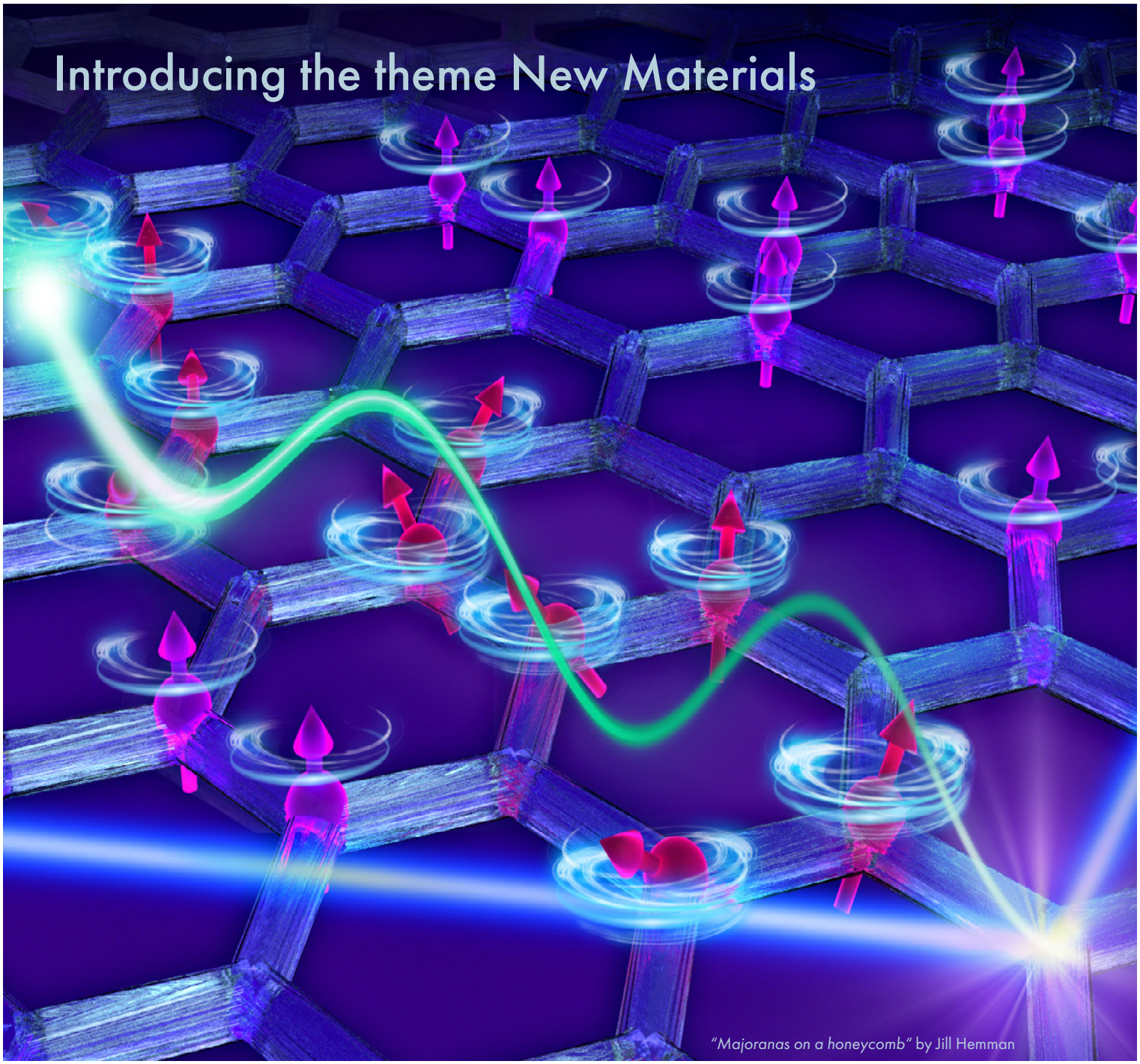
LINXS LUND INSTITUTE OF ADVANCED NEUTRON AND X-RAY SCIENCE

LINXS Annual Report 2020 Highlights



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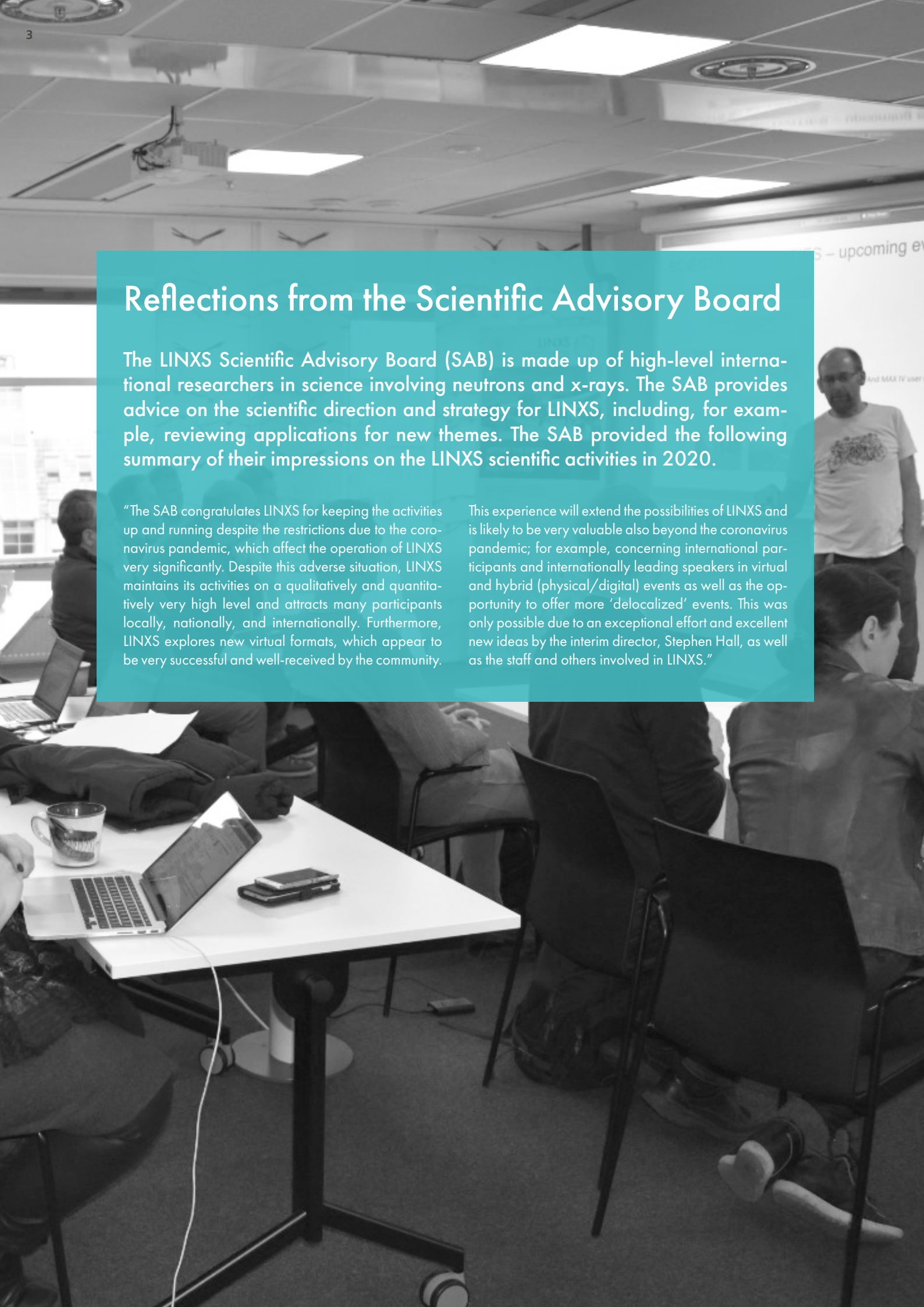


