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Synergies between ESS and MAX IV

Maximising the potential of their co-location in Lund

Image: COBE
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Maximising the potential of their co-location in Lund

technopolis |group|, June 2017

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Executive Summary

Possible synergies could arise from the co-location of a neutron source, the European Spallation Source (ESS), close to a synchrotron facility, MAX IV in Lund, Sweden. ESS is a large scale Research Infrastructure (RI) which has been in the making for more than a decade and is planned to have its first call for users in 2023 and be in full operation from January 2026. Since 2015 ESS has been operating as European Research Infrastructure Consortium – a specific legal form to facilitate the establishment and operation of RIs with European interest. Eleven European countries act as founding members (with Sweden and Denmark as hosts) and three other countries have observer rights. Apart from the facility in Lund a super-computing data management and software centre will be built in Copenhagen. MAX IV is a synchrotron that opened in Lund in June 2016. It is the largest national RI in Sweden. The main part of base funding for MAX IV is provided from the Swedish Research Council; thus making fundamental research and the needs of the Swedish research community a main focus of this RI.

A synchrotron and neutron source are conceptually quite similar. They use similar techniques and theoretical principles for analysing matter (resp. photons and neutrons): they both accelerate charged particles to high energies with magnets. This extra energy is used to produce light (photons) or smash out neutrons from the nuclei of atoms (spallation) respectively. Their different outputs at the beamlines enable analyses that are sometimes analogous but give different – often complementary – information. This complementarity is for some studies and/or instrument categories more useful or obvious than for others as described in more detail in this report.

The main reason for scientists to go to specific RIs is their specifications, not co-location per se. Excellence and uniqueness of the facility and its beamlines are the most important factors. MAX IV and ESS are both world-class with specs better than any other similar RIs to date. A fundamental complementarity through differences exists between them enabling researchers to construct a full understanding of the samples that are being studied. At the moment several techniques for analysis at ESS and MAX IV are complementary and further additional synergies between the techniques can be realised in the future. When ensuring such complementary, it is, however, crucial to ensure that certain conditions are in place. A benefit of co-location is reaped where there is a common access for complementary techniques at both RIs and this access is assisted. Turning the Lund site into an international hotspot will benefit not only from synergy through science but also from synergy through support facilities, ranging from common entrance and reception, to guesthouses, conference centres, and common laboratories.

Location itself matters too. The advantage of Swedish researchers is that they are relatively close to both RIs. This may be beneficial in international cooperation and may also attract excellent international researchers to Sweden. To foster the benefits of (co-)location, the neutrons and synchrotron communities should be brought together. Here, training of researchers should focus on synergetic side aspects and support to young researchers – as future generation of users – should be prioritised.

Unawareness among the Swedish researcher community of using this unique opportunity is probably a major problem at the moment; followed by a lack of skills. It is important, therefore, to tackle such barriers and promote connections between the potential users and the facilities. While longer-term strategic decisions can take time, there are smaller things that can be implemented already now around building the capacity of existing researchers, supporting future researchers, and growing a combined neutron/synchrotron research community, not necessarily restricting it within set geography.

For the site to become a thriving international hub a vision and strategy for the development over the next 20 years needs to be prepared and communicated. This should include the vision and steps on how to support the existing potential, how to bring up a new generation of researchers, and how to use the potential synergy through science and support facilities. The MAX IV synchrotron facility and the European Spallation Source in Lund are here to stay. Therefore, it is important to take certain steps NOW to ensure a successful use of these resources in the FUTURE.
1 Introduction

1.1 The context of this study

This report presents the results of a study on the possible synergies that could arise from the co-location of the European Spallation Source (ESS) close to the MAX IV synchrotron facility in Lund. The Swedish Research Council commissioned this study and Technopolis Group completed it during January-May 2017 with support from the Swedish Research Council. The key objective was to collect views from a selected number of researchers working in the research fields where the two research infrastructures (RIs) can be used. The assumption here was that personal experience of researchers expressed in interviews could add a valuable dimension to further discussions with other stakeholders like universities and industry. Care was taken to include researchers that have used complementary technologies that will be available at the two facilities. The questions in the interviews ranged from details about instrument complementarity to strategic experiences of developing research infrastructures.

The authors thank all the contributors for their time and valuable input provided during the study.

The report was compiled so that it can also be discussed with a wider audience not necessarily closely associated with ESS and MAX IV. For that matter, it starts with a brief introduction about the two facilities and then continues discussing the synergies of ESS and MAX IV through science and facilities and avenues for further strategic development.

1.2 The European Spallation Source

The European Spallation Source (ESS) is a neutron source that is currently being built in Lund (Sweden). It had been in the making for more than a decade when in 2009 Lund was chosen as the site with Sweden and Denmark as host countries. Apart from the facilities in Lund, a super-computing data management and software centre (DMSC) will be built in Copenhagen (Denmark). Work on the site in Lund started in 2014 under the auspices of ESS AB, a company formed under the Swedish law and owned by Sweden and Denmark. In parallel, work on forming an organisation with all the European partners continued.

In 2015 ESS AB was replaced with ESS ERIC, a European Research Infrastructure Consortium (ERIC) which is an EU legal entity for international RIs. The founding members are 11 European states: Czech Republic, Denmark, Estonia, France, Germany, Hungary, Italy, Norway, Poland, Sweden and the United Kingdom. Additionally, it includes three other EU member states – Belgium, Spain and the Netherlands – as founding observer countries which plan to become members in the near future. Once ESS is fully operational (which is planned for after 2025), two to three thousand research users from international universities, institutes and industry are expected to come to ESS annually.

The original mission of ESS is “to design, build and operate the world’s leading research facility using neutrons for science and innovation.” Technically speaking, neutrons are produced at ESS through a spallation process. High-energy protons are collided with atoms whose nuclei are rich in neutrons and thereby free neutrons are produced. In ESS protons are created from hydrogen gas and linearly accelerated with magnets to relativistic speed (close to the speed of light) and hit on a metal target material to produce several high-energy neutrons. A rotating tungsten target is used. The neutrons produced by spallation are directed to the beamlines where the scientific instruments are positioned. The more neutrons produced in the spallation process, the higher the luminosity (brightness) of the

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1. It is important to note that no companies were interviewed during this study. All the views and suggestions put forward in relation to industry engagement came from the researcher community and, thus, might have not captured all the nuances.
3. A new proposal for a vision will be addressed in early June. This proposal is: “Our vision is to build and operate the world’s most powerful neutron source, enabling scientific breakthroughs in research related to materials, energy, health, and the environment, and addressing some of the most important societal challenges of our time.”
spallation source. ESS will have the highest neutron peak brightness in the world, at least 30 times greater than current research facilities.

Currently 16 beamlines are in the development phase at ESS (see Table 1), with another seven planned before full operation starts. There will still be room for installation of future instruments in the operational phase. The beamlines enable to serve experiments in the fields of, for example, Energy, Materials, Life Sciences, Magnetics and Electronics, Fundamental Physics and Cultural Heritage.

