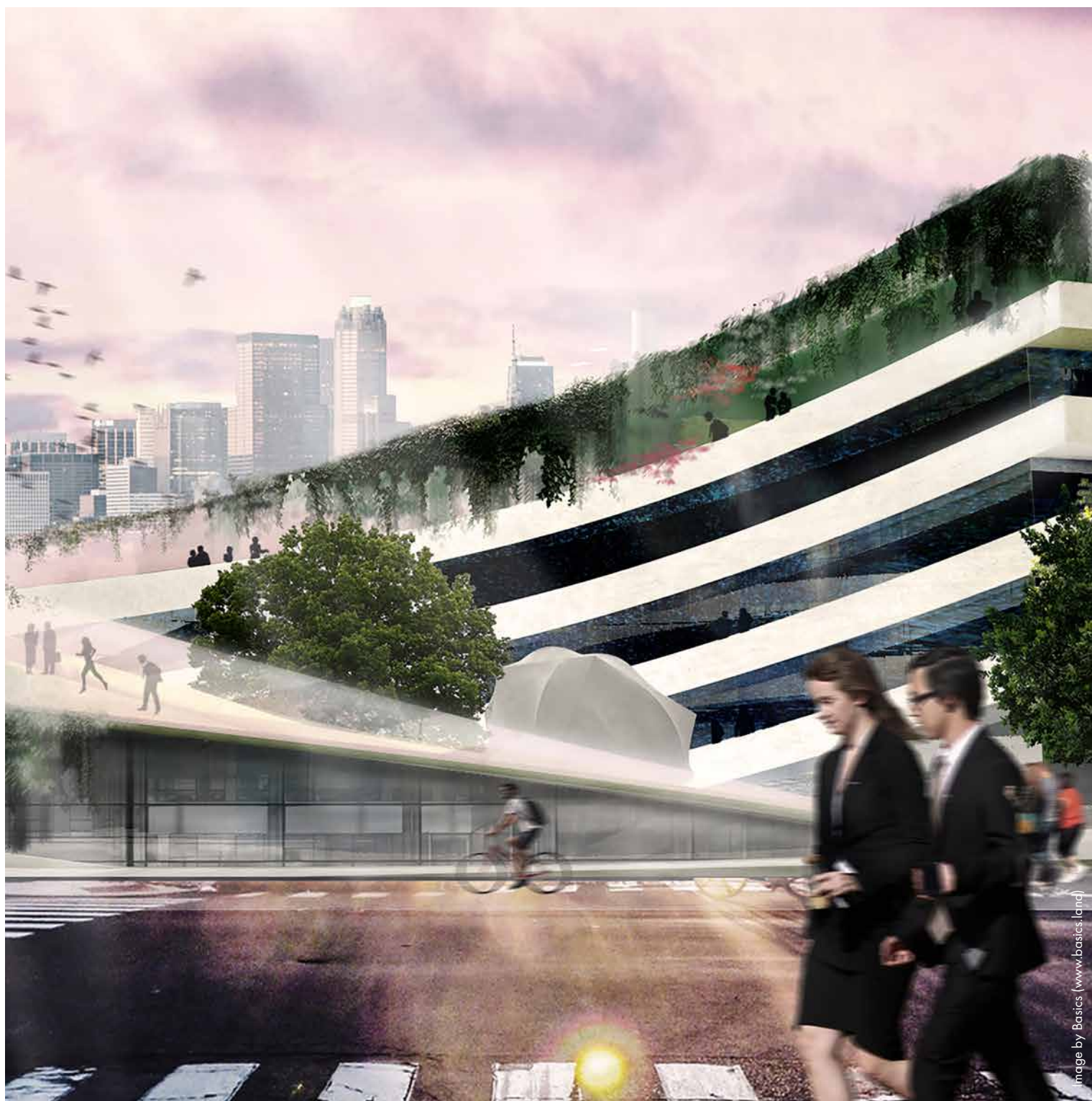




LINXS LUND INSTITUTE OF ADVANCED
NEUTRON AND X-RAY SCIENCE

LINXS Annual Report 2019



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, which includes reviewing applications for new Themes. The SAB provided the following summary of their impressions on the progress of LINXS 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.”