Reflections from the Scientific Advisory Board

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 coronavirus 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 coronavirus 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."

Director's word

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 funda-mental 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 comple-ment 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 webi-nar 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.

A milestone was reached when the RISE Large Scale Research Infrastructure (LSRI) team of technical experts located near or working closely with the new facilities in Lund joined the institute's membership programme as the first LINXS research group member. We welcome them to the LINXS community.

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 trans-disciplinary 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 Northern 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.

We would like to sincerely thank everyone that has contributed to the development of LINXS this year; our staff, board and SAB, LINXS fellows, visitors, as well as participants at our activities. We look forward to continue working with all of you to further develop LINXS in its aim to support and advance x-ray and neutron science.

Stephen Hall, LINXS Director

Svensk sammanfattning

Vi kommer att minnas 2020 som det år den globala coronaviruspandemin härjade. För LINXS var det också ett år av stora framsteg och utveckling av vår verksamhet, inte minst vad gäller de arbetsverktyg vi använder för att uppnå vårt uppdrag. Pandemin har lett till nya sätt att arbeta och interagera digitalt online. LINXS har anammat dessa nya arbetssätt i form av webbseminarier, zoommöten och hybridevenemang, där fysisk närvaro och digitalt deltagande blandas. Denna påtvingade verklighet har varit både utmanande, eftersom den begränsar fysiska möten och interaktion, och givande på så vis att den har drivit på vårt digitaliseringsarbete och gett upphov till nya perspektiv på LINXS roll och värde. Vi har framgångsrikt flyttat nästan alla våra aktiviteter och möten online. Vi har utvecklat god praxis för digitala aktiviteter, utrustat våra fysiska lokaler med digitala verktyg och ökat antalet aktiviteter totalt. Onlineaktiviteter lämpar sig väl för att skapa och dela innehåll via LINXS webbplats, och i många fall är det ett bra och hållbart format vad gäller att t.e.x minska resande i samband med aktiviteter. Därmed kan vi se att digitalisering och hybridaktiviteter fortsatt kommer att vara en viktig del av hur vi arbetar i framtiden – när det är lämpligt. Digitalisering gynnar även vårt arbete med att attrahera en bredare publik från olika tidszoner och länder. Emellertid är fysiska interaktioner en viktig hörnsten i LINXS verksamhet och vi ser fram emot att inom en snar framtid kunna ha fysiska möten här på LINXS.

Under hösten välkomnade vi ett nytt tema, "New Materials for energy and sustainability" och utlyste en ny temansökan för LINXS femte tema. Det nya temat kommer att undersöka ett antal banbrytande vetenskapliga frågor utifrån ett grundforskningsperspektiv men även koppla dem till globala utmaningar, samt verka för att utveckla forskarnätverk av röntgen- och neutronanvändare. Temat är ett utmärkt komplement till våra befintliga teman, med sitt fokus på hård materia, och utvidgar LINXS nätverk till att omfatta nya områden. I den andra änden av temacykeln skulle Imaging ha varit det första temat som avslutades 2020; aktiviteterna kommer dock att fortsätta fram till sommaren 2021 eftersom många av de planerade evenemangen behövde skjutas upp med anledning av coronapandemin.

En milstolpe uppnåddes när RISE Large Scale Research Infrastructure (LSRI) -teamet med tekniska experter som är placerade nära eller arbetar nära de nya anläggningarna i Lund gick med i institutets medlemsprogram som LINXS första forskargruppsmedlem. Vi välkomnar dem till LINXS-nätverket.

För att främja utvecklingen av LINXS pedagogiska uppdrag lanserade vi 2020 en kunskapsbank som är tillgänglig på vår webbplats och arbetet med vår wiki pågår som planerat. Våra två nya webinarieserier, "Let's Dive into the Atoms" och "CoWork", har belyst intresset för å ena sidan diskussioner på introduktionsinivå för nya användare av röntgen- och neutrontekniker och å andra sidan djuplodande utforskningar av ett nytt och banbrytande fält. Båda webinarieseriena attraherade deltagare från hela världen, något som vida överträffade våra förväntningar.

Under året kunde vi också konstatera att LINXS har spelat en viktig roll som inkubator av initiativ och tvärvetenskapliga forskarnnätverk utanför LINXS, på lokal, nationell och internationell nivå – framförallt via arbetsgruppernas verksamhet. Konkreta exempel är forskningsprogrammet "Antibodies in Solution" som har utvecklat starka internationella förbindelser, bland annat med NIST i USA, och nationella finansieringsinitiativ kring Northern Lights on Food inom arbetsgruppen Food Science and Technology. Dessutom har LINXS spelat en nyckelroll i utvecklingen av ett projekt för att ta fram ett svenskt strålrör vid ESS för GISANS. Dessa exempel, som visar hur LINXS aktiviteter kan utveckla nationella och internationella nätverk och bidra till att stötta långvariga externa projekt och samarbeten, är fantastiska att se, och nu överväger vi hur LINXS på bästa sätt kan fortsätta stödja deras utveckling så att de kan fortsätta växa utanför LINXS.

