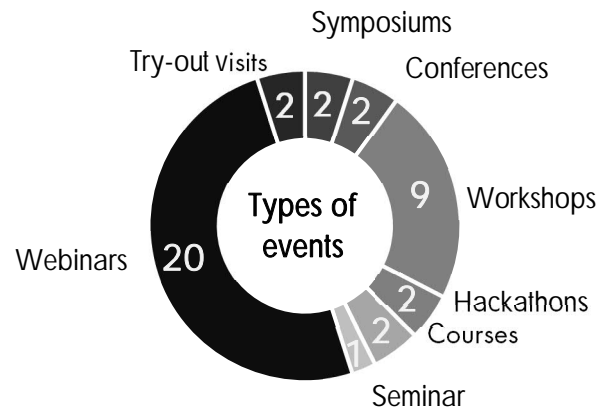
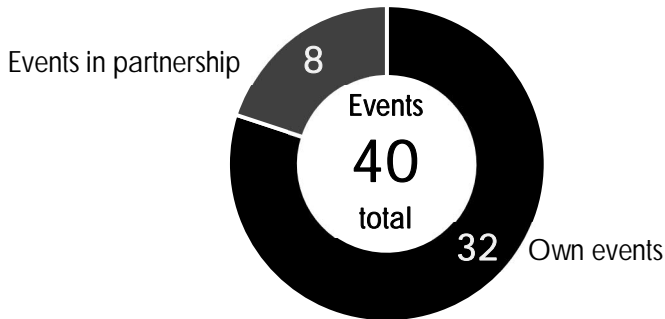
Connected to the overall communication work, was the launch of the LINXS YouTube channel where the recorded material and LINXS videos are posted and linked to the website.

The LINXS website had 18,694 visits in 2020, an increase of 32% compared with 2019. Among them, 14,682 were unique visitors (20% increase). The website had 44,794 page views, an increase of 17% compared to 2019. Most popular content in descending order were the Home page, the LINXS events, the Management page, the Educational page and the About page. Moreover, the LINXS LinkedIn page has been used to further promote all articles, newsletters and events, gaining increased number of followers (497 in 2020). It serves very well as a further communication tool to reach larger audiences and allows even more outreach through individual sharing/reposting.

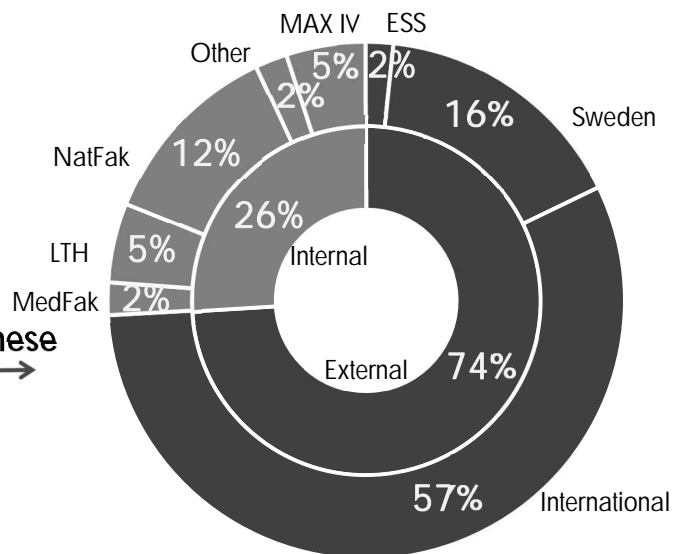
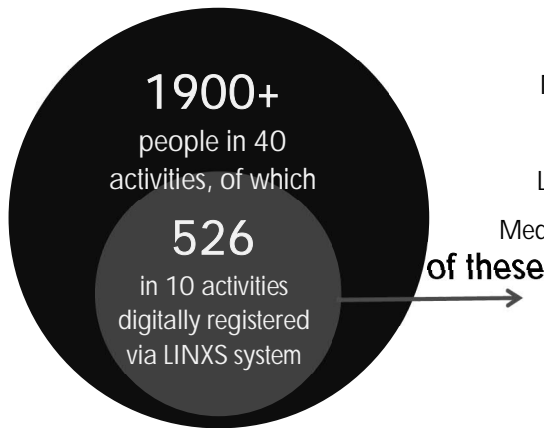
The new European Accessibility Act, enforced since September 2020, represents an important challenge for LINXS. The law obliges that digital material in the web is accessible to all, which means that subtitles should be included in all recorded material. Due to the high scientific vocabulary used, the automatic captioning that YouTube offers is not satisfactory. On the other hand, it is practically impossible for LINXS to provide budgetary resources for a captioning service. This creates an obstacle to the implementation of the LINXS educational mission in the future. The issue will be discussed with the LINXS board and possible solutions will be investigated.