Words 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”. LINXS activities gathered more than 900 participants, 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 a variety of 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. 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, LINXS clearly progressed well in its mission and delivered on the plan defined at the start of the year. Great progress has been made in anchoring LINXS in Lund as well as on the national and international level. We have established best practices to proactively 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 having MAX IV and ESS in Sweden. We also initiated the process of renewal and evolution of LINXS with the call for a new Theme and the start of recruitment of a new LINXS director. We also established a participatory model to open up LINXS to formal memberships and partnerships with other organisations. We welcome interested groups to contact us to be part of our drive to develop and promote science using x-rays and neutrons.

The great steps taken this year to establish LINXS as an international institute in Science Village Scandinavia would not have been possible without the active and engaged participation of our scientific community and the strong support of our staff, Board and SAB. I would like to thank everyone who has been involved in LINXS thus far and I look forward to working with you all in the coming years to further develop the institute and our community.

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

About LINXS

Established in 2017, LINXS is an advanced study institute whose mission is to advance science and education for all research activities that can benefit from the use of neutrons and x-rays. LINXS is dedicated to becoming a nucleus and think-tank for national and international scientific activities relating to research using neutrons and x-rays, both as a network and as a physical location providing an inter-

action hub in close proximity to the large-scale research facilities, MAX IV and ESS, in Lund, Sweden. LINXS brings together world-leading scientists for short-term focused research visits and creates international networks to be an international competence centre, research networking hub and focus-point for education of future generations of neutron and x-ray users.

LINXS mission

Establish

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

Attract

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

Promote

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

Create

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

Focus Areas

Soft Matter

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

Life Science

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

Hard Matter

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



Soil Science Workshop

Why join LINXS?

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

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

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

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

“For me it’s about the community and the knowledge exchange. That’s what LINXS can give me as a researcher. We were missing a physical place where we could meet and collaborate on x-ray and neutron science . . . LINXS gives me an opportunity to discuss techniques and methods with like-minded researchers, in a space which supports activities specifically aimed at pushing research and ideas forward.

Tommy Nylander, professor at Physical Chemistry, Lund University, and a LINXS Fellow





Dynamics Core Group meeting

LINXS themes and Working Groups 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

How LINXS works

Core group

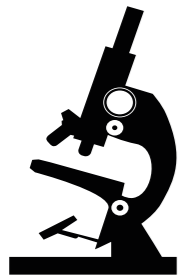
A theme is governed by a core group composed of prominent external and local researchers. One of the main missions of LINXS is to bring external excellence in to work with local and national researchers. The core group usually has an individual from the LINXS management group as a member. A core group suggests to the management group how resources should be allocated for that theme.

Working group

Under the core group there are working groups working on specific activities. These range from conferences, workshops and schools to specific research programmes aided by external research fellows. Working groups are also formed via an application procedure, though this is shorter and more quickly evaluated than that for themes.

Activities

Each working group has a palette of budgeted activities to draw from that can be useful to its defined goals. The nominal budget enables planning of the scientific scope in relation to the total LINXS budget. The activities can be: conferences, research programmes, workshops, hackathons, sabbaticals, schools, seminars and training & outreach, for instance.



1. THEME



2. CORE GROUPS



3. WORKING GROUPS



4. ACTIVITIES

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). 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 and on an international level. The WGs also worked to establish a strong programme 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.



Geoarcheology Working Group Meeting



Soil Science Workshop

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.

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 focused through the initiation of four research programmes. These research programmes are the outcome of some successful workshops during 2018, and their direction came from identified needs from the research community.

