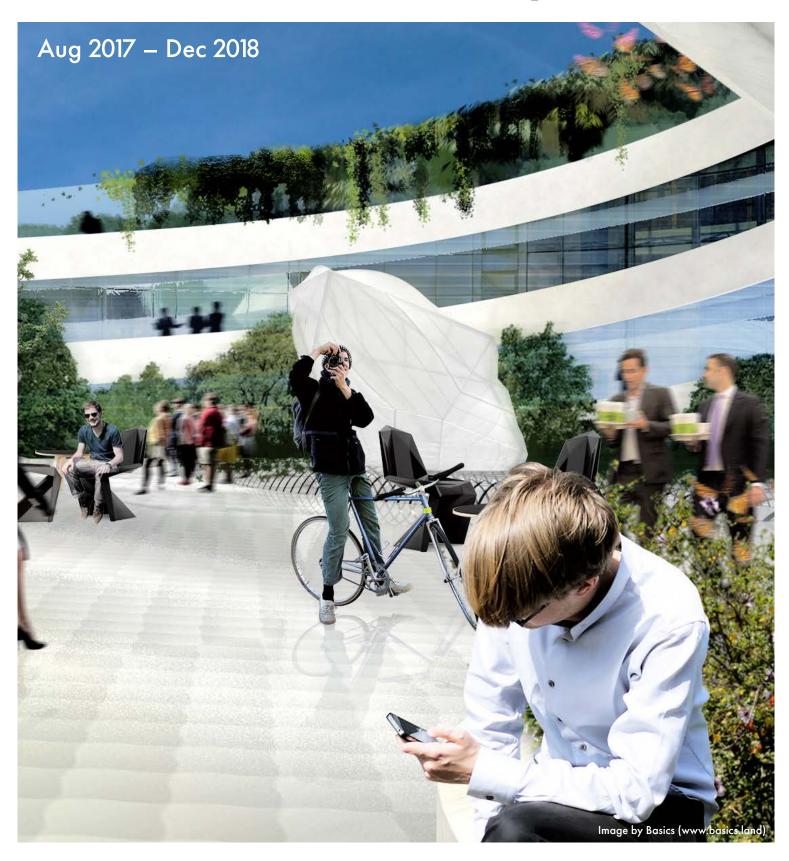
LINXS Annual Report



5 x 107 TbCatB crystals were

Small

MARCH 2012 | NATURE METHODS

Supporting LINXS is a new venture for Crafoord, as we do not normally fund research environments. But we got really excited about the idea to contribute to a new dynamic meeting place, where research and exchange are in focus.

I think LINXS has achieved a great deal in a short time; it's not only a physical place, but researchers and groups are already working here"

> Ebba Fischer, Board Chair, The Crafoord Foundation



Peter Schurtenberger, LINXS Founding Director



Stephen Hall, LINXS Director

"This is a very exciting time for LINXS"

Message from founding and current Directors

It is with somewhat mixed feelings that I write this short foreword for the first Annual Report of LINXS. It has been wonderful to help growing LINXS from a white paper that I had written in early 2011 (!) to a project granted by the vice chancellor of Lund university in 2016 that now has become a "real" institute with its own premises which opened in November this year. Many people have contributed to this successful development, and it was truly rewarding to see the very strong support and excitement that LINXS has created among fellow scientists locally, nationally and internationally.

The numerous excellent presentations and the lively discussions between the participants of the different events organised and hosted by LINXS are a strong testimony for the importance of a structure like LINXS. At the same time,

writing these words as my last official task as the founding director also carries a slight touch of sadness, probably similar to the feelings parents have when children leave their home to become independent.

I'm absolutely convinced that LINXS will see further rapid growth and become a true success story, helping researchers at Lund University and elsewhere to explore, use and further develop MAX IV and ESS to their full potential. I look forward to many more hours of exciting and rewarding scientific exchange that I will hopefully be able to enjoy as a scientist at LINXS in the future, and I wish my successor and the rest of the LINXS team all the best for the future.

> Peter Schurtenberger, **LINXS Founding Director**

This is a very exciting time for LINXS as we build up our scientific activities and expand our community. In the past year we have hosted a number of successful events facilitating interactions between researchers involved in exploiting neutrons and x-rays to address challenges in their respective fields. We have enjoyed presentations and lively discussions between experienced neutron and x-ray users from a wide range of scientific areas, as well as introducing less experienced researchers to a range of techniques and ideas that could lead to new ways to answer their scientific questions.