LINXS in Numbers 2020

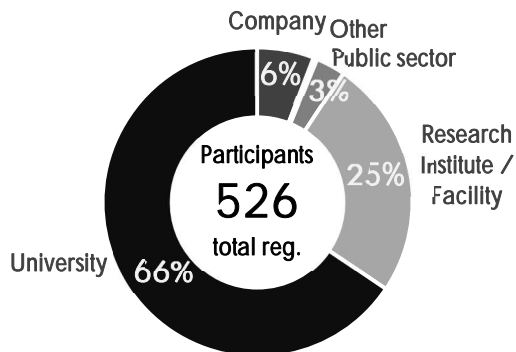
LINXS Activities and participation



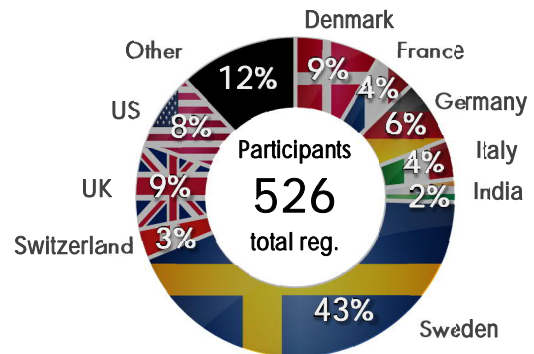
Participants



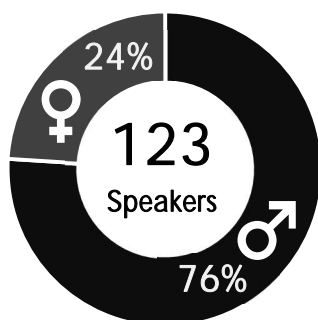
Organisational types



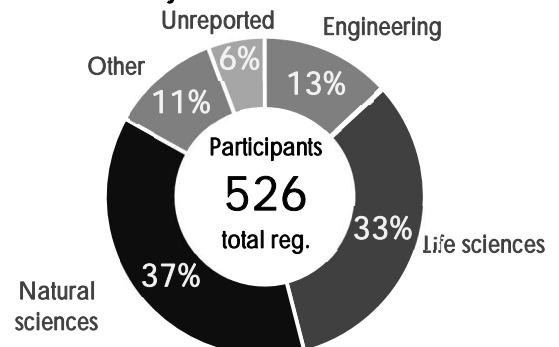
Country of origin



Keynote speakers gender balance

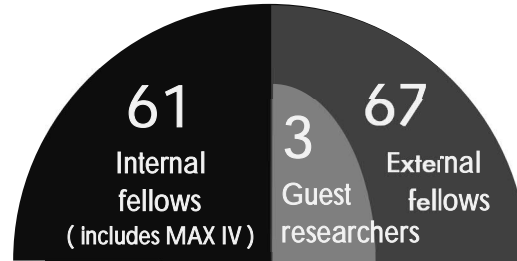


Main subject field



LINXS Community – fellows in 2020

131 LINXS fellows in 2020



LINXS Community - affiliations of LINXS fellows

48 organisations are involved in the LINXS core groups, working groups and visiting researcher programme.

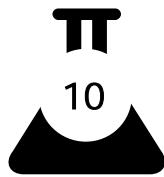
16 in Sweden (including Lund University)

32 international (AU:3, CH:1, DE:7, DK:3, ES:1, FI:1, FR:4, HR:1, IT:2, MX:1, NO:1, UK:3, USA:4)

these were,



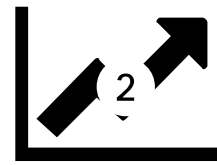
Universities



Research Institutes



Large Scale
Research Infrastructures



Companies

LINXS Community

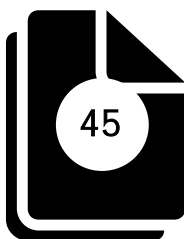


2 Core Partners (in addition to Lund University)

1 Member (Research Group)

9 Collaborations

Outcomes



Publications with
LINXS affiliation



Project applications

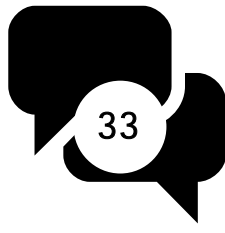


Project funded

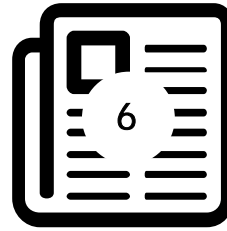
Communications



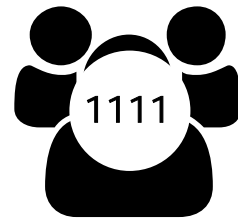
Outreach activities



Website news



Newsletters



Subscribers



497 followers in LinkedIn

Annual Financial Report 2020

Income	SEK
External funding	299,738
Partners contribution	9,000,000
Activities	2,995
Deferral 2020	-220,000
Membership fees	50,000
Total Income 2020	9,132,733
Expenditures	SEK
Activities	-351,158
Equipment	-129,117
Materials & consumables	-119,660
Premises	-1,209,093
Salaries	-4,899,232
Overhead	-2,082,838
Total Expenditures	-8,668,669
Annual Result	341,636

Partner contributions during 2020 was funding from the Lund University Central administration and the faculties of Science, Engineering and Medicine at Lund University. The faculty of Medicine also contributed in-kind with 50% of the salary of the LINXS vice-director (until July 2020), and with 20% of the salary of the co-director and 20% of the salary of the ISB theme leader (as of August 2020). External funding for the FORMAS project was deferred for project implementation in 2021. The final surplus will be moved to the budget of 2021 together with the accumulated agency capital from the previous years.

Detailed financial reporting is included in Annex 7.

Annex 1 – LINXS Themes and Working Groups in 2020

IMAGING

WG 1 - New Opportunities in Imaging with X-rays and Neutrons

WG 2 - GeoArCH: Geology, Archaeology and Cultural Heritage

WG 3 - X-ray and Neutron Imaging Applications in Soil Sciences

WG 4 - TBS: Tomography of Biological Samples

WG 5 - Food Science and Technology

WG 6 - QUANTIM: Image Quantification

DYNAMICS

WG 1 - Dynamics and Structure of Biological Macromolecules

- Research programme 1: Simulation, theory, and software development for anisotropic systems
- Research programme 2: Antibodies in Solution

WG 2 - Characterizing soft matter with X-ray Photon Correlation Spectroscopy (XPCS)

WG 3 - Dynamics and Structure of Membranes and their Constituents

- Research programme 1: Structure and dynamics utilizing the GISANS technique
- Research programme 2: Sample environment and data evaluation of biological membranes

INTEGRATIVE STRUCTURAL BIOLOGY (ISB)

WG 1 - Biocompute and Artificial Intelligence & Machine Learning

WG 2 - Time-Resolved Structural Biology - New possibilities in a time of new facilities

WG 3 - Amyloid: An integrative approach

WG 4 - Membrane Proteins - Structural resolution and homology modelling

WG 5 - Lund Integrative Structural Biology Centre Initiative

NEW MATERIALS

WG 1 - Functional Magnetic Materials

WG 2 - Charge Transfer Materials

WG 3 - Light Harvesting Processes

WG 4 - Catalysis

WG 5 - Nanostructures and Interfaces

Annex 2 – List of LINXS activities 2020

LINXS events and events organised in partnership:

1. LINXS Event - Mini-symposium by the Time-Resolved Structural Biology working group, January 24, 2020.
2. LINXS Event - LINXS Winter Science Day, February 12, 2020.
3. LINXS Partner Event - GeoArchaeology try-out workshop at the Elettra Sincrotrone in Trieste, Italy, February 13-14, 2020.
4. LINXS Event - Seminar with Prof. Christine Ziegler, Universität Regensburg, Germany, February 27, 2020.
5. LINXS Partner Event - GeoArchaeology try-out workshop II at Heinz Maier-Leinitz Zentrum of Technische Universität München, Germany, March 2-4, 2020.
6. LINXS Event - QUANTIM Hackathon: 3D visual annotations, March 12-13, 2020.
7. LINXS Partner Event: EUvsVirus - COVID19 hackathon, April 23-27, 2020.
8. LINXS Partner Event - PhD course on Grazing Incidence Scattering, May 18-20, 2020.
9. LINXS Event - User-friendly analysis of spectroscopy data with Quasar - multivariate statistics and machine learning, with Dr Ferenc Borondics, SOLEIL, France, May 22, 2020.
10. LINXS Event - Webinar "Let's dive into the atoms!" series - An introductory lecture on synchrotron-based X-rays, possible experiments at different beamlines, with Jens Uhlig – Synchrotron Experiments, Chemical Physics Lund University, Sweden, June 3, 2020.
11. LINXS Event - Webinar "Let's dive into the atoms!" series - How to exploit chemical sensitivity in X-ray spectroscopy, with Pieter Glatzel- HERFD-XAS and RIXS (ESRF), June 5, 2020.
12. LINXS Event - Webinar "Let's dive into the atoms!" series - Beyond the E0 state of nitrogenase: Spectroscopic studies of Intermediates in biological dinitrogen reduction, with Serena DeBeer - Max Planck Institute for Chemical Energy Conversion in Muelheim an der Ruhr, Germany, June 8, 2020.
13. LINXS Event - Northern Lights on Food Digital Workshop, June 10, 2020.
14. LINXS Event - Webinar "Let's dive into the atoms!" series - Science and data analysis at the European Spallation Source, with Thomas Holm Rod, ESS, June 15, 2020.
15. LINXS Event - Webinar "Let's dive into the atoms!" series - Small Angle Scattering Data Analysis with SasView, with Wojciech Potrzebowski, ESS, June 22, 2020.
16. LINXS Event - Webinar "Let's dive into the atoms!" series - EasyDiffraction: new easy-to-use software for analysis of diffraction data, with Andrew Sazonow, ESS, June 29, 2020.
17. LINXS Event - Northern Lights on Food Masterclass, September 1-3, 2020.
18. LINXS Partner Event - Large 3D and 4D image analysis workshop, September 8-11, 2020.
19. LINXS Partner Event - Workshop on the PETRA III Upgrade and Swedish Proposals, September 14, 2020.
20. LINXS Partner Event - GISANS Workshop, September 25, 2020. Satellite Meeting to ESS ILL User meeting, September 23-25, 2020.
21. LINXS Event - Webinar with Dr Christopher J. Garvey - Profiling flocculating and sedimenting particles with neutron dark field imaging, October 6, 2020.
22. LINXS Event - LINXS Virtual Town Hall and Discussion meeting, October 7, 2020.

23. LINXS Event - Webinar "Let's dive into the atoms!" series - Large scale facilities: neutrons for life science research, with Zoe Fischer, ESS, October 13, 2020.
24. LINXS Event - Webinar CoWork series - Introduction to coherent X-ray imaging, with Prof. Pablo Villanueva-Perez, Lund University, Sweden, October 16, 2020.
25. LINXS Event - Webinar CoWork series - CDI principles and algorithms with Dr Tomas Ekeberg, Uppsala University, Sweden, October 22, 2020.
26. LINXS Event - Webinar "Let's dive into the atoms!" series - Supra and Sub molecular investigation of pathology tissues by X-ray scanning microscopy, with Cinzia Giannini, National Research Council, Bari, Italy, October 26, 2020.
27. LINXS Event - Webinar CoWork series - An Introduction to hard X-ray forward ptychography and ptychographic computed tomography, with Maik Khant, MAX IV Laboratory, October 28, 2020
28. LINXS Event - Kick-off Symposium, New Materials for Energy and Sustainability, November 2, 2020.
29. LINXS Partner Event - BigScience@LU • Academic input in Big Science facilities, November 5, 2020.
30. LINXS Event - Webinar CoWork series - An Introduction to hard X-ray Coherent Diffractive Imaging in Bragg geometry and quantitative phase retrieval, with Dmitry Dzhigaev, Lund University, Sweden, November 6, 2020.
31. LINXS Event - Webinar CoWork series - Spatially resolving the structure of topological defects in ferroelectric nanocrystals, with Edwin B. Fohlung, Rensselaer Polytechnic Institute, USA, November 13, 2020.
32. LINXS Event - Webinar CoWork series - Three-dimensional coherent Bragg imaging of rotating nanoparticles, with Alex Björling, Max IV Laboratory, November 19, 2020.
33. LINXS Event - Time Resolved Structural Biology – Seeing the structure of motions, November 23-25, 2020.
34. LINXS Event - Webinar "Let's dive into the atoms!" series - XFEL science and introduction to beamline proposal writing, with Stefano Bonetti, Dept. of Physics, Stockholm University, Sweden, November 25, 2020.
35. LINXS Event - Webinar CoWork series - X-ray Bragg ptychography: principles, applications and perspectives for imaging crystalline properties in complex materials, with Virginie Chamard, Institute Fresnel Marseille, France, December 3, 2020.
36. LINXS Event - Webinar CoWork series - X-ray coherence-based imaging applied to 3D cellular biology, with Carla Cristina Pólo, Brazilian Synchrotron Light Laboratory (LNLS), Campinas, Brazil, December 8, 2020.
37. LINXS Event - Webinar "Let's dive into the atoms!" series - Introduction to table-top X-ray spectroscopy and Beamline proposal writing, with Jens Uhlig, Chemical Physics, Lund University, Sweden, December 9, 2020.
38. LINXS Event - Webinar CoWork series - New opportunities for materials science with coherent x-ray diffraction imaging with Stephan O Hruszkewycz, Advanced Photon Source, Argonne, USA, December 10, 2020.
39. LINXS Event - LINXS Antibodies working group Kick-off, December 2-4, 2020.
40. LINXS Event - LINXS Science Day, December 16, 2020.

