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LINXS LUND INSTITUTE OF ADVANCED
NEUTRON AND X-RAY SCIENCE

LINXS Annual Report 2021

Executive Summary and reflections from the LINXS Director

The continuation of the global pandemic meant that 2021 was again a year of mostly online activities. Nevertheless, we are very proud of the LINXS progress.

In the year the new theme “Integrative Pharmacology and Drug Discovery” was approved, focusing on pharmacology, going from structure-based drug design of both small molecules and macromolecular drugs to their interplay with tissue and its formulation, and macromolecular drugs such as antibodies. The initial 3 working groups active in the theme will explore the structure-function relationship of human drug target proteins and tissue both in vitro, ex vivo, and in vivo, utilizing X-rays and neutrons. The direction and topic of the Theme was marked as a priority of the Scientific Advisory Board and has turned out to be very timely in the face of the pandemic, with the CSO of Pfizer part of the Core Group.

As the statistics show, the activities of LINXS were predominantly hybrid and online because of the continuing pandemic, and due to the shift in LINXS’s strategy for achieving impact in the face of it. We were very pleased to host several schools, and continuation of the very successful Webinar series “Co-Work” dedicated to the exploitation of the coherence properties of X-rays, as well as “Science at large scale research facilities” introducing the latest capabilities, scientific breakthroughs, and developments at large scale research facilities globally.

We are seeing positive outcomes wider national collaborations as evidenced through national funding received by consortia connected to the Northern Lights on Food Theme, as well as the GISANS initiative, which came out of the Dynamics Theme.

A welcome side effect of the pandemic has also been an accumulation of educational material, as LINXS undertakes to preserve talks and presentations and to act as a structured repository for such information. This repository grew significantly during the year to 120+ items - and is still growing rapidly. Going forward, LINXS will work to further improve accessibility and expand this information as a part of strategic efforts in providing educational tools to the research community.

Finally, on the 1st of December 2021 the new LINXS Director Trevor Forsyth started his position. This marked the end of a 3-year strategic recruitment effort, unique in the history of the university, where two successive university leaderships and the faculties of Medicine, Science and Engineering, have all been instrumental in providing the basis. We are deeply grateful to all those involved for their unwavering vision and support.

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 2021.

The SAB thanks the outgoing director Stephen Hall (as well as the LINXS staff and others involved in LINXS) for all the effort during these taxing times. Despite the restrictions due to the COVID-19 pandemic, the LINXS activities remained on a qualitatively and quantitatively very high level and were successfully extended to new (previously not planned) directions, and in particular: different online formats, which we expect to be very valuable also after the pandemic. The SAB extends a warm welcome to the new director Trevor Forsyth and wishes him success with the further development of LINXS.

LINXS scientific achievements and impact

In 2021 there were three Themes active, and 2 in the process of concluding as planned. The recent theme "Northern Lights on Food" was ramping up its activities with 5 working groups starting up in the period, and "New Materials" was hitting its stride, also with 5 working groups active. "Integrative Structural Biology", with its 6 working groups, is concluding in 2022. The Themes of Imaging and Dynamics were extended due to the pandemic and only keeping a few activities ongoing, with most of their combined 9 working groups dormant, however, many of these have on their own accord been very active as detailed in the following.

Northern Lights on Food Theme outcomes and reflections

The Northern Lights on Food (NLF) theme was started with the aims to bring together expertise in food science and technology together with experts in characterization methods using neutrons and X-rays to generate new knowledge and cutting-edge technology within food science. The potential to advance food science by taking full advantage of the research tools provided by ESS and MAX IV will be explored and promoted.

Before the NLF theme was established a WG was established within the Imaging theme and a second Northern Lights on Food Workshop, was arranged June 9-11, 2021, as a fully digital event with financial support from Formas. The workshop was opened by the Vice Chancellor of Lund University, Professor Erik Renström and attracted 125 participants. Apart from the scientific talks, funding opportunities for advanced food research were presented by Sisse Marquina-Jonberg - Novo Nordisk Foundation, Denmark and Maria Öhman - Vinnova, Sweden. The workshop also featured a panel debate on the future of food research and how to utilize the infrastructures Max IV and ESS. The panel consisted of Elisabet Nielsen (Vinnova), Johanna van Schaik Dernfalk (Formas), Carina Knorpp (Näringsdepartementet), Rickard Öste (Aventure/Oatly), and Tommy Nylander (LU-LINXS) and was moderated by Pia Kinhult, ESS, Sweden.

The activities within the NLF LINXS theme were kicked off with an Inspirational symposium for new theme Northern Lights on Food on October 22, 2021. Presentations was given by Prof. Brent S. Murray, The University of Leeds, UK, Dr. Camille Loupiac, University of Burgundy, UB- AgroSup Dijon, France and Dr. Fabrice Cousin, Laboratoire Léon Brillouin, Université Paris-Saclay, France. The symposium attracted about 50 participants.

A 2nd Northern Lights on Food Masterclass was held 15-19 Nov 2021 and was arranged as a hybrid event. The Masterclass was funded by a FORMAS grant and attracted 15 attendees. The theme of the course was imaging and included hands-on experience at Stephen Hall's tomography lab at Lund University.

Northern Lights on Food was represented at the Nordic-US Food Summit that was organized by Business Sweden. A panel debate "Lab to Table" was arranged on 16 November with Christian Malmberg, Senior Research and Project Manager Food at Lantmännen, Tommy Nylander, Co-founder Northern Lights on Food Initiative & Professor at Lund University, Rickard Öste, Professor at Lund University, Co-Founder at Oatly & Founder Aventure, Susana C.M. Teixeira, SANS Instrument Scientist at University of Delaware & Guest Researcher at the NIST Center for Neutron Research and was moderated by Pia Kinhult, Head of Host States Relations at ESS.

The 5 Working Groups started the activities during the autumn 2021:

WG 1 - Structure of Food Raw Materials: Focus on the relationship between the structures of raw materials and process conditions. (Nick Sirijovski, Oatly; Maud Langton, SLU; Francesco Vilaplana, KTH)

WG 2 - Food Colloids: Focus on the colloidal and interfacial phenomena to build up the complex food matrix. (Ben Boyd, Copenhagen Uni; Jacob Kirkensgaard, Copenhagen Uni)

WG 3 - Structure of Food during Processing: (Stephen Hall, LU; Niklas Lorén, RISE)

WG 4 - Food Interactions on Surfaces: Focus on the interface between food and processing surfaces, attachments of microorganisms, as well as food and packaging materials. (Tommy Nylander, LU; Jenny Schelin, LU; Martin Adell, Tetra Pak)

WG 5 - Food and health: (Peter Spéjel, LU; Greg Smith, ISIS; Anna Ström, Chalmers)

Funding obtained for Northern Lights on Food Activities:

- Northern Lights on Food - knowledge and innovation for a green transition in the food sector. (Grant ID: 20307448, Swedish Agency for Economic and Regional Growth, EU European Regional Development Fund and Skåne Region)
- European Food Laboratory (EuFL) – Case study. (The research and innovation council of Skåne (FIRS))
- Strengthen food sector research and innovation by enabling use of neutron and synchrotron techniques. (2021-04909, Vinnova)

New Materials Theme outcomes and reflections

The New Materials for Energy and Sustainability 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.

Five working groups were defined at the start of the Theme, focusing on different types of material. Each group has now more clearly defined the spheres they are interested in, and some groups have focused on using LINXS to tackle community problems, whereas others have focused on education activities, or building networks. Although the year has presented challenges, primarily due to the pandemic, the different groups have trialled different approaches and have met many of their goals. Two grant applications to the Röntgen-Ångström Cluster programme were submitted, growing from partnerships developed within the working groups. Unfortunately, both proposals were rejected, but the collaborations are still growing.

A variety of different activities have been held throughout 2021 within the Theme, along with several jointly organized activities. Each of the working groups has adopted a different approach, targeting different areas and audiences. A brief description of each working group's approach and progress will now be given.

Functional Magnetic Materials

Throughout 2021, the working group met regularly. The initial focus was on combining micromagnetic simulations with scattering data (specifically neutron scattering data), and two workshops on this were organized in March and April 2020, involving ~60 individual participants. This resulted in a clear statement of the importance of being able to link well-

tested simulations to neutron scattering results, and that the end-goal should be that this becomes a normal, easy-to-use method of analysing relevant neutron data. Next steps were outlined, and work is moving forward by those interested to achieve this.

The working group has subsequently been exploring other areas, for example the issue of considering inelastic scattering specifically in the small momentum transfer regime, as well as examining the situation with relation to studies of magnetic materials at MAX IV. As a part of this, the working group organized a session at the MAX IV User Meeting looking at the broader field of quantum materials.

Charge Transfer Materials and Light Harvesting Processes

Over the course of 2021, it became clear that these two working groups were very closely linked and this has been formalized by merging the two groups. This working group pioneered innovative ways of building collaborations, by means of a weekly openLINXS meeting run through Microsoft Teams, that has led to several joint beamtime proposals, grant applications, and an LCLS campaign proposal.

An in-person school for 24 people specializing on X-ray absorption spectroscopy (including EXAFS and XANES) was organized by the working group, including experimental time provided by Balder at MAX IV, and proved to be very popular with the students. The group plans to continue running this school annually, and also to introduce a more advanced workshop for practitioners in the field.

Catalysis

The catalysis working group ran a series of webinars in the first half of the year, culminating in an in-person meeting in October, bringing together speakers from all over Europe. The group has also worked with the Charge Transfer Materials working group to discuss sample environment requirements where they overlap, together with representatives from MAX IV and ESS. A prototype flow cell has been constructed and will be tested in the coming year. One area in which the group is planning to develop in 2022 is in trying to establish greater contact between the current group and researchers using neutron scattering to address catalytic questions.

Nanostructures and Interfaces

This working group has been building up a network of collaborations and is developing some joint projects with other working groups, particularly with catalysis. A LINXS workshop on X-ray phase imaging was held in December 2021. Looking forward, the group plans to liaise more closely with the other working groups and outside partners at ESS.

Integrative Structural Biology (ISB) Theme outcomes and reflections

2021 was a year of many positive developments for the Integrative Structural Biology theme, and also the last year for the theme at LINXS. Unfortunately, the big showstopper - the COVID-19 pandemic, was still affecting the activities. 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 2021. Instead, the final symposium will take place the 4-6th of May in 2022. Despite the pandemic, ISB has managed several successful events (described below)

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 outcome of these meetings was the successful official formation of the Working group, identification key topics and suggestions for activities. During 2021, the group has had two successful workshops, the first one was focusing on protein expression and sample quality control, and the second focused on sample preparation for structural biology and structure determination by different methods such as X-ray crystallography, neutron crystallography and single-particle cryo-EM. Both workshops were held online with roughly 100 participants from all over the world.

Like the rest of the ISB theme activities, the activities of the amyloid working group have suffered badly from the pandemic. Thus, a meeting aiming to highlight and promote the application of SAXS (MAX IV) and SANS (ESS) for the characterization of amyloid systems was cancelled due to travel restrictions. However, a workshop focused on "User-friendly analysis of spectroscopy data with Quasar - multivariate statistics and machine learning" did occur as an online event in May 2020 and resulted in a follow up workshop on the 13-15th January 2021. This activity was based on a collaboration between the French Soleil light source, MAX IV and the Faculty of Medicine. A meeting entitled "Heart and Mind", focusing on the cardiomyopathy and neuropathy in relation to amyloidogenesis will be held on the 5th March 2022. In addition, as a follow up event, a further meeting of the "Heart and Mind" workshop will be in June 16-17, 2022.

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 LU medical faculty and LINXS Co-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".

The time-resolved working group has had working group meetings during 2021 focusing on a follow-up to the successful online workshop organized in November 2020. It was decided to aim on a physical meeting this time hoping the pandemic restrictions would ease but with the constantly changing restrictions it has not been possible to organize the workshop.