LINXS is now moving into its next phase with longer-term working group programmes. Furthermore, the move to our new premises is an important step towards further developing the LINXS community by hosting our working groups' activities and welcoming both local and visiting researchers for extended research stays. Everyone

involved in LINXS is working hard towards developing a dynamic, productive scientific environment and progressing towards our goal of becoming a national institute.

We would like to take this opportunity to thank the Crafoord Foundation, the Lund University leadership and the Science, Engineering and Medical faculties for their support of LINXS.

It was a great honour to be asked to take LINXS forward as Director. I am very much looking forward to interacting with the national and international neutron and x-ray communities and assisting researchers, from all backgrounds and both existing and new, to make the most of the potential of facilities such as MAXIV and ESS.

> Stephen Hall, **LINXS Director**

3

Attracting the best scientists in the world

LINXS is needed to maximise the value in having the large research infrastructures MAX IV and ESS in Sweden.

With MAX IV (in operation) and ESS (user operations in 2023) co-located on either side of Science Village Scandinavia, we have a unique opportunity to develop an internationally-leading research community. MAX IV and ESS will each be best-in-class infrastrucutres, but national and international return on this investment is not a given.

Previous experience shows that a high ouput in terms of academic excellence is contingent on active efforts to bring together user communities and to keep up lively interaction with these, as well as new potential users, academic and public/private.

In the long term, these community-building efforts will increase the scientific output and societal impact, as well as increase the lifetime of the infrastructures by helping to keep methods, techniques and beamlines relevant and state-of-the-art.

The infrastructures themselves are, by nature, focused on operations. Unless their presence is coupled with an institute whose express purpose is driving these issues, we risk falling into the same patterns repeated elsewhere. That is why Lund University is incubating LINXS, with the view towards a national and international, topical advanced study institute focused on bringing the best scientists in the world together to expand the realm of possible research and user communities utilising synchrotron and neutron sources.

New user groups ESS Annual visits at full operations 2000-3000 Average visit length 2-4 days Annual visits at full operations LINXS 2000-3000 Average visit length 3-5 days **MAXIV** 50-90 researchers any given day at full operations International excellence New user groups

Kickoff

27-29 sep 2017

Exciting! Party! Scientific Energy!

LINXS started with a bang! More than 160 people gathered for the kick-off to mark the beginnings of the institute's work, and to discuss the future of synchrotron- and neutron-based research, focusing on topics in life sciences, soft matter and hard matter.

Sven Lidin, Chair of the LINXS board, and Professor in Inorganic Chemistry, described the event as a testimony to the great dynamic and energy that exists in the fields of neutron and x-ray science.

"People that I have not seen in years were there. To me, that shows that both researchers and industry have been waiting for something like LINXS. We need a bridge between academia and MAX IV and ESS."

He notes that it is no longer enough to just have the research infrastructure in place.

"You need a physical place, a centre that is independent and that can offer a research context for exploration and practical experiments."

Sven Lidin highlights that the vision of LINXS has been properly established in the past year and that we have started to see the added value that LINXS can bring.

"LINXS can reach out to research fields not yet familiar with synchrotron and neutron science. We can lead in exploring matter with new methods. Working in a thematic fashion, where you bring researchers together around different topics, is a big part of this."

An example of how LINXS can enable the exploration of new research frontiers are the new working groups that have been established during the year, for instance in the area of geoarchaeology, and soil sciences. These groups gather researchers from fields not usually associated with using x-ray and neutron science, such as archaeology and geology.

According to Sven Lidin, LINXS' organisational set up is key in making the institute achieve its goals of creating new research collaborations. This is because all LINXS working groups have to include at least one international researcher - who comes to Lund for concentrated time periods to use MAX IV and ESS.

"You maintain the enthusiasm, and people's will and ability to share their knowledge and time with others. It is a great recipe to attract people who are leaders in their field.

Next steps will be about achieving results. To do more experiments and testing. But LINXS also needs time to grow and to do it organically.", he concludes.