Vi vill uppriktigt tacka alla som har bidragit till utvecklingen av LINXS i år; vår personal, styrelse och vetenskapliga rådgivande nämnd, LINXS fellows, besökare såväl som deltagare på våra aktiviteter. Vi ser fram emot att fortsätta arbeta med er för att vidareutveckla LINXS och uppnå vårt mål att stödja och avancera röntgen- och neutronvetenskap.

Stephen Hall, LINXS Director

About LINXS

Established in 2017, LINXS is an advanced study institute whose mission is to advance science and education for all research activities that can benefit from the use of neutrons and x-rays. LINXS is dedicated to becoming a nucleus and think-tank for national and international scientific activities relating to research using neutrons and x-rays, both as a network and as a physical location providing an interaction hub in close proximity to the large-scale research facilities, MAX IV and ESS, in Lund, Sweden. LINXS brings together world-leading scientists for short-term focused research visits and creates international networks to be an international competence centre, research networking hub and focus-point for education of future generations of neutron and x-ray users.

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.

Attract
outstanding 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.

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.

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.

Focus Areas

Soft Matter
Liquids, colloids, polymers, foams, gels, granular materials, liquid crystals, and a number of biological materials. These materials share an important common feature in that predominant physical behaviors occur at an energy scale comparable with room temperature thermal energy.

Life Science
Fields of science that involve the scientific study of living organisms – such as microorganisms, plants, animals, and human beings – as well as related considerations. While biology and medicine remains the centerpiece of the life sciences, technological advances in molecular biology and biotechnology have led to a burgeoning of specializations and interdisciplinary fields.

Hard Matter
Materials science and solid-state physics, the study of rigid matter, or solids, through methods such as quantum mechanics, crystallography, electromagnetism, and metallurgy. It is the largest branch of condensed matter physics. Solid-state physics studies how the large-scale properties of solid materials result from their atomic-scale properties. Thus, solid-state physics forms a theoretical basis of materials science. It also has direct applications, for example in the technology of transistors and semiconductors and all solid-state nanoscience.

How LINXS works

Core group

A theme is governed by a core group composed of prominent external and local researchers, as one of the missions of LINXS is to bring external excellence in to work with local and national researchers. The core group leads the theme and defines the general direction for theme activities. It also discusses with the management how resources should be allocated for that theme. The core group can have management group individuals as members.

Working group

A theme unites working groups for specific activities. These range from conferences, workshops and schools to specific research programmes aided by LINXS fellows. Working groups are also formed via an Application procedure, though this is shorter and more quickly evaluated than that for themes.

Activities

Each working group has a palette of typical Activities to draw from in order to reach its defined goals. The activities can for instance be: Conferences, Research Programmes, Workshops, Hackathons, Sabbaticals, Schools, Seminars and Training & Outreach, but are not strictly limited to these. The nominal budget enables planning of the scientific scope in relation to the total LINXS budget.

1. THEME 2. CORE GROUPS 3. WORKING GROUPS 4. ACTIVITIES

Why join LINXS?

All researchers whose work can develop through the use of x-ray and neutron methods can benefit from being part of the LINXS community and participating in LINXS activities. LINXS is a place to explore new ideas and research questions, to discuss methods and approaches, as well as meet and collaborate with scientists from around the world and from different disciplines and organisations. There are many ways to interact with and join the LINXS community:

- Attend LINXS activities and participate in the scientific discussions.
- Join existing themes and working groups.
- Initiate new themes, working groups and research activities connected to the LINXS focus areas through the LINXS membership and partnership scheme.

As a member of a LINXS working group or theme, you get an opportunity to organise research activities connected to your area of interest, and to create new contacts and networks. LINXS offers administrative support to organise and run activities, disseminate information, and create a setting to highlight and discuss research developing and exploiting x-ray and neutron methods, with an aim to further research collaboration within national and international research networks.

LINXS welcomes researchers from all disciplines and organisations worldwide to join the LINXS community.

"What excites me about leading a working group at LINXS is the possibility for more far-reaching and unconditional discussions, with both researchers and industry. Since the theme duration is relativley long, and open ended in its framing, it allows for broader perspectives to be brought to the table, than other type of research projects."

Sara Blomberg, assistant professor at the Department of Chemical Engineering at Lund University, and leader of the catalysis working group.

LINXS themes and Working Groups 2020

Imaging (Sep 2017 – Dec 2020)

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 (Dec 2017 – May 2021)

WG 1 – Dynamics 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) (Nov 2018 – Dec 2021)

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 (Sep 2020 – Dec 2023)

WG 1 – Functional Magnetic Materials
WG 2 – Charge Transfer Materials
WG 3 – Light Harvesting Processes
WG 4 – Catalysis
WG 5 – Nanostructures and Interfaces