During 2020 ISB started a new working group, Lund Integrative Structural Biology Centre Initiative (ISBC). The aim of this working group was to investigate if there is an interest, in the Lund area, of a future integrative structural biology centre placed at Brunnshög, and to help catalysing the discussion and development of these ideas. The first workshop was held in February 2021, with four invited speakers from integrative structural biology centers in

Europe. For this meeting, PIs that are directly working with structural biology in the Lund were invited. After the meeting the participants were asked to fill in a survey. One question was if the invited PIs thought that an ISB center should be established in Lund, and 93% of the participants were positive towards the establishment of ISBC. As the working group received such a positive response, the working group decided to go further with their plans and submitted a letter to the University management. The letter was also received very well from the management and currently there are ongoing discussions on how this will be funded. During 2021 the working group also had additional meetings and initiated a seminar series to strengthen the structural biology community in Lund. This has led to that we now are submitting a "letter of interest" to the University management to become one of the five scientific profile areas that LU will have in the future.

Dynamics Theme outcomes and reflections

'Antibodies in Solution' Research Programme (under the Dynamics Working Group 1, "Dynamics and structure of biological macromolecules")

The establishment of a close collaboration with the American National Institute of Standards and Technology (NIST) agreeing to act as a source for mAb material and as a partner in the programme followed by the 'Antibodies in Solution' online Kick-off Meeting at the end of 2020 paved the way for our 2021 activities: A detailed research Road Map describing the underlying research strategy, the four different research Work Packages as well as the research goals and timeline of this LINXS initiative has been established during the first quarter of 2021. This was accomplished by numerous zoom meetings of the entire Consortium, the individual Work Package members and the LINXS mAb Steering Group.

After the next hurdle - the establishment of a Material Transfer Agreement (MTA) and the respective negotiations between the legal departments of NIST and the different Consortium partners - a first load of the NIST antibody (NISTmAb) material was sent out to those partners whose submitted Materials Request Forms (MRF) had been evaluated positively by the Steering Group and subsequently by NIST. This has happened at the end of May / beginning of June. First experiments on the NISTmAb then started in early summer 2021, both at neutron and X-ray large scale facilities as well as in-house. The experimental and simulation results have been presented at our first Progress Report Meeting (November 2021; via zoom (25-30 participants)). Two of the most important achievements on the NISTmAb in 2021 are: i.) the identification and fixation of specific solvent conditions based on a systematic screening study and ii.) the establishment of a detailed sample preparation protocol.

Throughout the entire year of 2021, the individual Work Packages have had regular Zoom meetings, always in close collaboration and vivid exchange with interested NIST scientists.

Moreover, intense discussions with a second potential partner and mAb provider (Novartis, Switzerland) have been and are still ongoing.

The Dynamics Working Group 3, “Dynamics and Structure of Membranes and their Constituents”

In the last year of the dynamics theme the WG 3 initiated work started to make an impact in several ways. The publications as a product of the visiting fellows program 2020 started to appear and resulted in 7 publications. The WG 3 organized Neutrons in Life Science and Biomaterials, 14-18 June 2021 as a web-based graduate course within the SWEDNESS program with 20 participants. SwedNess is a graduate school providing research training in neutron scattering funded by The Swedish Foundation for Strategic Research (SSF). Here dynamics and structure of membranes and their constituents were an important part of the curriculum. A conclusive workshop focusing on biomembranes was planned for 2021 but was postponed to 2022. It is now planned as a hybrid LINXS Partner event - Lipid Bilayers at ESS- BESS in Lund, 13-15 June 2022. WG 3 leader Tommy Nylander was elected vice president and president elect of European Colloid Interface Society ECIS in September 2021. He was also appointed Specialty Chief Editor of Frontiers in Soft Matter, Self-Assembly and Self-Organisation.

Research programme 1: Structure and dynamics utilizing the GISANS technique

Swedish universities, institutes and companies collaborate on planning new instruments for installation at ESS, the world's most powerful research facility for neutron radiation, outside Lund. A dedicated Grazing-Incidence Small-Angle Neutron Scattering (GISANS) instrument will enable researchers to analyse in detail how a neutron beam spreads when reflected from a surface. Here LINXS has served as a meeting point and a hub to solidify the collaboration. The Swedish Research Council in November granted funding (2021-06230) for an interdisciplinary project “Preparing for a GISANS instrument at ESS – A Swedish Initiative” with Tommy Nylander as project leader. This project, SAGA, are jointly conducted by Lund University, Uppsala University, Malmö University, Linköping University and KTH. During 2022 a 3 year PostDoc will be appointed, placed at LINXS. During 2021 a SAGA GISANS workshop was held on 12 of May in connection with the Swedish Neutron week 10-12 of May.

Research programme 2: Sample environment and data evaluation of biological membranes

Quite some effort was made to secure to provide sample environment to increase the activities in this area. Here should be mentioned the successful proposal for renewed funding (2021-00159) from Swedish Research Council for the only Swedish operated and own neutron instrument, Super ADAM, placed at ILL in Grenoble France, and operated jointly by the universities in Uppsala, Lund and Linköping. Another successful grant application (2021-06151) for Swedish Research Council were dealing with growth and characterization of magnetic layers to develop new methodology for exploring soft matter and life sciences using neutron scattering. The project involved partners from universities in Linköping, Lund and Uppsala as well as ESS an STFC – ISIS neutron and muon source, UK. An important part of this project is to get new methodology to study biological membranes based on magnetic reference layers.

Imaging Theme outcomes and reflections

With the Theme concluding there were not many activities in 2021. However, the very successful Co-Work webinar series continued to provide a much-needed international forum for coherent imaging with X-rays.

The Theme also invited one of the few guest researchers who were able to come in the year: Prof. Adam Hitchcock from McMaster University in Canada, who spent 2 months in Lund supporting the SoftiMAX beamline at MAX IV in its start-up phase. We are looking forward to his planned return in 2022. The invitation was supported by the Working Group on Soil Science.

Imaging also hosted a collaborative project between LTH and ESS, a demonstration model initially being used as a prototype for the ODIN experimental station. This project was reported on in the LINXS news and laid the foundation for a larger initiative.

Within the framework of the GeoARCH working group, collaborations continued, including imaging of artefacts from the marine excavation of the Danish 15th century flagship "Gribshunden". The excavation is widely known from both American and Swedish documentary television. Collaborations were also initiated with the Lund University Historical Museum.

A very few activities will be carried over into 2022, but the theme is now considered closed and has entered "Legacy" status. The Annex for the Imaging Theme contains the "Legacy" statement, summarising the outcomes overall to the public.

Conclusion of the first LINXS Postdoc position

In 2021, Anurag Kawde worked on successfully moderating the webinar series that was focused on the sciences at large-scale facilities around the world. The scientific directors of various synchrotron and neutrons sources talked about different techniques used in their respective facilities and also shed light on how to explore different materials such as biological, battery related, green materials, fossils, and so on.

Anurag received the NanoLund young scientific researcher award for the year 2021 and 100K seed funding for the demonstration of novel solar catalytic material that can enhance solar absorption significantly for efficient solar energy harvesting and conversion. Anurag will now be working in close collaboration with Umea University, Max Planck Institute Germany, and Lund University to investigate the reaction mechanism in biohybrid devices for solar energy conversion. He will be actively using the research facilities such as NanoLund, MAX IV, Lund Laser center, Umea University "Nano For Energy " and Max Planck Institute for Chemical Energy conversion for further understanding of novel solar catalytic devices.

Anurag concluded his Postdoc position at LINXS in the end of May 2021 but continued to contribute to the LINXS webinar series he initiated.

LINXS Strategic & Operational Achievements

This section reports on progress according to the 2021 Strategic and Operational Plan, and follows its headings for strategic and operational objectives.

Strategic progress

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

LINXS has been further established globally, with further increased international exposure, thanks to the shift in working practices and emphasis on digital and online spaces due to the pandemic. LINXS has also involved itself intimately in helping organise meetings connected to the work on the MAX IV Strategy and supporting communities interested in in-kind contributions to ESS. This supports LINXS ambition to be a “go to” place for activities that want to exist in the context of a “neutral” platform between national and international actors.

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, as well as with a strong online presence.

LINXS has always strived to be an attractive and comfortable environment to do science in, and the long-term goal of establishing a physical presence in Science Village Scandinavia (SVS) has progressed, keeping all actors relevant to such a move, SVS AB, The LU Office for moving to Brunnsög (led by Eva Åkesson), and SKANSKA and Wihlborgs (via LU Estates). The two latter companies are building the first places that can offer a home for LINXS for the initial phase of its location in SVS.

The presence at IDEON is now well established and used as much as possible. During 2021 work progressed on making this a virus-safe environment to work in. LINXS door have consistently stayed open to all that need us.

Promote and extend LINXS’s scientific portfolio within and between the existing and new/developing themes

The concepts of “Town Hall” meetings, with updates between the Themes, as well as “Science Day” inspirational workshops have continued, and we refer to the earlier Theme reports for improvement of the working practices within the Themes.

Establish new themes and work towards further calls for themes

Northern Lights on food started its activities during the year, and 2021 saw the application of a new Theme “Integrative Pharmacology and Drug Discovery”. The “organic” practice of Themes developing from working groups and lively scientific interaction has continued, where several are now in the pipeline and expected to regroup for call(s) in 2022.

Expand and improve the visitors program integrated into the LINXS mission

While much progress was made in the digital sphere and digital communication capabilities and capacities were improved (see next section), there were very few guest researchers in 2021, due to the uncertainty caused by the pandemic. Emerging from this will have to be a priority going forward. Prof. Adam Hitchcock was a guest researcher able to come to Lund in autumn (see above under Imaging), as was Hilde Venvik, member of the Catalysis Working Group in the New Materials Theme.

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

This is one of the truly remarkable achievements of last year where the Educational material available grew to over 120 recorded talks and instructional videos. The main task going forward will be to structure this resource and take advantage of the possibilities engendered, by involving LINXS in projects to make this accessible, and by developing how the material is made available on the site.

Promote on-line interaction opportunities during the current restrictions imposed by the global pandemic

The dramatic increase in events during 2021 speaks for itself, LINXS has integrated its equipment and facilities for working online, and has inspired people to use them, be it using the in-house equipment or hiring in professionals. Going forward LINXS must strive to increase its capabilities, mobilise help and resources for self-help. It is the goal of LINXS to be able to be part of a solution no matter what the budget is.

Carry forward the on-line developments and established on-line presence of LINXS to further enhance LINXS's international interactions in the post-pandemic world, in conjunction with benefitting from the renewed possibility (and community need) for physical meetings.

Again, the record speaks for itself, LINXS increased the number of people involved and greatly improved its routines, so that the number of registered and classified participants has more than doubled, going from 526 people in 2020 to 1318 people in 2021. We estimate that as a conservative figure over 2000 people have been involved in LINXS in some way during 2021, which is an increase from the previous year's 1900. The relative proportions of engagement are roughly the same across the actor constellations, though we note an increase in the involvement from the LU Medical Faculty. While the relative percentages are the same, the absolute number show a huge increase in engagement across the board. See the "LINXS in numbers" section for more detail.

Operational progress

Appoint and integrate a new director

Delivered. Though the process was drawn out due to its complexity and the pandemic hampering travel, the incredibly successful recruitment of Prof. Trevor Forsyth was completed, with the help of the LU leadership and a recruitment package co-provided by the faculties of Medicine, Science and Engineering. Such a collaboration between the faculties and the LU leadership in recruitment is unprecedented in the history of the university. LINXS would like for the record to extend its deepest thanks to all those involved.