Focus Areas

LINXS works under strategic, long term focus areas reflecting broad research priorities. These are: Soft matter, Life Science and Hard Matter. These are areas where it is felt that a lot of progress can be made in opening up specific fields either by enhancing existing methods using synchrotrons and neutron facilities, opening up for users in new fields, or doing both simultaneously.

Soft Matter

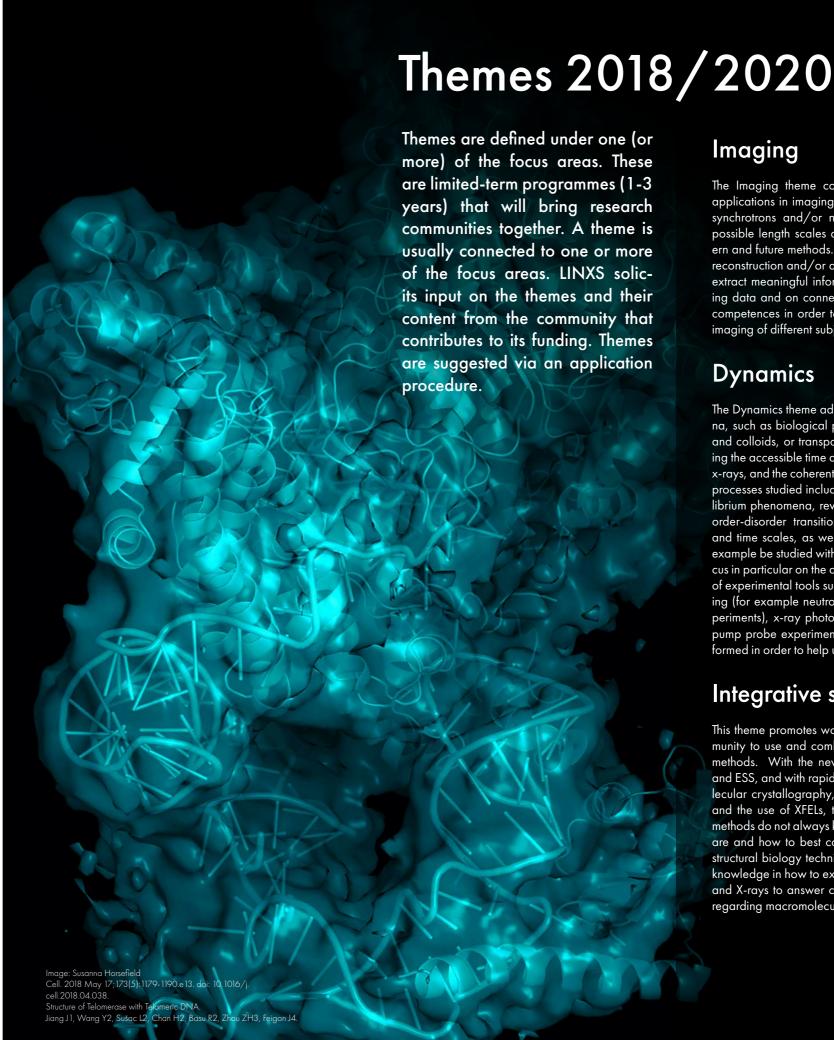
liquids, colloids, polymers, foams, gels, granular materials, liquid crystals, and a number of biological materials. These materials share an important common feature in that predominant physical behaviors occur at an energy scale comparable with room temperature thermal energy.

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.



Imaging

The Imaging theme covers acquisition, processing and applications in imaging that are relevant to systems using synchrotrons and/or neutron sources. We consider all possible length scales and subjects accessible with modern and future methods. The focus is on finding new image reconstruction and/or analysis techniques that can help to extract meaningful information from x-ray/neutron imaging data and on connecting different methodologies and competences in order to shed new light on challenges in imaging of different subject matters.

Dynamics

The Dynamics theme addresses time dependent phenomena, such as biological processes, motion of biomolecules and colloids, or transport processes in hard matter, utilizing the accessible time and length scales with neutrons and x-rays, and the coherent properties of MAX IV. Systems and processes studied include equilibrium as well as non-equilibrium phenomena, reversible and irreversible processes, order-disorder transitions, dynamics on different length and time scales, as well as transient states that could for example be studied with pump-probe experiments. We focus in particular on the application and future development of experimental tools such as quasi-elastic neutron scattering (for example neutron spin echo or backscattering experiments), x-ray photon correlation spectroscopy or fast pump probe experiments, and computer simulations performed in order to help und understand experimental data.