LINXS Hosted events:

1. LINXS Hosted event - Nanosafety Workshop "Safe by Design & NFFA", January 9-10, 2020.

2. LINXS Hosted event - Simulation software workshop, July 10, 2020.
3. LINXS Hosted event - Max IV Industry group Strategy Day, September 15, 2020.
4. LINXS Hosted event - Software workshop, October 15, 2020.
5. LINXS Hosted event - ESS Science directorship Management meeting day, October 13, 2020.
6. LINXS Hosted event - ESS Management Team Strategy day, October 27, 2020.

LINXS Outreach activities:

1. LINXS event - Framtidens forntidsforskning: tekniska möjligheter öppnar upp för nya arkeologiska frågor, October 15, 2020.
2. LINXS presentation at 32nd MAX IV User Meeting, "LINXS support in widening the user base", Stephen Hall, LINXS director, September 28, 2020.
3. Breakfast @LINXS with LU Collaboration, January 8, 2020.
4. Breakfast @LINXS - LU Research Services, February 13, 2020.
5. Lecture at SciLifeLab entitled "How to become a Life Science researcher that uses synchrotron light and neutron applications", Dr Oxana Klementieva, September 2020.
6. PhD course "MAX IV/ESS-based imaging for medical and biomedical research", Dr Oxana Klementieva, October 12, 2020.

Annex 3 – List of publications with LINXS affiliation 2020

LINXS affiliated publications that have been communicated to LINXS. LINXS fellows are encouraged but not obliged to use the LINXS affiliation, or to acknowledge LINXS when credit is due.

1. **Structural Characterization of the Microbial Enzyme Urocanate Reductase Mediating Imidazole Propionate Production**
Raminta Venskutonytė, Ara Koh, Olof Stenström, Muhammad Tanweer Khan, Annika Lundqvist, Mikael Akke, Fredrik Bäckhed, Karin Lindkvist-Petersson
Nature Communications In press
2. **Highly viscoelastic films at the water/air interface: α -Cyclodextrin with anionic surfactants**
Alberto S. Luviano, Jorge Hernández-Pascacio, Daniel Ondo, Richard A. Campbell, Ángel Piñeiro, José Campos-Terán & Miguel Costas, 2020 Apr 1, In : Journal of Colloid and Interface Science. 565, p. 601-613 13 p.
3. **Design and use of model membranes to study biomolecular interactions using complementary surface-sensitive techniques**
Luke A. Clifton, Richard A. Campbell, Federica Sebastiani, José Campos-Terán, Juan F. Gonzalez-Martinez, Sebastian Björklund, Javier Sotres & Marité Cárdenas, 2020, In : Advances in Colloid and Interface Science. 277, 102118.
4. **Super-Resolution Infrared Imaging of Polymorphic Amyloid Aggregates Directly in Neurons**
Oxana Klementieva, Christophe Sandt, Isak Martinsson, Mustafa Kansiz, Gunnar K Gouras, Ferenc Borondics Adv Sci (Weinh). 2020 Feb 7;7(6):1903004. doi: 10.1002/advs.201903004. eCollection 2020 Mar.
5. **Structure dynamics of ApoA-I amyloidogenic variants in small HDL increase their ability to mediate cholesterol efflux**
Oktawia Nilsson, Mikaela Lindvall, Laura Obici, Simon Ekström, Jens O Lagerstedt, Rita Del Giudice. J Lipid Res. 2020 Nov 24;62:100004. doi: 10.1194/jlr.RA120000920
6. **Apolipoprotein A-I primes beta cells to increase glucose-stimulated insulin secretion**
Oktawia Nilsson, Rita Del Giudice, Mototsugu Nagao, Caitriona Grönberg, Lena Eliasson, Jens O Lagerstedt. Biochim Biophys Acta Mol Basis Dis. 2020 Mar 1;1866(3):165613. doi: 10.1016/j.bbadis.2019.165613. Epub 2019 Nov 22.
7. **Targeting GLUT1 in acute myeloid leukemia to overcome cytarabine resistance**
Hannah Åbacka, Jesper S Hansen, Peng Huang, Raminta Venskutonytė, Axel Hyrenius-Wittsten, Giulio Poli, Tiziano Tuccinardi, Carlotta Granchi, Filippo Minutolo, Anna K Hagström-Andersson, Karin Lindkvist-Petersson. Haematologica, 2020 Jun 18;haematol.2020.246843. doi: 10.3324/haematol.2020.246843. Online ahead of print.
8. **On the interaction of softwood hemicellulose with cellulose surfaces in relation to molecular structure and physicochemical properties of hemicellulose**
Naidjonoka, P., Arcos Hernandez, M., Pålsson, G. K., Heinrich, F., Stålbrand, H., Nylander, T.
2020, In: Soft Matter. 16, p. 7063-7076 14 p
9. **Anomalous Salt Dependence Reveals an Interplay of Attractive and Repulsive Electrostatic Interactions in α -synuclein Fibril Formation**

- Ricardo Gaspar, Mikael Lund, Emma Sparr, Sara Linse, 2020: Published online by Cambridge University Press: 06 August 2020
QRB Discovery, 1, E2. doi:10.1017/qrd.2020.7
10. **The Effects of Chain Length on the Structural Properties of Intrinsically Disordered Proteins in Concentrated Solutions**
Eric Fagerberg, Linda K. Månsson, Samuel Lenton, and Marie Skepö, 2020: Journal och Physical Chemistry. B 2020, 124, 52, 11843–11853
 11. **More than protection: the function of TiO₂ interlayers in hematite functionalized Si photoanodes**
Anurag Kawde, Alagappan Annamalai, Anita Sellstedt, Jens Uhlig, Thomas Wågberg, Pieter Glatzel and Johannes Messinger, 2020: Physical Chemistry Chemical Physics, 22, 28459-28467
 12. **Sub-trabecular strain evolution in human trabecular bone**
Mikael J. Turunen, Sophie Le Cann, Erika Tudisco, Goran Lovric, Alessandra Patera, Stephen A. Hall & Hanna Isaksson, 2020 dec 1, I : Scientific Reports. 10, 1, 13788.
 13. **Bone Damage Evolution Around Integrated Metal Screws Using X-Ray Tomography: In situ Pullout and Digital Volume Correlation**
Sophie Le Cann, Erika Tudisco, Magnus Tägil, Stephen A. Hall & Hanna Isaksson, 2020 aug 5, I : Frontiers in Bioengineering and Biotechnology. 8, 10 s., 934.
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Annex 4 – Visiting researcher programme report 2020

LINXS hosted three international guest researchers in 2020. Additional guest researchers were scheduled, but the outbreak of the Covid-19 pandemic prevented their visit to Lund.