Secure medium and long-term funding, as well working towards new funding opportunities/applications (e.g., foundation funding and EU)

LINXS was written in to at least six proposals during the year, but needs to progress further. As detailed in the Theme report for NLF, most of the project-based funding that has come in has been related to that. However, LINXS has also been directly involved in the GISANS initiative, with a postdoc being placed at LINXS to carry out the work. Going forward LINXS will seek to increase its interface with European funding, not the least via engagement in schools & network – oriented funding, such as MSCA CoFUND and other initiatives.

Extend LINXS's community including collaborations, partnerships and memberships

Here again, the record (See LINXS in numbers section) shows that the community of LINXS has expanded significantly, the pertinent question is how this concretely has led to memberships and partnerships. We are proud to report that discussions with Uppsala University regarding partnership was significantly bolstered by a joint meeting at the level of the Vice Chancellors over Christmas Dinner. It was agreed that the two universities will appoint working groups to hammer out how such a partnership can be formed. Going forward this point will be of crucial importance for the future shape of LINXS.

Engage board and management group members

This work has progressed partially but needs to progress more. The need to clarify the roles and responsibilities of the Scientific Advisory Board remains and are underway, and the formal scope of the Board is set out in the statutes. LINXS has progressed in its description of roles and responsibilities, and this has been part of active discussions during the year. Any major changes in practices needs time to be properly worked through also with the new Director.

Establish theme development plans

During the year, LINXS continued activities such as Science Days and Town Hall meetings that seek to increase cross-Theme exchange of ideas and working practices. LINXS has also progressed in developing the model of what happens with a Theme when it is concluded and goes into "Legacy" status.

Focus on identifying and promoting the benefits, outputs and added value of LINXS

We refer to the report on LINXS communications as the main source for the outcomes of this. Significant informal discussions have been undertaken during 2021 to promote LINXS, and one of the fruits of this is the initiated discussion with Uppsala University regarding a partnership.

Actively encourage sustainability and gender-balance in LINXS's operations

LINXS continues to encourage sustainable working practices, not the least by making vegetarian food the default option at events, working digitally whenever appropriate, and carefully considering when to subsidise travel. The gender balance of keynote speakers at LINXS has improved significantly in 2021, with the ration of women to men being 36/64, up from 24/76 in the previous year. This is good progress toward the target of 60/40 either way. We recommend for people to influence what they can control, cognizant of the fact that there are very different gender ratio profiles on average in different disciplines.

LINXS communications as a pathway to impact

LINXS continued its efforts to use communications and outreach strategically towards realising the overall mission for LINXS.

As the activities of LINXS increases and extends to more areas and communities, the significance of capturing and giving value to the various outputs are growing. 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.

News highlights

The recruitment of a new LINXS Director, Trevor Forsyth, was a news item that was highlighted and spread in various channels, such as on Lund University, ESS and MAX IV websites, newsletters and the Lund University Magazine, LUM.

Launch of new theme Northern Lights on Food received attention and engagement, especially at the kick-off Food conference in June and activities throughout the fall of 2021.

A successful application for a GISANS instrument at ESS, in a joint collaboration of LINXS researchers and researchers at all the major Swedish Universities, was announced in a press release in collaboration with communication departments of all stakeholders.

Newsletters

Publication of the LINXS newsletter continued and the subscription list increased to 2179, increasing from 1111 in the past year and with very few un-subscriptions. 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 2021. On average, 664 persons opened each newsletter – ranging from 591 to 757, i.e., an average 39 % 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, 32 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.

Web

The LINXS website is the main tool for communication and transparency. It continued to be updated and expanded during the year, with a focus on supporting current and potential researchers at LINXS.

As the first LINXS themes were closed, a Legacy section was developed to archive and showcase the impacts of the Imaging, Dynamics themes and Integrated Structural Biology to close in early 2022.

The LINXS website had 28 078 visits in 2021, an increase of 50 % compared to 2020. Among them 19 232 were unique visitors (30 % increase). The website had 56 132 page views, an increase of 25 % compared to 2020. Most popular content in descending order were the Home page, the LINXS events page, the Management page, the Educational page and the Science at large scale facilities page.

Social media

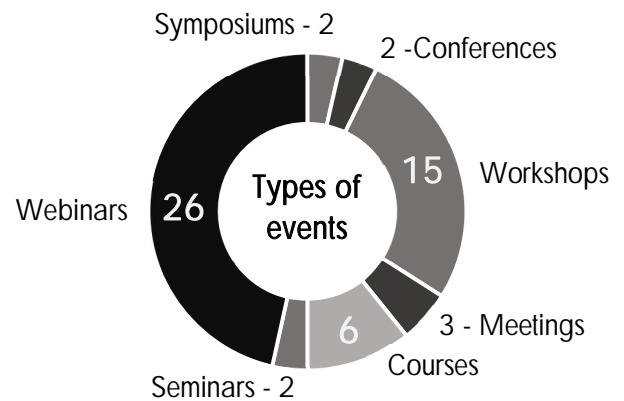
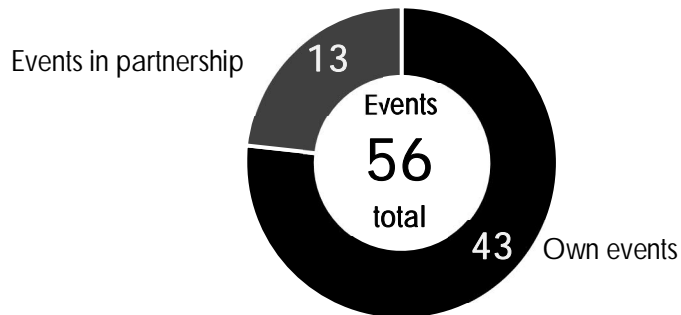
The LINXS YouTube channel was updated with a new introductory film about LINXS and recordings of webinars including the public panel debate on the future of ESS and MAX IV as part of the Futures Week at Lund University, which received a lot of interest.

The LINXS Twitter account @LINXS_Sweden expanded its follower base to 224 persons and organisations and is actively following 132 key actors and persons in the field. In the plans for 2022 is to use the Twitter platform more extensively as the communities and activities are increasing.

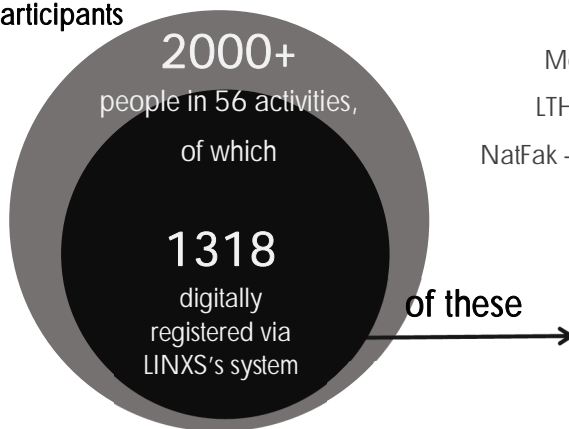
The LINXS LinkedIn page was used to further promote all articles, newsletters, and events, gaining an increased number of followers amounting to 811 persons (an increase of 63 % as compared to 2020). It serves very well as a further communication tool to reach larger audiences and allows even more outreach through individual sharing/reposting.

LINXS in numbers 2021

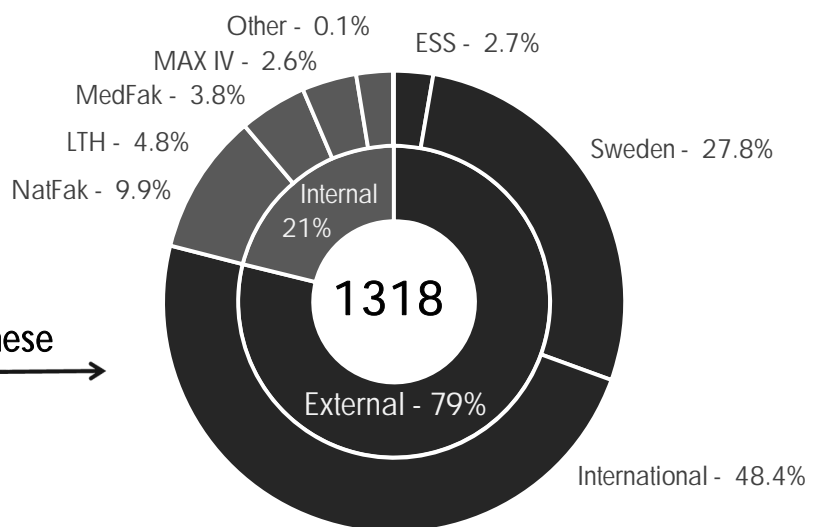
LINXS Activities and participation



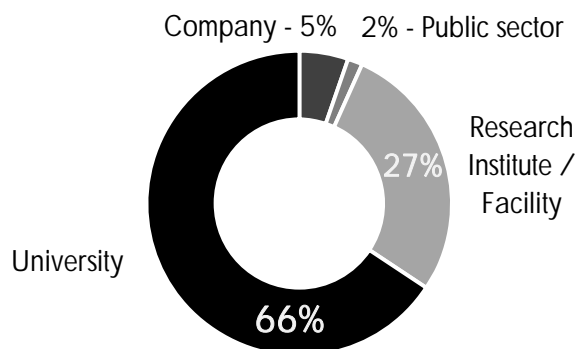
Participants



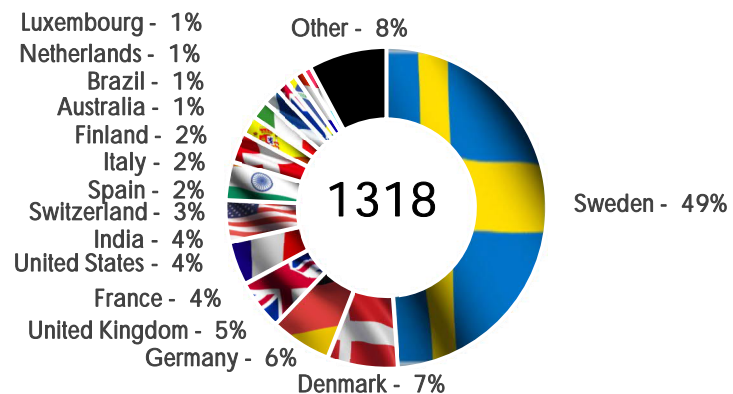
of these



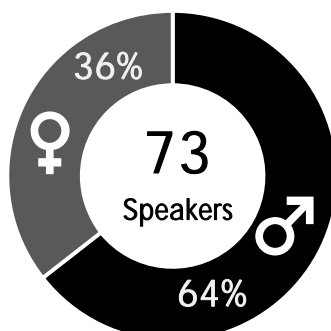
Organisational types



Country of origin

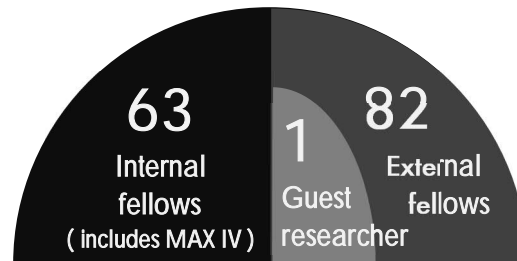


Keynote speakers gender balance



LINXS Community – fellows in 2020

145 LINXS fellows in 2021



LINXS Community - affiliations of LINXS fellows

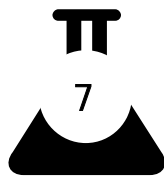
51 organisations are involved in the LINXS core groups, working groups and visiting researcher programme.