Integrative structural biology

This theme promotes work that enables the scientific community to use and combine a range of structural biology methods. With the new possibilities offered by MAX IV and ESS, and with rapid progress in the fields of macromolecular crystallography, Cryo-EM, small angle scattering and the use of XFELs, the scientists benefiting from these methods do not always know what the different possibilities are and how to best combine data from complementary structural biology techniques. There is an urgent need for knowledge in how to exploit combined data from neutrons and X-rays to answer completely new research questions regarding macromolecular structure and function.





1. THEME



Internal

External

2. CORE GROUP



3. WORKING GROUPS



4. ACTIVITIES

Activities

aug 2017 – dec 2018

During this period, LINXS worked out of its original office in the centre of Lund, where space was limited. We focused on bringing networks together through events and initialising our major themes and associated groups.

From august 2017 to december 2018 people active in LINXS have had:

- 3 Large meetings with >100 people
- 5 Smaller meetings (avg. 50-100 people)
- Themes and core groups initiated
- Working groups started
- 1 Hackathon

Established its interim location at the Delta 5 building in the Ideon science park

A doctoral school on neutron imaging co-organised with SWEDNESS

2 LINXS Postdoctoral Fellowships opened

On the following pages we present some examples of activities made possible by LINXS



Imaging Symposium

18th-19th dec 2017

The Imaging Symposium brought together 50 participants from the faculties of science, engineering, medicine and the humanities at Lund University and MAX IV - all with an interest in imaging with x-rays and neutrons. The aim was to establish a community, develop interactions and, above all, identifying working group activities within the LINXS Imaging theme.

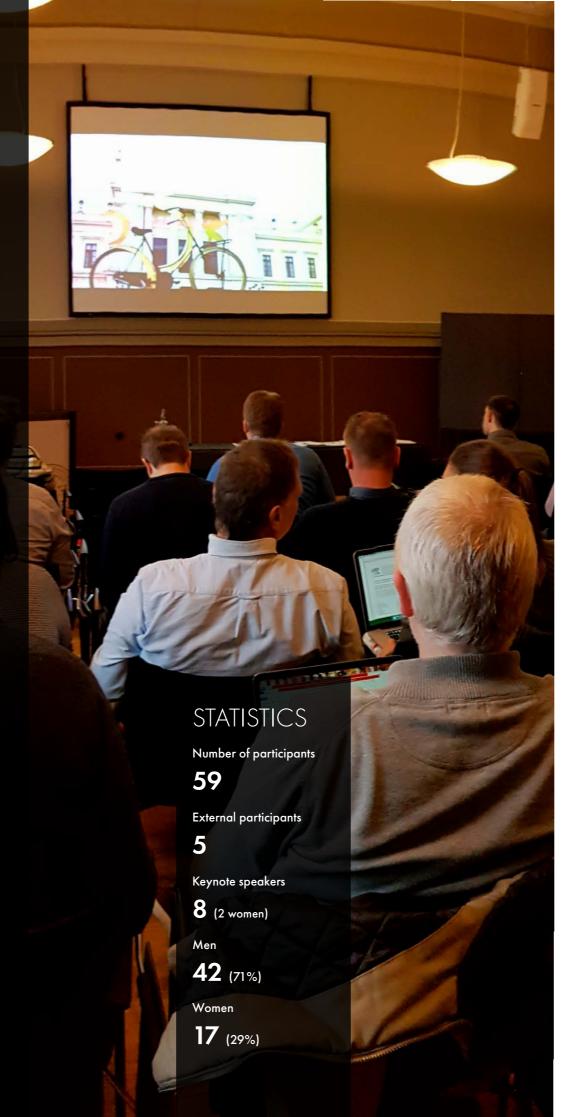
"It was an opportunity to create new research groups and make connections. There is always a language barrier to overcome when you bring different people together, especially when it comes to new methods, says Björn Nilsson, archaeologist the Department of Archaeology and Ancient History at Lund University, and part of an Imaging working group."