Dr Stefano Mezzasalma, a soft matter theorist at the Ruđer Bošković Institute in Zagreb, was a guest researcher with the “Time-Resolved Structural Biology” working group in the ISB theme between January and April 2020. Stefano explored what happens in protein crystals on the time scale of vibrations. During his visit Stefano worked, in particular, on studying protein dynamics by exploring the protein response to radiation fields in the THz frequency domain. His work at LINXS was, in collaboration with a number of researchers including from University of Gothenburg and Linnæus University.

THz pump/X-ray probe experiments are not routinely performed on protein crystals, therefore the team had to estimate what happens with protein atoms in thermal equilibrium and in out-of-equilibrium conditions. Stefano’s contribution was also invaluable for the statistical analysis of time-resolved X-ray diffraction data. Stefano’s visit ended in April at the height of the pandemic, but, with the support of the LINXS staff, he was able to travel back to his home institute. The collaboration that came out of Stefano’s visit has continued and shifted to virtual space with regular online meetings. This kind of intense interaction between theorists and experimentalists is essential for driving blue-sky research where scientific consensus has not been reached.

Professor José Campos Terán from Universidad Autónoma Metropolitana - Cuajimalpa (UAM-C), Mexico, and Dr Chris Garvey, Australian Nuclear Science and Technology Organisation (ANSTO), Australia, were already guest researchers at LINXS since 2019, working with the “Dynamics and Structure of Membranes and their Constituents” working group. Their stays at LINXS ended in August and December 2020, respectively, but they both continue to be LINXS fellows and active members of the WG. The results of the visiting researcher program are already reflected in a number of publications (see Annex 3). It is noteworthy that Prof. Campos Terán and Dr Garvey produced 9 papers out of the total 45 papers with LINXS affiliation in 2020 and more are expected to appear in 2021. During 2020 the number of seminars were limited, but the visiting researchers contributed to several webinars, as lecturers or as very active participants. Prof. Hellweg, who was guest researcher in 2019, and Campos Terán continued and expanded a collaboration started at LINXS on responsive hybrid lipid and polymer surface; this, also involving Mr Jonas Runge, a student of Prof. Hellweg, who was Erasmus student in Lund. The beamtime granted at The Heinz Maier-Leibnitz Zentrum in Germany was postponed to 2021, when Prof. Campos Terán is expected to return. The collaboration that Prof. Campos Terán established with researchers at the departments of Chemical Engineering, Biotechnology and Biochemistry at Lund University is now continuing also with activities at Prof. Campos Terán’s home university in Mexico, Universidad Autónoma Metropolitana. Prof. Campos also develops sample environment for reflectometry measurements. Dr Garvey, has, apart from intensifying the collaboration with Malmö University, developed a method to determine the crystallinity of cellulose coatings on surfaces together with researchers at Physical Chemistry and Applied Biochemistry, Lund University. The collaboration also extended to studies of blood cells with cellulose surfaces. In addition, he started a collaboration with Applied microbiology, Lund University on the interfacial behaviour of a particular polymer excreted from microorganisms. Other examples of the researchers’ activities at LINXS included taking very active part in the GISANS program with a talk at the workshop on 26 September 2021.

Annex 5 – LINXS Webinar Series report 2020

“Let’s dive into the atoms!” LINXS Webinar Series: - An introduction to x-ray and neutron methods

This first LINXS Webinar series introduced x-ray and neutron science from a methods perspective. The aim was to create a fundamental understanding of how researchers can use x-rays and neutrons in their own research. It was open to researchers from all over the world and no in-depth knowledge of x-rays and neutrons methods was needed.

In total, the series attracted 680 registrations. More than 481 participants from all over the world attended live, an impressive participation rate (71%) and a significant increase in participation compared to physical seminars. Participants were from academia, industry, and other research organisations.

The first group of webinars took place in June 2020. Six experts (3 each on x-rays and neutrons) gave lectures on the various techniques used at large-scale facilities such as synchrotron and spallation sources. The goal of the webinar series was to provide educational insight and guide potential users about the large-scale facilities. The feedback received was encouraging; overall, around 78 % of participants found the lecture content/level to be perfect, while about 15% felt that they needed something in between, while the rest found the lectures to be too advance. Participants wanted to learn about the direct/physical aspect of using such facilities. For instance, they were curious to know what they can do at such facilities which is not possible in the regular labs. Similarly, enormous interest was seen for the lectures on data analysis software. Participants were enthusiastic about learning the software and how it can be used for their data interpretations. They also expressed an interest in learning how to write successful proposals to acquire beamtimes at large-scale facilities.

With this in mind, the second group of webinars in the fall covered the neutrons research in life sciences, and most importantly the XFEL science, and aimed to provide educational insight and guide potential users on the large-scale facilities and on how to write a compelling beamtime proposal. Two female and two male experts (1 on neutrons and 3 on x-rays) gave lectures on the various techniques used at large-scale facilities such as synchrotron and spallation sources. All the invited speakers shared their experience on writing a successful beamtime proposal, the prerequisites required to make a successful proposal, as well as tips on what reviewers seek when they read beamline proposals. As the webinars were made available on the website, the number of registered participants for the live webinar decreased, while the viewings of the recordings in the LINXS website significantly increased. Moreover, the feedback received was encouraging; overall, around 78 % of participants found the lecture content/level to be perfect, while about 15% felt that they needed something in between and the rest found the lectures to be too advance.