20 in Sweden (including Lund University)

31 international (DE:8, DK:6, USA:4, FR:4, UK:2, IT:2, AU:2, NO:1, LU:1, ES:1), these were:



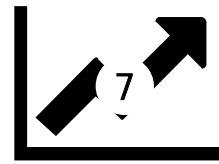
Universities



Research Institutes



Large Scale
Research Infrastructures



Companies

LINXS Community

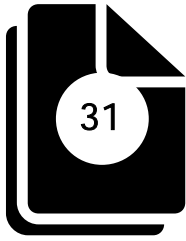


2 Core Partners (in addition to Lund University)

1 Member (Research Group)

10 Collaborations

Outcomes



Publications with
LINXS affiliation



Project applications

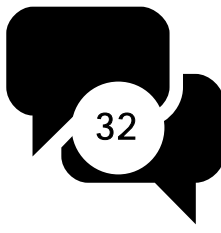


Projects funded

Communications



Outreach activities



Website news



Newsletters



Subscribers



LinkedIn



Twitter

Annual Financial Report 2021

Income	SEK
External funding – FORMAS deferral	34,715
Partners contribution	8,000,000
Activities	0
Membership fees	50,000
Total Income 2021	8,084,715
Expenditures	SEK
Activities	-232,032
Equipment	-92,612
Materials & consumables	-99,281
Premises	-1,181,452
Salaries	-4,204,527
Overhead	-1,736,123
Total Expenditures	-7,546,026
Annual Result	538,689

Partner contributions during 2021 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 20% of the salary of the LINXS co-director and 20% of the salary of the ISB theme leader. External funding for the FORMAS project was deferred for project implementation in 2021. The final surplus will be moved to the budget of 2022 together with the accumulated agency capital from the previous years.

Detailed financial reporting is included in Annex 5

Annex 1 – LINXS Themes and Working Groups in 2021

NORTHERN LIGHTS ON FOOD

Theme and Core Group Leader: Selma Maric, Lund University, Sweden

WG 1 - Structure of food raw materials

Leader – Francisco Vilaplana, KTH, Sweden

WG 2 - Food colloids and structured interfaces

Leaders – Ben Boyd and Jacob Kirkengaard, Copenhagen University, Denmark

WG 3 - Structure of food during processing

Leaders – Stephen Hall, Lund University and Niklas Lorén, RISE, Sweden

WG 4 - Food interactions on surfaces

Leader – Jenny Schelin and Tommy Nylander, Lund University, Sweden

WG 5 - Food structure and health

Leader – Peter Spéjel, Lund University, Sweden

NEW MATERIALS

Theme and Core Group Leader: Elizabeth Blackburn, Lund University, Sweden

WG 1 - Functional Magnetic Materials

Leader – Elizabeth Blackburn, Lund University, Sweden

WG 2 - Charge Transfer Materials (ended)

WG 3 - Light Harvesting Processes

Leader – Jens Uhlig, Lund University, Sweden

WG 4 - Catalysis

Leader – Sara Blomberg, Lund University, Sweden

WG 5 - Nanostructures and Interfaces

Leader – Maria Messing, Lund University, Sweden

INTEGRATIVE STRUCTURAL BIOLOGY (ISB)

Theme and Core Group Leader: Karin Lindkvist, Lund University, Sweden

WG 1 - Biocompute and Artificial Intelligence & Machine Learning (concluded)

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

Leader – Thomas Ursby, MAX IV, Lund University, Sweden

WG 3 - Amyloid: An integrative approach

Leader – Oxana Klementieva, Lund University, Sweden

WG 4 - Membrane Proteins - Structural resolution and homology modelling

Leader – Urban Johanson, Lund University, Sweden

WG 5 - Lund Integrative Structural Biology Centre Initiative

Leader – Karin Lindkvist, Lund University, Sweden

DYNAMICS (CONCLUDING)

Theme and Core Group Leader: Marie Skepö, Lund University, Sweden

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

IMAGING (CONCLUDING)

Theme and Core Group Leader: Stephen Hall, Lund University

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

Annex 2 – List of LINXS activities 2021

LINXS events and events organised in partnership:

1. LINXS event - WEBINAR: CoWork series - Coherent X-ray imaging of 3D magnetic systems with Claire Donnelly, Jan 12, 2021 (Imaging)
2. LINXS event - Amyloid Workshop: User-friendly analysis of spectroscopy data with Quasar - multivariate statistics and machine learning, Jan 13-15, 2021 (ISB)
3. LINXS event - WEBINAR: CoWork series - The Atomic beamline at the Upgraded Advanced Photon Source with Ross Harder, Jan 28, 2021 (Imaging)
4. LINXS event - WEBINAR: CoWork series - ID01 in light of the ESRF - EBS with Steven Leake, Feb 12, 2021 (Imaging)
5. LINXS event - Workshop "Integrative Structural Biology Centre Initiative", Feb 18, 2021 (ISB)
6. LINXS event - WEBINAR: CoWork series - Effectiveness of Phasing Algorithms in Bragg Coherent Diffractive Imaging with Ian Robinson, Feb 25, 2021 (Imaging)
7. LINXS event - Catalysis Working group Webinar - "Research in Catalysis at MAX IV" by Andrey Shavorskiy, March 2, 2021 (New Materials)
8. LINXS Event - Amyloid Workshop - Heart and Mind: linking in vitro science to the clinical context, March 5, 2021 (ISB)
9. LINXS Event - Workshop - Magnetic materials: linking scattering data to magnetic simulations, Part I, March 25-26, 2021 (New Materials)
10. LINXS event - WEBINAR: CoWork series - The new Carnaúba beamline at the new Brazilian synchrotron source with Carlos Sato Baraldi Dias, March 25, 2021 (Imaging)
11. LINXS Event - Workshop Magnetic materials: linking scattering data to magnetic simulations, Part II, April 8-9, 2021 (New Materials)
12. LINXS event - WEBINAR: CoWork series - Characterization and mapping of nanostructure using ptychographic 3D nanoscale imaging and small angle X-ray scattering at the cSAXS beamline, with Manuel Guizar Sicaire, April 8, 2021 (Imaging)
13. LINXS event - WEBINAR: Science at Large Scale Research Facilities - The European XFEL: new science opportunities, start of user operation and first results, April 14, 2021
14. LINXS event - WEBINAR: Science at Large Scale Research Facilities - Science with the ESRF EBS, April 21, 2021
15. LINXS event - WEBINAR: CoWork series - Playing with coherence in soft X-ray scattering, with Claudio Mazzoli, April 22, 2021 (Imaging)
16. LINXS partner event - Webinar - How can researchers at MAX IV benefit from LINXS? April 23, 2021
17. LINXS event - WEBINAR: CoWork DUO webinar: Holographic tomography as a new tool for bioimaging and 3d Virtual Patho-Histology of Lung Tissue from Covid-19 Patients based on Phase-Contrast X-ray Tomography, April 29, 2021 (Imaging)
18. LINXS event - WEBINAR: Science at Large Scale Research Facilities - Neutron Sciences at the Oak Ridge National Laboratory, May 5, 2021
19. LINXS event - WEBINAR: CoWork series - Investigating the early life on Earth with nanoscale X-ray coherent imaging, with Lara Maldanis, May 6, 2021 (Imaging)
20. LINXS Event - Everything you want to know about applying for and managing a Theme at LINXS! May 6, 2021

21. LINXS Partner event - Swedish Neutron Week 2021, May 10-12, 2021
22. LINXS Partner event - Early Stage Researcher (ESR) Career Day, May 11, 2021
23. LINXS Partner Event - SWEDNESS/LINXS Doctoral-level course on neutron imaging, May 17-20, 2021 (Imaging)
24. LINXS event - Catalysis Working group webinar - Oxide formation at Pt-Sn model catalyst surfaces, with Lindsay Merte, May 18, 2021 (New Materials)
25. LINXS event - WEBINAR: Science at Large Scale Research Facilities - Neutron scattering and imaging at the Swiss Spallation Source SINQ, May 19, 2021
26. LINXS event - WEBINAR: CoWork DUO webinar: X-ray ptychographic topography, a new tool for strain imaging - Diffraction of X-ray by thin perfect crystals, May 20, 2021 (Imaging)
27. LINXS Event - Membrane Protein workshop: Structural Resolution of Membrane Proteins: From Expression to Sample Preparation, May 25-26, 2021 (ISB)
28. LINXS event - WEBINAR: Science at Large Scale Research Facilities - Revealing the hidden structure and dynamics of matter: opportunities for research at the ISIS Neutron and Muon source, May 26, 2021
29. LINXS Partner Event - SwedNESS PhD school: Small Angle Neutron Scattering (SANS), May 31-June 4, 2021
30. LINXS event - WEBINAR: Science at Large Scale Research Facilities - Scientific opportunities at Sirius, the new Brazilian synchrotron light source, June 2, 2021
31. LINXS event - WEBINAR: CoWork series - Probing dynamics with X-ray Photon Correlation Spectroscopy: achievements & outlook, with Dina Sheyfer, June 4, 2021 (Imaging)
32. LINXS event - Northern Lights on Food (NLF) II, June 9-11, 2021 (Imaging)
33. LINXS Partner Event - SwedNESS PhD school: Neutrons in Life Science and Biomaterials, June 14-18, 2021
34. LINXS event - WEBINAR: CoWork series - XPCS: A powerful technique to study the dynamics on colloidal length scale, with Antara Pal, June 17, 2021 (Imaging)
35. LINXS Town Hall meeting, June 21, 2021
36. LINXS event - WEBINAR: CoWork DUO webinar: Upscaling x-ray nanoimaging to macroscopic objects - Ptychographic image reconstruction using automatic differentiation: first and second order methods, June 24, 2021 (Imaging)
37. LINXS Partner Event - Workshop on a Future μ -Spectro-microscopy Beamline, Aug 26, 2021
38. LINXS Partner event - Strategy workshop for IR spectromicroscopy beamline MIRARI at MAX IV, Sep 3, 2021
39. LINXS event - WEBINAR: Science at Large Scale Research Facilities - The SLS 2.0 Upgrade, Sep 22, 2021
40. LINXS event - WEBINAR: Science at Large Scale Research Facilities - The Institut Laue Langevin - 50 years of neutrons, science and innovation, Sept 29, 2021
41. LINXS Partner event - HELIOS International Graduate School, Lund Retreat, Oct 4-8, 2021
42. LINXS event - WEBINAR: Science at Large Scale Research Facilities - Science at the Diamond Light Source and future plans for a major upgrade of the facility with the Diamond-II programme, Oct 13, 2021
43. LINXS event - Seminar with LINXS Guest fellow Prof. Adam Hitchcock, McMaster University, Canada, Oct 14, 2021 (Imaging)

44. LINXS Partner Event - Workshop on synchrotron tomography for future MAX IV experiments, Oct 20, 2021
45. LINXS Partner event - MAX IV and ESS as engines for breakthrough science, Oct 20, 2021
46. LINXS event - WEBINAR: Science at Large Scale Research Facilities - Science at the research neutron source Heinz Maier-Leibnitz (FRM II), Oct 20, 2021
47. LINXS event - Lund Integrative Structural Biology Seminar Series, Oct 21, 2021 (ISB)
48. LINXS event - Inspirational symposium for new theme Northern Lights on Food, Oct 22, 2021 (Food)
49. LINXS Partner event - Quantum and advanced materials (MAX IV User meeting), Oct 26, 2021 (New Materials)
50. LINXS event - Catalysis workshop, Oct 28, 2021 (New Materials)
51. LINXS Event - XAS-School 2021, Nov 1-5, 2021 (New Materials)
52. LINXS Partner event - BECC - LINXS mini-symposium: Chemical imaging of soil and other environmental samples with synchrotron based soft X-ray STXM and ptychography, Nov 1, 2021 (Imaging)
53. LINXS event - 2nd Northern Lights on Food Masterclass, Nov 15-19, 2021 (Food)
54. LINXS Town Hall meeting, Dec 3, 2021
55. LINXS event - 2nd Membrane Protein Working Group Workshop, Dec 7-8, 2021 (ISB)
56. LINXS event - Workshop: Introduction to PyPhase - a Python package for X-ray phase imaging, Dec 9-10, 2021 (New Materials)

