

LINXS Annual Report 2019

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Executive Summary and reflections from the LINXS Director

In 2019, LINXS made strong progress in its mission to become a nucleus for x-ray and neutron based research. This was achieved through a significant number of successful, high quality scientific activities, including hackathons, workshops, symposia and conferences, as well as a solidification and extension of the LINXS scientific portfolio within and between the existing themes, including new working groups (WGs) and the development of “research programmes” (RPs). Participants in our activities number in the hundreds, and the visibility and identity of LINXS was strengthened by participation in strategic outreach events at the local and national level. The LINXS visiting researcher programme was initiated and we welcomed our first guest researchers; this is a key mechanism for attracting high profile researchers to LINXS, who, in turn, attract other researchers. The first LINXS post-doc was also recruited, in part towards developing the participation of early stage researchers in LINXS. We have also started seeing research publications from our researchers with the LINXS affiliation in different academic journals. Most importantly, LINXS is developing as a place (physical and philosophical) where researchers from different institutes around the world and different scientific domains and perspectives come together to interact, discuss and develop new ideas.

2019 has also been a year of developing and clarifying our operational and working procedures to professionalise and improve our support to the LINXS community and to provide a strong foundation for the realisation of our overall strategic objectives and mission. Central to this work has been involving the community in the discussion on how LINXS should develop and how it can best enable the advancement of science using neutrons and x-rays.

As we look back on the year, it is clear that, in relative terms, LINXS progressed well in its mission and delivered according to the strategic and operational plan defined at the start of the year. Good progress has been made in anchoring LINXS in Lund as well as on the national and international level. We have established mechanisms for working proactively to bring researchers together and in promoting interactions within and across disciplines to fertilise research in x-ray and neutron science. Moreover, LINXS has contributed to the growing national discussion on how to maximise the benefits of the large-scale research x-ray and neutron infrastructures in the country, i.e., MAX IV and ESS. We also initiated the process of renewal and evolution of LINXS with the call for a new Theme and the search for a new LINXS director.

As we head into 2020, we look forward to welcoming a new theme and WGs, and to continue solidifying the interaction within and across the LINXS community, attract new users, create new networks and to further promote science and education focusing on the use of neutrons and x-rays.

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 2019.

The SAB commends LINXS for its progress and achievements in 2019, especially in developing the scientific environment around research using neutrons and x-rays, encouraging exchanges between researchers with different backgrounds and bringing together international, national and local researchers. LINXS's three themes have been successfully initiated and developed over the past two years. LINXS activities are already of a high scientific quality and have stimulated scientific discussion focusing on the use of neutrons and x-rays in a range of scientific areas. LINXS is, thus, working well towards achieving its mission.

Scientific quality is of the utmost importance and a successful visiting researcher programme plays an important role in this; the SAB would like to see this further developed in the coming years and to see an even greater integration of LINXS in the local, national and international scientific landscape. In 2020, the SAB would like LINXS to further define its scope, develop strategic collaborations and work towards mitigation of identified risks.

LINXS scientific achievements and impact

During 2019, LINXS had three running themes with 12 associated working groups (WGs), within which there are four Research Programmes (RPs) (see Annex 2). The increase in the number of WGs during the year and the breadth of science represented is a testament to the growing interest in exploiting x-rays and neutrons in an increasing range of research areas and

LINXS role in catalysing this interest. In the following, the scientific activity in the three current themes is summarised and some representative cases are presented in Annex 5.

Imaging Theme

The Imaging theme ramped up its activity in 2019 within its six WGs. This included a reorganisation to form a new WG on “New Opportunities in Imaging with X-rays and Neutrons” plus two new WGs in “TBS: Tomography of Biological Samples” and “Food science and Technology”; the latter has evolved to be a cross-theme WG with the Dynamics theme.

Key moments of the year include the GeoArCH symposium in January, which brought together experienced users of x-rays and neutrons, in particular from the Munich neutron source, FRMII, and the Elettra Synchrotron in Trieste, with a large group of potential new x-ray and neutron users from around Sweden, Denmark and beyond. Several new collaborations were established at this event and plans were made for, amongst other activities, try-out workshops at the two facilities, which will take place in 2020. GeoArCH also organised a special session at the MAX IV user meeting in the autumn to highlight the large potential for the use of x-rays in the areas of geology, archaeology and cultural heritage.

The “QUANTIM” WG held hackathons where image analysis experts and researchers from different fields with tomographic data analysis challenges spent 2-3 days of intense collaborative work to extract quantitative data from 3D and 4D image sets. This has led to new collaborations with, for example, the QIM project (a collaborative project between DTU, UCPH, LU and MAX IV: <http://qim.compute.dtu.dk>). A number of focused workshops/seminars were also held by the QUANTIM and “new opportunities” WGs, including on “Inverse problems in X-ray phase retrieval and tomography”.

Midsummer was marked by a very successful workshop on “x-ray and neutron imaging applications in soil sciences”, which introduced new users from soil science and related areas to x-ray and neutron methods, established new national and international connections and highlighted the activities in this area in Sweden on an international level. The WGs also worked to establish a strong program for 2020, which will be the final year of the Imaging Theme. The conclusion of the theme will be marked with a symposium in December 2020, where the progress, outcomes and perspectives will be presented and discussed by the community.

Reflections and insights from the “Workshop for x-ray and neutron imaging applications in soil sciences” is included in Annex 5 as a representative LINXS story for 2019.

Dynamics Theme

The LINXS dynamics theme progressed very well through 2019 with an intensification of the research activities. The WGs have been extended with new fellows and the work was focussed through the initiation of four RPs. The RPs are the outcome of some very successful workshops during 2018, and their direction is based on the round table discussions and identified needs from the research community. These four RPs form the core of the Theme work and are described in more detail below. The first two RPs belong to the “Dynamics and structure of biological macromolecules” WG and the latter two to the “Dynamics and structure of membranes and their constituents” WG.

1. Simulation, theory, and software development for anisotropic systems

Solving the structure of complex molecular systems, such as anisotropic colloids, proteins and viruses, poses a particular challenge due to intermolecular interactions between solutes, co-solutes and the solvent. In October 2019, a first planning meeting for the RP was held with eight invited participants, including chemists, physicists, experimentalists, theoreticians and software developers from three Swedish universities, two international universities and ESS in Denmark and Sweden. Three overall focus topics were identified: (i) software development and model implementation in SasView; (ii) calculation of scattering patterns from interacting biomolecules; (iii) effects of biomolecular concentration on stability and dynamics. The first research project is in progress and involves, primarily, LU and Århus University with a focus on calculating water solvation contributions in concentrated protein solutions.

Reflections and insights from the RP's work: "Expanding the toolbox for neutron and X-ray experiments – a snapshot of the work of LINXS research programme: Simulation, theory, and software development for anisotropic systems" is included in Annex 5, as a representative LINXS case for 2019.

II. Antibodies in Solution

The characterization and understanding of the static and dynamic properties of antibody solutions received particular attention at the round table discussions of the LINXS workshop on the "Dynamics of Biological Macromolecules" in June 2018. This hot topic clearly emerged as one where LINXS could, and should, play a central role. It was decided that LINXS should coordinate a concerted effort in this area based on assured access to sufficiently large quantities of high-quality anti-body material and by leading an internationally coordinated research program using this material. The RP "Antibodies in solution" was thus created with the first task, in 2019, of securing sufficient quantities of one or more monoclonal antibodies. Chances are high that the ongoing negotiations will come to a successful end in the beginning of 2020. The RP has also brought together leading experimentalists, theoreticians and simulators in the field from all over the world, who have committed to work on the characterisation of these antibodies in a coherent, efficient and synergistic way. A kick-off meeting with these key scientists is in its planning phase and will most probably take place in the second half of 2020 at LINXS, once the antibody material supply has been secured.

III. Structure and dynamics utilizing the GISANS technique

During 2019, LINXS led an initiative to bring the Swedish community together to form a Swedish-led consortium around the GISANS techniques and the future instrument (SAGA) at ESS. A strategy document was developed and submitted to the Swedish Research Council in September. This strategy was very well received and a follow up meeting was held at LINXS in December. The action plan involves obtaining funding for a postdoc shared between Swedish universities and ESS: it was proposed by the community that this postdoc be placed at LINXS. The focus of the RP is on developing the science and the community around GISANS and not on the building of the instrument, which is a longer term objective of the Swedish-led consortium that the RP will feed into.

IV. Sample environment and data evaluation of biological membranes

The main activity of the RP has been developing a new concept to study non-lamellar lipid phases and to be able to monitor transitions of lipids due to lipase activity. This work has focussed around the visiting LINXS fellows Prof. Campos Terán and Dr. Garvey. Outreach activities have involved participation and presentations at the Biophysical Society meeting in

Baltimore and the dedicated biomembrane session at ACS in Orlando, as well as the Bilayers at ILL meeting in Grenoble. The core members of the WG are working to put the activity of the WG in a larger perspective, i.e. extending the collaboration with the ISB and Imaging themes at LINXS.

In the context of the activities described above, the Dynamics Theme had the privilege to welcome their first guest researchers as visiting LINXS fellows: Prof. Jan Dhont from Forschungszentrum Jülich, Germany; Prof. Thomas Hellweg, Bielefeld University, Germany; Prof. José Campos Terán, Universidad Autónoma Metropolitana Unidad Cuajimalpa, Mexico; and Dr. Chris Garvey, from the Australian Nuclear Science and Technology Organization, Australia. The visiting researcher programme report is included in Annex 4.