In general, the “Let’s Dive into the Atoms” series has been much appreciated for its practical aspects behind neutron and x-ray science, including information on how to run experiments and apply for beam-time. This focus fills an important gap in terms of bringing in new users to our facilities.

“CoWork” LINXS Webinar Series – Inversion of Coherent X-ray Data

The “CoWork” webinar series was dedicated to the exploitation of the coherence properties of x-rays for advanced materials characterization, with a special focus on inverse microscopy techniques, such as Coherent Diffraction Imaging (CDI), Ptychography and Holography.

As a positive externality of the pandemic, the series grew out of a cancelled Coherence Workshop originally planned for October 2020 and has blossomed into a strong forum for the discussion of coherence-based inverse microscopy techniques.

Lectures and tutorials, delivered by national and international experts and tailored for beginners, provided a basic understanding of existing approaches and an overview of their capabilities and limits. The final goal was to increase awareness about these methods and to create the basis for a larger user community that will exploit and develop them.

Target audience were all scientists interested in the exploitation of the coherence properties of the radiation produced at modern synchrotron sources, of which MAX IV is the first example in operation. With the final aim to increase the user community.

Nine webinars were organised in 2020 and more than 356 participants from all over the world registered, and attendance on average was 20 to 70 persons per webinar.

The Webinar series has managed to meet part of the scope of the "parent" workshop, that was "to increase awareness towards the capabilities offered by coherence-based x-ray techniques and create the basis for a larger user community that will exploit and develop them". The keynote lectures and the tutorials offered from national and international experts have succeeded in illustrating the capabilities a variety of Inverse microscopy approaches to newcomers, teaching basics data analysis with the most diffused inversion approaches and showing scientific results from scientists from different fields.

The success of the initiative can be measured by (i) the large number of people who have followed to multiple seminars, (ii) the steady increase of the number of participants, (from initial 40 to 174 subscribers today) including also an international community of experts in the techniques proposed; (iii) the participation to the Q&A sessions and the availability of up to 50% of the audience to continue further for an informal discussion; (iv) the increasing number of speakers (from 5 originally planned to 15 of today, of which 80% are invited and 20% are self-proposed). No refusal is counted as of today.

The large participation to this event might reflect an increased interest of the scientific community towards the exploitation of coherence properties of x-rays, in view of the many source upgrades planned at several facilities worldwide. But also, a need of researchers to keep in touch with other scientists, and their results, in absence of occasions to meet in person.

In this sense, this event has proved to meet the values of LINXS, to put people in contact. In a couple of occasions, during the "informal" discussion session, a proposition of collaboration has been proposed between two attendees. Which is certainly more than one could expect from a webinar!

Following the positive feedback from many attendees, CoWork continues in 2021 with a frequency of about 2 webinars per month and, upon request, a new time – 3:30pm CET, to facilitate the participation to people from USA. Along with scientific contributions on results, experimental and analysis methods and approaches, this 2021 edition will feature the presentation of Beamlines worldwide that provide coherent x-rays – and related set-ups and expertise – for materials research.

One direct outcome of this activity is the publication of the (recorded) webinars. These are available as educational material in the LINXS webpage and have already been accessed by many people. This will certainly continue with the continuation of this series in 2021.

Depending on the world pandemic, a physical workshop could be organised in Lund in Sept-Oct 2021, with the aim of fostering collaborations, and even creating a working group or future theme application within LINXS, centred on Coherent X-Rays. This could lead to various outcomes, including a contribution to the long-term Science Strategy of MAX IV, the formation of one or more collaborative teams that can further the development of coherence-based approaches (including setups at beamlines, analysis tools, etc.), the application to grants and the writing of common proposals.

Annex 6 – Reflections and voices from LINXS cases in 2020

IMAGING – MAKE A SMALL COMMUNITY LARGER – NEW LINXS WEBINAR SERIES ON COHERENT X-RAYS (November 5, 2020)

A new LINXS webinar series aims to make the community of researchers using techniques based on coherent x-rays larger and more diverse. It is organised under the Imaging theme.

– We want to encourage more researchers to explore these techniques and tease out how we can broaden the scope of advanced material characterisation, says organiser Gerardina Carbone, beamline scientist at MAX IV, and member of the working group: New opportunities in Imaging with x-rays and neutrons.

The webinar series focuses on the exploitation of the coherence properties of x-rays for advanced materials characterisation, with a special focus on inverse microscopy techniques, such as coherent diffraction imaging -CDI, ptychography and holography. These approaches can be used to analyse different types of materials, from biological materials and cells all the way to crystals, passing through diverse materials for applications such as cement, batteries, and catalytic nanostructures, to cite a few.

– An easy way to explain it, is that the use of coherent x-ray data establishes a clear mathematical relation between sample and diffracted data. This can be enforced within a "phasing" algorithm to recover a complete sample description only from the data, with no other assumptions.

The first three webinars in the series have already taken place. Gerardina Carbone says that the overall idea behind the initiative is to increase the community of researchers using coherent x-rays and bring in more discussion of how to expand its uses into new fields.

– Because of limited access to coherent x-ray sources in the past years, the community using coherence has been quite small up to now. At first, we wanted to organise a workshop, to allow people to meet and discuss in person, but because of the pandemic we had to settle on the webinar approach.

Another aim of the webinar series is to link researchers from various fields, including people that are experienced and people who are just curious to learn more about coherence, and to really focus on transfer of knowledge in an interactive way. Therefore, the webinar series also welcomes more open talks, where people bring ideas for topics that could be explored with coherence.

– Of course the webinar format can be quite challenging but we hope to develop ways to exchange ideas and encourage discussions. We aim for shorter contributions with a longer discussion on how to make the experiments. That is the important goal – to have these discussions.

Highlight practical aspects and limitations

The webinars will also have a strong focus on "how to make the experiments". Since the field is still developing, Gerardina Carbone emphasises that it is important to show, not just tell. One aspect is to discuss practical aspects such as writing beamtime proposals, and how to prepare samples so that researchers are prepared ahead of the experiments.

– Often it is not that complicated. The samples might need to be cut or placed on a tip to be firmly held or placed on a membrane. One just needs to keep this in mind before the measurements begin.