LINXS fellows in 2020 came from the following 48 organisations

Aarhus University, Denmark

Australian Nuclear Science and Technology Organisation (ANSTO), Australia

Australian Synchrotron, Australia

Bielefeld University, Germany

Centro de Física de Materiales (CSIC-UPV/EHU), Spain

Chalmers University of Technology, Sweden

CNRS, France

Deutsches Elektronen-Synchrotron DESY, Germany

Elettra – Sincrotrone Trieste SCpA, Italy

European Molecular Biology Laboratory (EMBL) Hamburg, Germany

European Spallation Source ESS AB, Sweden

Forschungszentrum Juelich GmbH, Germany

Fritz Haber Institute Berlin, Germany

Georgetown University, USA

Inria / CNRS, France

Institut de Biologie Structurale – Grenoble, France

Institut Laue Langevin (ILL), France

ISIS Facility, STFC, United Kingdom

Johnson Matthey Formox AB, Sweden

Karlstad University, Sweden

Karolinska Institutet, Sweden

KTH Royal Institute of Technology, Sweden

La Trobe University, Australia

Linköping University, Sweden

Linnaeus University, Sweden

Lund University, Sweden

Malmö University, Sweden

MAX IV, Sweden

Northwestern University, USA

Paul Scherrer Institut (PSI), Switzerland

Rensselaer Polytechnic University, USA

Research institutes of Sweden (RISE), Sweden

Ruđer Bošković Institute, Croatia

Sense Unlimited, Denmark

Stockholm University, Sweden

Swedish University of Agricultural Sciences (SLU), Sweden

Tampere University, Finland

Technical University Munich (TUM), Germany

Technical University of Denmark (DTU), Denmark

The "Abdus Salam" Int. Centre for Theoretical Physics, Italy

Universidad Autónoma Metropolitana – Cuajimalpa (UAM-C), Mexico

Universität Regensburg, Germany

University of Bari, Italy

University of Copenhagen, Denmark

University of Florida, USA

University of Gothenburg, Sweden

University of Nottingham, United Kingdom

Uppsala University, Sweden

Imaging theme

The Imaging theme had a strong programme for the year and got off to a good start with two "try-out workshops" in the GeoArCH working group. These workshops were caried out in collaboration with the Elettra Sincrotrone (Trieste, Italy) and the Heinz Maier-Leinitz Zentrum (Technische Universität München, Germany) and enabled researchers to get direct hands-on experience at large-scale facilities imaging their own samples.

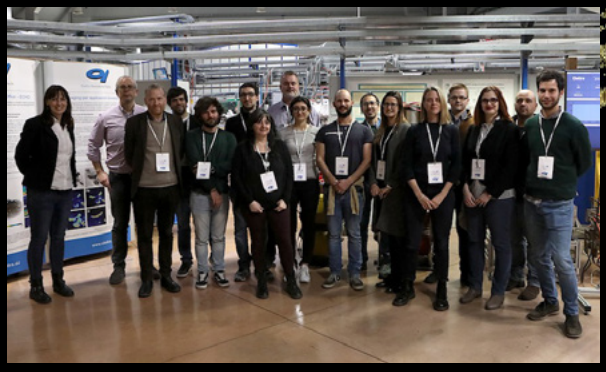
Unfortunately, the closure of Europe due to the coronavirus pandemic hit many events. First was the 3rd hackathon under the QUANTIM working group. Only about 6 of the 30 registered participants could be present in person. However, we were able to arrange that the experts gave their tutorials remotely in LINXS's first (unplanned) hybrid event. Further hackathons have been postponed until physical meetings are possible. The 2nd LINXS/SWEDNESS neutron image course also had to be postponed until 2021. The ambitious programmes of the Soil Science working group, as well as those of the TBS: Tomography of Biological Samples working group (including workshops around Sweden) were cancelled, but certain aspects will hopefully still be realised in 2021.

In addition to the hackathon, the QUANTIM working group partnered with DTU on the "Large 3D and 4D image analysis workshop" online (that was part of a series of workshops in the framework of the "Mummering" EU ITN network).

The Food Science and Technology working group quickly adjusted to the "new normal" and held a "Northern Lights on Food" digital workshop in June. Online meetings also enabled national (Swedish) food science and advanced technology experts, from both academia and industry, to come together 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. Fellows in the working group were also successful in getting funding from the Lindqvist Stiftelse for a new research project, connected to LINXS on "Dietary regulation of Gut and Blood Brain Barrier function".

The improved situation over the summer enabled the Food working group to go ahead with the planned Northern Lights on Food "Masterclass", a first (planned) 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.

The Masterclass on Food organised by the Northern Lights on Food of the Food Science and Technology working group.



Try-out workshop at the Elettra Sinctrotrone in Italy organised by the GeoArch: Geology, Archeology and Cultural Heritage working group.

A clear theme highlight of the year and a positive result of the coronavirus 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. 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.

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.

Make a small community larger – new LINXS webinar series on coherent x-rays

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 theme

The LINXS Dynamics theme progressed very well in 2020 and focus has been on the working group research activities within their research programmes. 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.

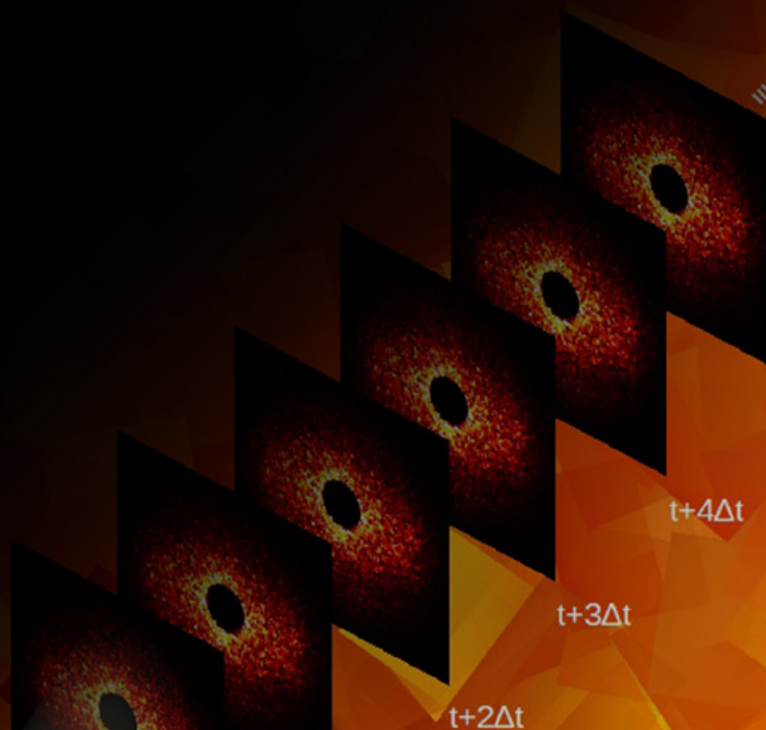
The Dynamics and Structure of Biological Macromolecules working group, include two research programmes. The Simulation, Theory and Software Development for Anisotropic Systems expanded its computational toolbox for predicting scattering functions from computer simulations and used this in a comparative experimental (SAXS) and theoretical study to understand the solution behaviour of enzymes. Two new projects 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. 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".

A milestone in the Antibodies in Solution research programme 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 for all the members of the programme could finally take place in December.