Table 1 Currently planned beamlines at ESS

<table>
<thead>
<tr>
<th>#</th>
<th>Beamline</th>
<th>Technique</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>LoKI</td>
<td>Small-Angle Neutron Scattering (SANS)</td>
</tr>
<tr>
<td>2</td>
<td>NMX</td>
<td>Macromolecular Diffraction</td>
</tr>
<tr>
<td>3</td>
<td>ODIN</td>
<td>Imaging</td>
</tr>
<tr>
<td>4</td>
<td>BEER</td>
<td>Materials and Engineering Diffraction</td>
</tr>
<tr>
<td>5</td>
<td>ESTIA</td>
<td>Reflectometry</td>
</tr>
<tr>
<td>6</td>
<td>DREAM</td>
<td>Powder Diffraction</td>
</tr>
<tr>
<td>7</td>
<td>C-SPEC</td>
<td>Direct Geometry Spectroscopy</td>
</tr>
<tr>
<td>8</td>
<td>SKADI</td>
<td>Small-Angle Neutrons Scattering (SANS)</td>
</tr>
<tr>
<td>9</td>
<td>VOR</td>
<td>Direct Geometry Spectroscopy</td>
</tr>
<tr>
<td>10</td>
<td>BIFROST</td>
<td>Indirect Geometry Spectroscopy</td>
</tr>
<tr>
<td>11</td>
<td>FREIA</td>
<td>Horizontal Reflectometry</td>
</tr>
<tr>
<td>12</td>
<td>HEIMDAL</td>
<td>Powder Diffraction</td>
</tr>
<tr>
<td>13</td>
<td>MAGIC</td>
<td>Single Crystal Diffraction</td>
</tr>
<tr>
<td>14</td>
<td>MIRACLES</td>
<td>Backscattering Spectroscopy</td>
</tr>
<tr>
<td>15</td>
<td>T-REX</td>
<td>Time-of-flight Spectroscopy</td>
</tr>
<tr>
<td>16</td>
<td>VESPA</td>
<td>Vibrational Spectroscopy</td>
</tr>
</tbody>
</table>

Source: European Spallation Source website [https://europeanspallationsource.se/section/ess-instrument-suite](https://europeanspallationsource.se/section/ess-instrument-suite) accessed in April 2017

1.3 The MAX IV synchrotron

MAX IV is a synchrotron that opened in Lund in June last year. It is built at the new Brunnshög research campus that will be shared with ESS and with some other research facilities of the University of Lund and potentially other organisations too located in Science Village Scandinavia. MAX IV is part of the Swedish MAX-Lab and is the largest national research infrastructure that is hosted by Lund University. The mission of MAX IV is “to enable research by providing photon-based experiments to all areas of natural sciences in which Sweden has an interest”.

The main part of base funding for MAX IV is provided from the Swedish Research Council. It will therefore focus on fundamental research and the needs of the Swedish research community – although MAX IV is also open to applied research by and with industry, charging an additional fee or requesting complementary funding. Beamtime can be obtained in competition based on scientific excellence and project feasibility. Users who will publish the results of their study in open access journals can get beamtime free of charge. From 2026 MAX IV expects 3,000 users per year.

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In synchrotrons, like MAX IV, electrons are accelerated with large magnets and brought into a so-called storage ring of the synchrotron. In this ring electrons travel at relativistic speeds (i.e. near the speed of light) in short straight sections followed by bends that are controlled by special magnetic structures. The bending of the electron beam is associated with an energy loss that is converted into light, the so called synchrotron radiation. The resulting beam of synchrotron radiation has some favourable properties: high flux (high intensity photon beams), high brilliance, high stability, polarised and pulsed. MAX IV has the highest brilliance of all currently existing synchrotrons in the world. The specs of MAX IV are considered world-class.

The MAX IV facility consists of two storage rings – a larger 3 GeV ring and a smaller 1.5 GeV ring – and a linear accelerator that serves as the electron injector to the rings and is also the light source for the Short Pulse Facility. The linear accelerator allows for a future upgrade towards a free electron laser. In order to stay a world-class RI, MAX IV will be regularly upgraded and updated during its lifetime. MAX IV can accommodate up to 32 beamlines, of which 14 (see Table 2) have already been funded and selected through an international review. These beamlines are currently being prepared, with only two already being operational – BioMAX and NanoMAX. The goal of MAX IV is to have 25 beamlines operating or under construction by 2026. At least nine of these beamlines will (have to) be internationally funded (from non-Swedish sources) or funded by industry. The beamlines enable to serve experiments in the fields of Life Science, Chemistry, Physics, Environmental Science, Engineering, Materials Science (incl. Nanotechnology) and Cultural Heritage.

Table 2 Currently planned beamlines at MAX IV

<table>
<thead>
<tr>
<th>#</th>
<th>Beamline</th>
<th>Accelerator</th>
<th>Technique</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ARPES</td>
<td>1.5 GeV</td>
<td>Angle resolved photoelectron spectroscopy (ARPES) including spin resolution (SPIN-ARPES) for detailed studies of the electronic structure of solids</td>
</tr>
<tr>
<td>2</td>
<td>Balder</td>
<td>3.0 GeV</td>
<td>Hard X-ray absorption and emission spectroscopy (XAS, XES) and X-ray diffraction (XRD) with emphasis on in-situ and time resolved studies</td>
</tr>
<tr>
<td>3</td>
<td>BioMAX</td>
<td>3.0 GeV</td>
<td>Macromolecular crystallography with a high degree of automation and remote access</td>
</tr>
<tr>
<td>4</td>
<td>CoSAXS</td>
<td>3.0 GeV</td>
<td>Small and wide angle X-ray scattering (SAXS, WAXS) and coherent techniques for soft matter and bio materials</td>
</tr>
<tr>
<td>5</td>
<td>DanMAX</td>
<td>3.0 GeV</td>
<td>Powder diffraction and tomographic imaging of hard (energy) materials</td>
</tr>
<tr>
<td>6</td>
<td>FemtoMAX</td>
<td>Linac</td>
<td>Time-resolved hard X-ray scattering and spectroscopy for studies of ultrafast processes</td>
</tr>
<tr>
<td>7</td>
<td>FinEstBeaMS</td>
<td>1.5 GeV</td>
<td>Electron spectroscopies and luminescence methods for studies of low density matter and solids</td>
</tr>
<tr>
<td>8</td>
<td>FlexPES</td>
<td>1.5 GeV</td>
<td>Soft X-ray spectroscopies for studies of low density matter and solids</td>
</tr>
<tr>
<td>9</td>
<td>HIPPIE</td>
<td>3.0 GeV</td>
<td>Near ambient pressure photoelectron spectroscopy on solids and liquids</td>
</tr>
<tr>
<td>10</td>
<td>MAXPEEM</td>
<td>1.5 GeV</td>
<td>Aberration corrected photoelectron microscopy for investigation of surfaces and interfaces</td>
</tr>
<tr>
<td>11</td>
<td>NanoMAX</td>
<td>3.0 GeV</td>
<td>Imaging with spectroscopic and structural contrast techniques and nanometre resolution</td>
</tr>
<tr>
<td>12</td>
<td>SoftiMAX</td>
<td>3.0 GeV</td>
<td>Scanning transmission X-ray microscopy and coherent imaging methods</td>
</tr>
<tr>
<td>13</td>
<td>SPECIES</td>
<td>1.5 GeV</td>
<td>Resonant inelastic X-ray scattering (RIXS) with high resolving power and near ambient pressure photoemission</td>
</tr>
<tr>
<td>14</td>
<td>VERITAS</td>
<td>3.0 GeV</td>
<td>Resonant inelastic X-ray scattering (RIXS) with unique resolving power and high spatial resolution</td>
</tr>
</tbody>
</table>

Source: MAX IV Laboratory, 2016
# 2 Synergies through science

## 2.1 Complementarity between analyses with X-rays and neutrons

A synchrotron and neutron source are conceptually quite similar. They use similar techniques and theoretical principles to generate particle beams (resp. photons and neutrons) for analysing matter: they both accelerate charged particles with magnets. Their different particle outputs at the beamlines enable analyses that are sometimes analogues, but give different – often complementary – information. This complementarity is for some studies more useful or obvious than for others.

### 2.1.1 Fundamental complementarity through differences

X-rays and neutrons both interact with matter, but in a different way. All matter is built of elements with a nucleus surrounded by a shell of electrons. Neutrons interact with the nucleus of the elements, while X-rays interact with their electrons. The nucleus and the electrons determine different properties of matter and so X-rays and neutrons can probe these different properties as well. Probing these different properties enables researchers to construct a full understanding of the sample that is being studied.

Matter consisting of light elements is generally better analysed with neutrons, as they contain few electrons and therefore produce a weak signal with X-rays in synchrotrons. For example, hydrogen – a common element in biological samples (soft matter) – is very light and has only one electron. It is therefore not easily detected with X-rays (weak signal), but neutrons that interact with the nucleus can detect hydrogen very well. In fact, neutrons can even discern the difference between hydrogen (\(^1\)H) and deuterium (\(^2\)H), i.e. neutrons are sensitive to isotopes\(^5\). That isotope resolving effect is used for markers in soft matter samples: through a process called deuteration some hydrogen atoms in the sample are replaced by deuterium so that parts of the sample can be marked for analysis. X-rays are not sensitive to isotopes (different number of neutrons in nucleus) but are sensitive to the atomic number (different number of electrons and protons). To get a full picture, both neutrons and X-rays could be used.