Integrative Structural Biology (ISB) Theme

2019 was a year of many positive developments for the Integrative Structural Biology theme. Following the 1st ISB symposium in late 2018, new WGs were formed with foci on very timely and highly relevant scientific areas and research questions. All WGs met in the beginning of the year to share and discuss ideas and potential interaction points. One outcome was that the Biocompute WG was expanded to also include artificial intelligence and machine learning. The new “Amyloid: an Integrative Approach” WG had its first workshop with focus on gaps in amyloid fiber structure analysis. Discussions were focused on a wide range of topics ranging from sample acquisition over structure determination modalities to data processing and integration of results. The workshop also identified additional areas of interest which resulted in the planning of several, focused workshops in 2020, for example on clinical aspects.

The “Membrane Proteins – Structural Resolution and Homology Modeling”¹ WG 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 WG, identification key topics that will be addressed and suggestions for activities. The WG is looking forward to launching its first activities during 2020, including a workshop in November with a focus on Sample preparation and Quality Control.

The Time Resolved Structural Biology WG was formed during 2019 and had a few meetings including video meetings during the year involving different constellations of the WG members who are spread over the world. The work concentrated on the organization of an up-coming workshop in May 2020 starting with discussions on how we can best contribute to the development of structural biology – what areas of research will benefit from time-resolved studies and how different techniques can be combined in the best way. The WG arranged for a guest researcher visit during 2020, Stefano Mezzasalma, who will in particular use his sabbatical to work on theoretical aspects of time-resolved experiments.

The theme arranged the 2nd ISB symposium in October 2019. While the 1st symposium demonstrated the roles different techniques can play for integrative structural biology, the 2nd symposium concentrated more on the science. The theme core group (CG) received a lot of positive feedback including that the mix of young speakers and keynote speakers contributed to the vivid discussions and promoted collaborations. The Integrative Structural Biology theme look forward to an exciting 2020.

¹ Not included in Annex 2 pending formal approval.

Reflections and insights from the “2nd Symposium - Integrative Structural Biology” as a representative LINXS story for 2019 is included in Annex 5.

LINXS Strategic & Operational Achievements

LINXS set a specific strategic and operational plan in the beginning of 2019 which helped to guide and streamline efforts in consolidating LINXS as an institute, in realising the LINXS activities and in developing conditions to allow future growth towards the realisation of its mission. The following summarises the development of LINXS in 2019 with respect to this strategic and operational plan.

Strategic objectives

- ***Establish LINXS as a nucleus for x-ray and neutron-based research in Lund***

During 2019, LINXS WGs further developed their scientific programs with a diversification of activities from workshops to focussed research activities, such as hackathon and RPs; the aim being to develop activities adapted to the different communities that stimulate interactions, discussions and development of ideas. LINXS has also developed its premises towards providing an attractive, comfortable and stimulating environment to work in.

A total of 28 activities, of which 17 were organised by LINXS and 11 in partnership with other organisations, attracted around 900 participants (see Annex 1). A total of 447 participants were registered digitally through the Indico system and provide a good statistical base for the LINXS indicators (see “LINXS in Numbers” below).

Documentation of “output” commenced to show that the activities have yielded results. A standard reporting template was drafted with the aim of capturing what happened at events, who was involved, the findings and conclusions, as well as any impact potential. Activity reports are being collected to help the definition of the next steps and way forward, based on the outcomes of the activity.

Guidelines on the use of LINXS affiliation and acknowledgement of LINXS support were issued and the first scientific publications with LINXS affiliations have been published (see list in Annex 3). LINXS fellows have started to use the affiliation at their discretion and a growing interest in its usage is noted, contributing to the aim to grow a “quality stamp” reputation.

LINXS widely communicated activity results through a series of news articles following its communication strategy (see “LINXS Communications as a pathway to impact” below).

New WGs were established. In Imaging, the “Tomography of Biological Samples” and the “Food Science and Technology” WGs were initiated, the latter as a direct result of the successful “Northern Light on Food” collaborative activity. Moreover, the “New Opportunities in Imaging with X-rays and Neutrons” WG was defined based on combining existing elements, such as the Fluorescence WG. In the ISB theme, the “Time Resolved Structural Biology” and “Amyloid: An integrative approach” WGs were established. In addition, the “Membrane Proteins - structural resolution and homology modelling” WG was developed and formally accepted within the ISB theme after a series of meetings and intense scientific deliberations at the end of the year. The idea for the formation of the WG was conceived during discussions at the LINXS Integrative Structural Biology Symposium (ISB) in November 2018.

WGs increased their external networking and collaboration opportunities. The “Food Science and Technology” WG achieved project funding from FORMAS and a “Northern Lights on

Food” international network project will be implemented in 2020. The project will explore the unique opportunities for Swedish food research and production presented by MAX IV and ESS. The WG also submitted an application to NordForsk for the project “Photons and neutrons for elucidation of sustainable extrusion” (ExtruLight) and formal decision is pending.

LINXS initiated a “Networking Initiative” effort aiming to increase Swedish utilisation of photon- and neutron-based technologies and support other Swedish universities to increase their user base. As part of this effort, LINXS applied for funding to Vinnova/VR for a series of workshops at other universities in Sweden.

Good connections with key relevant actors, such as MAX IV, ESS, NNSP, SNSS, FASM and SWEDNESS were further developed in 2019 and a MoU was signed with the Elettra large-scale facility in Italy. In addition, formal contact with a number of Swedish universities was established and a growing number of researchers from other parts of Sweden have been involved in both WGs and activities. The 11 LINXS outreach activities during the year reached a large number of people at national and international level and significantly contributed to this end, not least by increasing the LINXS visibility and contributing towards anchoring LINXS at a national level (see list in Annex 1).

LINXS visiting researcher programme

LINXS is founded on the idea of bringing researchers together and promoting interactions within and across disciplines to fertilise research. To this end, LINXS launched its visiting researcher programme in 2019 as part of its work to attract world-leading scientists. The programme brings international researchers to LINXS for short- and long-term research visits. During their time at LINXS, they share their expertise and knowledge with the LINXS network and support the development of international and regional networks and collaboration in the field.

Four guest researchers were hosted by LINXS in 2019: Prof. Jan Dhont, Director at Forschungszentrum Jülich, and Professor at Heinrich-Heine University in Germany for one month; Prof. Thomas Hellweg from Bielefeld University in Germany for two months; Prof. José Campos Terán from Universidad Autónoma Metropolitana – Cuajimalpa in Mexico for a year; and Dr. Chris Garvey, from the Australian Nuclear Science and Technology Organisation in Australia for one year. Dr. Garvey’s visit is a collaboration between Malmö University and LINXS, and he is also a visiting Professor at Malmö University.

The results of the visiting researcher program are already reflected in a number of publications (see Annex 3) and seminars, but, most importantly in new research collaborations. To name a few, Prof. Hellweg and Terán established a new collaboration to prepare functional and responsive hybrid lipid and polymer surface, which has resulted in at least one approved beamtime application at The Heinz Maier-Leibnitz Zentrum in Germany. Prof. Terán also established working relationships with researchers at the departments of Chemical Engineering, Biotechnology and Biochemistry at Lund University. Dr. Garvey, has, apart from intensifying the collaboration with Malmö University and extending existing collaborations on cellulose and cellulose surfaces at Physical Chemistry at Lund University, also started working with researchers at Applied Biochemistry at Lund University. Other examples of the researchers’ activities at LINXS include the coordination of two PhD schools on neutrons and small angle scattering in Germany and Malmö, teaching on two courses on biomembranes and membranes and a series of seminars for the LINXS network. An analytic report of the visiting researcher programme is in Annex 4.

- So far, the visiting researcher programme is a great success. It has had exactly the outcome we would like to see going forward, says Stephen Hall, Director of LINXS. The guest researchers have all been very active in promoting LINXS activities and have established an impressive number of contacts within a rather short time. They have also worked to attract new users of x-rays and neutrons. It is clear that the programme is key to LINXS and we will further develop this in the coming years.

Post-doctoral programme

Dr. Anurag Kawde became the first LINXS postdoctoral fellow in June. Dr. Kawde works with Prof. Tõnu Pullerits and Prof. Marie Skepö at the Chemical Centre and NanoLund, at Lund University, on artificial photosynthesis and x-ray spectroscopy. Since he began at LINXS, he has established an international collaboration between Sweden, Denmark, Norway and Finland for a next generation renewable energy project studying and designing nanomaterials at the atomic level using Synchrotron facilities. He has also received a MIRAI scholarship, a joint initiative between Japanese and Swedish government to promote sciences at the large-scale facilities like synchrotron and spallation sources. Through this scholarship, he has worked on the possibility of organising schools like MIRAI at LINXS in Lund. The initial plan is to organize an “x-ray and neutron school” in collaboration with MAX-IV, ESS, Uppsala and Chalmers University. Dr Kawde initiated a young researcher network to discuss advanced x-ray and neutron science.

The successful integration of the postdoctoral fellow plays an important role in increasing the LINXS community with young researchers and in animating LINXS’s activities.

- *Establish the LINXS premises as a vibrant, active and attractive work/meeting/interaction space*

To achieve the goal of bringing researchers together and promoting interactions, LINXS, as an organisation and as a physical location, needs to be an attractive place to work and meet fellow researchers. The physical location is, thus, very important; In 2019, LINXS became well established in its interim location at IDEON, which fits well the desired profile, with flexible meeting and socialising spaces, offices and technical support. However, LINXS also requires people and activities at the premises to function as envisaged. With regards to people, in 2019, LINXS encouraged a greater presence of its guest researchers, as well as WG and CG members at the new premises to promote interaction. The idea is to create a positive feedback scenario – the more people and activities present at LINXS, the more people will want to work and take part in activities at the premises. The Science Day on August 26th was the first time that researchers engaged across different Themes and WGs at LINXS met with each other to brainstorm about how LINXS should develop in the future in order to fulfil its potential in advancing science. The WGs shared their progress and plans, explored synergies and discussed the science. The Science Day included a scoping exercise to explore present and future visions for LINXS. The questions explored where: “What is LINXS for you?”, “What do we want LINXS to be in 5-10 years?”, and “How do we get there?”. Discussions resulted in valuable insights, strategic proposals and scientific synergies. All researchers agree that LINXS has an important, strategic role in catalysing communities around large-scale research infrastructures (LRIs) – a role which has been neglected historically in other locations.