The Characterizing soft matter with X-ray Photon Correlation Spectroscopy (XPCS) working group helped initial feasibility measurements in October 2020 during measurements of the coherent flux at CoSAXS and MAX IV. In addition, a proposal for an expert commissioning experiment on CoSAXS was accepted, as well as a Röntgen-Ångström Cluster grant proposal, with Peter Schurtenberger as the PI for the Swedish partners, starting in 2020.

The Dynamics and Structure of Membranes and their Constituents working group also include two research progammes. The Structure and Dynamics Utilizing the GISANS Technique research programme intensified its community building during 2020. A key activity has been a virtual workshop at LINXS, with 124 registered participants. 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.

The Sample Environment and Data Evaluation of Biological Membranes research programme has been successful in attracting scientists for research visits to contribute to the science of the programme, 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.



The 'Antibodies in Solution' research programme – aims to plug a crucial research gap

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.

– 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 specialised 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, 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.

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, concludes Peter Schurtenberger.

Integrative Structural Biology (ISB) theme

2020 was a year of many positive developments for the Integrative Structural Biology theme, despite the big showstopper of the coronavirus 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. Despite the pandemic, ISB held a number of the planned events during the year. 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 stay in January, the working group organised 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.

The main activity of the Time-Resolved Structural Biology working group during 2020 was a digital workshop in May. The three-day workshop had 18 speakers, six posters, a panel discussion and around 170 registered participants. The event provided a good overview of the subject and allowed the participants to learn about methods they were not familiar with.

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. 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.

The strong programme of the Amyloid: an integrative approach working group was, obviously, curtailed, but the group was determined to progress and organised a successful online workshop in May focused on "User-friendly analysis of spectroscopy data with Quasar – multivariate statistics and machine learning". The workshops resulted in a new collaboration between the French Soleil light source and the Lund University Physics department. A meeting aiming to highlight and promote the application of SAXS and SANS for the characterization of amyloid systems is planned for 2021. Members of the amyloid group have also been involved in outreach activities, delivering seminars and teaching.

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. Several joint activities were initiated, including a joint online seminar series. Another joint activity involved two local coronavirus 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. 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.

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 Brunnshög, between MAXIV and ESS, and to help catalyse the discussion and development of these ideas.

Professor Karin Lindkvist active at Medical Structural Biology at Lund University is new core group leader of the Integrative Structural Biology theme.

Reflections from the time resolved structural biology working group workshop in November

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 stimulations.

– 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.

Participants at the online workshop, Time Resolved Structural Biology – Seeing the Structure of Motions, in November.

New Materials theme

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 characterisation 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.

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.

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.

The Functional Magnetic Materials working group held a first network meeting in December and will continue on a monthly basis next year. The first activity will be a workshop on micromagnetic simulations and their use in analysing scattering data planned for late March/early April 2021. The Charge Transfer Materials working group and the Light Harvesting Processes working group have struck up a collaboration and have set up a weekly open LINXS meeting, running since early December. So far, joint beamtime proposals have been discussed. The Light Harvesting Processes working group has also been working to prepare an EXAFS workshop 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.

The Catalysis working group, meanwhile, had a kick-off meeting in December to introduce the members of the working group to each other. So far, two LINXS seminars have been planned for spring 2021. Finally, the Nanostructures and Interfaces working group is waiting to develop its activities 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.

Elizabeth Blackburn, Professor in Physics at the Division of Synchrotron Radiation Research at Lund University is theme leader of the New Materials theme.

"*Neon Nano Art Micrograph*", by Yana Sychikova and Serhii Kovachov

Working group on catalysis aims to deepen the understanding of chemical processes

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 centered 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 discuss with other researchers in the field! Networking and collaborations is important, and often an efficient way to solve problems and achieve new insights, she concludes.

LINXS activities in 2020

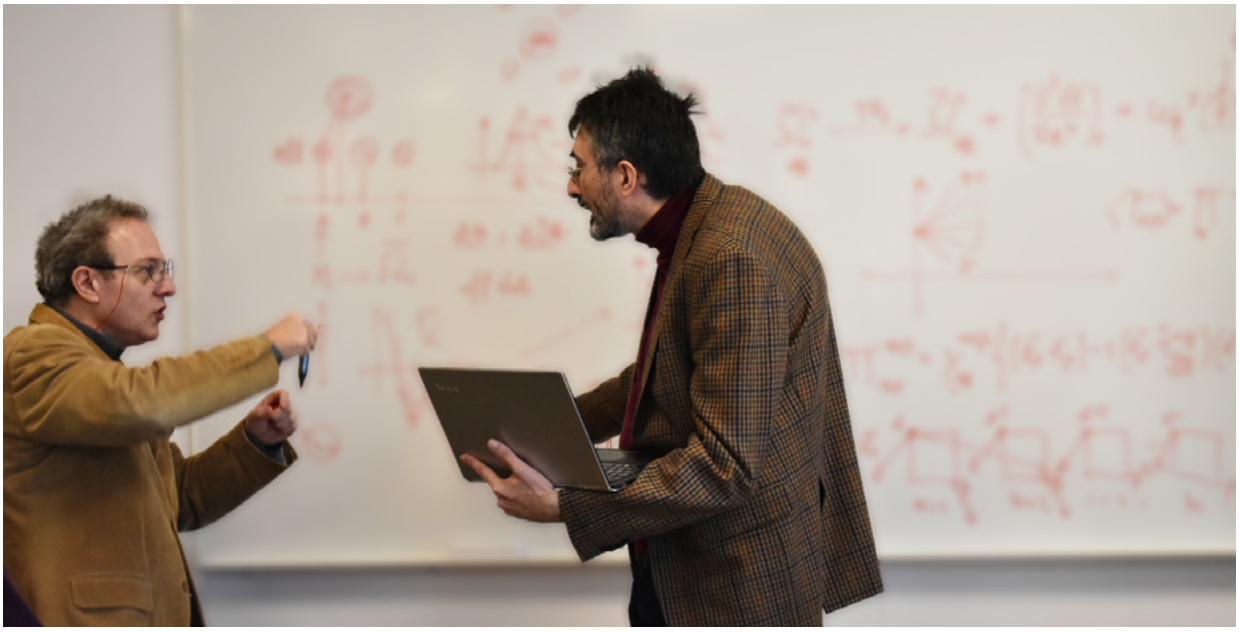
LINXS events and events organised in partnership

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.