Neutrons are also important for the analysis of magnetism and related phenomena such as superconductivity\(^6\). Unlike photons (X-rays), neutrons have a magnetic moment that strongly interacts with magnetic materials. Neutron sources are therefore often used to analyse magnetism, although several synchrotron techniques have been developed to analyse magnetism as well. Magnetism is an effect that is related to electrons and therefore X-rays are useful too. The difference is that with magnetism neutrons can give an overall picture and the immediate response of the system, while with X-rays one can refine these aspects to look at specific details (e.g. tuning to specific elements). Researchers studying magnetism thus complementary use synchrotrons and neutron sources to improve their understanding of magnetic samples. It gives them the opportunity to form a full picture of the materials system.

A fundamental property of neutrons is that they are not electrically charged – they are neutral. Due to that property they generally interact weakly with matter and can have a deep penetration into materials. Therefore, one can analyse large samples and dense materials with neutrons. This would allow for studies in engineering on, for instance, strain and stress in larger objects. The interactions that neutrons have with nuclei can however result in a slight radioactivity of the sample (neutron activation). Photons are not charged nor do they have a mass. X-rays therefore scatter more easily, with a fast response, and have a small penetration depth. Very thin and small samples can therefore be

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\(^5\) Isotopes are variations of the same element, i.e. they have the same atomic number, but with a different number of neutrons in their nucleus and thus a different mass. The atomic number is related to the number of protons, which is for uncharged atom identical to the number of electrons.

\(^6\) Superconductivity is a quantum mechanical phenomenon in which specific materials – called superconductors – reach zero resistance when they are cooled below a critical temperature. More so, they demonstrate some unique magnetic effects: full expulsion of the magnetic field (the Meissner effect), magnetic vortices and critical magnetic fields above which magnetic vortices appear or the superconducting state disappears.
analysed with X-rays, while this is not feasible with neutrons. This would, for instance, allow studies in nano chemistry on the formation of materials, reactions (e.g. oxidation) and interactions. The interaction of X-rays with electrons leads to shifts in energy levels, allowing to identify elements. Although X-rays do not make samples radioactive, they can be destructive to the sample.

As analyses with X-rays can be performed on small samples, synchrotrons are useful for samples that can only be produced in small amounts. This is sometimes the case in biological or chemical studies on macromolecules or small samples of soft matter like proteins. Biological samples often contain hydrogen and therefore sometimes a larger amount of the sample is studied with neutrons as well, since hydrogen is practically invisible with X-rays.

The response of X-rays is generally faster than those of neutrons. X-rays are therefore better to study the fast response of materials, although this could also be done with neutrons. Due to this fast response and the need for small samples, X-rays are better equipped to look at the ‘birth’ of materials, while neutrons may look better at the ‘life’ of materials (being applied). ESS is however said to have better specs to do analyses that need a fast response than other neutrons sources. An example from the interviews is the functional response of bones under mechanical loading.

2.1.2 Specific complementary techniques

Several techniques for analysis at ESS and MAX IV are complementary. The ones mentioned during the interviews are discussed here. At both MAX IV and ESS there is room for additional beamlines and instruments. Through these beamlines additional synergies between the techniques available at both RIs can be realised in the future.

On macromolecular crystallography there is a good complementarity between ESS and MAX IV. This technique is used to study more complex biological molecules such as proteins, DNA, RNA and viruses. The BioMAX beamline at MAX IV is used for these types of experiments and at ESS the NMX beamline will use this technique. The beamline at ESS will have the highest brilliance for macromolecular crystallography with neutrons. A common access to these beamlines (which is currently being discuss between MAX IV and ESS) will be beneficial in utilising these synergies. For the neutron analysis one would then need a larger sample of which a smaller part is used for the X-ray analysis. For this type of biological research there is a clear benefit in being co-located and therefore both research facilities strive to realise a common access mode, so that users can apply for beamtime at the macromolecular crystallography beamlines of both RIs.

Inelastic scattering is another technique that is available at both ESS and MAX IV. With inelastic scattering the dynamics in materials can be analysed, such as lattice dynamics (e.g. phonons) and electron dynamics (e.g. excitations and density of states). At MAX IV the beamlines SPECIES and VERITAS will use this technique. Neutron inelastic scattering can for example identify the movements in materials due to heating, but also magnetic excitations can be observed. X-ray inelastic scattering can observe for example electron excitation. Both techniques are complementary as neutrons can observe the larger effects, while X-rays can observe the smaller effects. Both can do this with a high brilliance, resulting in a good resolution. Complementary use of both RIs regarding inelastic scattering techniques is expected.

Small-angle scattering is a complementary technique that will be available at both MAX IV and ESS. SAXS and SANS are small-angle scattering techniques with X-rays and neutrons respectively. Several interviewees indicated to have used SAXS and SANS and to use these complementary techniques in the future as well. Small-angle scattering techniques do not need a crystalline sample, making them especially useful for (structural) biological research, such as research on proteins and colloids. SANS and SAXS give structural information on nanometre sized macromolecules. At MAX IV the beamline CoSAXS will use the SAXS technique and at ESS the beamlines LoKI and SKADI will use the SANS technique. SAXS measurements are much faster than SANS measurements, therefore researchers often analyse first the samples with SAXS and select interesting areas in phase space and then look for more details at those areas with the slower SANS technique. One interviewee mentioned that at Grenoble they often use 24h beamtime at the synchrotron and then 24h beamtime at the neutron source to do these
analyses. With MAX IV and ESS there is also a clear potential to offer common access to these beamlines at both RIs to exploit the synergy of this technique.

**Powder diffraction** is another set of complementary techniques that will be available at MAX IV and ESS. Generally, powders or microcrystalline samples are analysed with both X-rays and neutrons. With powder diffraction researchers can observe diffraction rings from which they can determine for instance the lattice parameters\(^7\) of the crystals in the powder, the materials in the powder, the phase of the crystals and their crystallinity. It gives valuable information on the content and the structure of the powder. At MAX IV the beamline DanMAX will use this technique and at ESS the beamlines DREAM and FREIA will use this technique. The reason why often both neutrons and X-rays are used for powder diffraction is that the crystals in the powder often consist of light elements (e.g. Hydrogen, Carbon, Nitrogen, Lithium and Oxygen) combined with heavy elements (e.g. Gallium, Yttrium, Strontium and Niobium) – neutrons observe the light elements better, while X-rays observe the heavier elements better.

**Imaging and tomography** are also done complementary with neutrons and X-rays. With these techniques images of objects can be created, even of microscopic size, in 2D (imaging) and 3D (tomography). A full picture can be constructed with both RIs, as X-rays and neutrons have a different absorption per element. Neutrons penetrate deeper in the object and visualise light elements better; X-rays do not penetrate deep in the object and visualise heavier elements better. The beamlines DanMAX, NanoMAX and SoftiMAX at MAX IV and the beamlines BEER and ODIN at ESS will use this technique. An example of application mentioned in one of the interviews is the imaging of metal prostheses on bone. With X-rays the bone is well-imaged, but there appear artefacts around the metal implants. The metal is better visualised with neutrons. Together they help to construct a full picture of the bone and the implant. This image can be constructed in 3D with computers using tomography.

### 2.1.3 Complementary aspects related to techniques

For most techniques to analyse specific samples dedicated set-ups are needed. The set-ups for experiments with neutrons and X-rays are generally similar if complementary techniques are used. If a specific set-up is needed for a sample at MAX IV, it might be transferrable for a similar experiment at ESS. Facilities on-site to characterise and prepare samples (chemical and biological labs, cleanrooms, deuteration labs), store and move (glove boxes, vacuum chamber etc.) samples as well as prepare a specific sample set-up (workshop) may be shared by both RIs contributing to their synergy. Some interviewees even suggested more advanced facilities in which samples could be fully prepared and characterised with equipment that not all universities or research institutes may have at their own labs (e.g. XRD, magnetometer and e-beam techniques).