For Björn Nilsson, the symposium paved the way for the creation of a new working group, GeoArchaeology, within the Imaging theme. It will bring together archeologists, geologists, cultural heritage researchers and political scientists with the aim to explore how their different disciplines can be brought closer together through the use of synchrotron and neutron based methods.

"LINXS is a springboard. Our group now has an opportunity to explore the relationship between geological and biological material at a nano level. This has not been done before."

He is looking forward to the work ahead. Not least because LINXS' organisation enables the different working groups to invite internationally renowned researchers, and provides professional support in organising activities such as workshops and seminars.

"Maybe we can identify questions we didn't even know existed. This is the challenge for all research fields: finding new areas and new answers. Now we have a way to start"



WORKSHOP

Dynamics of Biological Macromolecules

4th-6th jun 2018

According to Professor Emeritus, Dr. Dieter Richter, Dynamics Core Group Member, and External LINXS Fellow, the Dynamics workshop that took place in June 2018 had just the right mix of people and activities to spark the necessary interest and ambition to push the research field of soft matter forward.

"The discussions were very good. With more than 80 people attending, it is clear that the interest is there.", he says.

The workshop on Dynamics of Biological Macromolecules brought together leading scientists from different fields such as soft matter physics, biology and pharmaceutical sciences, with expertise in experiments, theory and computer simulations. The aim was to discuss how neutrons and x-rays can be used in the development of new technology and to discuss experimental techniques. Topics covered included dynamics of proteins in crowded and confined geometry, dynamics of intrinsically disordered proteins, antibody dynamics and internal motion in proteins and protein dynamics and drug discovery.

"I see LINXS and our theme as something that can be a catalyst to create long term research collaboration between countries. There is a lot of potential. Now you have to take it in your hand and really go with it."

Dr. Dieter Richter says that the flexible and inclusive working methods of LINXS are favorable to support longevity in collaboration and research. Having a small core group of people working closely together mean that careful consideration can be put into organising activities that really give something back to the participants.

"We have to continue working like this. Explore what we can do and not do. And most importantly, not lose the momentum. And here is where LINXS can really come in. You need a centre that can attract people and create an environment where research can flourish."

The right people together



Prof. Dieter Richter

STATISTICS

Number of participants

95

External participants

54

Keynote speakers

13 (3 women)

Mer

60 (63%)

Women

35 (37%)



15

The Integrative Structural Biology Theme

Started in Nov 2018

First Symposium

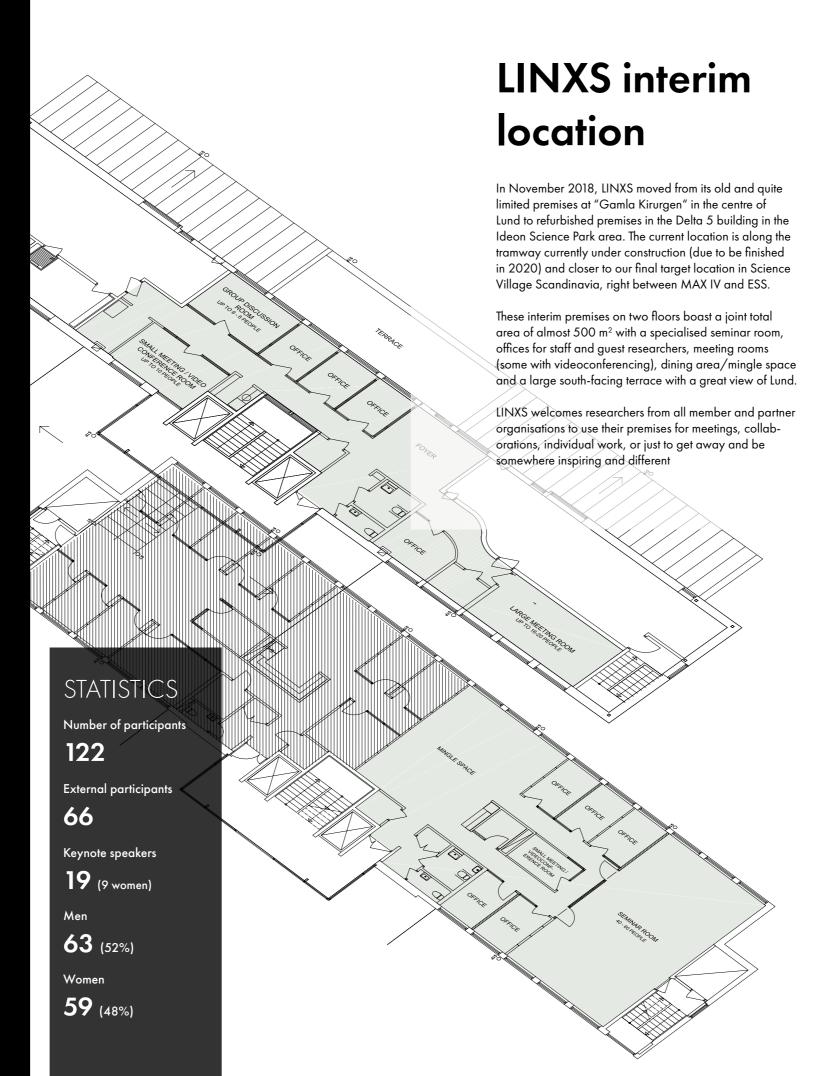
In November, the theme Integrative Structural Biology (ISB) had its very first symposium. The aim was to highlight cutting-edge research in the field of structural biology, with an emphasis on recent development in combining different structural biology methods, and to encourage new and old members of the structural biology user community to utilise these methods to address key scientific questions.