ESS management team meeting hosted in October 2020 at LINXS.

31. LINXS Event – Webinar CoWork series – Spatially resolving the structure of topological defects in ferroelectric nanocrystals, with Edwin B. Fohtung, 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 visiting researcher programme



Dr Stefano Mezzasalma, a soft matter theorist at the Ruđer Bošković Institute in Zagreb, together with Gergely Katona from Gothenburg University pictured at LINXS Winter Science Day in 2020.

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 by attracting three prominent researchers in 2020. 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. 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.

The guest researchers shared their expertise and knowledge with the LINXS network and supported the development of international and regional networks and scientific collaborations. The success and impact of the visiting researcher programme is reflected in a number of research publications with LINXS affiliation, as well as active participation in LINXS activities and initiatives such as the GISANS programme.

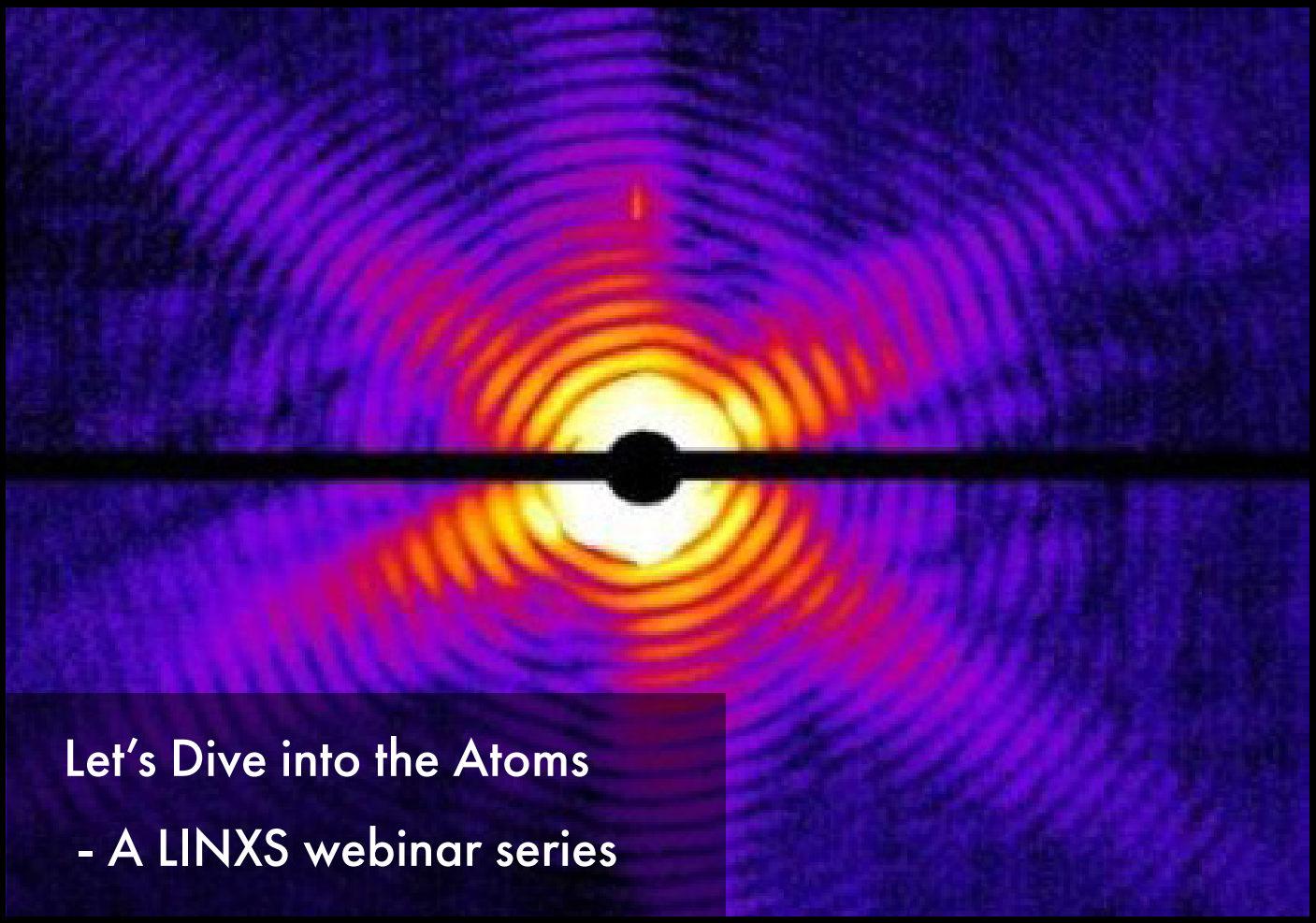
LINXS webinar series and educational resources

A major development for LINXS in 2020 was the launch of two new webinar series.

Let's dive into the atoms! The aim of this webinar series 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. The 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 facilities such as MAX IV and ESS.

The **CoWork** webinar 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. It aims to gather researchers interested in the field of CDI, and has succeed in attracting and growing an international community of experts. The final goal is to increase awareness about CDI methods and to create the basis for a larger user community that will exploit and develop them.

Both webinar series have been very well received, and have attracted participants from all over the world. Webinars are recorded and made available on the LINXS website where an "educational materials" section was developed contributing to the LINXS mission to educate on x-rays and neutrons, as well as increasing the LINXS digital presence, international outreach and visibility.


Let's Dive into the Atoms
- A LINXS webinar series


Inversion of Coherent x-ray data
- the CoWork webinar series

Timeline

2020
First LINXS member RISE – LSRI
Regular Call for themes
Renewal of SAB Mandate
New Theme Starting

2021
Regular Call for themes
New Theme Starting
Conclusion of two LINXS themes
Instalment of new Director

2022
Regular Call for themes
New Theme Starting
Conclusion of LINXS themes

2023
Long term funding secured
Regular Call for themes
New Theme Starting
Conclusion of LINXS themes
LINXS partnership offering updated

2024
Permanent location to SVS
Regular Call for themes
New Theme Starting
Conclusion of LINXS themes

2025
Steady state operations achieved at 16M/24M a year.

"LINXS is becoming established as a world leading advanced studies institute and we are now working on the next stage of our evolution, to be physically positioned at the centre of the activity at Science Village Scandinavia (SVS), close to MAX IV and ESS, as soon as the first buildings are completed, hopefully by 2024. We believe that being placed in close vicinity to MAX IV, ESS and future planned research laboratories, will enable LINXS to enhance its role as an interaction hub for researchers from all over the world to catalyse ground-breaking transdisciplinary research using x-ray and neutrons."