The Strategy meeting on September 27th brought together, also for the first time, representatives of all the stakeholders in LINXS to discuss the strategic development of LINXS; this included representatives from the Scientific Advisory Board, the Board, the Management

and Theme representatives. The goal was to discuss the future of LINXS and how to strategically attain it. Participants brainstormed on the LINXS vision and worked on short and long-term strategies that will allow LINXS to succeed in its mission, reach its goals and fulfil its potential. The strategy discussions were based on three possible development contexts: local, national, international, representing three avenues for LINXS, namely: 1. LINXS as an "LU institute fully funded by LU"; 2. LINXS as a "National institute co-funded by Swedish universities"; and 3. LINXS as an "International institute co-funded by international organisations". The strategic recommendations captured at the meeting will gradually feed into LINXS future strategic and operational plans.

Furthermore, a mingle organised on June 12th brought the LINXS community together at the LINXS premises in a more social environment, to strengthen the social aspect of LINXS community and foster relations between the LINXS national and international fellows.

Following the strategic plan, LINXS developed its premises as a venue for LINXS activities and meetings, including CG, WG, and RP meetings, the Board and SAB meetings etc. Moreover, LINXS welcomed and hosted a significant number of meetings and activities falling within its scope and contributing to its mission, but organised by external parties (see Annex 1). The aim of such "hosted events" is to strengthen and contribute to the further development of the ecosystem of actors and actions, both national and international, around neutron and x-ray related science, ESS and MAX IV. Examples of hosted meetings are those organised by NanoLund, LU's SVS project group, ForMAX, SWEDNESS, FIRS, DEUNET network, the Swedish-German Röntgen-Ångström Cluster MEDISOFT, MAXESS, ESS, and ILL. An increased interest in using the premises, particularly from MAX IV and ESS was noted.

"On 25 April 2019 the ESS organized and hosted a Deuteration Network meeting at LINXS in Lund. There were participants attending from all the major deuteration labs from every corner of the globe - from Japan to Sweden. LINXS provided us with a fantastic meeting space and the staff were helpful and supportive of our group during the event. The DEuteration and MAcromolecular Xtallization lab (DEMAX) at ESS really values the support and possibilities that LINXS offers to us here in Lund." Zoë Fisher, Group Leader for Deuteration and Macromolecular Crystallisation

The increased number of activities, the visiting researcher and the post-doctoral programmes, as well as the hosted events and meetings brought many to the LINXS premises and contributed to making a more active and vibrant venue. However, more work needs to be done to attain the level of ambition that LINXS has set for itself in terms of the daily presence of researchers in the premises and a more dynamic interaction. Moreover, usage of the new premises in 2019 gave insight on the most important aspects in attracting researchers on an average day, i.e. outside activity and meeting days. Aspects such as the possibility to work uninterrupted as well as in a group, having spontaneous interactions with the LINXS community and guests around a good cup of coffee, participating in parallel scientific activities organised at the premises, are just some examples of factors that need to be considered.

Much was accomplished but relevant work can never be completed and will of course continue and intensify in 2020.

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

During 2019, three themes ran in parallel, with a total 12 WGs including four RPs (see list in Annex 2).

A first step towards both solidifying the existing WG programmes and to establish new ones was to formalise the procedures for establishing, managing and operating a WG. To this end, LINXS has developed and implemented a formal application and decision process for all new WGs. A LINXS handbook, with information for WGs and CGs, has also been developed, described in more detail in the section on LINXS operations.

LINXS internal meetings and the 1st Science Day played an integral role in building the LINXS community and developing cross-WG and cross-theme interactions. New and already established WGs had the opportunity to meet, discuss and exchange experiences. Researchers were also afforded opportunities to explore synergies.

In addition to the ongoing work under the themes, LINXS also supported activities to highlight the possibilities afforded by x-ray and neutron science to new audiences that represent an unexplored potential. One such activity was the workshop “Northern Lights on Food”, a joint initiative with MAX IV and RISE, to bring together experienced x-ray and neutron users with researchers from food science and practitioners from the food industry. The aim was to identify common challenges and start new collaborations on how to develop and improve food and food processes by exploiting x-ray and neutron techniques. The workshop laid the ground for the formation of a new LINXS WG on food under the Imaging theme, but with clear cross-theme relevance to the both the Dynamics and ISB themes. Other important outcomes were the establishment of a network of companies and researchers interested to explore food and food processes, in the context of x-ray and neutrons science, and a draft White Paper on “The Use of X-ray and Neutron-Based Techniques in Food Research and Development” that will be published in 2020.

Reflections from “Northern Lights on Food” as a representative LINXS story for 2019 are included in Annex 5.

- ***Establish a path towards the development of new themes***

Themes at LINXS usually run for three years. The current Imaging Theme will be concluded at the end of 2020 and a new theme will be initiated during 2020. In preparation for this renewal phase a procedure for selection of new Themes has been established to ensure a transparent, independent and efficient selection process. The call process has been established with a call text, application template, defined evaluation criteria and other supporting documents. The selection process is primarily based on external expert evaluation by the LINXS SAB, with the remit to ensure scientific excellence and complementarity within LINXS. The selection process has two stages, the first is based on a brief Theme description and plan and a small number will then be selected to proceed to a more detailed theme definition before a final decision is made. The SAB have the possibility to suggest modifications of theme proposals before submission to the second stage and can even suggest the combining of proposals, if appropriate.

At the end of the 2019, LINXS launched its renewal process and put out a call for a new theme, with a deadline February 28th, 2020 (Reg.nr F 2019/1697). The SAB was closely involved in the process, and advised on the subject of the call assure to complementarity and strengthening of LINXS's science profile and to steer the process towards proposals that encourage multi- and trans-disciplinary interactions and to include more than one of the LINXS focus areas. Following the SAB recommendations, the call is for “a new LINXS Theme in the areas of hard condensed matter, materials, and related areas”. The call is open to applicants

from partner organisations and this is currently Lund University. The call was widely communicated through the LINXS website and contact list, as well as LU and relevant faculty newsletters and official communications.

Operational objectives

- ***Develop clear and transparent working practices***

In 2019 we worked to develop clearly defined and transparent working practices, which are essential to LINXS as a young institute. These practises have been developed and implemented gradually through the year. The LINXS operational processes (for applications, fellowships, appointments and decisions) were designed to ensure integrity, accountability and transparency in decision-making. The objective is also to make them efficient and to avoid unnecessary burden to the researchers. Part of this work is also to clearly communicate the processes to the LINXS community, which includes establishing concise terminology. The processes reflect the current state of the institute's development and will be updated as LINXS develops. LINXS acknowledges the valuable contribution and collaboration with the Lund University "Department of organisational development and change management" in the process mapping design.

The LINXS Statutes were updated (STYR 2019/1016) to better reflect the LINXS mission and openness to a wider national and international participation, the LINXS roles were defined (STYR 2019/1010) and formal decisions related to the LINXS management and Board were made. In addition, "back-office" processes for archiving and document registration have been established and implemented (including working on a backlog of such tasks from before the processes were implemented).

The SAB mandate period formally ended in the end of 2019 and membership to the SAB new mandate period 2020-2022 was formally processed and completed.

The LINXS website is a key tool for communication and transparency and has been significantly updated and expanded during the year, with a focus on supporting current and potential researchers at LINXS. A handbook targeted at WGs and CGs has also been developed and published on the website. The handbook is continuously updated and contains information on how to organise, communicate and report on activities, plus other information relating to working at LINXS. A Library has been added to store LINXS templates, documents and publicity materials. Publications with LINXS affiliation are also listed. The LINXS website also features regular and timely news articles on WG activities to highlight the research activities at LINXS.

- ***Extend LINXS's remit beyond Lund University***

LINXS has the objective to grow from the solid foundation provided by Lund University to an institute supported by a number of national and international partner organisations and foundations. Therefore, LINXS has worked on the development of a "model" for LINXS memberships and partnerships, advised by the Board and SAB. The focus in this respect during 2019 was to prioritise establishing contacts, discussions and anchoring with other Swedish universities and organisations, as well as within national policy. A variety of actions were pursued to this end. LINXS WGs also encouraged the involvement of non-LU researchers in WGs and activities.

During 2019, LINXS has strengthened its identity and visibility through outreach activities to new audiences and potential partners, both nationally and internationally (see Annex 1). A significant outreach activity was the participation in Almedalen, which resulted in strengthening

the contacts with a number of Swedish universities. A significant insight was the importance of highlighting what LINXS can offer to Swedish universities in terms of enhancing their existing and new user communities, promoting research in x-rays and neutrons, networking and bringing people together. LINXS needs to engage with the Swedish universities in an optimal way and work with their existing structures around x-ray and neutron science. Several Swedish organisations and institutes visited LINXS (e.g. RISE and SciLifeLab) and discussions will continue. Furthermore, events at various Swedish universities jointly organised by local researchers and LINXS are planned and potentially supported by Vinnova/VR. The aim of these is to probe and increase the potential user base for MAX IV and ESS in Sweden.