Research programmes

“Simulation, theory, and software development for anisotropic systems” looks at how one can solve the structure of complex molecular systems, such as anisotropic colloids, proteins and viruses, this is a particular challenge due to intermolecular interactions between solutes, co-solutes and the solvent. During the year, work was undertaken to identify focus topics: (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 as part of the programme is in progress and involves, primarily, Lund University and Århus University with a focus on calculating water solvation contributions in concentrated protein solutions.

“Antibodies in Solution” was formed in response to the round table discussions at LINXS workshop “Dynamics of Biological Macromolecules” in June 2018. This hot topic emerged as one where LINXS could, and should, play a central role. In 2019, the work focused on securing sufficient quantities of one or more monoclonal antibodies. The research programme brings 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.

“Structure and dynamics utilising the GISANS techniques”, aims to develop the science and the community around GISANS and the future instrument (SAGA) at the European Spallation Source (ESS). It was formed as a result of LINXS’s initiative to bring the Swedish community together to form a Swedish-led consortium in connection to the GISANS

techniques. A strategy document was developed and submitted to the Swedish Research Council in September 2019.

“Sample environment and data evaluation of biological membranes” has its main aim in developing a new concept study on non-lamellar lipid phases and to be able to monitor transitions of lipids due to lipase activity. This work has focused 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 the ILL meeting in Grenoble.



GISANS meeting.



Meeting of the LINXS research programme simulation, theory and software development of anisotropic systems.

Expanding the toolbox for neutron and x-ray experiments

A snapshot of the 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 a 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 experimental design and make precious beam time much more efficient.

t+4Δt

t+3Δt

t+2Δt

Integrative Structural Biology (ISB) Theme

2019 was a year of many positive developments for the Integrative Structural Biology theme. As a result of the 1st ISB symposium in late 2018, new WGs were formed with focus on very timely and highly relevant scientific areas and research questions. One outcome was that the “Bio-compute and Artificial Intelligence & Machine Learning” 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” 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 (formally approved in 2020), identification of key topics that will be addressed and suggestions for activities. The “Time Resolved Structural Biology – New Possibilities in a Time of New Facilities” WG was also formed during 2019. The work has concentrated on the organisation of an upcoming workshop, 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 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.



ISB second symposium.



ISB working group meeting.

“By meeting others, you get inspired in your own research, and can identify future collaborators

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 collabora-

tions. 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, associated with Institut Laue Langevin in France, and Keele University in the UK, is also a member of the Integrative Structural Biology Theme. 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 of science in human health 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”, concludes Trevor Forsyth.

LINXS Activities in 2019

LINXS events and events organised in partnership

1. LINXS Event: Geology, Archaeology and Culture Heritage studies in a new light, Jan 15 – 17, 2019
2. LINXS Event: Welcome to afternoon coffee and a seminar by Prof Hans J Vogel from University of Calgary, Feb 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, Aug 27, 2019
20. LINXS Partner Event: 8th Scandinavian Symposium, Amyloid Diseases and Amyloid Mechanisms (ADAM 8), Aug 28–30, 2019
21. LINXS Partner Event: Doctoral school: Neutrons for membrane biophysics, Sept 16–20, 2019
22. LINXS Event: 2nd Symposium – Integrative Structural Biology, Oct 9 – 11, 2019
23. LINXS Event: Research program Simulation, theory, and software development for anisotropic systems, Oct 22–24, 2019
24. LINXS Partner Event: All-day Symposium: Language technology in Medicine and Life sciences, Nov 8, 2019
25. LINXS Partner Event: Seminar on funding opportunities for artificial intelligence and digitalization in medicine and life sciences, Nov 15, 2019
26. LINXS Event: Amyloid Workshop: “Mind the gaps in amyloid fibre structure analyses”, Nov 21 – 22, 2019
27. LINXS Event: GISANS meeting at LINXS, Lund, Dec 3, 2019
28. LINXS Event: Seminar with Dr Garib Murshudov, MRC Laboratory of Molecular Biology in Cambridge, UK, Dec 6, 2019



Some of LINXS visiting guest researchers.