LINXS Hosted events:

1. BigScience Sweden meeting, April 15, 2021
2. Dept. Of Chemistry Board meeting (15 people), Sept 16, 2021
3. Brain storming meeting, Sara Linse's Research Group (12 people), Oct 12, 2021
4. SNSS Board meeting, Nov 23, 2021
5. Brain storming meeting, Sara Linse's Research Group (12 people), Oct 12, 2021
6. Meeting Smile Incubator-ESS (20 pers) Oxana presenting LINXS, Nov 24, 2021
7. MAX IV - ALFA LAVAL Industry meeting (15 pers), Magnus Fredriksson, Nov 25, 2021
8. Dept. Of Chemistry Economy planning (Henrik Steen), Dec 1, 2021

LINXS Outreach activities:

1. Meeting ESS/MAX IV-office in Stockholm - LINXS (digital), Feb 12, 2021
2. Medicon Valley Alliance R&D Network Webinar, Focus on Research infrastructure (Kajsa M Paulsson), May 20, 2021
3. ESS/MAX IV Summit online, Oct 14, 2021
4. MAX IV and ESS as engines for breakthrough science, Oct 20, 2021
5. LINXS model och the national perspective, Oct 25, 2021
6. LINXS stand at TechConnect Europe in Malmö, Nov 15-17, 2021
7. Meeting with delegates from Uppsala University Management concerning future collaborations and partnership, Dec 17, 2021

Annex 3 – List of publications with LINXS affiliation 2021

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. *Physical and chemical properties of carbon nanotubes in view of mechanistic neuroscience investigations. Some outlook from condensed matter, materials science and physical chemistry*, Stefano A. Mezzasalma, Lucia Grassi, Mario Grassi. 2021, December. In: Materials Science and Engineering
2. *Tailoring plasmonic resonances in Cu-Ag metal islands films*, Matej Bubaš, Vesna Janicki, Stefano A. Mezzasalma, Maria Chiara Spadaro, Jordi Arbiol, Jordi Sancho-Parramona. 2021 October 30. Applied Surface Science
3. *Comprehensive multidimensional study of the self-assembly properties of a three residue substituted β 3 oligoamide*, Buchanan, C., M. G. Hinds, L. Puskar, C. J. Garvey, and A. Mechler. 2021 October. Pure and Applied Chemistry.
4. *C-amidation of substituted β 3 oligoamides yields novel supramolecular assembly motif*, Buchanan, C. E., L. Ljiljana Puskar, C. J. Garvey, and A. Mechler. 2021, 22 October, In: Nanotechnology.
5. *Estimation of pre-dolomitisation porosity and permeability of a nummulitic carbonate reservoir rock using the Multi-Component Architecture Method (MCAM)*, A. Mangione, H. Lewis, S. Geiger, Z. Jiang, G. D. Couples, J. Buckman, S. Beavington-Penney & S. A. Hall, 2021 Oct, In: Marine and Petroleum Geology.
6. *Photoelectrochemical Oxidation in Ambient Conditions Using Earth-Abundant Hematite Anode: A Green Route for the Synthesis of Biobased Polymer Building Blocks*, Kawde A, Sayed M, Shi Q, Uhlig J, Pullerits T, Hatti-Kaul R. August, 2021. MDPI, Catalysts.
7. *Deuterated Bacterial Cellulose Dissolution in Ionic Liquids*, Vikram Singh Raghuwanshi, Yachin Cohen, Guillaume Garnier, Christopher J. Garvey & Gil Garnier, 2021 Jul 27, In: Macromolecules.
8. *Correlative optical photothermal infrared and X-ray fluorescence for chemical imaging of trace elements and relevant molecular structures directly in neurons*, Nadja Gustavsson, Agnes Paulus, Isak Martinsson, Anders Engdahl, Kadda Medjoubi, Konstantin Klementiev, Andrea Somogyi, Tomas Deierborg, Ferenc Borondics, Gunnar Keppler Gouras & Oxana Klementieva, 2021 Jul 22, In: Light, science & applications.
9. *Dual modality neutron and x-ray tomography for enhanced image analysis of the bone-metal interface*, Elin Törnquist, Sophie Le Cann, Erika Tudisco, Alessandro Tengattini, Edward And, Nicolas Lenoir, Johan Hektor, Deepak Bushan Raina, Magnus Tägil, Stephen A. Hall & Hanna Isaksson, 2021 Jul 7, In: Physics in Medicine and Biology.
10. *Stochastic modelling of 3D fiber structures imaged with X-ray microtomography*, Philip Townsend, Emanuel Larsson, Tomas Karlson, Stephen A. Hall, Malin Lundman, Per Bergström, Charlotta Hanson, Niklas Lorén, Tobias Gebäck, Aila Särkkä & Magnus Röding, 2021 Jun 15, In: Computational Materials Science.

11. *Morphologies and Structure of Brain Lipid Membrane Dispersions*, Alfredsson, V., Lo Nostro, P., Ninham, B. & Nylander, T., 2021 June 14: *Frontiers in cell and developmental biology*. 9, 675140.
12. *The Brittle-Ductile Transition in Porous Limestone: Failure Mode, Constitutive Modeling of Inelastic Deformation and Strain Localization*, Patrick Baud, Stephen Hall, Michael J. Heap, Yuntao Ji & Teng fong Wong, 2021 May, In: *Journal of Geophysical Research: Solid Earth*.
13. *The Protein Corona Leads to Deformation of Spherical Micelles*, Cheng Cao, Lin Zhang, Ben Kent, Sandy Wong, Christopher J. Garvey & Martina H. Stenzel, 2021 Apr 26, In: *Angewandte Chemie - International Edition*.
14. *Effect of non-Gaussian end-to-end distributions on shear and elastic gel moduli: theoretical and experimental approach*, Stefano Mezzasalma, Michela Abrami, Gabriele Grassi and Mario Grassi. 2021.
15. *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*, 2021 Apr 1;106(4):1163-1166.
16. *Amyloid Structural Changes Studied by Infrared Microspectroscopy in Bigenic Cellular Models of Alzheimer's Disease*, Agnes Paulus, Anders Engdahl, Yiyi Yang, Antonio Boza Serrano, Sara Bachiller, Laura Torres-Garcia, Alexander Svanbergsson, Megg Garcia, Gunnar Keppler Gouras, Jia-Yi Li, Tomas Deierborg & Oxana Klementieva, 2021 Mar 26, In: *International Journal of Molecular Sciences*.
17. *Review of life science applications using submicron O-PTIR and simultaneous Raman microscopy: a new paradigm in vibrational spectroscopy*, Mustafa Kanziz, Alice Spadea, Jayakrupakar Nallala, Cassio Lima, Howbeer Muhamadali, Joanna Denbigh, Jayne Lawrence, Gorkem Bakir, Peter Gardner, Nick Stone, Roy Goodacre, Kathleen Gough & Oxana Klementieva, 2021 Mar 5, In: *Advanced Chemical Microscopy for Life Science and Translational Medicine*.
18. *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*. 2021 Mar 1;12(1):1347.
19. *3D X-Ray Diffraction Characterization of Grain Growth and Recrystallization in Rolled Braze Clad Aluminum Sheet*, Torkel Stenqvist, Johan Hektor, Sara Bylund, Robert Moberg, Märten O.M. Edwards, Stephen A. Hall & Lars Åke Näslund, 2021, In: *Advanced Engineering Materials*.
20. *Anisotropic dynamics of magnetic colloidal cubes studied by X-ray photon correlation spectroscopy*, Antara Pal, Md Arif Kamal, Thomas Zinn, Jan K.G. Dhont & Peter Schurtenberger, 2021, In: *Physical Review Materials*.
21. *Bicontinuous cubic liquid crystalline phase nanoparticles stabilized by softwood hemicellulose*, Polina Naidjonoka, Marco Fornasier, David Pålsson, Gregor Rudolph,

- Basel Al-Rudainy, Sergio Murgia & Tommy Nylander, 2021, In: Colloids and Surfaces B: Biointerfaces.
22. *Impact of arginine–phosphate interactions on the reentrant condensation of disordered proteins*, Samuel Lenton, Stefan Hervø-Hansen, Anton M. Popov, Mark D. Tully, Mikael Lund & Marie Skepö, 2021, In: Biomacromolecules.
 23. *Innovatively processed quinoa (Chenopodium quinoa Willd.) food: chemistry, structure and end-use characteristics*, Ramune Kuktaite, Ritva Repo-Carrasco-Valencia, Cesar C.H. de Mendoza, Tomás S. Plivelic, Stephen Hall & Eva Johansson, 2021, In: Journal of the Science of Food and Agriculture.
 24. *Localised strain in fissured clays: The combined effect of fissure orientation and confining pressure*, Erika Tudisco, Claudia Vitone, Cristina Mondello, Gioacchino Viggiani, Stefanos Athanasopoulos, Stephen A. Hall & Federica Cotecchia, 2021, In: Acta Geotechnica.
 25. *Membrane Protein Structures in Lipid Bilayers: Small-Angle Neutron Scattering With Contrast-Matched Bicontinuous Cubic Phases*, Charlotte E. Conn, Liliana de Campo, Andrew E. Whitten, Christopher J. Garvey, Anwen M. Krause-Heuer & Leonie van 't Hag, 2021, In: Frontiers in Chemistry.
 26. *Editorial: Membrane Structure and Dynamics Studied with Neutron Scattering*, Holderer, O., Koutsioubas, A., Garvey, C.J. and Nylander, T. 2021. In: Front. Chem.
 27. *Controlling Phase and Rheological Behaviours of Hexagonal Lyotropic Liquid Crystalline Templates for Nanostructural Administration and Retention",*, Wang, G., Garvey, C.J., Gu, S., Gao, W., O'Dell, L.A., Krause-Heuer, A.M., Darwish, T.A., Zhigunov, A., and Tong, X J. Coll. 2021, In: Journal of Colloid and Interface Science.
 28. *Solid state polymer architecture of empty fruit bunches of the African oil palm*, Jarrett, K., Buckley, C., and Garvey C.J. 2021. In: Rev. Adv. Chem., in press (2021).
 29. *Micro/nano-structural evolution in spruce wood during soda pulping*, Ahmed Wagih, Merima Hasani, Stephen A. Hall & Hans Theliander, 2021 Jan 6, In: Holzforschung.
 30. *Conformation of Myoglobin-Poly(Ethyl Ethylene Phosphate) Conjugates Probed by SANS: Correlation with Polymer Grafting Density and Interaction*, Daniela Russo, Christopher J. Garvey, Frederick R. Wurm & José Teixeira, 2021 Jan 4, In: Macromolecular Bioscience.
 31. *Building polymer-like clusters from colloidal particles with isotropic interactions, in aqueous solution*, Sara Haddadi, Marie Skepö, Patric Jannasch, Sophie Manner & Jan Forsman, 2021, In: Journal of Colloid and Interface Science. 581, p. 669-681 13 p.
 32. *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, 2021, In: Journal of Lipid Research. 62, 100004.
 33. *The Effects of Chain Length on the Structural Properties of Intrinsically Disordered Proteins in Concentrated Solutions*, Eric Fagerberg, Linda K. Mansson, Samuel Lenton & Marie Skepo, 2021, In: Journal of Physical Chemistry B. 124, 52, p. 11843–11853