As a result of the above efforts, discussions were concluded with one Swedish organisation which is expected to become the first external LINXS member in the beginning of 2020.

Other examples of LINXS strategic outreach include LINXS participation in the VR Workshop on ESS and Max IV, as well as a presentation at the MAX IV reference group, and a stand at the MAX IV user meeting. Furthermore, contacts have been established with a number of international universities and large-scale facilities. Representatives, including from University of Grenoble, Imperial and ILL, visited LINXS through the year and a MoU was signed with Elettra (the x-ray synchrotron facility in Trieste, Italy). In addition to the participation of many researchers from around Sweden, there has been good participation from neighbouring Danish universities in LINXS WGs and as participants to various activities.

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

- ***Secure long-term funding***

During 2019 LINXS has consistently worked towards securing long-term funding, and to plot a sustainable path forward. There has been a consolidation and clarification of the support from Lund University for which LINXS continues to be very grateful. This has largely been in response to a discontinuation of the initial seed funding from The Crafoord Foundation who have felt that LINXS' trajectory is already on a good footing. During the year contact has been ongoing with VINNOVA and The Swedish Research Council, especially their unit for Research Infrastructures. LINXS and its mission and role in the Swedish ecosystem around the facilities MAX IV and ESS has been more established and communicated to national stakeholders and a specific effort to engage other Swedish universities was started. Coming into the next year, LINXS will increase its efforts to receive longer-term funding, specifically for a visiting researcher and postdoc programme. LINXS will also seek to expand the number of national and international partners and members. LINXS has also solicited and is receiving help from the LU Development Office in approaching Swedish Foundations. Approaching international foundations will be revisited in conjunction with the appointment of a new Director.

- ***The search for a new director***

Since Peter Schurtenberger stepped down from his role as director of LINXS in 2018, Stephen Hall has taken on the role of interim director. Ensuring the long-term future of LINXS requires the appointment of a new director with a strong international standing in science using x-rays and neutrons to succeed the current interim director. Therefore, a priority in 2019 was to establish a strategy for the recruitment of a new director, which was carried out in coordination

with the Board and the faculty partners (i.e., the faculties of Science, Engineering (LTH) and Medicine at Lund University).

It was identified that it is important that the position is anchored both at LINXS and within a host academic institution (which should be at Lund University, as this is currently the sole partner) to be able to offer a professorial post with the director position. The director will be 50% at LINXS and 50% at the host institute. This requires a commitment from the host faculty to support the director for 50% during the mandate and to commit to host the person after their mandate at LINXS. It is envisaged that directors will hold the position for 5 years, which is renewable.

A Search Committee was formed with key representatives from Lund University. The search committee defined the profile for the position which included the requirements for a strong research profile in x-ray and neutron related science and a broad international (and national) network in the area. The director should also have a broad scientific interest and, whilst they will clearly have a strong personal research area, they should have a more general understanding of the science around LINXS and associated network. Ideally, the director should have knowledge of both x-ray and neutron methods.

The call was formally announced in October with a deadline on December 1st 2019. LINXS promoted the call widely through various channels, including the LINXS and ESS websites, Nature Careers, Science Careers, CERN Courier, LinkedIn, as well as through the LINXS contact list and personal networks and recommendations of several key neutron and x-ray scientists. The call attracted 24 applicants, the majority of which were senior high-level international scientists with very impressive records of scientific accomplishments and experience. LINXS considers this as a confirmation of the international appeal of the LINXS concept and a stamp of approval by the international scientific community of the LINXS potential. The formal recruitment process will commence in January 2020 with an evaluation committee that includes representatives from LU and the LINXS SAB.

Communications as a pathway to impact

LINXS communication and outreach activities are strategic pathways for LINXS to achieve scientific and societal impact in the short, medium and long term.

In 2019, LINXS developed its first communication plan and associated communication procedures, which were aligned to the overall LINXS mission and goals. In particular the communication goals for 2019 were: to establish, create and identify communication channels to highlight LINXS's work; to identify and establish strong networks and research groups that can be associated with LINXS; to promote a strong research profile at LINXS; to establish internal communication channels within the LINXS community.

A major tool in the LINXS strategic communication work is the LINXS newsletter. This was established to create a shared internal and external communication channel for the LINXS community, where the work of LINXS themes and WGs can be highlighted, as well as news from LINXS and from the field of x-ray and neutron science. In total, LINXS issued five newsletters in 2019, featuring articles, interviews and information on events, plus messages from the Director. All newsletters have had higher than 50% opening rate, which is a testament to the perceived relevance of the newsletter. The number of people opening the newsletters has been around 400, for the last two newsletters.

Other examples of the communication strategy are the numerous popular science articles in the LINXS website about LINXS themes and WGs. Through strategically highlighting different researchers, events and activities, LINXS aims to highlight the diversity of science taking place

at the Institute, as well as the type of discussions and topics the LINXS community is pushing forward. The articles also aim to attract new user groups and interested researchers to LINXS. One example of a direct positive outcome is two researchers (one already involved at LINXS and the other from outside) have come together to work on joint research project as the result of an article in the newsletter.

LINXS strategic outreach activities (see Annex 1) also served to strengthen the LINXS identity in both a local and national context as described previously.

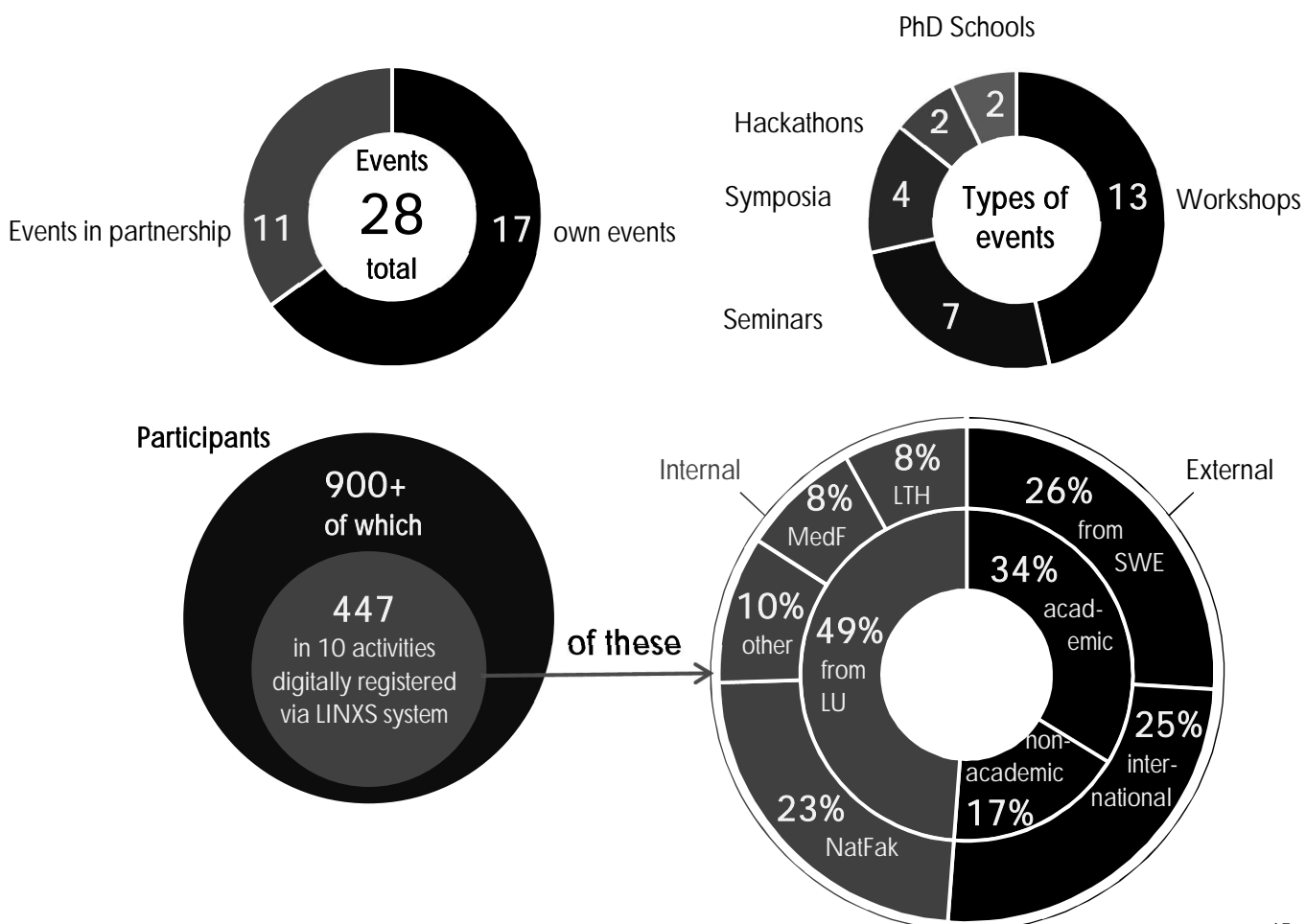
As mentioned, the LINXS website has been continuously updated and expanded during the year and a LINXS profile was created on LinkedIn serving as a further communication tool to reach larger audiences. News articles and activities are also communicated regularly via the LINXS LinkedIn page.

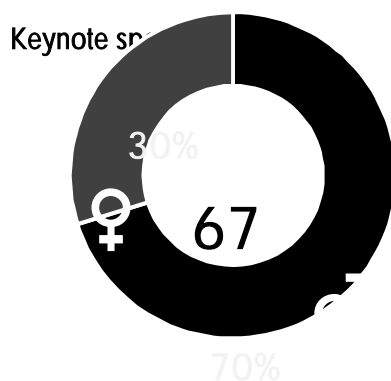
To summarise, LINXS has made a good start on developing and making use of strategic communications and outreach activities to help realise its mission. In 2020, this work will intensify, as the number of LINXS activities increases and the work of the WGs and themes develop and mature. External communication will receive a special focus, in an effort reach audiences outside the LINXS community.