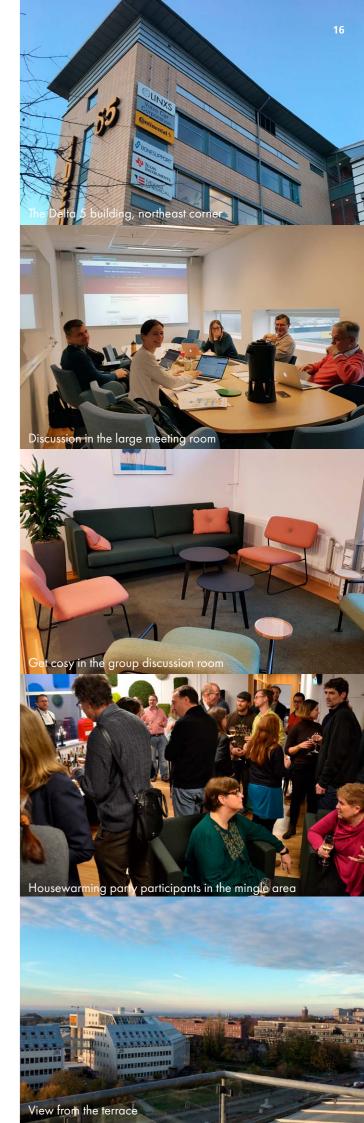
More than 120 people attended the event, which attracted a very high interest. Participants represented researchers at different levels from national and international universities as well as industry.