A few interviewees suggested that there may be a well-conditioned sample transfer arranged between MAX IV and ESS. This might facilitate complementary use and reduces risks of contamination and degradation of samples. Samples going from ESS to MAX IV might be slightly radioactive (neutron activated), that should then be taken care of properly. Generally, such samples may not be brought into synchrotrons, but for synergy it might be worth considering expertise or conditions at MAX IV to do so. On the other hand, several interviewees explained that a smart experimental design can usually circumvent the need for doing the analysis on the (full) same sample. In a synchrotron one would just need a part of the sample that was analysed with a neutron source.

For many experiments at MAX IV and ESS special conditions and equipment are needed. These often concern conditions such as ultra-low temperatures, vacuum or low pressure and high magnetic fields. Both RIs need cooling for the magnets in their storage rings as well. The cryogenics needed for this cooling of the system and experiments can be shared among both RIs. The cryogenic system will use the expensive liquid Helium (\(^4\)He) for cooling. Currently there are plans for a line between MAX IV and the ESS Helium liquifying plant to recover and liquify the used Helium for reuse. This reduces cost,

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\(^7\) Lattice parameters determine the spacing of the atoms in the crystal and thus give structural information on the crystals in the powder.
increases efficiency and can be shared among the RIs. Other expensive equipment for experiments at both RIs may be shared as well.

Most techniques at MAX IV and ESS are generic or multidisciplinary. The advantage of generic techniques is that they are useful to users from many disciplines doing all kinds of studies. The disadvantage is however, that the configuration of instruments at beamlines need to be adapted all the time for specific user groups. A thematic focus of some instruments would reduce that need to change configuration, which would reduce the time needed for experiments. One interviewee mentioned that this is especially relevant for biologists, as they are less trained to build these kinds of experimental set-ups for multipurpose instruments than physicists and chemists are. It would therefore be good to have at both RIs beamlines that solely – or at least for an extended period of time – operate in a specific mode. For example, the SANS and SAXS instruments could both operate for two months in a mode optimised for structural biology experiments to facilitate quick complementary experiments at both RIs. During this period these beamlines could be supported by specialised beamline scientists.

Quite often interviewees mentioned that both RIs have very good specs to do time-resolved experiments to study dynamics. Some even have high expectations of these capabilities in terms of new research. If both RIs are good at time-resolved experiments, this could be promoted and synergies could be sought there. In this respect, also in-vivo experiments could be positioned. In-vivo experiments – with living animals – could be done with neutrons and X-rays, but an interviewee stated that there are so far no capabilities for that type of research.

2.2 Scientific importance of co-location

The main reason for scientists to go to a specific RI is its specs, not co-location per se. They go for the RI where they can do their experiment best. Excellence and uniqueness of the facility and its beamlines are the most important factors. MAX IV and ESS are both world-class with specs better than any other similar RI to date. To stay attractive, it is important to update the specs – as is planned for both ESS and MAX IV – so that both RIs stay world-class. Access and funding for travel and access to the RI is also an important factor to choose a specific RI. Funding schemes may be developed that promote the synergetic use of both co-located world-class RIs.

Co-location is however an interesting factor for scientists. Given the fact that there are several neutron and X-ray techniques that are often complementary used, co-location is beneficial indeed. This benefit is reaped if there is a common access: researchers can apply for beamtime for complementary techniques at both MAX IV and ESS during the same stay. That would prevent them from additional traveling (and associated costs), reduce the risks of contamination, degradation or other damage to the sample and could enable new experimental designs. One example that was mentioned, was synchronised experiments at both RIs. Such an experiment could be interesting for studying time-related effects of the same batch, for example, at the same time after a chemical reaction, so that the studied effects can be compared.

As the purpose of this project was to look at the synergies of the co-location of MAX IV and ESS specifically, quite a few examples of complementary use were identified. However, for many studies there is no need or benefit of using both ESS and MAX IV. Complementary use really depends on the field of study and the research questions of the study. Therefore, some fields of science benefit from the co-location of both RIs more than others.

Two fields of science that benefit from the co-location of ESS and MAX IV that were mentioned most often in the interviews are (structural) biology and materials science. In structural biology research on proteins, colloids and peptides have been mentioned to benefit from neutron and X-ray analyses. They often use small angle scattering (SAXS and SANS) and macromolecular crystallography. Materials science is a broad field in which some studies benefit more from co-location than others. Studies regarding magnetic materials and superconductors have been mentioned to benefit clearly from neutron and X-ray analysis, but also studies on meta materials and powders have been mentioned. In materials science inelastic scattering and powder diffraction are techniques that are often used.
In the field of structural biology, the synergy between both RIs is so obvious that researchers from the University or Lund have spontaneously set up a collaboration with both ESS and MAX IV. Both RIs have dedicated some funding to facilitate this collaboration to do analyses at both RIs related to structural biology. Structural biology is also strongly related to pharmaceutical research (e.g. pharmaceutical proteins). Pharmaceuticals can, for instance, be modelled using experimental data from X-ray and neutron analyses. In this field there is also a clear potential to involve industry.

Other fields that can benefit from complementary use mentioned in the interviews are biomechanical engineering and chemistry. In biomechanical engineering an example from research on bone prostheses was given: with X-rays the bone is well-imaged, but there appear artefacts around the metal implants. The metal is better visualised with neutrons. Together they help to construct a full picture of the bone and implant. For these studies imaging using X-ray and neutron tomography were used. Such studies are close to medical studies, but the medical field is not yet familiar to the use of these kinds of RIs. In chemistry research can be done on the formation of molecules and proteins and their interaction with membranes. It was mentioned that it would be interesting in chemistry to synchronise experiments in ESS and MAX IV, so that the sample is analysed at the same time after a chemical reaction.

But not only fields benefit, location matters as well. The advantage of Swedish researchers is that they are relatively close to both world-class RIs. This benefit is even more pronounced for the researchers at Lund University. This may be beneficial in international cooperation and may also attract excellent international researchers to Sweden. It is easier to develop a relation with people at the RI and to take over beamtime if there is an unexpected cancellation. Also, MAX IV is primarily a Swedish research facility, so that Swedish researchers can benefit most from the synergy. Some interviewees also indicated that they have priority access to certain beamlines at MAX IV as they were involved in developing the beamline.

The disadvantage for Swedish researchers is that there is currently limited experience with neutron analysis in Sweden and the neutron community is rather small. ESS is an international facility and will bring in neutron experience to Sweden. A Swedish beamline at ESS in which Swedish research groups are heavily involved is mentioned as an essential means to improve the knowledge of and access to neutron analysis in Sweden.

2.3 Foster synergy through science

The users of neutrons and synchrotron sources have their own communities. To foster complementary use, these communities should be brought together. In Denmark this is already done through DANS-SCTTT, the user community for synchrotron and neutrons sources providing funding and organising knowledge sharing to their members. Such an organisation is non-existent in Sweden, instead there are different user organisations for the two communities. Recently a Research School, SWEDNESS, has been set up in Sweden to organise training in neutron analyses. About 40 PhD students participate in this school. One interviewee assessed this number of students as too low, since generally only a fraction of PhD students continues in Swedish academia. The curriculum will contain an introductory course that will also address X-ray techniques, but an introductory course generally lacks sufficient detail for practical application.

A school that trains in analyses with X-rays and neutrons and reveals their complementarity could be a means to increase the future complementary use of both ESS and MAX IV. This might be just a change in curriculum. This training could very well be organised at ESS and MAX IV site in Lund, with the benefit that users often tend to do their experiments at the RIs that they are trained or familiar with. To create a community, it was suggested that supervisors should be from several Swedish universities, so that the community is not local but national.

Training of researchers could also focus on synergetic side aspects. An example would be scientific computing, since both RIs produce lots of data and issues on data analysis, modelling, programming and visualisation are quite similar for the users of both RIs. But scientific computing may extend beyond training: there could also be a shared department between the two RIs that assists researchers in data analysis and data visualisation. A research group on scientific computing or data science on
site could be involved in these trainings and assistance. Data analysis is currently done with different tools in different fields that need to be up to date and sometimes need to be tailored. Work related to developing such data analysis tools could help users in their publications, but could also result in publications in its own right. Data scientists at such a group need to be multidisciplinary, as knowledge of the field of which they analyse data or assist in analysis is important. They could also work on quick data visualisation during measurements.