LINXS' visiting researcher programme

The LINXS visiting research programme brings international researchers to LINXS for short-term research visits. During their time at LINXS, they share their expertise and knowledge with the LINXS community and networks and support the development of regional and international 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; Prof. Thomas Hellweg from Bielefeld University in Germany; Prof. José Campos Terán from Universidad Autónoma Metropolitana – Cuajimalpa in Mexico; and Dr Chris Garvey, from the Australian Nuclear Science and

Technology Organisation in Australia. Dr Garvey's visit is a collaboration between Malmö University and LINXS, and he is also a visiting Professor at Malmö University.

“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.”

LINXS' first post-doc

Dr Anurag Kawde became LINXS first postdoctoral fellow in June. Dr Kawde works 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.

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.



Anurag Kawde, PhD



FASEM doctoral school.

Timeline

“ The great steps taken this year to establish LINXS as an international institute in Science Village Scandinavia would not have been possible without the active and engaged participation of our scientific community and the strong support of our staff, board and SAB. I would like to thank everyone who has been involved in LINXS thus far and I look forward to working with you all in the coming years to further develop the institute and our community.

Stephen Hall, LINXS Director

Location 2022+

Science Village

MAX IV



Location 2018-2022



Tramline

ESS

Background image by Lund City Council / Arrow

Visiting programme started
 Fellows active from 37 different organizations and 10 countries
 First call for theme
 Opening for additional member organisations
 First LINXS post-doc

2019

Regular calls for themes
 Renewal of SAB mandate period
 First member organisation
 New Theme starting

2020

New Theme starting
 Conclusion of 2 first Themes
 Instalment of new Director

2021

Long term funding secured

2022

Permanent location in SVS established

2023

Steady state operations reached at 16-24 MSEK/year

2024

MAX IV
13 BEAMLINES available

MAX IV
16 BEAMLINES available

ESS
Start of User Operations

Finances 2019

Statistics 2019

INCOME



Detailed income (kSEK)

| | |
|--|-------|
| Partner contribution ⁱ⁾ | 8 000 |
| Fees..... | 129 |



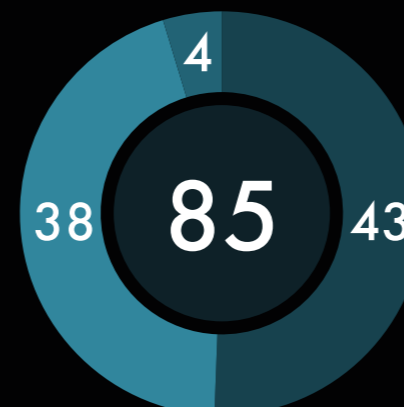
EXPENSES



Detailed expenses (kSEK)

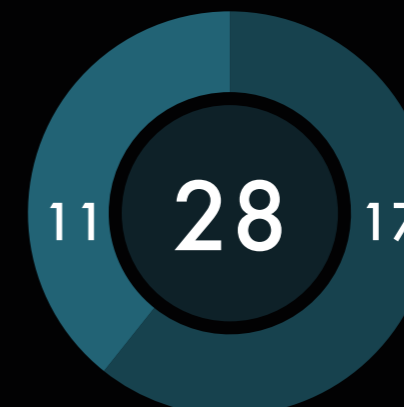
| | |
|---|-------|
| Salaries ⁱⁱⁱ⁾ | 5 316 |
| Activities ^{iv)} | 1 584 |
| Premises ^{v)} | 1 350 |
| Equipment ^{vi)} | 226 |
| Materials & consum. ^{vii)} | 193 |

LINXS Fellows



43 internal, 38 external,
4 guest researchers

LINXS Events



17 own, 11 in partnership

LINXS Event types



13 workshops, 7 seminars,
4 symposia, 2 hackathons
2 PhD schools

Communication & outreach

- 11 outreach activities
- 31 newsitems
- 5 newsletters

Participants at events

791 subscribers

228^{ix)} External participants in LINXS system

447 Registered in LINXS system

900+ Attendees in total

67 (20)♀ Keynote speakers

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

ⁱⁱ⁾ The expenses overshooting the income in the period are deferred to next year's budget.