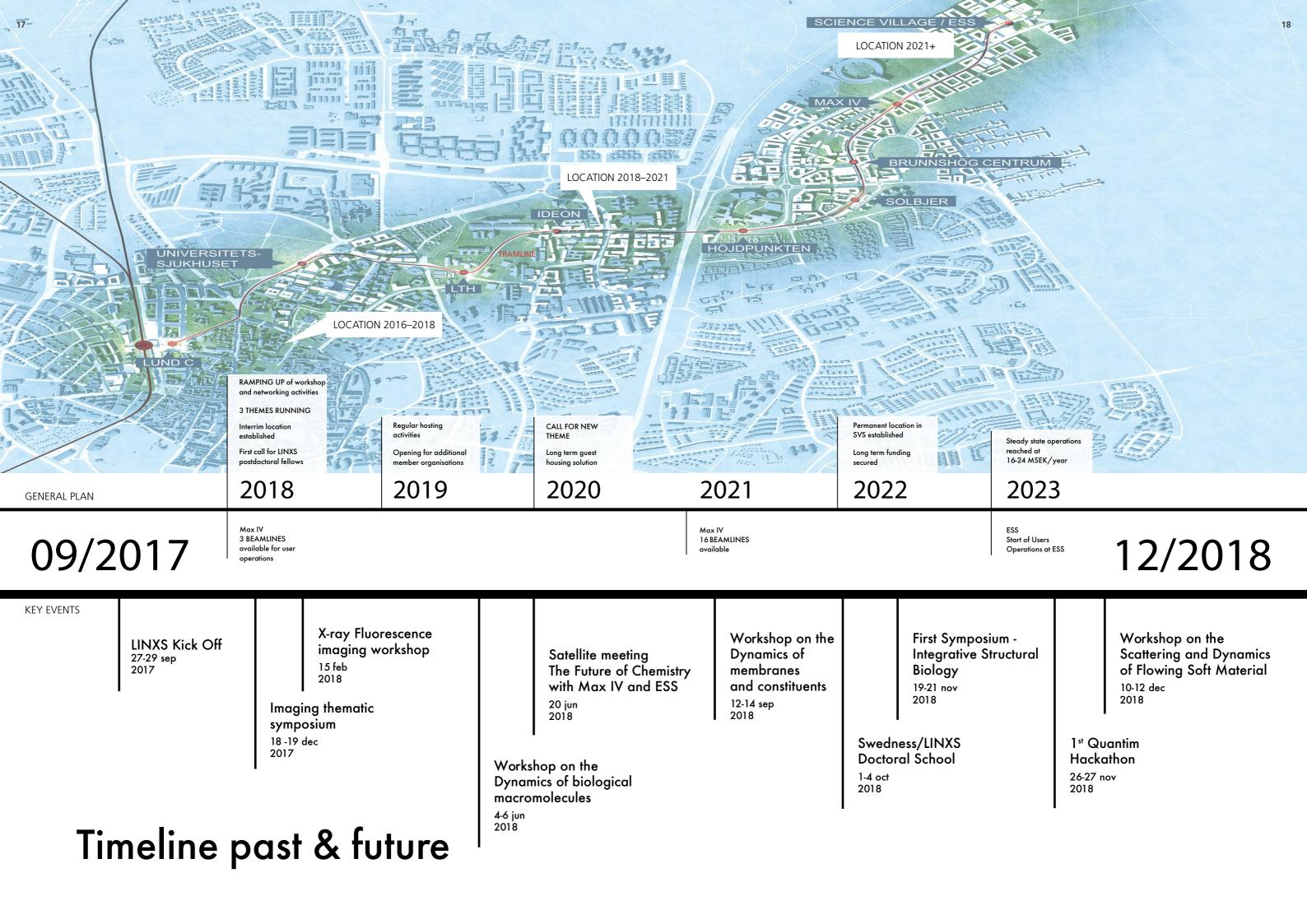
"It was a great opportunity to hear inspirational presentations, highlighting cutting-edge research in integrative structural biology as well as to discuss key challenges within the field. These challenges include the need for validation methods and education of scientists in an evolving cross-disciplinary field. With the help of working groups in complementary areas, our theme aims to help address these challenges", says Susanna Horsefield, Professor in Biochemistry at Lund University, and Core Group theme

The symposium ended with a fruitful discussion on ways forward for the research field, and how LINXS can help to promote and strengthen integrative structural biology. Suggestions included a service where researchers can post a problem, courses in methods and integrative approaches, and to provide a platform and network where issues are continuously discussed and addressed and success stories can be shared and learnt from.









19

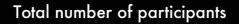
Finances

Statistics

















External participants

327



- il 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.
- 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.
- vi) 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.
- vii) Materials and consumables mainly include office supplies and printing equipment.

Keynote speakers

84 (26)

SCIENTIFIC ADVISORY BOARD

LINXS has a Scientific Advisory Board with two international experts covering each focus area. The SAB advises the Management in all scientific matters, evaluations, and on the long term scientific development of the institute. This initial Scientific Advisory Board has been active since Jan 2017 and has convened five times since then.



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. Dagn 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. 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 modellina.



Prof. Christian Rüegg SAB MEMBER - AREA HARD MATTER

Christian is the Head of the Division for Research with Neutrons and Muons at the Paul Scherrer Institute and a Professor in the Department of Quantum Matter Physics of the University of Geneva. 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. 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 as well as flows of solvents and solutes through porous matrices.



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.

Organisation

With the vision of becoming a national and international institute, LINXS is incubated by Lund University, and as such is currently a Lund university Centre with a Management Group which answers to the Board. The Board level makes strategic decisions, while the Management Group makes scientific decisions. The Scientific Advisory Board issues recommendations to the Management Group on Themes and and the Management Group decides.