MAX IV and ESS are user facilities. Scientists come there to do their experiments, but there are no scientists with only research as responsibility at the RIs – the facilities are not research institutes. Synergy through science could however be realised by having scientists permanently working at the shared site of ESS and MAX IV. A research centre, institute or laboratory that has a close relation with both RIs is expected to strengthen a shared science environment between the facilities. This could be located in the Science Village Scandinavia, at the land between both RIs, for which plans are currently being developed by the region. There are plans to indeed move labs and groups from Lund University to Science Village Scandinavia. Other universities in Sweden could also consider a hub in Science Village Scandinavia; although this is not looked at as a priority within the universities given a good connectivity to Lund. However, a link with universities in one form or another was stressed as important.

The scientific work at RIs is characterised by collaboration. The experiments at RIs are generally never done alone. This creates an opportunity to learn from others, to share experiences, to discuss science and analyses, to build connections and to form new communities. Having an interaction with other scientists at RIs stimulates creativity, changes the way of thinking and promotes excellence. Creating such an environment, shared by both ESS and MAX IV, is often mentioned in interviews as important, especially for young researchers. Such an environment, shared by both ESS and MAX IV, may inform researchers about the opportunities of another RI for their research and may challenge them to also use this other RI. This could very well contribute to increased complementary use if that is also practically supported. In that respect funding for studies with complementary use of ESS and MAX IV would be stimulating. For young researchers, exchange programmes for doing a long-term research project at both ESS and MAX IV was suggested as a valuable programme to promote excellence and to exploit synergies. Another option would be joint staff positions at MAX IV and ESS.

Research is not done in academia alone; many companies also do research. These companies can also benefit from experiments at MAX IV and ESS. The interaction between companies and scientists is considered mutually interesting, as they can learn from each other. It may improve the transfer of knowledge to companies and attract companies to the region. In that respect intermediary companies have been mentioned in the interviews as companies that may be located in Science Village Scandinavia. Intermediary companies would be specialised in experiments at both MAX IV and ESS and offer their expertise as a service to other companies that have no experience with these RIs. These companies can do the experiments and give the results of the analyses and further interpretation back to their clients. Their clients could be SMEs or larger companies that do not have a (large) R&D department.

Apart from attracting companies, some interviewees suggest also to think about creating companies or commercial activities related to ESS and MAX IV. Incubation of start-ups could be arranged at the Science Village Scandinavia. This could be start-ups related to instrument development or techniques that have been developed at ESS and MAX IV and could be used elsewhere at other RIs and research facilities or applied in other sectors and products. This would create a high-tech engineering environment related to technologies used at both RIs, such as scientific instrumentation, optical components, magnets, read-out electronics and other electronic components, but also data analysis and visualisation software. It would contribute to creating an international hotspot.
3 Synergies through support facilities

3.1 Common needs at ESS and MAX IV

Synergies between ESS and MAX IV can be exploited by looking at their common needs in support facilities, which can be shared between both RIs. With that idea in mind the region is developing the area between MAX IV and ESS into Science Village Scandinavia. The interviewees have identified several common needs which are presented further.

Both MAX IV and ESS need a reception and user office for their guests. This is something that they can share to improve synergies. A common entrance and reception will also strengthen the look and feel of one site. Also, common access can be arranged here as well if both user offices collaborate closely.

Almost every interviewee mentions the shared need for a good guesthouse. In order for the users of the RIs to invest their time efficiently, housing in direct vicinity to ESS and MAX IV is important. For instance, there is a need for an on-site guesthouse that is close to the beamlines at MAX IV and ESS so that researchers can optimise their time with the instruments. One interviewee refers to the guesthouses in Grenoble as a good example, where the guesthouse is in walking distance from the beamline. This gives researchers a possibility to have some rest, while still being very close to their experiment should any action is needed.

Short-stay housing on-site is being discussed but is currently missing at the MAX IV. The researchers using the RI are now relying on a guesthouse set up by a private entrepreneur, who will be competing with the region that plans to invest in short-stay housing later in the Science Village. This housing is currently delayed due to radiation permits needed for the detailed planning process. This means that the site is currently lacking basic infrastructure for its users, which is not expected to be improved in the near future. This is not so much of an issue for the current users at MAX IV, since there is some private housing in the neighbourhood, but it is for the researchers who will come to ESS to build their instruments. They will arrive before sufficient housing is in place.

Additional practical needs that have been mentioned are the availability of drinks and food 24/7. This catering can be shared among both RIs. Besides the obvious advantages of common lunch places, restaurants, cafés and activity places, these facilities give researchers an opportunity to meet informally and to share ideas. This social function is considered very important also for gaining interest in the other RI on the site. Often researchers have to run long experiments and have little sleep during their stay. It is therefore important to have access to drinks and food – especially strong coffee is seen as important by some interviewees. There is a need for these services to be available on-site close to the experiments so that researchers do not have to leave their experiment for too long. This is relevant for both RIs.

Each beamline at MAX IV and ESS have experts that help the users with their experiments. These beamline scientists are experts in experiments with the research instruments at the beamline. The techniques and beamlines at MAX IV and ESS are to a certain extent equivalent as described in earlier part of this report. These beamline scientists can share their knowledge between both RIs or even work at both RIs to improve synergies and to promote synergetic use among the users of the RIs.

Both RIs produce lots of data that users need to access and analyse afterwards. For that storage and on-site computing power is needed for some of the data processing and preliminary analyses. This IT infrastructure and support is something which in principle can be shared. For ESS this has already been arranged with a datacentre in Copenhagen; and MAX IV has its own datacentre and collaborates with SNIC to cover some pieces further. It would however be wise to explore if there can be a practical cooperation regarding IT, for example, on (the development of) software tools for analysis, visualisation, but also practical IT support on-site. Another aspect would be strategies for handling data and developing common or specific tools for experiments. Both RIs may cooperate around such common problems or challenges – some coordination on this between MAX IV and ESS has started for tomography. Expertise on data manipulation, data analysis and data visualisation of experimental data from neutron and X-ray experiments can be realised on-site by a scientific group on data science or scientific computing. The users of both RIs could benefit from that.
To make the Lund site an international hotspot for researchers, knowledge transfer is important for the users of both RIs. For that a small joint conference centre would be interesting. Apart from conferences, the organisation of workshops and seminars could be valuable as well. This could improve the knowledge transfer between the scientists working at either of the RIs or with/between their users. Especially knowledge related to techniques or that are problem oriented could be of value to the users of both MAX IV and ESS. An example that was given in the interviews were joint user meetings between both RIs as a means of effective knowledge transfer. On a broader level knowledge transfer to the general public was also mentioned. This could very well be done together with both RIs, for instance by opening a public science house or a science museum in Science Village Scandinavia explaining the history, importance, working and scientific use of both RIs.

For some scientific users it is important to have some shared laboratories on-site. This is mainly important for the field of biology, as some samples might be degraded during travel or need to be prepared on-site. Sample preparation labs have therefore been mentioned as important for both facilities. Biologists noted the importance of an on-site deuteration lab (isotope labelling) and biological lab, for other fields a general physics and chemical lab is sometimes mentioned as relevant. Sample analysis labs are also viewed as potential shared facilities. Such a lab would have instruments to characterise and analyse the sample before and after measurements. It would consist for example of (electron) microscopes, magnetometers, calorimeters, AFM, STM, XRD etc. Others indicate that most researchers do these analyses in the labs of their own institute. Apart from such labs, well-conditioned storage facilities are needed to store the samples, such as desiccators, fridges, freezers and glove boxes. These facilities could be shared, although some interviewees mention that they should be close to the beamline – while ESS and MAX IV are still about a kilometre apart.