34. *The Crystal Field Plasmon Splitting*, Stefano Antonio Mezzasalma, Marek Grzelczak, and Jordi Sancho-Parramon. 2021. ACS Photonics.
35. *Aquaglyceroporins and orthodox aquaporins in human adipocytes.*, Huang P, Hansen JS, Saba KH, Bergman A, Negoita F, Gourdon P, Hagström-Andersson A, Lindkvist-Petersson K. Biochim Biophys Acta Biomembr. 2022 Feb 1;1864(1):183795.
36. *Analyses of the complex formation of Staphylococcal Enterotoxin A and human gp130 cytokine receptor*, Sibel Uzunçayır, Arturo Vera-Rodriguez, Paulina Regenthal, Hannah Åbacka, Cecilia Emanuelsson, Christopher D. Bahl, Karin Lindkvist-Petersson. FEBS Lett. 2022 Jan 21. doi: 10.1002/1873-3468.14292. Online ahead of print.
37. *Neutron crystallography reveals mechanisms used by Pseudomonas aeruginosa for host-cell binding*, Lukas Gajdos, Matthew P Blakeley, Michael Haertlein, Trevor Forsyth, Juliette M Devos, Anne Imberty. Nat Commun. 2022 Jan 11;13(1):194. doi: 10.1038/s41467-021-27871-8.
38. *Conformation of poly(ethylene glycol) in aqueous cholinium amino acid hybrid solvents*, Brunner, M., Garvey, C.J., Warr, G.G. and Atkin, R. J. Coll. Interfac. Sci., 602, 334 (2021). doi: 10.1016/j.jcis.2021.06.015

Annex 4 – LINXS Community

In 2021 LINXS fellows came from the following organisations:

1. Aarhus University, Denmark
2. Alfa Laval Sweden
3. Arwa Foodtech AB, Sweden
4. Australian Synchrotron, Australia
5. Centro de Física de Materiales (CSIC-UPV/EHU), Spain
6. CFEL, Germany
7. Chalmers University of Technology, Sweden
8. CNRS, France
9. Deutsches Elektronen-Synchrotron DESY, Germany
10. Elettra - Sincrotrone Trieste SCpA, Italy
11. European Molecular Biology Laboratory (EMBL) Hamburg, Germany
12. European Spallation Source ESS AB, Sweden
13. Forschungszentrum Juelich GmbH, Germany
14. Fritz Haber Institute Berlin, Germany
15. Georgetown University, USA
16. Hamburg University, Germany
17. Inria / CNRS, France
18. Institut de Biologie Structurale - Grenoble, France
19. Institut Laue Langevin (ILL), France
20. ISIS Facility, STFC, United Kingdom
21. Johnson Matthey Formox AB, Sweden
22. Karolinska Institutet, Sweden
23. KTH Royal Institute of Technology, Sweden
24. La Trobe University, Australia
25. Linköping University, Sweden
26. Linnaeus University, Sweden
27. Lund University, Sweden
28. Malmö University, Sweden
29. MAX IV, Sweden
30. Northwestern University, USA
31. Norwegian University of Science and Technology, Norway
32. Novozymes, Lyngby, Denmark
33. Oatley, Sweden
34. Rensselaer Polytechnic University, USA
35. Research institutes of Sweden (RISE), Sweden
36. Sense Unlimited, Denmark
37. Stockholm University, Sweden
38. Swedish University of Agricultural Sciences (SLU), Sweden
39. Tampere University, Finland
40. Technical University Munich (TUM), Germany
41. Technical University of Denmark (DTU), Denmark
42. The "Abdus Salam" Int. Centre for Theoretical Physics, Italy

- 43. Tetra Pak, Sweden
- 44. University Düsseldorf, Germany
- 45. Universität Regensburg, Germany
- 46. University of Copenhagen, Denmark
- 47. University of Florida, USA
- 48. University of Gothenburg, Sweden
- 49. University of Luxemburg
- 50. University of Pavia/University College London, United Kingdom
- 51. Uppsala University, Sweden

Annex 5 – Financial reporting 2021

Income statement	Categories	Description	SEK
	Activities	Conference fee	0
	Activities Total		0
	Partners contribution	LTH-funding	2,000,000
		Medfak-funding*	1,000,000
		Natfak-funding	3,000,000
		LU Central-funding	2,000,000
	Partners contribution Total		8,000,000
	External Funding	Formas deferral	34,715
	External Funding Total		34,715
	Membership fees	Membership RISE	50,000
	Membership fees Total		50,000
Income Total			8,084,715
Expenditure	Activities	Conference cost	-92,862
		Hotel & housing	-58,324
		Other (filming, services)	-27,130
		Representation external	-24,611
		Travel	-29,104
	Activities Total		-232,032
	Equipment	Depreciation	-92,612
	Equipment Total		-92,612
	Materials & consumables	Office supplies	-32,059
		Other	-11,260
		Print material	-20,615
		Services	-20,799
		Travel	-14,549
	Materials & consumables Total		-99,281
	Overhead	OH	-1,736,123
	Overhead Total		-1,736,123
	Premises	Cleaning	-101,460
		Premises rent	-1,079,992
	Premises Total		-1,181,452
	Salaries	Salaries	-4,204,527
	Salaries Total		-4,204,527
Expenditure Total			-7,546,026
Annual Result			538,689

* In addition, the Lund University faculty of Medicine contributed in-kind with 20% of the salary of the LINXS co-director and of that of the ISB theme leader.

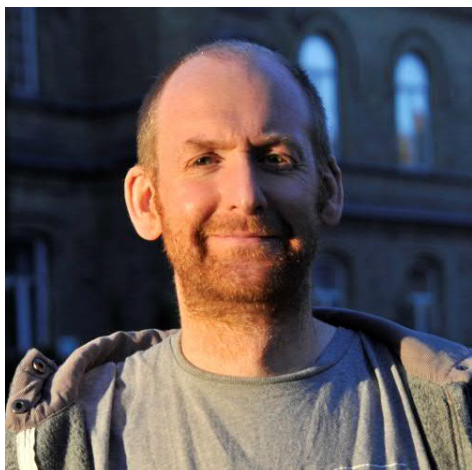
** Deferral of FORMAS project funding implemented in 2021.

Annex 6 – Highlights and Legacy statements

Legacy statement – Imaging

CREATING NEW COMMUNITIES - THE LEGACY OF THE IMAGING THEME

Reaching large research communities



“The imaging theme was first and foremost about opening up the potential of using x-ray and neutron imaging techniques to new communities”, says theme leader, and outgoing LINXS Director, Stephen Hall.

He led the theme from 2017 – 2021. Officially the theme should have concluded at the end of 2020, but various activities, that were delayed by the pandemic, have continued through 2021.

As he reflects back on the achievements of the theme’s core and working groups, one thing is clear: the greatest legacy of the theme overall is how it has sparked interest and curiosity to use X-ray and neutron imaging techniques to advance science over a broad spectrum of research areas, and involving many researchers who are completely new to the subject.

Stephen Hall gives some key examples of how the theme engaged a large group of researchers from different fields during its time at LINXS.

One such example was the very first workshop the theme organised back in 2017 on X-ray fluorescence imaging, which paved way for a new user group at NanoMAX at MAX IV and the building of a new working group, “New opportunities in Imaging with X-rays and Neutrons”.

The GeoArcheology and Cultural Heritage (GeoArCH) working group attracted new users and sparked interest in imaging techniques among, for example, archeologists and paleontologists, whereas the Soil Science working group connected biologist and soil experts to explore new methods and applications.

The hackathons, organised by the QuantIm working group, brought data analysts from around Europe, in particular from the [QIM project](#), together with researchers from many different research fields to discuss options and alternatives for improved data analysis and image quantification. This led to many new collaborations, as well as a template for a new way of collaborative working (the hackathons) at LINXS.

The working group on Food Science and Technology, reached out to food researchers in the region, including from industry and food companies, a group not connected to LINXS previously and not common users of X-rays and neutrons. Late in the Theme, an activity within the “New opportunities in Imaging with X-rays and Neutrons” working group developed (due to corona restrictions) into the webinar series, Co-Work, which focused on coherent diffraction imaging and Ptychography and Holography. This

webinar series brought together experts from all over the world for focused discussions on how to plan, conduct and analyse experiments exploiting the coherence properties of X-rays for advanced material characterization. This took place during the corona pandemic and was a great success due to responding to a real need to meet and discuss, even if it was on-line.

A strong ambition to introduce imaging techniques

– It has been great to see how new people and scientific fields have become interested in imaging with X-rays and neutrons during this time. I think it has to do both with working practices, and with the actual scientific direction of the working groups. We have also had a clear ambition to reach out to large communities who are less familiar with x-rays and neutrons, which has led to many new researchers coming into the field. Imaging is a very visual technique, which of course helps in attracting new users!

The overall effect of the theme is actual quite significant, says Stephen Hall. Both locally and on an international level one can start to see lasting impacts, way beyond the duration of the theme.

Consolidated communities around MAX IV and ESS

For example, locally, the theme has helped create a strong user group for fluorescence imaging in Lund, Sweden and in Denmark, as mentioned above. Based on theme's very first workshop on X-ray fluorescence imaging, MAX IV saw a great increase in applications to use fluorescence in experiments.

The hackathon concept, as a method to capture interest and initiate focused discussions, has also taken off and inspired other themes and working groups. The food working group, meanwhile, has not only gone on to form its very own theme at LINXS, Northern Lights on Food, but has also secured independent funding and is progressing with plans to establish a European Food Laboratory to be located in Science Village Scandinavia.

The theme has also helped to consolidate communities around MAX IV and ESS. Especially when it comes to pushing tomography as technique. For example, the theme helped in forming the communities around proposals for new imaging beamlines at MAX IV. Furthermore, connections made within the GeoArCH working groups led to a pan-european proposal towards supporting multi-model imaging at the future ODIN beamline at ESS. The theme, and LINXS, have also been instrumental in increasing the capacity and knowledge of early career researchers, e.g., with the organisation of doctoral schools on neutron imaging in collaboration with SwedNess and the first Northern Lights on Food master class.

Themes should not be afraid to follow new directions

When asked what he would do differently if he was to start the Imaging theme today, Stephen Hall responds that better planning and organisation are important, as is the need to follow new directions and not be afraid to stop activities that are not developing.

– Our theme grew organically which is great, but to ensure that you hit the ground running once the theme starts, planning in advance is good. Of course, the current

LINXS application process ensures that our new themes are better organised.

With better planning one can include more hands-on activities on part of the working groups, says Stephen Hall. For example, experiments at X-ray and neutron facilities, and more hands-on analysis of data. Such activities can in turn help push the advanced aspects of imaging forward – an aspect which he would have liked to see further developed during the theme.

– For example, one could have hackathons extended over a couple of weeks, bring people together over longer time periods, and work more long term in building up the understanding and capacity of the user communities. This way of working, I think, could have had a greater impact in terms of creating opportunities to discuss more, and do more science.

Potential for having shorter running themes could be explored

A faster working pace could also be something for new themes to explore, he reflects. While three years is a good time to get things started, it could also be too long – if it is the case that people have achieved what they want to achieve.

– In that sense, having working groups running for a shorter time could be a way forward – to enable people to go where the passion is, and focus efforts onto one

question. It would also allow the theme, and in extension LINXS, to be more dynamic and respond to changing scientific needs, that can lead on to targeted applications for beamtime at facilities or new grant applications.

People and their engagement at the core of LINXS

A final question is how one keeps the momentum of the themes going – especially when the activities within the working groups are very much based on interest, passion and ideas, as opposed to financial recompense.

– With a place like LINXS, it will always be about the people and their engagement. Going forward, there needs to be more discussion of how LINXS can support themes to develop to their full potential, and how researchers involved in themes can have more structure in terms of organising activities and developing their ideas.

– One has to remember, that there are very few arenas that support X-ray and neutron science in the way LINXS does, in terms of organising and funding collaborative events and activities, and providing a platform to meet. This is at the core of LINXS, and is a great precursor for successful themes, as long as we continue to get enthusiastic people; with a vision and passion to push forward scientific ideas, he concludes.