BOARD

Sven Lidin Board Chair

Dean of the Faculty of Science and Professor in Inorganic Chemistry. Member of the Nobel Prize Committee for Chemistry since 2003 and its chair 2014-2016.

Ulf Olsson Board Member

Ulf Olsson represents the Faculty of Science at Lund University. He is a Professor of Physical Chemistry, with special interest in soft matter systems.

Kajsa M. Paulsson **Board Member**

Antigen presentation Group

Leader at Experimental Medical Science. Kajsa represents the Faculty of Medicine at Lund University.

Sindra Petersson Årsköld **Board Member**

pean Spallation Source ERIC and representing it in the Steering Committee. Research background in membrane proteins, bioenergetic systems, metals in biology and proton transfer.

Axel Rüter **Board Member**

Graduate student representative. In his research he studies of the model peptide system AnK. A and K are amino amino acid alanine.

Senior Advisor at the Euro-Student Union (LUNA). Marianne Sommarin

the self-assembly behaviour

acids and n denotes a certain number of the hydrophobic

Hanna Sjö **Board Member** Student representative and President of the Science

Board Member Senior advisor to the Vice-Chancellor of Umeå University for research infrastructure and Professor in plant biochemistry at UPSC. Member of the MAX IV &

Marjolein Thunnissen **Board Member**

Life Science Director at MAX IV and represents MAX IV in the LINXS Board. Marjolein is an expert in structural biology using synchrotron radiation and her first use of synchrotrons dates back to the late 1980s.

Erik Swietlicki **Board Member**

Vice Dean at the Faculty of Engineering (LTH) at Lund University and representing LTH. Professor and leading scientist within the Aerosol Group at the Division of Nuclear Physics at Lund University.

MANAGEMENT

Stephen Hall LINXS Director

LINXS Director and Core Group leader for the Imagina 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

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.

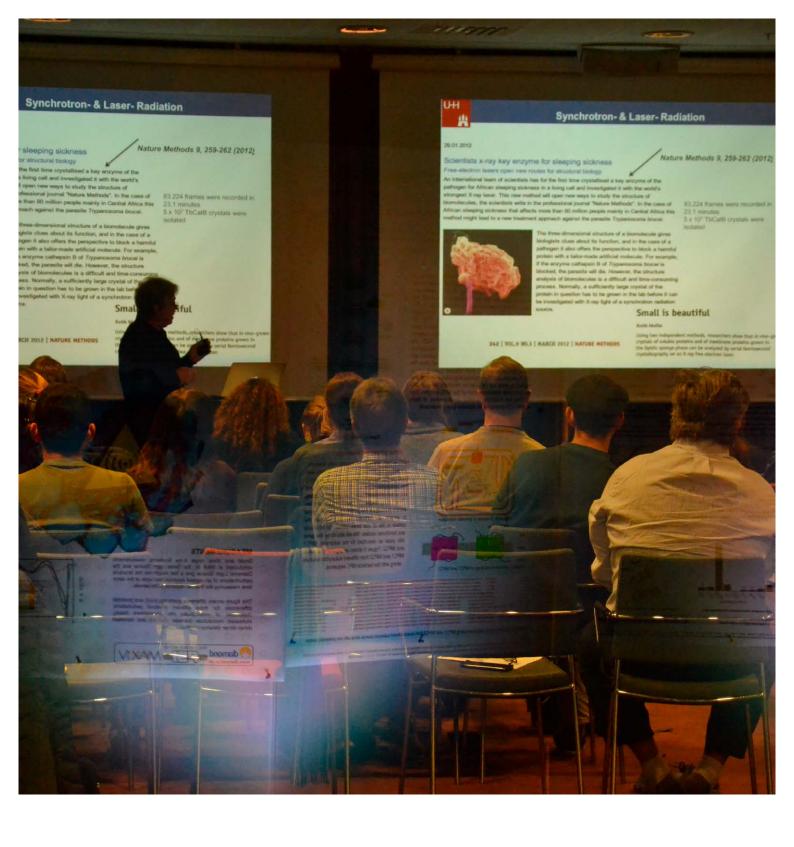
Marie Skepö LINXS Co-Director

SciLife boards

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 **Head of Administration**

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



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