Interviewees also stressed the importance of permanent research groups on-site using these labs and sharing their facilities. Grenoble was mentioned as an example. A big scientific group is there on-site that can help researchers to use the facilities efficiently. It is important for the users of the RIs that there are other scientists on-site with expertise to help using the facilities to their full potential. This is good for the interaction and knowledge transfer between scientists and for the state of the labs. Lund University has the ambition to be the host university and might share some of its labs with the users of both RIs. Some of the facilities of Lund University might be moved to Science Village Scandinavia. The Nanolab is planned to move to ESS and MAX IV site and the moving of some research groups is currently being discussed within the university. Other Swedish universities might have an on-site shared lab or group as well but moving research groups from other locations in Sweden to ESS/MAX IV was not considered by the interviewees as a positive direction.

There are several other support facilities and services that can be shared among the RIs and interviewees considered important or interesting. Some of these are related to physical activity: running tracks and other exercise facilities. Others concern basic things such as a good internet connection, which is not always available at the beamline, and some office space for scientists to work. On a more technical level maintenance and technical staff can be shared, but also a workshop for reparations and making parts for instruments.

### 3.2 The potential of shared services

Some of the services that both RIs would offer their users can be shared. They can help in improving synergies between MAX IV and ESS. Most of the services mentioned are related to data and IT.

**Data collection, data storage and data analysis** are activities that are at the basis of the research at both RIs. These can be quite complex. Interviewees have mentioned several services to facilitate these activities. When synergetic or complementary use is offered, the data from the one RI should be accessible at the other RI as well. For that local computing power is needed, which can be shared among both RIs. Currently the backups and computing power at MAX IV is in collaboration with Lund University. ESS has this arranged with its own computing centre in Copenhagen; MAX IV might investigate a potential collaboration with this centre. Some interviewees suggested that in the future
researchers might need to apply for both beamtime and computing power. This could be an application to ESS and MAX IV. **Cloud computing** could be another solution.

**Software** and data should be accessible online. Currently the PReSTO project is working on high-performance computing software and data accessibility on-site and off-site. Some interviewees expressed a need for **user-friendly open source applications** for data analysis that are updated and that are accompanied with support. These should have suites specifically for certain fields of sciences and certain experiments within either one of the RIs. It would be interesting to have data-analysis tools available on an online platform. These could have scripts or **online tools for specific analyses**, for instance, for spectroscopy data; as well as tutorials or instructions on these data analyses.

**Scientific data experts** could be available on-site for advice, assistance and training. They might be part of an on-site **research group on scientific computing**. This service could be complemented with offering **support** or **short trainings** on data manipulation, data analysis and data visualisation for specific types of experiments. Many researchers have difficulties with this and sometimes it is solved **ad hoc** without a thorough standard approach. It often takes lots of time; one interviewee stated that more than 50% of the time for experiments is spent on data analysis. Organising this data support and short trainings could be in collaboration with both RIs and could make MAX IV and ESS more interesting to potential users. It could, however, be quite an effort to deliver this support.

The data from previous experiments at ESS and MAX IV can be stored long-term for reuse by other scientists. The sharing of data may be useful for new research to build upon or to test theories without doing new experiments. Currently, only meta data are stored but it would be valuable to have the raw data saved as well for analysis by others. The researcher who collected the data can then first do his/her analysis and write planned publications, after which the data can become open for others to (re)use (**open data**). For that a **data policy** should be developed by both RIs together, so that data of samples analysed with both RIs can be accessed by researchers. **Standardisation** of tools and data output from instruments at both RIs is welcomed as well.

The users of both RIs will receive support during their measurements. **Beamline experts** help researchers to use the analysis instrument and to tailor the setup for their experiment. Some of these experts could be employed at both RIs to facilitate complementary use. There may also be experts specifically for experiments that both use ESS and MAX IV and that can guide in using complementary instruments, such as SANS and SAXS, or even synchronised experiments at both RIs. They could help in the **logistics** and practicalities associated with complementary use to make the process more efficient. **Workshop technicians** help the researchers in, for instance, making specific holders for instruments at both RIs. This could reduce costs.

Other services at ESS and MAX IV that can be shared are more of a practical nature. For instance, the **security, maintenance and cleaning service** can be shared. The potential would be a reduction in cost. Security is also related to safety; it would also include the security clearance for samples that are being brought from one RI to another. **The user office and administrative support** to users can be coordinated, which could make complementary use of the RIs more efficient and interesting for users.

For companies that would like to do experiments at ESS and/or MAX IV a **special point of contact** could be appointed. This point of contact can arrange the coordination and financing and can direct companies to **intermediary companies** if they lack the knowledge and skills to do experiments themselves. Such companies can do experiments at the RIs to solve a product related problem of a company and report the analysis or solution back to the company. Such intermediary companies can be located in Science Village Scandinavia and can make use of the shared lab facilities on-site.

### 3.3 The potential of shared facilities

The potential and importance of shared facilities is rated differently by interviewees. Mainly biologists find some shared facilities important. Physicists are less enthusiastic about shared facilities. This is largely due to the fact that some biological samples need to be prepared on-site for experiments (e.g.
some cannot travel fully prepared); while physicists often bring their sample fully prepared. Further characterisation on-site was considered interesting by some, but others mentioned that they have the needed instruments at their institute and would naturally prefer to do their analyses there. Nonetheless, certain potential of shared facilities is visible.

**Sample preparation labs** are considered interesting to have on-site. This facility can be shared among both RIs, reducing costs and increasing interaction between the users of both RIs. Sample preparation could for instance be the aligning, cleaning, etching or cutting of samples, the isotopic labelling of samples (**deuteration lab**) and the preparation of biological samples. Interviewees active in the field of structural biology referred to the **structural biology labs** in Grenoble as being relevant both for ESS and MAX IV.

Facilities for **storing samples** are also very important. These facilities may be shared to a limited extent. Samples are often stored temporarily and close to the beamline. Samples that have been sent ahead or need to be analysed later (e.g. when other beamtime is available) can be stored centrally and can be shared. Storage would for instance consist of desiccators, fridges, freezers and glove boxes. Some of these could be portable to move from one RI to another or from a beamline to another beamline – **well-conditioned sample transfer** may be relevant if both RIs are complementary used. The latter is, however, relevant for a small user group.

A **sample characterisation lab** could be relevant for some users as well. Generally, users are making preparations at home a long time before they go to an RI. They have fully characterised their sample. A small user group may not have certain characterisation equipment at home and may use that on-site. This could also be the case after the experiment or if there is some time-related effect that is being studied or if samples deteriorate over time. However, the interviews give the impression that only a small group would use a sample characterisation lab. Such a lab could, however, be shared to reduce costs (also from the user perspective) and increase the interaction between the scientists of both RIs. Experimental techniques in such a lab could be (electron) microscopes (SEM), STM, XRD, AFM, magnetometers, spectrometers, calorimeters etc. Such a lab could be shared with the local university and may very well already be part of the **Nanolab of Lund University** that is expected to move to the site of MAX IV and ESS.

For **industry** the concept of shared facilities may be interesting as well. Science Village Scandinavia might have some experimental facilities that companies cannot afford and may rent for their experiment at either one of the RIs. Also **intermediary companies** could benefit from these facilities. Although industry is a small user group of RIs, it could be relevant for the regional economy or for the financing of the RIs. Companies on site or interactions of researchers with companies could stimulate the transfer of knowledge and technology to the market.

Other shared facilities have a strong relation with services that have already been mentioned. **A shared user office, restaurant, cafe, meeting places, shared offices and conference facilities** could stimulate complementary use due to lowering the administrative burden, facilitating interactions between researchers from both RIs and organising knowledge transfer between and among users and beamline scientists. **A (technical) workshop** may also be shared among the RIs to reduce costs, as sometimes specific sample holders or changes to equipment are needed. This may also be useful for the maintenance and further development of instruments on-site. As many instruments will be built over time for both RIs, such a workshop or environment for instrument construction and testing may be useful – although large parts of that work will be done elsewhere.

When combined in the most beneficial way to the users these various facilities and services in combination with the best up-to-date instruments will contribute to making the site in Lund a thriving international hotspot.
4 Strategic development

For a Lund site to become a thriving international hotspot it has to be a place where different users want to come and spend time. It has to be a world-leading scientific location with unique facilities. The instruments and the equipment need to be built and work well. In view of some interviewees, there are some concerns at the moment but if all works out well, the key researchers in the fields will come. The place should also be a melting pot of ideas from various generations of researchers exchanging experiences and industry of different size and purpose. This way it will create a special and vibrant environment, where there is no desire to sleep but instead a burning wish to stay up discussing the experiments and collected data. An active, open and welcoming campus is needed connecting different parts and disciplines together. An international dimension needs to be kept and nurtured in the minds of all users and from the very beginning of the journey.