LINXS 2019 in Numbers

LINXS Activities and participation

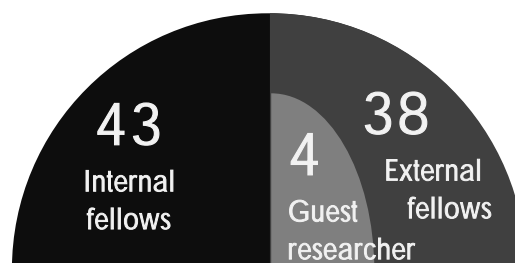
LINXS Events





LINXS Community – fellows in 2019

85 LINXS fellows in 2019



LINXS Community – organisations

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

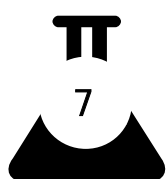
13 in Sweden (including Lund University)

24 international (5DE, 3DK, 3USA, 3AU, 3IT, 1MX, 4FR, 1HR, 1UK)

these were,



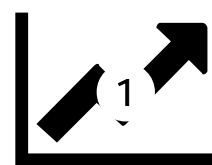
Universities



Research Institutes

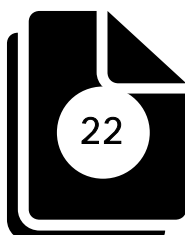


Large Scale
Research Infrastructures



Company

Outcomes



Publications with
LINXS affiliation

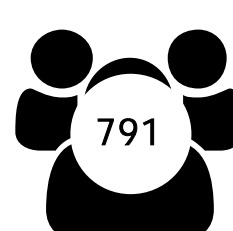
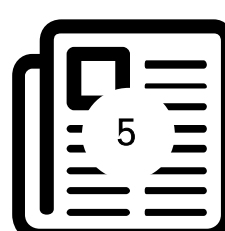
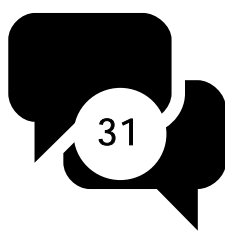


Project applications
submitted



Project funded

Communications



[Outreach activities](#)
[Website news](#)
[Newsletters](#)
[Subscribers](#)

Annual Financial Report 2019

Income	SEK
External funding	500,000
Partners contribution	8,000,003
Activities	128,580
Deferral 2020	-500,000
Total Income 2019	8,128,583
Expenditures	SEK
Activities	-1,406,318
Equipment	-200,748
Materials & consumables	-171,544
Premises	-1,199,006
Salaries	-4,720,044
Overhead	-971,009
Total Expenditures	-8,668,669
Annual Result	-540,086

Partner's contribution during 2019 was funding from the Lund University Faculties of Science and Engineering. In addition, the Lund University Faculty of Medicine contributes in-kind with 50% of the salary of the LINXS Vice-Director.

External funding was deferred for project implementation in 2020.

The final deficit was covered with the accumulated agency capital from the previous year.

Detailed financial reporting is included in Annex 6.

Annex 1 – List of LINXS activities

LINXS events and events organised in partnership

1. LINXS Event: Geology, Archaeology and Culture Heritage studies in a new light, January 15-17, 2019
2. LINXS Event: Welcome to afternoon coffee and a seminar by Prof. Hans J Vogel from University of Calgary, February 21, 2019
3. LINXS Partner Event: Magnetism, Correlated Systems and X-rays, March 14-15, 2019
4. LINXS Partner Event: Symposium - Lipid self-assembly - structure, function and applications, March 14, 2019
5. LINXS Event: QUANTIM Hackathon, Theme - cellular materials in 3D and 4D20, March 21-22, 2019
6. LINXS Event: Workshop - Tomography of Biological Tissue, March 25, 2019
7. LINXS Partner Event: Northern Lights on Food, March 26-27, 2019
8. LINXS Event: Inverse problems in X-ray phase retrieval and tomography, April 4, 2019
9. LINXS Event: Welcome to afternoon coffee and a seminar by Prof. Richard Neutze from Gothenburg University, April 10, 2019
10. LINXS Partner Event: BigScience@LU – addressing the need of academic input in building and maintaining Big Science facilities!, April 24, 2019
11. LINXS Partner Event: French and Swedish School on Energy Materials (FASEM), May 13-17 2019
12. LINXS Event: Roundtable discussion "AI in structural biology, x-ray and neutron science", May 23, 2019
13. LINXS Partner Event: LINXS @ Nordic AI Powwow, Lund, May 23, 2019
14. LINXS Event: Welcome to afternoon coffee and a seminar by Prof. Jan K. G. Dhont from Forschungszentrum Jülich GmbH, "Non-uniformly Flowing Suspensions - Non-local stresses, shear-gradient induced mass transport, and a shear-banding instability in systems with a yield stress", May 23, 2019
15. LINXS Partner event: X-ray Imaging workshop at Syddansk Universitet (SDU) in Odense, Denmark, June 4, 2019
16. LINXS Event: Welcome to afternoon coffee and a seminar by Dr Sylvain Bohic from STROBE and ESRF, June 5, 2019
17. LINXS Event: Workshop for X-ray and neutron imaging applications in soil sciences, June 17-18, 2019
18. LINXS Event: Software Hackathon (Mikael Lund), July 10, 2019
19. LINXS Event: Welcome to morning seminar with Dr Thomas Hellweg, Dep. of Physical and Biophysical Chemistry, Bielefeld University in Germany, August 27, 2019
20. LINXS Partner Event: 8th Scandinavian Symposium, Amyloid Diseases and Amyloid Mechanisms (ADAM 8), August 28-30, 2019
21. LINXS Partner Event: Doctoral school: Neutrons for membrane biophysics, September 16-20, 2019
22. LINXS Event: 2nd Symposium - Integrative Structural Biology, October 9-11, 2019
23. LINXS Event: Research program Simulation, theory, and software development for anisotropic systems, October 22-24, 2019 Oct
24. LINXS Partner Event: All-day Symposium: Language technology in Medicine and Life sciences, November 8, 2019

25. LINXS Partner Event: Seminar on funding opportunities for artificial intelligence and digitalization in medicine and life sciences, November 15, 2019
26. LINXS Event: Amyloid Workshop: "Mind the gaps in amyloid fibre structure analyses", November 21-22, 2019
27. LINXS Event: GISANS meeting at LINXS, Lund, December 3, 2019
28. LINXS Event: Seminar with Dr. Garib Murshudov, MRC Laboratory of Molecular Biology in Cambridge, UK, December 6, 2019

LINXS Hosted events:

1. LINXS Hosted event: a non-specialized summer school: Imaging of 3D-structures, September 30 – October 4, 2019
2. LINXS Hosted event: PhD course: Small angle scattering, October 21-22, 2019

LINXS Outreach activities:

1. LINXS stand at HALOS kick-off!, Lund, April 3, 2019
2. LINXS presentation at MAX IV Reference Group meeting URG, May 28, 2019
3. LINXS at Almedalen, Jul 1-4, 2019
4. LINXS stand at 31st MAX IV User Meeting, Sep 23-25, 2019
5. LINXS stand at Protein Science Day 2019 with HALOS speed-dating/matchmaking, October 15, 2019
6. LINXS participation in the VR Workshop om den Europeiska Spallationskällan, ESS och Max IV, Göteborg, October 17, 2019
7. LINXS presentation to ScilifeLab meeting,
8. LINXS Stand at MVA R&D Network Meeting, Lund, November 21, 2019
9. LINXS Stand at Big Science Sweden Conference 2019, November 26, 2019
10. LINXS presentation at Future by Lund, November 27, 2019
11. LINXS presentation at RISE User Community meeting - photons and neutrons, Gothenburg, November 28, 2019

Annex 2 – LINXS Themes and Working Groups in 2019

IMAGING

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

WG 2 - GeoArCH: Geology, Archaeology and Cultural Heritage

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

WG 4 - TBS: Tomography of Biological Samples

WG 5 - Food Science and Technology

WG 6 - QUANTIM: Image quantification

DYNAMICS

WG 1 - Dynamics of Biological Macromolecules

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

WG 2 - X-ray Photon Correlation Spectroscopy (XPCS)

WG 3 - Dynamics and Structure of Membranes and their Constituents

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

INTEGRATIVE STRUCTURAL BIOLOGY (ISB)