Another thing is to make sure to highlight who to contact in order to make an experiment, and what to ask them: what do you really need to know before you start?

– We want to help people who have never done this before. We hope that this type of approach will give a bit more practical information than just reading a scientific paper.

Early career researchers to the take lead

Many of the webinars will be presented by early career researchers as opposed to established experts. Gerardina Carbone explains that with more time to plan the schedule, she aimed to look beyond just contacting people who are already ahead in their research career.

– To really open the field, you also have to make the actual format more inclusive. You cannot always rotate around the same big names, and in fact many experts gladly pushed for their younger colleagues to take part.

More webinars to follow

Finally, Gerardina Carbone highlights that this series might be one of more to come. She sees a development where one could focus on other topics and perspectives related to the exploitation of coherent x-rays.

– This webinar is just the start, she concludes!

DYNAMICS – THE ‘ANTIBODIES IN SOLUTION’ RESEARCH PROGRAMME – AIMS TO PLUG A CRUCIAL RESEARCH GAP (December 19, 2020)

The Antibodies in Solution research programme at LINXS aims to increase the fundamental understanding of antibodies, and in time create simulation models and experimental tools that can test and predict antibody behaviour in solutions up to high concentrations.

Anna Stradner is a Professor at the Division of Physical Chemistry at Lund University, and leader of the research programme.

– Up to now, we have rather had a cook and look scenario based on past experience when formulating solutions with antibodies. We lack a fundamental understanding of how antibodies behave in solutions, and at higher concentrations, says founding Director of LINXS, Peter Schurtenberger, Professor at the Division of Physical Chemistry at Lund University.

Antibodies are specialised, Y-shaped proteins, that can protect the body against viruses, bacteria, and fungi. The antibody sticks to a protein called an antigen. The antibodies find and attach to the antigen and can make the immune system destroy the cells containing the antigen. Monoclonal antibodies are becoming of increasing interest to the pharmaceutical and medical industries for their potential to be used as disease treatments, including some types of cancer. Industrially produced antibodies are usually made from mouse proteins, a combination of human and mouse protein, and mouse protein attached to a human protein.

Expensive to produce and many unanswered research questions

Yet, many questions on how antibodies behave in solution, particularly at higher concentrations, remain to be solved. Another aspect is that antibodies are currently very expensive to produce. This has to do with the need of extensive preproduction efforts to ensure that the antibody can be produced in great quantities, and that it is stable, and not contaminated. The production also requires high-quality specialized technical equipment. This has severely hampered systematic fundamental studies by individual research groups.

It exists a clear need for a major collective effort in order to secure sufficient amounts of well-defined antibodies and perform a concerted research investigation that covers all relevant length and time scales needed to understand the physical properties of individual antibodies as well as those of concentrated solutions. At LINXS, a research programme on antibodies was thus created two years ago, in 2018, to tackle these problems. The research programme gathers 14 international research groups, with four groups from Lund University, as well as pharmaceutical companies and the American National Institute of Standards and Technology (NIST). In mid-December, they had a kick-off for all the members of the programme.

– We have been working together since 2018 but our main challenge has been to get hold of an appropriate set of antibodies to use for our experiments. Access to sufficient amounts of high

quality antibody material is the basic prerequisite for our programme. Now, finally, we are hoping to receive antibodies from NIST in 2021, says Anna Stradner, Professor at the Division of Physical Chemistry at Lund University, who is leading the programme.

Anna Stradner and Peter Schurtenberger explain that an overarching aim of the programme is to investigate the step between antibody production and drug development. Currently there is no coherent study of how antibodies behave on a fundamental level in solution at higher concentrations. For example, what happens to the antibodies when additives and chemicals are added, or when the pH-value or the storage temperature change?

– This type of research is very important in terms of understanding how to use antibodies, and in what concentrations. If you inject a medicine, you cannot administer too large volumes, meaning you have to go for relatively high antibody concentrations in order to provide a physiologically effective dose in one shot. Similarly, you do not want the solution to be too viscous since it can be difficult and painful to inject, says Peter Schurtenberger.

Study behaviour with different techniques

Once the programme receives the antibodies, the research groups will start to apply different complementary methods to investigate the behaviour of the antibodies under carefully predefined conditions and characterize them.

– Antibodies are very complex proteins. Using different techniques will therefore be key to understand their behavior on a fundamental level. We will use x-ray and neutron scattering techniques together with relevant complementary methods and advanced data analysis tools to get as broad a picture as possible, says Anna Stradner.

Ideal result for the research programme – from individual antibodies to model systems

When asked what they would like to see as the outcome of the research programme, Anna Stradner and Peter Schurtenberger emphasise two things: simulation models and tools.

– We want to be able to test individual antibody behaviour at an early stage of development, where only small amounts of the precious antibody are available. Can we predict how the antibody will behave in solution at higher concentrations based on what we have learned from the model systems that we have developed? says Anna Stradner.

More fundamental knowledge on antibody solution behaviour can in time revolutionize drug development and use of antibodies believe the researchers.

– What we are doing here is a fairly unique effort in terms of filling a research gap of broad societal interest. We are gathering theorists and experimentalists from across the world, to look into an area that is yet under researched, says Peter Schurtenberger.

LINXS has played a crucial part in making the work possible.

– The power of LINXS is to act as a good broker. It gave us a platform to gather researchers from different fields to work together on this project. This is a classic example of what an organisation such as LINXS can do for science, in terms of supporting this type of bottom-up initiative to grow, concludes Peter Schurtenberger.

ISB – REFLECTIONS FROM THE TIME RESOLVED STRUCTURAL BIOLOGY WORKING GROUP WORKSHOP IN NOVEMBER (December 18, 2020)

LINXS asked Martin Weik, member of the Time Resolved Structural Biology working group, and researcher at the Institut de Biologie Structurale in Grenoble, France, to share his experiences of organising and attending the three-day online workshop, Time Resolved Structural Biology – Seeing the Structure of Motions, in November.

– The workshop beautifully showcased the diversity of time-resolved methods and methodologies to study biological macromolecules at work: time-resolved x-ray scattering in solution and on crystals at synchrotrons and XFELs, time-resolved neutron spectroscopy, time-

resolved single-particle cryo electron microscopy, NMR, electron diffraction and molecular dynamics simulations.