ⁱⁱⁱ⁾ Salaries include staff, management and emoluments.

^{iv)} Activities mainly includes costs for the organization of LINXS events, accommodation, travelling and outreach.

^{v)} Premises include costs for rental, network and services such as cleaning, and necessary refurbishment of the new LINXS interim location, such as upgrade of the ventilation system to enable events for more people.

^{vi)} Equipment mainly includes costs and depreciation for computers, equipment for the operation of scientific activities, and furniture – a cost in large part related to the establishment of LINXS in its interim location.

^{vii)} Materials and consumables mainly include office supplies and printing equipment.

^{viii)} "Internal" refers to people affiliated to partner organisations of LINXS, "External" is anyone else.

^{ix)} Of these 228, 113 are international participants from outside Sweden, and 115 are from Swedish organisations other than Lund university or MAX IV.



Quantim Hackathon



Almedalen 2019

LINXS Community



ISB working group meeting



Peter Schurtenberger and Sven Lidin, Lund University



Seminar with guest researcher Jan Dhont



Seminar with Dr. Garib Murshudov



LINXS Science Day



Doctoral school on imaging 3D structures



LINXS fellows in 2019 came from the following 37 organisations

- Aarhus University, Denmark
- Australian Nuclear Science and Technology Organisation (ANSTO), Australia
- Australian Synchrotron, Australia
- Bielefeld University, Germany
- Chalmers University of Technology, Sweden
- CNRS, France
- Elettra – Sincrotrone Trieste SCpA, Italy
- European Molecular Biology Laboratory (EMBL) Hamburg, Germany
- European Spallation Source ESS AB
- Forschungszentrum Juelich GmbH, Germany
- Georgetown University, USA
- Inria / CNRS, France
- Institut de Biologie Structurale - Grenoble, France
- Institut Laue Langevin (ILL), France
- Karolinska Institutet, Sweden
- La Trobe University, Australia
- Linköping University, Sweden
- Linnæus University, Sweden
- Lund University, Sweden
- Malmö University, Sweden
- MAX IV, Sweden
- Northwestern University, USA
- Novozymes, Denmark
- Rensselaer Polytechnic University, USA
- Research institutes of Sweden (RISE), Sweden
- Ruđer Bošković Institute, Croatia
- Stockholm University, Sweden
- Swedish University of Agricultural Sciences (SLU), Sweden
- Technical University of Denmark (DTU), Denmark
- Technical University of Munich, Germany
- The "Abdus Salam" Int. Centre for Theoretical Physics, Italy
- Universidad Autónoma Metropolitana - Cuajimalpa (UAM-C), Mexico
- Universität Regensburg, Germany
- University of Bari, Italy
- University of Copenhagen, Denmark
- University of Gothenburg, Sweden
- Uppsala University, Sweden

Organisation

LINXS Board



Sindra Petersson Årsköld
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(LUNA), Lund University

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(LTH), Lund University

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Board Member
Faculty of Medicine, Lund
University

Ulf Olsson
Board Member
Faculty of Science, Lund
University

LINXS Management

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

Jens Lagerstedt
LINXS Vice-Director and Core Group leader for the theme Integrative Structural Biology. Principal investigator and Docent (Eng. Reader or Associate Professor) in Medical Protein Science, Faculty of Medicine. Moved to Lund University in 2009 after postdoctoral training at University of California and at Sahlgrenska Academy.