WG 1 - Biocompute and Artificial Intelligence & Machine Learning

WG 2 - Time Resolved Structural Biology

WG 3 - Amyloid: An integrative approach

Annex 3 – List of publications with LINXS affiliation 2019

1. Dainius Jakubauskas, Łucja Kowalewska, Anna V. Sokolova, Christopher J. Garvey, Kell Mortensen, Poul Erik Jensen & Jacob J. K. Kirkensgaard., 2019, Ultrastructural modeling of small angle scattering from photosynthetic membranes., Scientific Reports volume 9, Article number: 19405 (2019)
2. Guang Wang, Christopher J Garvey, Juan Zhang, Luke A O'Dell, Anwen M Krause-Heuer, Maria Forsyth, Tamim A Darwish, Steinhart Miloš and Lingxue Kong., 2019, Evolution of structural dimensions in mesoporous template precursor from hexagonal lyotropic liquid crystals, Journal of Physics: Condensed Matter, Volume 32, Number 7
3. Athanasopoulos, S.D., Hall, S.A. and Kelleher, J.F., 2019, A novel multiscale neutron diffraction based experimental approach for granular media, Géotechnique Letters 2019 9:4, 284-289
4. Tudisco, E., Etxegarai, M. Hall, S.A., Charalampidou, E.M., Couples, G.D. Lewis, H. Tengattini, A. and Kardjilov, N., 2019, Fast 4D imaging of fluid flow in rock by high-speed neutron tomography, *Journal Geophysical Research: Solid Earth*, 124, 3557– 3569.
5. Johan Hektor, Micha, J. S., Stephen A. Hall, Srinivasan Iyengar & Matti Ristinmaa., 2019, Long term evolution of microstructure and stress around tin whiskers investigated using scanning Laue microdiffraction, *Acta Materialia*. 168, p. 210-221 12 p.
6. Zhai, C., Herbold, E.B., Hall, S.A. and Hurley, R.C., 2019, Particle rotations and energy dissipation during mechanical compression of granular materials, *Journal of the Mechanics and Physics of Solids*. 129, 19-38.
7. Pettersson, S., Engqvist, J. and Hall, S.A., Toft, N. and Hallberg, H., 2019, Peel testing of a packaging material laminate studied by in-situ X-ray tomography and cohesive zone modeling, *International Journal of Adhesion and Adhesives*. 95, 102428.
8. Marian Cors, Oliver Wrede, Lars Wiehemeier, Artem Feoktystov, Fabrice Cousin, Thomas Hellweg & Julian Oberdisse., 2019, Spatial distribution of core monomers in acrylamide-based core-shell microgels with linear swelling behaviour, *Scientific Reports (Nature Publisher Group); London Vol. 9, (Sep 2019): 1-11.*
9. Brändel T, Dirksen M, Hellweg T., 2019, Tuning the Swelling Properties of Smart Multiresponsive Core-Shell Microgels by Copolymerization, *Polymers* 11: 1269.
10. Stenqvist, B. & Mikael Lund., 2019, On short-ranged pair-potentials for long-range electrostatics, *Physical Chemistry Chemical Physics*. 21, 44, p. 24787-24792 6 p.
11. Maria Valldeperas, Andrea Salis, Justas Barauskas, Fredrik Tiberg, Thomas Arnebrant, Valdemaras Razumas, Maura Monduzzi, Tommy Nylander., 2019,

Enzyme encapsulation in nanostructured self-assembled structures: Toward biofunctional supramolecular assemblies, *Current Opinion in Colloid & Interface Science*, Volume 44, Pages 130-142.

12. Jennifer Gilbert, Maria Valldeperas, Surender K. Dhayal, d Justas Barauskas, Cedric Dicko and Tommy Nylander., 2019, Immobilisation of β -galactosidase within a lipid sponge phase: structure, stability and kinetics characterisation, *Journal Nanoscale*, issue 44, 2019.
13. Linda K. Månsson, Tym de Wild, Feifei Peng, Stefan H. Holm, Jonas Tegenfeldt, and Peter Schurtenberger., 2019, Preparation of colloidal molecules with temperature-tunable interactions from oppositely charged microgel spheres, *Soft Matter*, issue 42.
14. Nicholas Skar-Gislinge, Michela Ronti, Tommy Gating, Christian Rischel, Peter Schurtenberger, Emanuela Zaccarelli, Anna Stradner., 2019, A Colloid Approach to Self-Assembling Antibodies, *Mol. Pharmaceutics*: 2019: 16, 6, 2394-2404,
15. Feifei Peng, Stefan Holm, Linda Månsson, Somnath Ghosh, Jérôme Crassous, Peter Schurtenberger and Jonas Tegenfeldt., 2019, A Droplet-Based Microfluidics Route to Temperature-Responsive Colloidal Molecules, *Journal of Physical. Chemistry*. 123, 43, 9260-9271
16. Maxime J. Bergman, Gating, T., Peter Schurtenberger & Anna Stradner., 2019, Experimental Evidence for a Cluster Glass Transition in Concentrated Lysozyme Solutions, *Journal of Physical Chemistry B*.123,10,s. 2432–2438
17. Sofi Nöjd, Christopher Hirst, Marc Obiols-Rabasa, Julien Schmitt, Aurel Radulescu, Priti S. Mohanty and Peter Schurtenberger., 2019, Soft particles in an electric field – a zero average contrast study, *Soft Matter* 15, 6369 (2019)
18. Jasper N. Immink, Erik Maris, Jérôme J. Crassous, Joakim Stenhammar, and Peter Schurtenberger., 2019, Reversible Formation of Thermoresponsive Binary Particle Gels with Tunable Structural and Mechanical Properties, *ACS Nano*, 13, 3292–3300.
19. Brijitta Joseph Boniface and Peter Schurtenberger., 2019, Responsive Hydrogel Colloids: Structure, Interactions, Phase Behaviour and Equilibrium and Non-equilibrium Transitions of Microgel Dispersions, *Curr. Opin. Colloid Interface Sci.* 40, 87-103.
20. Maria Jansson & Marie Skepö., 2019, Polyelectrolyte-nanoplatelet complexation: Is it possible to predict the state diagram?, *International Journal of Molecular Sciences*. 20, 24, 6217.
21. Jansson, Maria; Lenton, Samuel; Plivelic, Tomás S. and Skepö, Marie., (2019), Intercalation of cationic peptides within Laponite layered clay minerals in aqueous suspensions : The effect of stoichiometry and charge distance matching, *Journal of Colloid and Interface Science* 557. P.767-776.

22. Tommy Garting and Anna Stradner., 2019, Synthesis and application of PEGylated tracer particles for measuring protein solution viscosities using Dynamic Light Scattering-based microrheology. Colloids and Surfaces B: Biointerfaces; Volume 181, 1 September 2019, Pages 516-523.

Other Research Output 2019

1. Alberto Sánchez, Jorge Hernández, Daniel Ondo, Ángel Piñeiro, Richard Campbell, Miguel Costas, José Campos., 2019, Highly Viscoelastic Films at the Water/Air Interface: α -Cyclodextrin-anionic surfactants complexes
Poster
2. Jonas Engqvist, Stephen Hall & Maria Fredriksson, 2019, A miniaturised pressure plate cell for in-situ X-ray imaging of water distribution in wood, p. 130-131.
Contribution to conference › Abstract
3. Jonas Engqvist, Matti Ristinmaa, Stephen Hall, Tomás Plivelic & Jackson, A., 2019, In-situ X-ray scattering experiments to measure deformation on multiple scales, p. 52.
Contribution to conference › Abstract
4. Stefanos Athanasopoulos & Stephen Hall, 2019, Multiscale Mechanics of Quartz Sand Under Load with Neutron Diffraction and Digital Image Correlation, p. 21. 21 p.
Contribution to conference › Abstract

Annex 4 – Visiting researcher programme report 2019

LINXS had four international guest researchers within the “Dynamics and Structure of Membranes and their Constituents” WG. Jan Dhont, who is a Director at Forschungszentrum Jülich (Institute of Complex Systems) and a full Professor at the Physics Department at the Heinrich-Heine University in Düsseldorf is a regular guest to LINXS and has been important in building up LINXS. We had the pleasure to have him at LINXS as a visiting fellow for a month during the spring. During this period, he shared his deep insight in soft matter systems and scattering techniques with many academics at Lund University. He gave a well-attended LINXS seminar (see Annex 1). Professor Thomas Hellweg (Bielefeld University, Germany), Professor José Campos Terán from Universidad Autónoma Metropolitana - Cuajimalpa (UAM-C), Mexico and Dr. Chris Garvey, Australian Nuclear Science and Technology Organisation (ANSTO), Australia are also visiting fellows. Professor Hellweg stayed for 2 months and Professor Campos Terán and Dr. Garvey are both with LINXS for more than a year. Dr Garvey is jointly appointed as a Professor at Malmö University. All three have been very active in promoting LINXS activities and have establish an impressive number of contacts within a rather short time, promoting also new users of x-rays and neutrons. Professor Hellweg and Dr. Campos Terán established a new collaboration to prepare functional and responsive hybrid lipid and polymer surface, which resulted in at least one approved beamtime application (MLZ, Garching). This collaboration involves activities on responsive particles at Physical Chemistry at Lund University. Professor Hellweg has also strengthen the collaboration with Prof. Lise Alerth's group at Copenhagen University. Professor Campos Terán has established new collaborations with Professor Frank Lipnizki, Chemical Engineering, Professor Rajni Hatti-Kaul, Biotechnology, Professor Henrik Stålbrand, Biochemistry at Lund University. Dr Garvey has apart, from intensifying the collaboration with Malmö University, and extending present collaboration on cellulose and cellulose surfaces at Physical Chemistry, established collaborations with Professor Leif Bülow, Dr Johan Svensson Bonde and Dr Cedric Dicko at Applied Biochemistry; and Dr Tommy Cederwall at Biochemistry at Lund University. He has benefitted from the LINXS fellowship which has enabled the extension of existing work by collaborations with Professor's Juan Colmenero and Angel Alegria (Materials Physics Center, San Sebastian) and Dr Patrick Judeinstein (Laboratoire Léon Brillouin). New areas for collaboration with Professor Kell Mortensen and Associate Professor Jacob Kirkensgaard at Copenhagen University have been with the melt processing of sustainable biopolymers and dairy gels respectively. Professor Hellweg gave a LINXS seminar in August. Dr. Garvey coordinated 2 PhD Schools: Neutrons for membrane biophysics SINE2020 (16-20 Sep 2019 in Garching, Germany); and in Malmö “Small angle scattering – a tool for revealing structure at the nanoscale”, and gave a number of presentations with LINXS/Malmö as an affiliation. Professor Campos Terán was teaching on two courses, one PhD Summer School – Nanotools at Biomembranes at Malmö University 26-30 Aug 2019 and at MIRAI short course “Membranes for a sustainable future” at Chemical Engineering, Lund University 17 – 21 Nov 2019. He also presented a poster with LINXS affiliation at the 33rd Conference of The European Colloid and Interface Society, 8-13 September, Leuven, Belgium. Professor Campos Terán and Dr. Garvey participated with oral contributions at the “Material Compatibilization”

workshop organized by Dr. Cedric Dicko and sponsored by STINT, LINXS and LU , 4 Sep 2019. Furthermore, an application was realized and two days of neutron reflectometry was obtained at ILL for the spring 2020 period in collaboration with Dr. Richard Campbell (University of Manchester). All three guest researchers have published or are going to publish papers with LINXS affiliation (see Annex 3).