Stephen Hall, LINXS Director

ESS

Location 2024+

Science Village

MAX IV

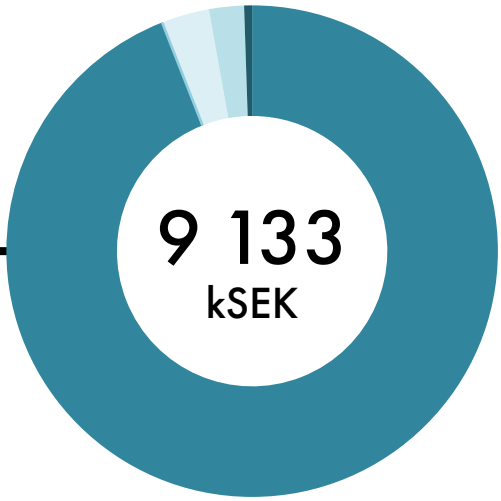
Location 2018 – 2024

Tramline

Background image by Lund City Council / Arrow

Finances 2020

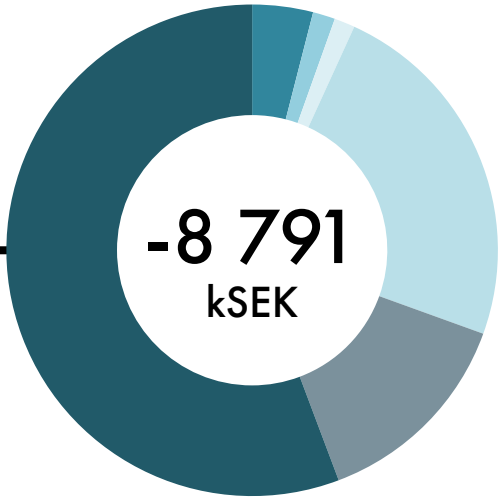
INCOME



Detailed income (kSEK)

Partners contribution [I]	9 000
Activities fees	3
Project External funding	300
External funding deferral 2021	-220
Membership fees	50

EXPENDITURE



Expenditure (kSEK)

Activities costs [II]	-351
Salaries [III]	-4 899
Premises [IV]	-1 209
Equipment [V]	-129
Materials & consumables [VI]	-120
Overhead	-2 083

I. Current partner is Lund university and contributions are from the Central administration, the Faculty of Science, Faculty of Engineering and Faculty of Medicine.

II. Activities mainly includes costs for the organisation of LINXS events, accommodation, travelling and outreach.

III. Salaries include staff, management and emoluments.

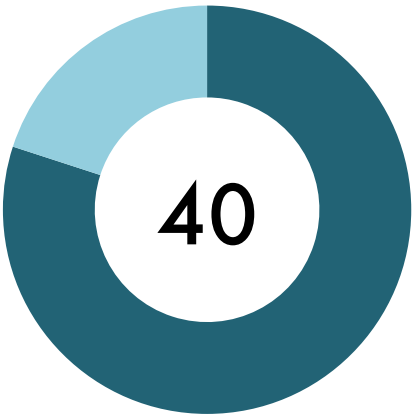
IV. Premises include costs for rental, internet connection and cleaning services.

V. Equipment mainly includes costs and depreciation for computers, equipment for the operation of scientific activities and furniture.

VI. Materials and consumables mainly include office supplies and printing equipment.

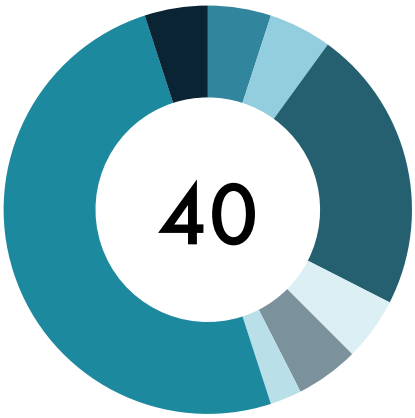
Statistics 2020

LINXS Activities



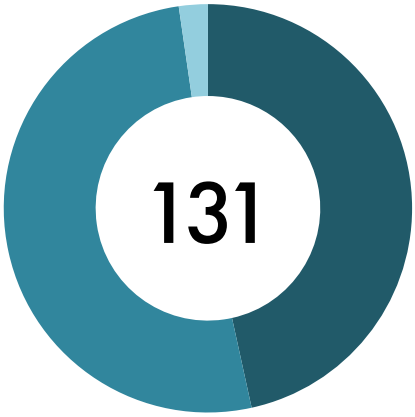
- LINXS Events 32
- Events in partnership 8

Type of Activities



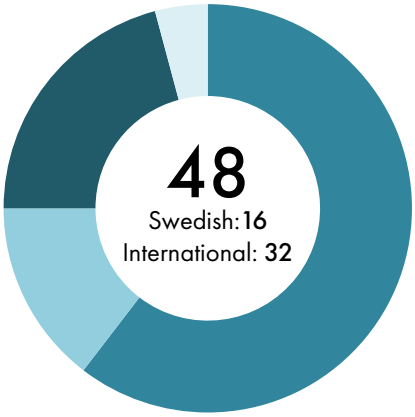
- Symposiums 2
- Conferences 2
- Workshops 9
- Hackathons 2
- Courses 2
- Seminar 1
- Webinars 20
- Try-out visits 2

LINXS Fellows



- Internal/Partner organisations 61
- External 67
- Guest researchers ... 3

Organisations involved in LINXS core and working groups and visiting researcher programme



- Universities 29
- Large Scale Infrastructures 7
- Research Institutes 10
- Companies 2