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Legacy statement – Dynamics

TACKLING RESEARCH QUESTIONS AT THE ABSOLUTE FOREFRONT – THE IMPACT OF THE DYNAMICS THEME

Antibodies, XPCS, Simulation, theory, and software development

“The Dynamics theme made it possible for research groups to focus on research questions that are much bigger than one researcher can tackle alone”, say theme leader, Professor Marie Skepö, and founding LINXS Director, Professor Peter Schurtenberger.

The Dynamics theme was one of the two first themes to form at LINXS back in 2017. As its activities are coming to an end, Peter Schurtenberger, and Marie Skepö reflect on some of the main achievements, and the importance of LINXS as a strong incubator for neutron and X-ray science.

The creation of the *Antibodies in solution* research programme within the working group “Dynamics and Structure of Biological Macromolecules” is a major milestone for the Dynamics theme. The idea for the programme grew out of an



Professor Peter Schurtenberger

early workshop on dynamics of biological macromolecules. A need to secure sufficient amounts of well-defined antibodies was identified – in order to perform research that covers relevant length and time scales to understand the physical properties of individual antibodies as well as those of concentrated solutions. Today, the research programme gathers 14 international research groups, with four groups from Lund University, as well as a pharmaceutical company and the American National Institute of Standards and Technology (NIST).

– Without LINXS as an incubator, the programme would not have been successful. We needed an independent broker that could gather us researchers under common goals, and to help us sustain the effort. For me, this is a prime example of what can be achieved if you have genuine support for a bottom-up approach, says Peter Schurtenberger, professor in Physical Chemistry at Lund University.



Professor Marie Skepö

Marie Skepö, professor in Theoretical Chemistry at Lund University, adds that other significant achievements include the take-off of the research programme on *Simulation, theory, and software development for anisotropic systems*, where researchers came together to share ideas and advance the methodological toolbox for analysing, understanding, and predicting experiments with X-rays and neutrons. This programme has now merged into the Antibodies programme's efforts. Researchers from the Dynamics theme have also been involved in other LINXS initiatives such as the Northern Lights on Food theme.

Another example is the outcomes from the working group on *Characterizing soft matter with X-ray Photon Correlation Spectroscopy (XPCS)*. Based on the group's work, in 2020, funding was granted for a large-scale international research project, *Dynamics of proteins in crowded environments on multiple length and time scales*, in the frame of a so-called Röntgen-Ångström Cluster, led by Professor Christian Gutt from the University of Siegen in Germany and Peter Schurtenberger. Another side-effect is that it has helped to boost the corresponding interests and activities at MAX IV, which has now also led to a successful application to VR for a new detector more suitable for using the technique.

– The knock-on effects of our initial work are great, because XPCS is different to other comparable techniques since you can measure motion of nanoparticles on small length scales. In the case of proteins, the distances you can measure actually correspond to the size of the protein, and how it moves until it encounters a neighboring protein. XPCS is therefore the only technique that can currently reveal slow motion of proteins in highly

concentrated solutions on these length scales, says Peter Schurtenberger.

Impacts that will last long beyond the theme

The research programme on utilizing the Grazing-Incidence Small-Angle Neutron Scattering (GISANS) technique that started within the "Dynamics and Structure of Membranes and their Constituents" working group is another example of long-term impact. It has been instrumental in creating a concerted national effort for the design and construction of a GISANS instrument that could provide unique knowledge of surface layers for potential use in a large variety of areas such as developing new medicines, packaging, batteries and other applications. The Swedish Research Council VR has now granted funding for a feasibility study for such an instrument at ESS.

At its core, the Dynamics theme - and its legacy- is about the people. Both the many researchers involved, as well as the inspiring guest researchers who have been connected to the theme over the years, say Marie and Peter.

– Our theme has paved the ground for setting up new constellations of people and focused on research questions that are much bigger than one researcher can tackle alone. By combining different experimental and theoretical techniques and backgrounds of the people involved, we become stronger. Now, theoreticians and experimentalists work together with research questions at the absolute forefront, both regarding scientific questions as such, as well as method development, says Marie Skepö.

Peter Schurtenberger adds that the combination of people with different

backgrounds has served the antibodies programme well. It was essential in creating a strong research consortium and plan that finally convinced NIST to provide the programme with their well-defined antibody, successfully ending an effort of more than two years to secure the required large quantities of material that was initially identified as the most important obstacle by the community. Since the programme will continue its work under the newly accepted LINXS theme: Integrative Pharmacology and Drug Design (IPDD) which will start in 2022, the expertise built up during the Dynamics theme will continue to feed into new LINXS initiatives, and by extension help to further develop X-ray and neutron science.

– The legacy of our theme, which can be seen on a local, national, and international level, in terms of the many important collaborations we have managed to establish, will only continue to grow as the years pass, says Peter Schurtenberger.

How can LINXS support future themes?

Both Peter and Marie are in strong agreement that LINXS should continue to be a place that can offer researchers an interdisciplinary environment free from the pressures of grant writing and funding expectations – as a way to enable themes and science to grow.

– Researchers are busy and they always have a lot on their agenda. Therefore, it is important that LINXS continues to offer a relaxed environment without demands, where researchers can meet and discuss interesting problems. The drive for researchers in general is curiosity, and LINXS should be a place where they can meet and discuss freely, without being

busy thinking: When is my next meeting?
says Marie Skepö.

Peter Schurtenberger adds:

– There is already so much steering of research on a political level. Great ideas come out of free research, and for that reason, I believe that the best way LINXS can support researchers is by maintaining a bottom-up approach, where themes are formed based on a genuine interest. That is also why some of our theme's early endeavours failed, because they were not based on what the scientists were actually curious about.

Apart from a free and open environment, Peter adds that LINXS should continue with the current support structures.

– LINXS offers an infrastructure for new concerted efforts. And this is important, because funding is not everything. LINXS has helped to push themes and should continue to find out what researchers need beyond funding. You need this willingness on behalf of the organisation to help. Things like administrative and technical support, catering and help to organise workshops cannot be underestimated, says Peter Schurtenberger.

In the future, Marie and Peter believe that digital efforts need to be further developed, both for the climate, and for the potential they represent for LINXS to expand to new audiences.

– A message that I would like to pass forward to new themes, is that the possibility to reach out has increased a lot with digital meetings, and in the future, I foresee that a combination of in person meetings and digital meetings is very good. In that way, LINXS becomes

inclusive and open to everyone that is interested, says Marie Skepö.

– Yes, we need to act responsibly in terms of our climate, and here LINXS could possibly create an important profile as an institute that really pushes both digital and hybrid ways of working, Peter Schurtenberger concludes.

Highlight – Collaboration

From kitchen tomography to a cutting-edge neutron imaging beamline

Link to original article, published Oct 11th, 2021:

[From kitchen tomography to a cutting edge neutron imaging beamline — LINXS](#)



Emanuel Larsson illustrates how the latest version of his kitchen-based light tomography (KBLT) scanner works. Photo: Noomi Egan.

A late Friday night in December 2018, Emanuel Larsson, who was working at RISE Research Institutes of Sweden at the time, started to assemble a small-scale tomography scanner in his kitchen, made up by everyday objects such as a camera, a water bottle, Lego pieces, and a flashlight. Why? To be able to better teach tomographic imaging to Swedish industry representatives and students.

Today, his model is used as a prototype to help prepare for future neutron beamlines at ESS - as part of a collaborative project between LTH and ESS, hosted by LINXS this summer.

– I had noticed that it was quite hard for people to grasp the basic principle of tomographic imaging. That made me want to build a model where you can actually show what is going on. I used stuff I found in the house, and I realised that they worked well to illustrate how one can scan, reconstruct and render a sample in 3D, says Emanuel Larsson.

Neutron tomography is an imaging technique that allows visualisation of samples in three dimensions. The sample rotates in the beam and multiple 2D radiography images are recorded with high-speed digital cameras.

A 3D representation of the volume of the object can be reconstructed using a mathematical algorithm. The technique also enables the visualisation of fluids, such as water or oil in large metal objects.

Neutron tomography is pivotal to many future breakthroughs since it is non-destructive and can thus be used to investigate the temporal and spatial resolution down to the micrometre scale in samples of both soft and hard matter- for example energy- and engineering materials, biological and geological samples and cultural heritage artefacts.

The model has evolved over time

Emanuel Larsson's first model was very basic. He used a paper screen, a light, a camera, and a sample. He took a photo of the sample, for example a water bottle, then he rotated it and took a new image, until he had captured the sample over 360 degrees. Three years later, that very first model has evolved – and now Emanuel is on version 25. The new model is refined but is still using the same flashlight and is now connected to a single board Raspberry Pi 4 computer. The sample can rotate 200 steps over 360 degrees, which should be compared to tomography setups at large scale research facilities where often thousands of radiographic images are captured of a sample over 360 degrees. In addition, Emanuel has also set

up user-friendly image reconstruction and analysis pipeline which can be applied both on the acquired and reconstructed data sets.

– Even though the model is quite basic it does the job. We did a comparison where we scanned a Lego figure with my model, and with real x-rays with the lab tomograph in the 4D Imaging Lab at the Division of Solid Mechanics at Lund University. And the results were not that different! The regular light could of course not penetrate through the plastic, as with the x-rays, but in both experiments you can see the outline of the figure in 3D.

The model is used as a prototype for ODIN at ESS

Today, Emanuel's model is not only used in the teaching he does in his new positions as a Method Expert in X-ray and Neutron Imaging at the Division of Solid Mechanics and as an Application Expert in Tomographic Imaging and Image Analysis at LUNARC, the Center for Scientific and Technical Computing at Lund University, it is also used as a prototype for the test beamline YMIR for the future imaging beamline ODIN, which will be built at ESS. This is because the techniques employed in

the model can be used to test both hardware and software pipelines both with light tomography and neutron tomography – even though Emanuel's model fits on two tables, and a neutron beamline fits in a very large room!

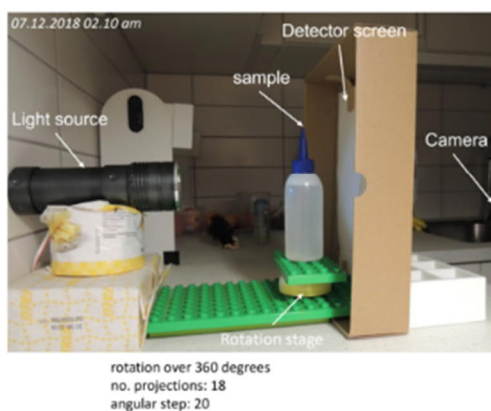
Samuel Staines, a master student at the Division of Solid Mechanics, is responsible for designing a replica of the model which can be compatible with what is needed for the new YMIR test beamline and the future ODIN beamline at ESS. He explains that it works just as well to use normal light as it would to use neutrons in order to test out how the beamline might behave. Before the ODIN beamline is built, the techniques will be tested in the test beamline, YMIR.

– There is a huge amount of work you need to do to develop a new beamline. That is why you need to test the platform, including hardware and software pipelines in multiple ways. One way is to refine and test in a smaller scale to get ideas on where the challenges and pitfalls will lie with the new instrument, says Samuel Staines.

Improving data collection strategies

Stefanos Athanasopoulos, who is a Guest Researcher at the Division of Solid

Setup of kitchen-based light tomography (KBLT) v.1.0



*The very first version of the KBLT scanner was very basic and built of objects such as a paper screen, a light, a camera and a sample such as a water bottle.
Credit: Emanuel Larsson.*

Mechanics is also involved in the project with ESS. His work is focused on improving the data collection strategies for future experiments at large scale research facilities.

– A big part of developing a new beamline is also about testing optimal ways for data collection. How will it actually work when a user comes in and runs an experiment? At the moment a lot of data is acquired from the experiments, says Stefanos Athanasopoulos.

– The ideal solution would be to build a single log file with all the data and information about the experimental setup so that you get everything in one place. That file can then be used by different researchers, not just the person conducting the actual experiments.