4.1 Building a thriving international scientific hub

4.1.1 Supporting existing potential

In view of several interviewees all researchers can benefit from using ESS and MAX IV. Ignorance among Swedish researchers of using this unique opportunity is probably a major problem at the moment; followed by a lack of skills. It is important, therefore, to tackle such barriers as much as possible and promote connections with researchers at the facilities. One way to encourage the use of these RIs and increase an interest of researchers is to offer researchers to run a test experiment. Such test experiments can be offered by the scientists working at the beamlines or through some research institutes located on-site.

Several interviewees pointed out that having some permanent institutes located in close proximity to the RIs is one approach to building a vibrant scientific community. Some parts of Lund University will be based on-site with ESS and MAX IV. However, some interviewees have bigger ambitions in mind. For example, it would be good to have a Fraunhofer spin-off on site, which is likely to happen if interesting research at Lund (e.g. nanoscience, accelerator physics etc.) is moving to the site too. In Lund the LINXS initiative has started mainly focusing on basic science within the Soft Matter, Life Sciences and Hard Matter and combining experimental and theoretical activities. The projects that will be granted access through this initiative will enable groups of researchers to come over for a predefined period of time to engage in a targeted research programme. It is undoubtedly a welcoming step. However, some interviewees mentioned a need for more established structures.

Establishment of interdisciplinary research centres is one of the ways to build international scientific community freely conversing in the lingo of these two user facilities. The DESY site in Hamburg has two such centres – CFEL (Centre for Free Electron Laser) and CSSB (Centre for Structural Systems Biology). Two conditions are paramount in the success of such centres: first, making them reasonably broad making as many researchers curious as possible; and second, strategically recruiting global level researchers as ‘anchors’ to these centres. Such star researchers most often are extremely expensive but if that works out then the benefits for the facility and the scientific community in the region and indeed the country are huge. Two factors are usually critical here – excellent scientific facilities and robust funding. The former should be in place once ESS and MAX IV are up and running. The latter is often a challenge and needs to be discussed. The appointment of the star researchers can be dual between the ESS facility and one of the Swedish universities, thus also bringing direct benefit to a community of researchers in a ‘host’ university.

Another thought which was put forward by the interviewees was around joint positions of scientists between the two RIs. Although some think that it does not make sense because it is important to equip researchers with very specific deep knowledge; others strongly feel that if a researcher has a dual position it will change the level of engagement between the facilities. It does not need to be 50/50. The majority of a position should be at one RI and a small part at another.
While longer-term strategic decisions on hiring are taking time, there are smaller things that can be implemented to support the development of the existing researchers. One such idea is around **sabbaticals or exchange programmes for visiting scientists**. Through this programme international researchers can come to Lund and use it as a base for their work but at the same time exploit scientific opportunities and use the resources available not only in Lund and Copenhagen but also in other Swedish universities working in the fields where MAX IV and ESS can be of use. Such sabbaticals can be funded by the universities where these researchers come from.

More short-term visits should be supported too, thus contributing to the setting up of an academic campus with researchers from various universities. **Mobility grants for researchers** can be helpful here. One possible scenario for Swedish researchers was suggested during the interviews. Once the researcher gets beamtime at ESS, s/he sends the decision letter to a Swedish funding agency (for example, the Research Council) requesting some funds from a programme to cover travel and subsistence. Such an approach could potentially lower the barriers for applying for the beamtime as the researcher knows that in case of a successful application it will not cost her/him to go and use the RIs. In particular, that could be of huge help for younger scientists. To make it work well, such programme should ensure a quick turn-around via an open call approach. Such mobility grants can first target ESS but can later be extended and allow Swedish researchers to visit all types of large scale Research Infrastructures in Europe. This way it will promote Swedish researchers abroad and also make researchers think about using the facilities.

**Some grants can cover not only travel but also beamtime.** For example, Denmark has national money that pays for beamtime; whereas many other European researchers are in a less luxurious situation. These can be organised at ESS and MAX IV, i.e. part of their funds can be used for that or they can organise a setting up of such funds for users. In case of ESS, perhaps with the support from the European Commission – either as a new mobility tool or linking it to the Erasmus+ and Marie Curie actions. In case of MAX IV, from within the Swedish universities and with the support from the Research Council.

### 4.1.2 Bringing up a new generation of researchers

A particular focus should be put on developing the skills and competences of future researchers. These are currently studying or researching in the fields where the MAX IV and the ESS facilities can be of use. They are the future users of ESS and MAX IV both within academia as well as in the private sector.

To build a potential of a new area within a university, these areas need to be incorporated into the curriculum and methods used at the two facilities need to be thought in parallel. Once this is in place, efforts need to be put in attracting new young people into these fields. That is for sure a very long-term approach but if this does not happen soon, years will be lost in trying to build a community of researchers who understand and can use both ESS and MAX.

Certain things can be put in place in relation to existing students. **Summer Schools** similar to the one at CERN could be an excellent tool. Students can come and work at the facility for a few months with courses from regional universities. This can apply to Bachelor and Master students studying physics, chemistry and biology as well as to PhD students in their early stage of research.

To further encourage the **PhD students** from Swedish universities working in scientific fields where the two RIs can be used, incentives can be prepared to allow them to **spend several months at the RIs**. This is set to be addressed by the SSF graduate school in neutron scattering. It will further strengthen the international profile of Lund as a location as the PhD students will be coming from various countries. One interviewee thought that perhaps a similar approach (i.e. with a dedicated PhD school) is needed for MAX IV. In case of such PhD schools when the graduate students do not necessarily ‘belong’ to a host university, these graduates will spread across Europe if not the world, bring a part of their ESS experience with them and in their future work will feel warm about ESS.

What is important then is for the PhD graduates to build their international scientific profile. This requires a well-thought-through long-term planning but which needs to be planned already now. Recent
graduates should be encouraged to do their post-docs abroad, build their international networks, capture more knowledge. The plan, however, should be for Sweden to attract the larger part of these post-docs back. This can be achieved if dedicated tenure track positions are created at Swedish universities. These young researchers will bring all their international experience back to Sweden and help further build the research capacity in the universities across the country and use the synergistic effects of ESS and MAX IV.

Further, a programme similar to the CERN fellowship can be set up acknowledging high achievements from young researchers. A joint ESS-MAX IV fellowship in material science was suggested as an example. This should be something that gives status, it should be prestigious and very selective.

4.2 Building an international innovation hub

ESS and MAX IV should also play a role of an innovation hub with large and small industry present at the site too. This innovation aspect (in view of international interviewees) needs to be integrated from the very beginning and deliver a clear message that these facilities can be used by industry. Building a momentum and nurturing links with industry can take time but it is truly important. There should be an interaction at those facilities between researchers and industry. The sooner this starts, the easier it will be in the years to come and the larger spillover effects such engagement will have on the region.

In most cases, industry will not use these research facilities on their own. First it should be about getting these techniques to be used and set up a research environment with the universities around that; have the universities use it and then bring it in practice with the industry collaborations. Scientists can then act as ambassadors and help mature the industry users to do experiments themselves or with the help from researchers. Availability of funding to facilitate this process can make it smoother. One interviewee expressed an opinion that access to companies can be shared between several international facilities. Another approach to innovation is to look into the research generated on site. DESY, for example, has recently set up an Innovation & Technology Transfer Group and created a position of a Chief Technology Officer leading a group of 15 people with a budget of €2m.

Attraction of companies – especially if these are well known and ideally large companies – could also draw attention to Skåne and Lund as a region. These can be companies not only directly interested in using the two RIs but many companies with interest in serving the equipment, the facilities, the companies and the wider campus.