Annex 5 – Reflections and voices from LINXS cases in 2019

SOIL SCIENCE WORKSHOP: *"IT WAS GOOD TO GET INSIGHT INTO ISSUES AND QUESTIONS THAT PARTICIPANTS ARE INTERESTED TO FIND OUT MORE ABOUT"*

In June 2019, the Soil Sciences WG had its first major event, a workshop spanning two days and gathering more than 50 participants.

The aim of the workshop was to push the research frontier in the most pressing questions in soil sciences: such as connecting biotic and abiotic processes, soil organic matter dynamics, and utilizing X-ray and neutron techniques to answer these questions. Another aim was to provide basic knowledge about different X-ray and neutron imaging techniques and to compare the pros and cons of the different approaches.

– We wanted to invite people who work with different aspects of soil to cover as many angles and techniques as possible. One goal was to establish a network between international soil scientists and beamline scientists, say Edith Hammer and Milda Pucetaite, members of the Soil Sciences WG.

As part of the workshop, four discussion groups were hosted: a newbie group, a nano- to micro-spectroscopic imaging group, a bulk spectroscopy group and a X-ray/neutron tomographic imaging group.

– It was good to get insight into issues and questions that participants are interested to find out more about. The variety of points brought up in the discussions highlight how big the interest in the area is.

Two areas that received a lot of attention were sample preparation and data analysis, plus there was much interest in the complementary use of different techniques.

– We think it was very useful for the people who attended the workshop to hear from experts about the importance of sample preparation in relation to experiments; are they compatible with beamline hardware? Talking to beamline scientists about the study before you apply for beam time is also important, as well as the need for you, as a scientist, to have thorough knowledge about your sample, maybe even using conventional techniques before you go further.

– Use of complementary techniques were also a major discussion point throughout the workshop, and something which all the speakers highlighted in their talks. It is very seldom that you can solve your questions with only one technique. Again, we think it is good that this is stressed, even though some scientists may feel that you have to have loads of technical expertise.

Edith Hammer and Milda Pucetaite see much potential for scientific development of soil science questions with the help of X-ray and neutron techniques. Especially in the field of physical stabilization of soil carbon, microplastics in soil and microsite conditions for biogeochemical processes including the fate of toxins.

– But, it is also clear that we need to focus on education and training in how to use the techniques and, especially, in how to use a range of different techniques. This is where we think that LINXS and us, as a WG, can help: by bringing scientist and experts together so that they can form connections and expand their knowledge.

All of the members in the WG were very satisfied with the workshop:

– We are happy with how the event went. Everyone seemed really keen in participating in discussions and making new connections. We have heard some feedback as well, about how excited people are about the new facilities in Lund, MAX IV and ESS, and the very cool science that they will be able to (and already does) produce.

The workshop was the first step to reach out to the wider community and to make new collaborations.

– Next on our list is to organise more events – workshops and smaller meetings – to address more specific scientific interests of the soil science community in using X-ray and neutron imaging techniques in their research, conclude Edith Hammer and Milda Pucetaite.

Voices from the Workshop

Aurora Patchett, Gothenburg University,

“I’m only at the start of my PhD. I am trying to define what methods to use. For me, it was useful to hear about the different applications since I work in a field setting where I use large soil samples, for example, biological soil crust. During the workshop, I met with people who are working on the same things as me, so I can see that there is room for collaboration.”

Emanuel Larsson, RISE

“I’m a tomography expert. I work with both neutrons and x-rays. The samples I see in my work range from food, to metals, to wound care dressings, but also soil sciences. The application does not actually matter. The techniques used to detect things in soil sciences can be transferred to other areas. For me, being at the workshop is about picking up ideas to see how I can use them in my overall work. I can see many similarities, for example, you can study the uptake of water in both plants and wound care dressings with neutron imaging.”

EXPANDING THE TOOLBOX FOR NEUTRON AND X-RAY EXPERIMENTS – A SNAPSHOT OF THE WORK OF LINXS RESEARCH PROGRAMME: SIMULATION, THEORY AND SOFTWARE DEVELOPMENT OF ANISOTROPIC SYSTEMS

The data generated from experiments at large scale research infrastructures is often vast and very complex to analyse and interpret. Meanwhile, it is becoming increasingly important to find out more about protein behaviour – to develop new types of food, more effective medicines and more knowledge about the human body.

Mikael Lund, professor in theoretical chemistry at Lund University, is leading a research programme at LINXS concerned with how to make data analysis both easier and more effective. The aim is to build computer simulations and models of protein experiments to help researchers analyse and predict protein behaviour. In October 2019, the programme had a three day workshop on the topic of scattering in anisotropic systems, where participants identified scattering in concentrated protein solutions as an area to further develop.

– Different types of computations can help researchers understand and work with their data in new ways. Ultimately, it is about making research at large infrastructure more insightful and efficient, says Mikael Lund.

He explains that researchers are faced with the twofold problem of length and time scales when they conduct scattering experiments on protein solutions.

– Today, many experiments are limited in terms of spatial and temporal resolution. Computer simulations can complement these with a broader set of time and length scales and become part of loop to extract as much information as possible from a scattering experiment.

The programme’s work is split into two parts: one part is focused on creating interaction models for proteins; the other on creating an analysis tool to link computer simulations to experimental data.

To develop their models and simulations, Mikael Lund and his colleagues will need input from experiments conducted at large scale research infrastructures. They will therefore work together with another WG at LINXS, namely Antibodies in Solutions, and use their protein sample data.

– Using a large set of well-defined samples is key for training our computer code and create descriptive models of the experiments. It will help us make predictions and analyse the experiments since the samples present a broad set of data, conducted under a well-defined set of sample conditions.

So far, Mikael Lund and his group have created a prototype model and a simulation tool for predictive scattering experiments. However, some of the analysis is still very demanding, even for the computer simulations.

– A major challenge is to create tools that can be used more broadly by researchers. You need tools that are both efficient and user friendly. One problem we need to solve is how to handle large data sets. In our simulations, we want to look at many interacting proteins as found in concentrated samples. Before, it was more common to only analyse one, perhaps two, proteins at a time.

The long-term ambition of the research programme is to include the computational tools in already established software and make them widely available. This is important because timeslots at large scale research infrastructures are often limited and could be used more effectively. An accurate computational toolbox could guide researchers in the experimental design and make precious beam time much more efficient.

"BY MEETING OTHERS, YOU GET INSPIRED IN YOUR OWN RESEARCH, AND CAN IDENTIFY FUTURE COLLABORATORS" - REFLECTIONS ON THE INTEGRATIVE STRUCTURAL BIOLOGY THEME'S SECOND SYMPOSIUM

The Integrative Structural Biology theme had its second symposium in October 2019 - an event that gathered close to a hundred researchers from different universities.

- It is really interesting to hear the stories behind other researchers' results and publications. By meeting others, you get inspired in your own research, and can identify future collaborators, says one of the keynote speakers, Professor Nieng Yan, from Princeton University.

An explicit aim with the symposium was to highlight advanced, cutting-edge research in structural biology and showcase the possibilities within the field.

According to Nieng Yan, the Integrative Structural Biology Theme represents the frontier areas of research, since it has a focus on multiple approaches and techniques.

– I see the whole field as entering a new era. We have started to use already established techniques, such as X-ray crystallography and electron microscopy, in new and different ways. It is exciting both for the research and for us researchers.

Veronica Lattanzi, a PhD student in biochemistry and structural biology at Lund University, agrees that the symposium was a great inspiration in terms of creating networks and to get another view of what you can do in the field. In particular, she is eager to learn more about scattering techniques.

– My key reflection is that the future of science is interdisciplinary and that we need to meet across disciplines. LINXS can help merge different fields and different techniques. In short, help us get new things done!

Theme members Jens Lagerstedt, researcher at the Department of Experimental Medical Science, Thomas Ursby, beamline scientist at MAX IV, and Susanna Horsefield, researcher at Biochemistry and Structural Biology, were very pleased with the second symposium:

– The mix of young speakers and keynote speakers contributed to the vivid discussions and promoted collaborations. We were also keen to emphasise how an integrative structural biology approach can be used to tackle difficult research questions, such as the determination of high-resolution structures of macromolecular complexes, of amyloids and of membrane proteins, and so on, say Jens Lagerstedt, Thomas Ursby and Susanna Horsefield.

– Another focus of the symposium was to highlight the importance of the use of complementary techniques using neutrons and x-rays. It is becoming more and more obvious that we need to use integrated approaches to push the research forward. The symposium also turned out to be a very good platform for bringing researchers together to initiate WG activities that focuses on specific scientific areas in structural biology.

Trevor Forsyth, from Institut Laue Langevin in Grenoble, France, and Keele University in the UK, is also a member of the Integrative Structural Biology Theme and he noted that,

– With this second symposium, I feel that people are really starting to identify with this theme that brings a wide range of people and different approaches together. I see a great deal of potential in exploring different scientific areas relating to human health.