The model makes techniques available to more students

Emanuel Larsson is also planning to make the code of his model freely available to students across the world – with the help of LINXS and Stephen Hall, outgoing Director of LINXS, and Senior Lecturer at the Division of Solid Mechanics at LTH. The idea is to publish an article on the kitchen tomography lab scanner, along with making the code available to download from the platform GitHub. If this plan succeeds, the cost of teaching students tomography techniques can be reduced drastically. Today, x-ray tomography scanners in laboratories can cost between 40 k€ to 1 M€. In comparison, the kitchen tomography scanner model can be built with readily available materials for between 100€ to 1000€, depending on which version of the KBLT scanner the students would like to build.

– Hopefully, the model can help inspire more students to start using imaging techniques in their research early on. It

allows them to play around with samples and sample environments – for example what will happen if you point a heat gun onto a rotating sample, and image the change in 3D over time, thus meaning 4D?



Stefanos Athanasopoulos, Samuel Staines and Emanuel Larsson have collaborated on the project which aims to help prepare for future neutron beamlines at ESS, hosted at LINXS this summer. Photo: Noomi Egan.

While using the model, students will also learn important skills in engineering, image reconstruction, analysis and 3D-rendering. Skills that will come in handy for future imaging experiments both at ESS and MAX IV.

– In a few years models like the kitchen tomography scanner could have huge impact in terms of increasing the user base of people using the techniques offered at large scale research facilities. It is all about inspiring people and making it easy to learn, test things and have fun at the same time, Emanuel Larsson concludes.

Researchers from ESS who are involved in the project:

- Kenan Murić, Data Acquisition Scientist, ESS.
- Robin Woracek, Instrument Scientist, ESS.
- Søren Schmidt, Senior Scientist, ESS.
- Tobias Richter, Group Leader for Experiment Control and Data Curation, ESS



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NEUTRON AND X-RAY SCIENCE

Highlight – Northern Lights on Food Theme

Link to original article, published June 21st, 2021:

<https://www.linxs.se/news/2021/6/21/the-northern-light-on-food-conference-highlights-the-need-for-a-food-network-for-scientists>

THE NORTHERN LIGHTS ON FOOD CONFERENCE HIGHLIGHTS THE NEED FOR A FOOD NETWORK FOR SCIENTISTS

The Northern Lights on Food II conference brought together researchers from academia and industry with the aim to establish a food network that will enable researchers to take full advantage of the new tools provided by large scale research infrastructures such as the ESS and MAX IV in Lund, Sweden. It was organised by the Food Science and Technology working group at LINXS.

A close to 140 participants, as well as keynote speakers and panelists, gathered for the online event, which took place over three days. It was opened by introductory remarks from the Lund University vice-chancellor, Prof. Erik Renström. In this interview, some of the keynote speakers and participants, share their reflections on the conference - which is a follow up activity on the successful Northern Lights on Food workshop in 2019.



Benjamin Boyd is professor at Monash University, Australia, and soon to commence a Novo Nordisk Laureate Research Fellowship at the University of Copenhagen. He is also core member of the new Northern Lights on Food theme at LINXS. Mario Martinez-Martinez is tenure-track assistant professor at Aarhus University (Denmark) with a focus on carbohydrates. Photo.

– The great science, collegial nature of the participants, and the many future potential intersections really highlighted the timeliness and need for a food network for researchers. This was not so much a surprise but a great validation of the concept we are trying to establish, says keynote speaker, Benjamin Boyd, professor at Monash University, Australia,

and soon to commence a Novo Nordisk Laureate Research Fellowship at the University of Copenhagen. He is also core member of the new Northern Lights on Food theme at LINXS.

– Especially bringing together such a great array of scientists across the food and scattering communities was brilliant: the speakers and also the attendance list was really a who's who from the Oresund region and beyond, so I was very impressed.

Mario Martinez-Martinez, tenure-track assistant professor at Aarhus University (Denmark) with a focus on carbohydrates, participated in the conference:

– The scientific rigor of the talks was at the highest level, covering the entire spectrum of structuring food macromolecules. I really enjoyed the talks. One interesting observation is that many of the researchers work on systems that might be too pure to resemble reality. This can represent a limitation that we need to be aware of going forward.

Research frontiers in food

When asked what Benjamin Boyd sees as research frontiers in food science, he responds.

– I think it is fair to say, that in the past, a large part of the food science spectrum has been too empirical. As approaches to study the structure in food systems are developed and matured, these new levels of understanding of how structure dictates performance, will enable true engineering of foods that are not only optimal from a composition perspective, but where structure is a much more important design feature.

– I also believe that understanding the interplay between structure and interactions with gut biology will be crucial for understanding the positive and negative impact of food, and x-ray and neutron scattering techniques are at the appropriate length scales to make a huge impact in this regard.

Mario Martinez-Martinez adds that, as a society and food scientists, we are now in an exciting time for science, since finding the crossover between nutrition and sustainability will dictate the most important aspects of food production and consumption.

– As an example, having livestock as the primary source of protein globally, considering the growing population, could be argued to potentially result in serious consequences for global protein security in the near future. But it is difficult to engineer those palatable and indulgent structures with the complex and diverse biopolymeric plant tissues.

He continues:

– Likewise, fighting chronic diseases, such as type-2 diabetes, obesity and cancer, through strategies emphasising individual willpower and personal responsibility is not enough unfortunately. Developing structured carbohydrate foods with the right dietary fiber and associated metabolites will become paramount, whose engineering principles would have to be built on clear structure-function relationships.

Mario Martinez-Martinez believes that the successful re-integration of fruit and vegetable waste is a good example of a strategy to move forward, yet the structuring and colloidal properties of such by-products needs to be understood at different length and processing scales.

– Because maintaining health is not only about reaching for that apple in the basket. We need indulgent foods that are more nutritious, healthy and sustainable.

Next steps

Going forward, Benjamin Boyd would like to see the development of a joint roadmap produced by both industry and academics.

– It would be great if we could get industry and academics together to develop a roadmap of what problems are unsolved, what areas are underdeveloped, and where the intersections are to develop new techniques/experimental formats to answer those questions. For me, this is clearly the next step, and the working groups within the coming theme Northern Lights on Food are in a good position to focus on these objectives.

It will also be key to start meeting in person, and not only online, he emphasises.

– Getting people together in person and not virtually is crucial. It is also very important to provide industry with a very clear picture of how scattering science can help them to solve problems - in a language understood by industrial scientists.

Mario Martinez-Martinez agrees that all the sectors that have an interest in food should be brought together with a clear understanding of their strengths and weaknesses.

– On the one hand, we have the small companies that are agile enough to materialise new ideas. Then we have the large companies, that have money and a scientific workforce, but whose size-derived inertia could halt new ideas to see the light.

– Above all, big and small companies, together with academics and policy makers, should jointly prioritise human and environmental health moving forward, he concludes.

The working group Food Science and Technology was formed under the Imaging theme but has now progressed and formed a new theme at LINXS, Northern Lights on Food. The theme will start in August 2021 and run for three years. One long-term goal is, thanks to the collaboration established through LINXS activities, to establish an interdisciplinary European Food Laboratory next to Max IV, ESS and the future location of LINXS at Brunnshög. These aspects were discussed in a panel debate at the conference, moderated by Pia Kinhult.

– To meet the need to transform the food systems we have to establish inclusive, efficient, sustainable, nutritious and healthy food systems capable of achieving the SDGs. The Northern Light on Food initiative is making one vital effort to make this happen by increasing the awareness in the research community of new and advanced techniques and also building bridges between academia and industry. Innovation in technologies, policies and new institutions will be critical. I am looking forward to the European Food Laboratory taking on this role in the future.

Pia Kinhult, Head of Host States Relations, ESS

Highlight – New Materials Theme

Link to original article, published Feb 1st, 2021:

<https://www.linxs.se/news/2022/2/10/58fuufjfe60tl3z0f0jxw59umd320v>

XAS SCHOOL PROVIDES PRACTICAL AND USEFUL SKILLS – WILL BE REPEATED ANNUALLY

In the first week of November 2021, an intensive hands-on crash course in the planning, performance and evaluation of X-ray absorption spectroscopy was conducted. Inspired by the success of a long running course, the course team, headed by Jens Uhlig, Lector at Lund University at Chemical Physics, modernised the approach and in close collaboration with MAX IV, developed a new concept.

The design consisted of one third part lectures, another third on data Analysis and the last third part on practical work, including sample preparation and a mini beamtime. The course was given by teachers from Lund university, Malmö university and MAX IV and received great interest from the very beginning.

Limited by practical aspects, much less than 50 percent of the applications could be accepted to this first round. 20 participants could join and based on an anonymous course evaluation the participants were very happy with both the concept and this year's course and are looking forward to using their newfound skills in future work.

“Through such intensive and practical training session we are forming a new generation of scientists that can propose and perform better experiments at our facilities. This course will be repeated annually and will form the first of multiple training opportunities provided to national and international researchers by scientists under the egis of LINXS”, says Jens Uhlig.



XAS School 2021 participants at LINXS facilities

Highlight – Integrative Structural Biology Theme

Link to original article, published January 24th, 2021:

[Great response to second workshop on Membrane Proteins — LINXS](#)

GREAT RESPONSE TO SECOND WORKSHOP ON MEMBRANE PROTEINS

In December 2021, the Membrane Proteins Working group held their second workshop, following up on the very successful one in May with more than 200 participants from a range of disciplines. The topics for the winter workshop was related to “Structural Resolution of Membrane Proteins: From Sample Preparation to Structural Resolution”.

In the first online workshop in May 2021, several aspects of expression systems, protein purification, membrane solubilization and other preparation methods were discussed. In December more topics were covered such as multi-protein complexes, detergent trials and crystallization strategies such as LCP and Hi-LIDE.



Erika Tóth, coordinator of the Membrane Protein workshops.

“In addition, we had also invited scientists to introduce their best practices on Cryo-EM and neutron structures, scattering techniques, and data collection and processing, says Erika Tóth, postdoc at Lund University and coordinator of the workshops. “The production of high-quality membrane protein crystals is always very challenging. We were able to cover many steps of the processes and get good advice on how to figure out the best way to prepare samples, which methods to use, understand more about data models and new software as well as how to conduct experiments at MAX IV.

NEW TECHNIQUES AND HOT TOPICS

The range of participants from PhD students to senior researchers was valuable. The younger researchers could talk in more detail about technical aspects from their lab work which many found very useful. The senior researchers contributed with perspectives on what they see ahead from decades of experience in the field.

“We had really good discussions and got a broad overview of new techniques and hot topics. In this field negative results do not get published and that can lead to that people might try to the same things. With this kind of open sharing, we can learn also what does not work so well. Everyone gets stuck somewhere in this pipeline”, explains Erika Tóth.

The workshop offered both longer keynote presentations and smaller talks, promoting interaction and Q&A sessions. Speakers included Maria Marta Garcia Alai and Christian Löw from EMBL, Hamburg, Petra Fromme, Arizona State University, Gisela Bränden, University of Gothenburg, Alessandra Luchini, PSI and Erik Lindahl, Stockholm University.

VALUABLE KNOWLEDGE EXCHANGE

An important part was to connect people and although the ambition was to hold a hybrid meeting, it had to be an online event in the end as the omicron version of the corona virus was spreading everywhere. On the positive side it made it easy for a broad international participation and speakers from the US to join over the two-day schedule.

“People really wanted to reach out, to be able to share data and find potential collaborations. Many have overlapping study subjects and can benefit from different approaches and methods to try. For those who are new to the field this kind of opportunity is very useful. We hosted a friendly environment where you could ask any questions you wanted. It was two days of really good networking opportunities, concludes Erika Tóth.

([Membrane proteins: advanced level problem solving without “one size fits all” solution — LINXS](#))