Industry can be involved already at the planning stage. Ideally, some instruments (or even beamlines) can be (co-)funded by companies. In such cases (and this is already present at some large scale facilities in the USA) the beamline can probably be used only by the company itself; but this needs to be negotiated with a company before going into this arrangement. It is important to note that these companies would probably be large from well-established industries (e.g. pharmaceuticals) which can afford such an investment; whereas the mid- and small-size companies are also important. For that matter, a close collaboration between industry and academia already as funders of instrument would be a good start. This, as interviewees pointed out, is already happening in Sweden around the forest industry. KTH received funding from the Swedish Government to do a feasibility study on ForMAX – a tool customised for the needs of the forestry industry on the topics linked to bio-composites, nano-cellulose and dissolving wood pulp process. It is too early to talk about the industry’s potential financial contribution to this tool, but having a part of the MAX IV facility planned to target the research needs of the whole sector (rather than individual companies) is a step in the right direction.

Such collaboration with industry could also turn into a platform that is used not only for science but also for training of young researchers from industry. If there is a substantial commitment from industry already at the beginning, the later stages will be easier. This will also help to address the current problem of industry having a low interest in the RIs. It is important to develop a local culture and shake hands with the industry. These are two parallel worlds. Right information presented at the right time is crucially important. Explaining to the companies in different sectors what the facilities can do for them is the least that can be done. Steel companies and forest industry were mentioned in the interviews as examples. One interviewee asked if perhaps the research institutes (rather than
universities) could have a task of linking industry with research facilities. They can have personnel performing a knowledge transfer mission and having appointments linked to the RIs. It will also enable the institutes to get the expertise. Swerea and Kinap dealing with metals and materials were mentioned as possible interesting partners.

**Provision of everyday support to ESS** is another way to engage companies. If possible, more Swedish companies should be involved here; thus bringing extra economic benefit from the ESS location to the country. These are not necessarily all high technology companies, but also include service organisations. Actions in this direction should start already now in order to position Sweden for this role and prepare the companies. Certain training for some companies might be needed, which will also require time.

Over the years the research performed at ESS and MAX IV, the facilities themselves and proximity of established companies will also attract the attention of smaller companies. To capture those, **places for incubation of start-ups** in technologies for instruments etc. need to be planned. In view of some international interviewees, companies should be put together and have a building or centre that will be inspirational to other companies as well. ‘Company ambassadors’ from universities can sit there too. They will be a link between the companies and universities. Looking at this from the Swedish perspective, Vinnova should have a role to play here.

### 4.3 Building capacity within the country

In view of many interviewees, Sweden should ensure that both RIs exploit the region and remain embedded. The user community in Scandinavia is quite small compared, for example, to the UK and France where there is a lot of knowledge, a large community and lots of training readily available. In Sweden this is all relatively small and new; hence it is important to grow this community, its experience and knowledge. The Lund site needs to be nationally important to be beneficial for the national community. Having a **strong national community which can share their experience** with others is also important for international users. When national researchers act as champions and demonstrate what can be done on site it will make the site more attractive to international users too. If some records or unique experiments are done using both facilities, then that will attract researchers to do similar work.

For Sweden not to fall behind international developments, a community using neutron sources on their own or in combination with X-rays should be grown. Currently the neutron community is small. **Building capacity of users who can benefit from both MAX IV and ESS** is one of the most urgent tasks. The community does not need to be restricted by geographical boundaries and focus purely on Lund. Expertise of X-ray and neutron scientists across the country needs to be used. This in return could attract international collaborators to universities across Sweden. The **universities across the country need to be actively involved**; and this does not mean them re-locating some of their laboratories to Lund. Some of the possible developments were discussed earlier around the development of a new generation of researchers.

What needs to be done is the increase in research fields linked to the two RIs and which can use the instruments at the two facilities. In Denmark, for example, the approach is towards creating centres of excellence related to the fields of the RIs. This will empower researchers (especially junior) who do experiments at Danish universities and on the site in Lund. Over the years these researchers will boost the science at the Danish universities as well as industrial users. One practical way to address this question is through launching a **dedicated programme to fund the research utilising opportunities through synergies** offered by ESS and MAX IV. Challenge the researchers to tackle problems with the techniques available at both RIs! That was an advice from several interviewees. It could be a programme run by the Swedish Research Council, targeting MAX IV (as a national facility) but with an aim to link the two RIs. This way the behaviour of researchers can change over time, e.g. they will start talking to the beamline users to understand what can be done.

For some visiting scientists **specialised training and education** might be needed. To address this need, a training centre connected to either local or national universities can be set up. The same centre can be used for preparing skills in industry, which is another important user group of the two facilities.
A ‘Maxlab for Dummies’ course was suggested as an example of a bridging step for users who come to the facility for the first time. Many users from outside the academia (i.e. whether private sector or hospitals) show interest in the facilities but are reluctant to use them (too technical environment, hard to understand were often mentioned as bottlenecks). These potential users need help to get over that threshold. Once they have seen how the facilities work and what the experiments can bring, returning for more experiments will mentally become much easier. Funding schemes that give small money for collaborating with facilities or even to challenge and encourage the use of both RIs in an experiment could help to expand the user base. To create a joint community and to make people move seamlessly between the two RIs, training can be organised collaboratively between ESS and MAX IV.

Once all is set, some interviewees suggested to spread the word of excellence and exciting research happening at Science Village Scandinavia through a tradition of high level and unique annual international conference.
5 Concluding remarks

Sweden has invested substantial resources into the MAX IV synchrotron facility and the European Spallation Source in Lund. It gives lots of obligations to a small country like Sweden but at the same time proves that also such small countries are good for a European facility. It also provides enormous opportunities to create a truly international hotspot and bring benefits to the international as well as national research community, industry and in the long run a wider society. The facilities are here to stay for several decades and it is important to take certain steps now to ensure a successful use of these resources. The interviewees who contributed to this piece of work strongly believe that both MAX IV and ESS are the best tools in the world. It is just a matter of imagination and putting forward interesting research questions for the investigation with the help of these facilities.

What is crucial now is to remember that sites with large scale research infrastructures like ESS will not evolve on its own. The interviewees with strong international experience highly recommended to have a strategy and a roadmap for such a place. A strategy on how the site will look like in 20 years and later is essential for a long-term success. A strategy that will answer two questions: Where do we want the site to be in 20 years? How do we get there? Organisation(s) which are in charge of the overall development of the site should be driving such strategy forward.

A couple of ideas helping to answer the second question are presented in this report. They are not repeated as a list here; instead, the reader is referred to earlier parts of this report to read various observations and short recommendations.

What is emerging clearly is a strong need to start early in collaboration between the two RIs. There is a clear potential for complementarity and this needs to be communicated in a coherent way to different users – especially those who have not yet looked at the two facilities together. There is also a need to communicate and promote the site in Lund as a single campus to Swedish and international users. For all the users the site has to offer attractive research opportunities – which both facilities are undoubtedly set to achieve – and convenient location to be in. This will help to create a vibrant environment and an international hotspot.

In concluding this short qualitative study, it is important to note that the thoughts described in this report present the views of 15 interviewees. Although the number is limited, these various researchers are renowned in their respective fields nationally and internationally. They have been active users of various X-ray and neutron facilities in Europe and have shared their experiences from these various locations.
Appendix A List of interviewees

A.1 Interviews in Sweden

- Prof Andreas Schreyer, European Spallation Source ERIC and University of Hamburg/Helmholtz Centre Geesthacht
- Dr Hanna Isaksson, Lund University
- Prof Jens Birch, Linköping University
- Prof Maria Sunnerhagen, Linköping University
- Dr Martin Månsson, KTH
- Prof Nils Mårtensson, Uppsala University
- Prof Sara Snogerup Linse, Lund University
- Dr Tomas Lundqvist, MAX IV Laboratory and Swedish University of Agricultural Sciences
- Prof Aleksandar Matic, Chalmers University of Technology
- Prof Björgvin Hjörvarsson, Uppsala University

A.2 Interviews abroad

- Prof Andrew Boothroyd, University of Oxford, United Kingdom
- Prof Caterina Petrillo, University of Perugia, Italy
- Prof Helmut Dosch, DESY and University of Hamburg, Germany
- Prof Lise Arleth, University of Copenhagen, Denmark
- Dr Matthias Wilmanns, European Molecular Biology Laboratory Hamburg, DESY, Germany