Communication & outreach

1111 Subscribers to the LINXS newsletter

6 newsletters

497 followers at Linkedin

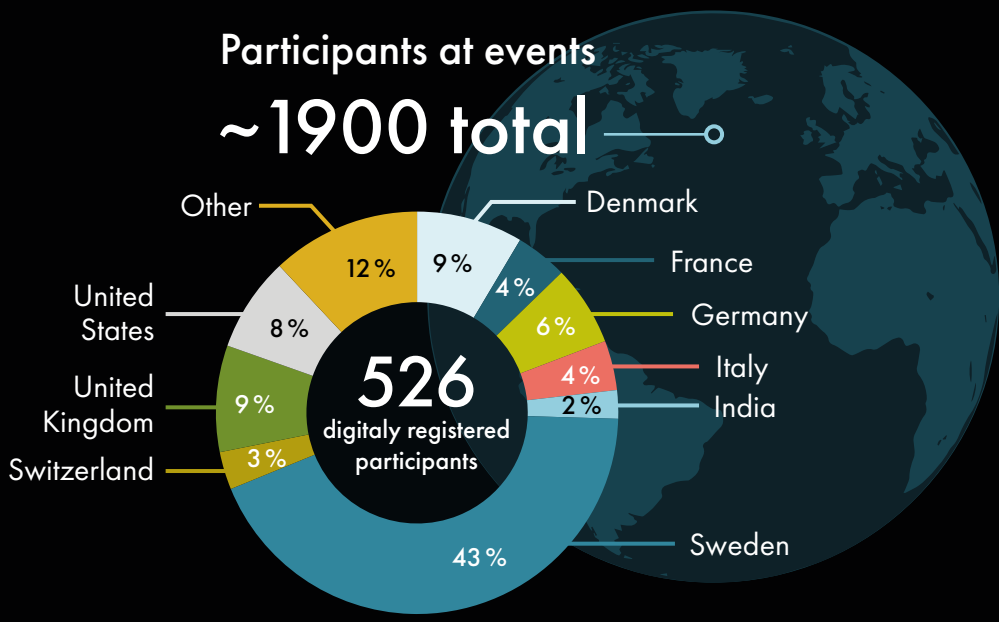
Keynote speakers

123 total

♀29 ♂94

Participants at events

~1900 total



Organisation

LINXS Board

Board members with LINXS staff in November 2020.

Sindra Petersson Årsköld
European Spallation Source ERIC

Hanna Sjö
Science Student Union (LUNA), Lund University

Marjolein Thunnissen
MAX IV

Marianne Sommarin
Umeå University

Sven Lidin, Board Chair
Faculty of Science, Lund University

Erik Swietlicki
Faculty of Engineering (LTH), Lund University

Kajsa M. Paulsson
Faculty of Medicine, Lund University

Ulf Olsson
Faculty of Science, Lund University

Veronica Lattanzi
The Science Doctoral Student Council (NDR), Lund University

LINXS Management

Stephen Hall
LINXS Director and Core Group leader for the Imaging theme. Associate professor at the Dept. of Solid Mechanics at the Faculty of Engineering (LTH), where he is also in charge of the 4D-Imaging Lab x-ray tomography facility. Came to Sweden in 2011 after moving from Laboratoire 3R in Grenoble, France.

Oxana Klementieva
LINXS Co-Director and Working group leader for the ISB WG 3, Amyloid: An Integrative Approach. Since June 2018 she is an associate senior lecturer and the head of the Medical Microspectroscopy research group at the Medical Faculty at Lund University. Her goal is to establish a cutting-edge research team and using multi-dimensional research strategy and synchrotron-based microspectroscopic techniques work on understanding the nature of neurodegenerative disorders.

Marie Skepö
LINXS Vice-Director. Professor and Deputy Head of Division of Theoretical Chemistry at Lund University. Research interests include: intrinsically disordered proteins (IDPs) – self assembly and interfacial behaviour, structural and thermodynamical properties of clay, polyacrylic acid in hard water, intermolecular interactions of PEG solutions, melting of DNA, and the adhesion of fermented milk to packaging surfaces.

Anna Ntinidou
Anna Ntinidou is the head of administration responsible for operations and supporting future development. She is a senior project manager with long experience in implementing EU and nationally funded transdisciplinary projects. She is a civil engineer with a Masters in innovation, speaks four languages and has lived and worked in four European countries.

Scientific Advisory Board

Prof. Lise Arleth
SAB Chair – Area Life Sciences
Lise is a Professor and Head of the The Structural Biophysics Group at the Niels Bohr Institute, Faculty of Science, Denmark. Her main research topics include biophysics and physical chemistry with the main focus on structural investigations of macromolecules and their aggregates in solution.

Prof. Christiane Alba-Simionesco
SAB Member – Area Hard Matter
Christiane is the Head of the Laboratoire Léon Brillouin (LLB). Her research focuses on the thermodynamics, structure and dynamics of molecular condensed phases, liquid, solid and amorphous. She is a leading expert in several experimental techniques and methods bridging the gap between time and space scales, improving theoretical concepts and analytical modelling.

Prof. Stefan U. Egelhaaf
SAB Member – Area Soft Matter
Stefan is a full professor (Soft Condensed Matter Physics) at the Heinrich-Heine University Düsseldorf. Interested in the physics of soft condensed matter, in particular its non-equilibrium behaviour. His research focuses on the behaviour of colloidal systems under external fields, their relaxation to equilibrium, and metastable states.

Prof. Daan Frenkel
SAB Member – Area Soft Matter
Daan is a former Head of the Department of Chemistry at Cambridge University and the current Director of Research. The Frenkel group focuses on the numerical exploration of routes to design novel, self-assembling structures and materials. In particular, the group is interested in the possibilities that bio-molecular recognition and motor action offer to create complex, nano-structured materials.

Prof. Christian Rüegg
SAB Member – Area Hard Matter
Christian is the Director of the Paul Scherrer Institute and Professor of physics at the University of Geneva, ETH Zurich and EPF Lausanne. His research projects focus on systematic studies of strongly correlated quantum phenomena in low-dimensional spin systems, single-molecule and frustrated magnets, and novel emergent materials.

Prof. Marco Stampanoni
SAB Member – Area Life Sciences
Marco is the Head of the SLS Tomography group and Professor for x-ray imaging at the ETH Zürich. With his team, he is working on novel X-ray based instruments and methods for non-invasive investigations of samples at various length scales, ranging from single cells up to humans. Research areas encompass a host of X-ray based imaging techniques for biosystems and clinical applications.

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