– Even more importantly, it was fascinating for me to see how various experimental and computational approaches are being combined in unique ways to address biological questions, such conformational changes in a particular enzyme during catalysis or light-driven processes connecting photochemistry and -biology in biological macromolecules.

What areas can time resolved techniques and methods push in health and medicine?

– The developments of drugs is often based on seemingly static protein structures. Taking into account conformational plasticity of drug targets might aid drug design and multiply opportunities to eventually diversify medical treatments. A small but growing number of startup companies have recognised this and base their design approach on both structural and dynamical characteristics of drug targets.

What where the most interesting discussion points brought up at the workshop?

– In round table discussions, panel members and participants exchanged their ideas about how to create new methodological synergies to tackle outstanding problems and how to further integrate experimental and computational approaches. Lively debated were also the pros and cons of single particle versus ensemble methods.

What about your work excites you the most, as a researcher?

– I am fascinated by the complexity of structural dynamics that animate each of the 20 000 different types of proteins in our body in such a unique and specific way. The precision with which each of the molecular processes is tuned in a protein is amazing to me and I am most excited by the opportunities to study protein dynamics that are generated when we combine and integrate various experimental and computational approaches.

NEW MATERIALS – WORKING GROUP ON CATALYSIS AIMS TO DEEPEN THE UNDERSTANDING OF CHEMICAL PROCESSES (December 18, 2020)

A new working group at LINXS, under the theme New Materials, aims to gain a deeper understanding of catalysts at an atomic level, and help solve the mystery of how catalysts actually work.

– No one really knows all the intricate details of how catalysts work. To try to resolve that, we are studying the catalytic processes on an atomic scale, “live”, i.e. when the catalyst is active and working, to identify what is happening and why, says Sara Blomberg, assistant professor at the Department of Chemical Engineering at Lund University, and leader of the catalysis working group.

A catalyst is a substance that enables a chemical reaction to proceed at a faster rate than usual or under different conditions. Catalysts are used in almost every industrial process today, and help turn raw materials to products such as plastics, paint and clothing. However, catalysts are expensive to produce, since they are made out of precious metals.

– In our working group, we want to tackle current challenges with catalysts. Can we, by gaining more in-depth knowledge, identify ways to make catalysts more efficient? Or identify new materials, with good properties, to substitute the expensive metals? The goal is to make industrial processes more efficient overall.

Key to accelerate transition to a fossil free society

According to Sara Blomberg, their work can be of crucial interest to industries and researchers working to accelerate the transition to a fossil free society. One example of the importance of catalysts is in the hydrogen production from renewable sources, such as wind, solar, biomass or water. Hydrogen can then be used in fuel cells to produce electricity that can power cars,

buses and commercial buildings –without any emissions, making hydrogen into a sustainable fuel alternative.

– The processes for producing hydrogen from renewables, need to be developed and made more cost and energy efficient for sustainable sources to be more widely used. Here, new types of catalysts can play a major role, in helping industries switch to renewable sources.

– We hope to contribute with more detailed understanding and knowledge, and in that way help industries. To do that, the industry needs to be engaged and participate in the working group, which is something we aim to do in our group.

LINXS – a space for far-reaching and unconditional discussions

Sara Blomberg says one aspect that excites her about the new working group is the possibility for more far-reaching and unconditional discussions, with both researchers and industry. Since the theme duration is quite long, and open ended in its framing, it allows for broader perspectives to be brought to the table, than other type of research projects.

– Within the theme and this working group, we have a unique possibility to discuss overarching questions centred around ways to improve catalytic processes in general.

Another area Sara Blomberg is exploring within the LINXS theme is on how to transfer industrial conditions to neutron and x-rays facilities.

– I am interested in how to perform experiments at synchrotrons and neutron spallation sources that mimic industrial conditions. For example, we are aiming to follow reactions on an atomistic scale while the catalyst is at work, so-called operando measurements. Many catalytic reactions occur at harsh conditions that requires robust reactors and challenging sample environments.

The fact that time is limited at the facilities is another factor researchers need to take into consideration, as well as different technological conditions from facility to facility.

– I believe that knowledge on the vast possibilities that MAX IV and ESS can offer is of crucial interest to industry researchers and society as a whole. If we can perform experiments on various catalytic reactions using both neutrons and x-rays, we expect to gain a much deeper understanding of how the processes work on an atomic level.

– I'm looking forward to discussing with other researchers in the field! Networking and collaborations are important, and often an efficient way to solve problems and achieve new insights, she concludes.

Annex 7 – Financial reporting 2020

Income statement	Categories	Description	SEK
	Activities	Conference fee	2,995
	Activities Total		2,995
	Partners contribution	LTH-funding	2,000,000
		Medfak-funding*	1,000,000
		Natfak-funding	4,000,000
		LU Central-funding	2,000,000
	Partners contribution Total		9,000,000
	Deferral	Deferral Formas**	-220,000
	Deferral Total		-220,000
	External Funding	Formas	299,738
	External Funding Total		299,738
	Membership fees	Membership RISE	50,000
	Membership fees Total		50,000
Income Total			9,132,733
Expenditure	Activities	Conference cost	-39,744
		Hotel & housing	-169,331
		Representation external	-8,915
		Travel	-133,168
	Activities Total		-351,158
	Equipment	Computer/screen/electronics	-35,006
		Depreciation	-94,111
	Equipment Total		-129,117
	Materials & consumables	Office supply	-13,831
		Other	-37,753
		Print material	-16,165
		Services	-51,910
	Materials & consumables Total		-119,660
	Overhead	OH	-2,082,838
	Overhead Total		-2,082,838
	Premises	Cleaning	-95,352
		Premises rent	-1,113,741
	Premises Total		-1,209,093
	Salaries	Salaries	-4,899,232
	Salaries Total		-4,899,232
Expenditure Total			-8,791,097
Annual Result			341,636

* In addition, the Lund University faculty of Medicine contributed in-kind with 50% of the salary for the LINXS vice-director until August 2020, and thereafter with 20% of the salary of the co-director and of that of the ISB theme leader.

** Deferral of FORMAS project funding for implementation in 2021.