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

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

Scientific Advisory Board



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



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



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



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



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



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

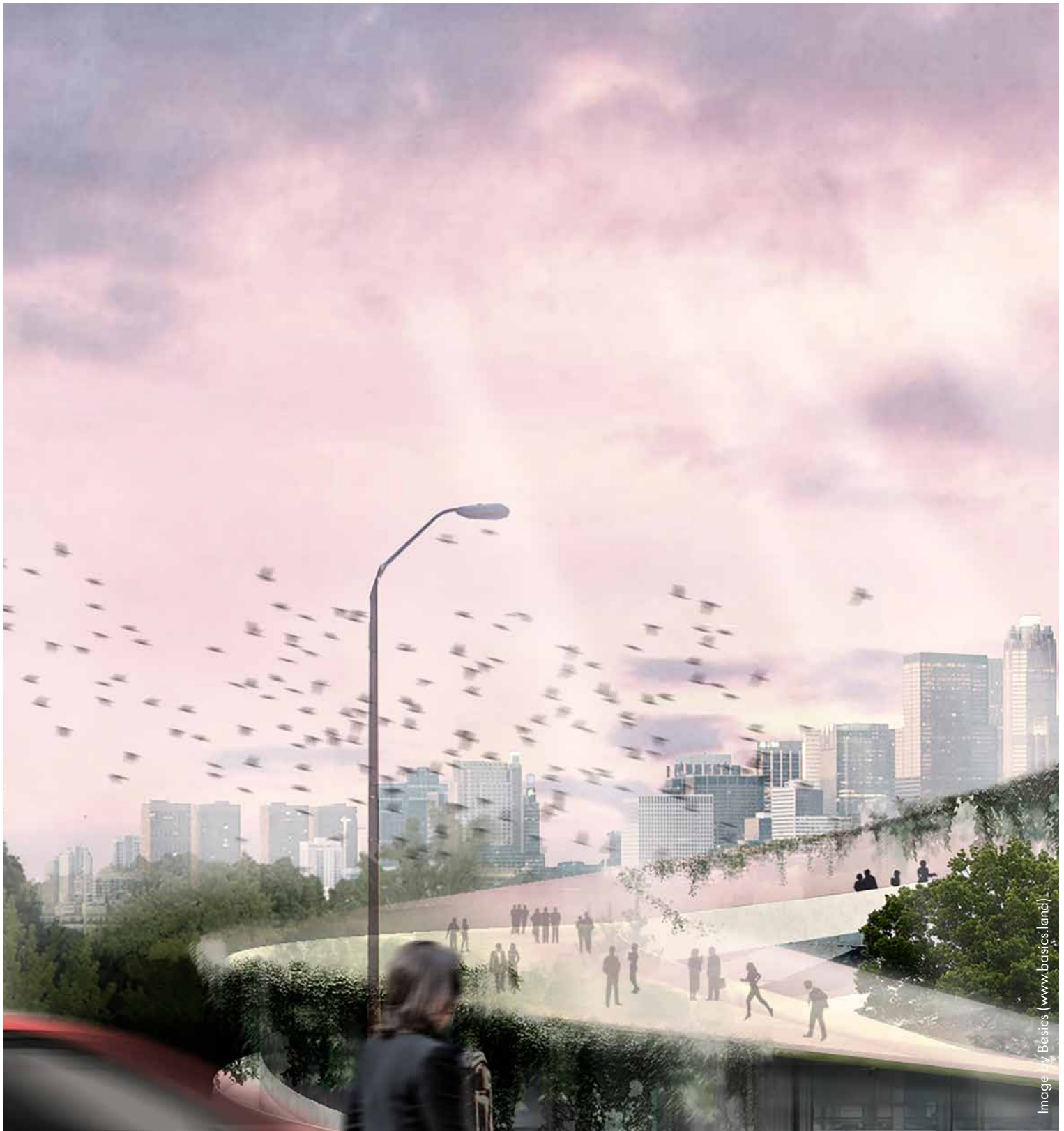


Image by Basics (www.basics.land)

A big THANK YOU to all those who have been active in LINXS and in particular to those who have contributed to our funding so far:



The Crafoord Foundation
ESTABLISHED BY HOLGER CRAFOORD 1980

www.linxs.se

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