Important examples include research on amyloid and related neurodegenerative diseases, membrane protein systems, connective tissue molecules, muscle contraction, and pharmaceutical and therapeutic issues where information of target proteins can guide the development of new drugs.

– In more general terms, we have an important underlying drive: to bridge the gap between the molecular and cellular levels of organisation. This is a priority where the broad range of capabilities at Lund (both existing and planned) can have a huge impact. Strong international link-ups with centres such as Grenoble in France (including the large-scale neutron and X-ray facilities at ILL, ESRF, and PSB) will be crucial in maximising the impact and exploitation for health.

Voices from the symposium:

Sudeep Karoki, University of Helsinki:

– I'm a structural biologist. I study protein structures, and I have been using synchrotrons at Grenoble, France and also in Diamond, United Kingdom. I'm interested in the X-ray crystallography technique and other techniques as a way to study the adhesion between neuron cells. I interested in structural based functional study of proteins and their implications neuronal disorders such as autism, epilepsy, and schizophrenia.

– At the symposium, I want to get new ideas and find out about functional studies. What are the general trends in science right now?

Veronika Nesverova, Lund University and Jennifer Roche, Copenhagen University:

– I think all the talks have had excellent quality. The selections of speakers have also been great. I feel inspired in my own research. I also enjoy the stories behind how people get their results. Hearing about how people work can help you in your own research, says Veronika Nesverova.

– The talks were interesting and so were the topics covered by the speakers. It was a good opportunity to network with the experts and hear about their experiences. In the future, I would also like to see a much wider community from universities within and outside Sweden, says Jennifer Roche.

REFLECTIONS ON NORTHERN LIGHTS ON FOOD: "IT'S CLEAR THAT INTEREST IN THIS AREA IS BUILDING, THERE'S A REAL PUSH TO UNDERSTAND FOOD TO MAKE IT BETTER"

A radical transformation of the food system is needed to provide a healthy, sustainable and affordable diet for all people. Research and development into how food can become more nutritious, taste better, and use less resources, have a key role to play.

In March 2019, MAX IV, LINXS and RISE organised a workshop to bring together x-ray and neutron researchers and the food industry. The aim was to identify common challenges and start new collaborations on how to develop and improve food and food processes.

More than 100 participants attended the event, including researchers from different institutes and universities, and industry representatives, ranging from smaller companies such as Kivik musteri, to larger ones such as Carlsberg and Tetra Pak.

– There was a fantastic range of people at the event who had no idea about x-rays and neutrons, and people who had no idea about food. Then we also had people who had some ideas of both. It's clear that interest in this area is building, there's a real push to understand

food to make it better, maybe in light of challenges such as life style diseases, climate change, and a desire to create more sustainable societies, says Stephen Hall, Director of LINXS.

During the workshop, many questions were raised around food and food structure, both from industry and from researchers. They included how to develop more sustainable foods, produced in ways that use less energy and resources, how to preserve foods, the development of alternatives to meat protein, and how to tailor food and nutrition to individual needs and health, to name a few.

– The intersection of food with health, taste, environment and safety was definitely the most prevalent focus during the workshop, says Selma Maric, researcher at Max IV, and one of the main organisers of the workshop. For me, it was especially interesting to hear about how methods from the Far East, especially fermentation, can be used to preserve foods, or that we need to develop new methods of preparing jellyfish so it is more edible!

Another topic was processing, and how it impacts on food structure, health, and on waste, for example the food that gets stuck in the processing machines. Packaging was also discussed at length; how can you maximize food safety while minimizing waste and environmental impacts? **HOW DO YOU MAKE A CUCUMBER CRUNCHIER?**

As researchers, Stephen Hall and Selma Maric can identify many areas where x-rays and neutrons can be used to address challenges or to advance specific knowledge about foods, especially about the structure of food, and how it behaves on the molecule and atom level.

For example, imaging techniques can be used to study how the food is broken down in the gut, says Stephen Hall. One could build an artificial gut to study how food is digested on the macroscale. Then you can also look at how proteins and other substances break down, to see how the body is interacting with the gut.

Diffraction techniques, with which you can look at the atom structure, can be used to study sense and taste receptors. It enables you to find out more about how sensors in the mouth react with the molecules in the food. The power of neutron scattering techniques can also be used to visualize only the protein or only the fat. This could be a way to monitor various processes involved in changing protein structure, for example to improve taste.

– Umami receptors and sweet receptors in the mouth seem to work together and share a common subunit. Can the umami taste be enhanced with sugar or can we make food taste sweet by exploiting the umami flavour without it actually containing sugar? These techniques open a wealth of opportunities. Likewise, we could combine new techniques with old traditions to make cucumbers more crunchy, last longer and still taste as good as they do fresh, says Selma Maric.

IDENTIFY WAYS OF WORKING TOGETHER

One of the outputs from the workshop is that MAX IV, LINXS, and RISE will write a white paper to summarise the findings from the discussions and presentations.

– Now we need to leverage the development and start thinking about how we can work together, says Selma Maric.

The collaboration between researchers and industry can take many forms, especially since there are differences between the companies in terms of expertise in using techniques, research and development capacities and resources.

– There are good examples from the forest and metal industries that we can look at. They work in large consortiums as a way to build capacity across the board. But there are many different ways people can gather, says Selma Maric.

From LINXS' perspective, next step will focus on the potential to start a new WG on food and x-rays and neutron techniques, as well as on the need for competence building workshops and initiatives.

– One main starting point is language. How do we speak to each other? There is scope to have an introductory workshop on the techniques. The industry has the questions but do not understand the technology yet, says Stephen Hall. After that, we follow up with maybe a WG, and education.

– For LINXS, it's all about creating a productive environment, working with people to develop new techniques, and to encourage new users of MAX IV and ESS, he concludes.

VOICES FROM THE WORKSHOP

A range of different people attended Northern Lights on Food.

Dr. Judith Houston was one of the speakers at the workshop. She works with neutron scattering at ESS.

– To date, I have yet to actually directly study food, but it is an interesting area to explore. Can we look at the dynamics of food? What useful information can you get from using scattering techniques? Things to look at could be how things store, how emulsifiers behave so can you make food last, taste better?

If she would start doing research on food, she wants to study chilli and how spicy foods react with receptors in the mouth.

– Is there a way to cure spiciness? What is the best natural ingredient? Maybe more people can get the goodness of chili if you could calm the spiciness.

Martin Adell from Tetra Pak was another speaker at the event.

– We want to use MAX IV and ESS to understand our processes better. We know a lot of them already: better quality, environmentally friendly, and safer.

For him, especially the material properties are important. How can you work with composites in the packaging such as plastics, foil, and printed cardboard? For companies it is important that their logos and other visual signifiers are visible on the packaging

– If we change the polymer layers in our packaging, how will it interact with the food? We need to know more about how food interacts with basic materials, so we can make our whole processing chain more sustainable, and above all, safe.

For me, personally, I would like to see a consortium being formed around food and the large infrastructures such as MAX IV and ESS. We need more focused efforts than only workshops or shorter initiatives.

Betül Yesiltas, post-doctoral researcher from the Technical University of Denmark and PhD student Mie Thorborg Pederson from University of Southern Denmark were two of the attendees at the workshop.

– I want to learn about applications in food in general, and in emulsions in particular. I'm working with emulsions in my research. We want to understand the oil/water interface; how we can work without disrupting the emulsion structure. Today, we do not know what makes the changes at the interface, says Betül Yesiltas.

– It is also interesting to find out more about MAX IV. How to get beam time for example.

Mie Thorborg Pederson has developed a method to preserve jellyfish to make it more palatable.

–I developed a technique involving soaking the jellyfish in alcohol and let the solvent evaporate to make the jellyfish crispy instead of gelatinous. I want to understand how the microscopic structure of jellyfish relate to the macroscopic mouth feeling, and therefore the talks are very interesting and relevant. It is interesting to hear about new techniques such as neutron scattering and the applications in food science. I have to think about if the different techniques are relevant for my future experiments.

Annex 6 – Financial reporting 2019

Income statement	Categories	Description	SEK
Income	Activities	Conference cost billed	63,700
		Conference fee	64,880
	Activities Total		128,580
	Partners contribution*	LTH-income	2,000,003
		Natfak-income	6,000,000
	Partners contribution Total		8,000,003
	Deferral	Deferral Formas	-500,000
	Deferral Total		-500,000
External Funding**	Formas	500,000	
External Funding Total		500,000	
Income Total			8,128,583
Expenditure	Activities	Conference cost	-609,756
		Hotel & housing	-296,781
		Participation conferences	-7,161
		Representation external	-67,624
		Travel	-424,995
	Activities Total		-1,406,318
	Equipment	Computer/screen/electronics	-4,655
		Depreciation	-94,111
		Furniture	-101,982
	Equipment Total		-200,748
	Materials & consumables	Office supply	-65,668
		Other (incl. currency exchange)	-9,720
		Print material	-24,443
		Services	-71,714
	Materials & consumables Total		-171,544
	Overhead	OH	-971,009
Overhead Total		-971,009	
Premises	Cleaning	-95,520	
	Installation premises	-20,978	
	Premises rent	-1,082,509	
Premises Total		-1,199,006	
Salaries	Salaries	-4,720,044	
Salaries Total		-4,720,044	
Expenditure Total			-8,668,669
Annual Result			-540,086

* In addition, the Lund University Faculty of Medicine contributes in-kind with 50% of the salary for the LINXS Vice-Director.

** Deferral of FORMAS project funding for implementation in 2020.