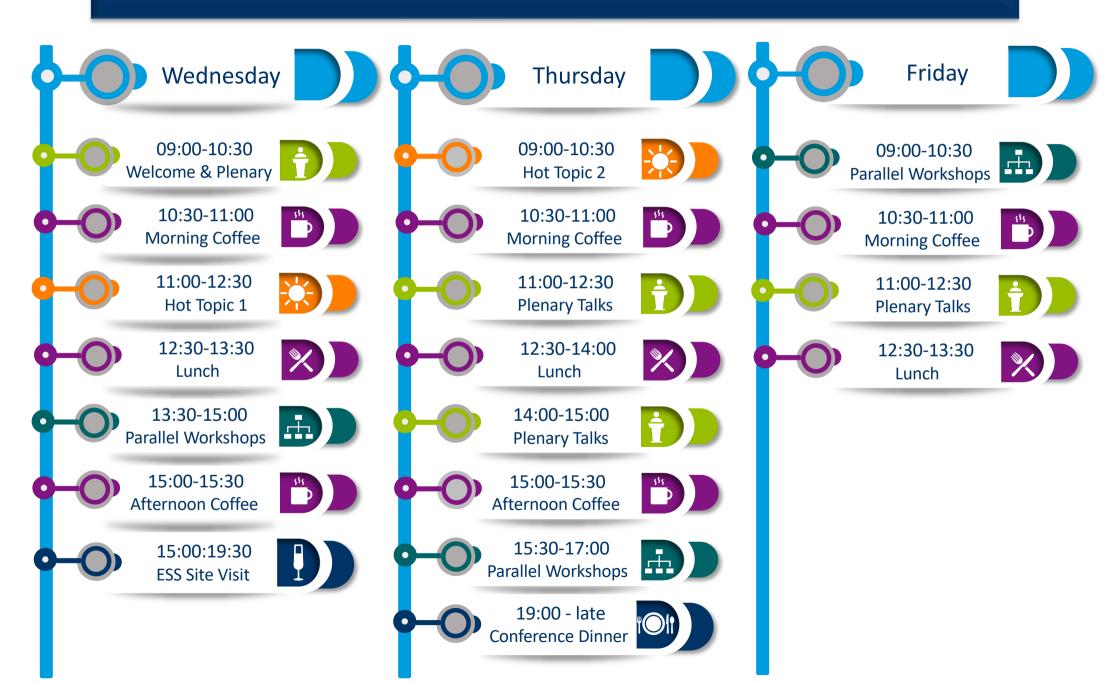


# Joint ESS ILL User Meeting

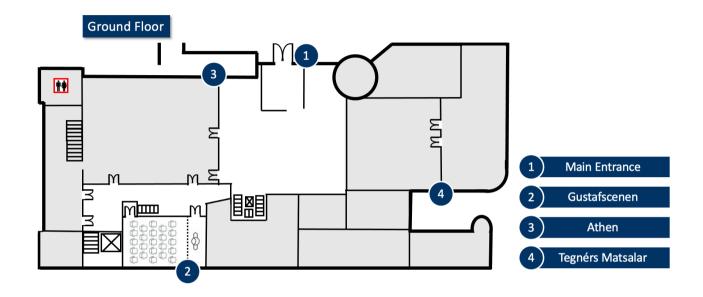
5-7 October 2022 Lund, Sweden

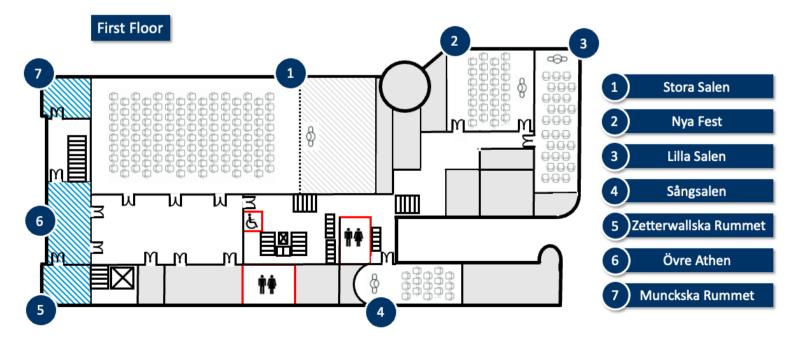
Programme Book

### Programme Overview

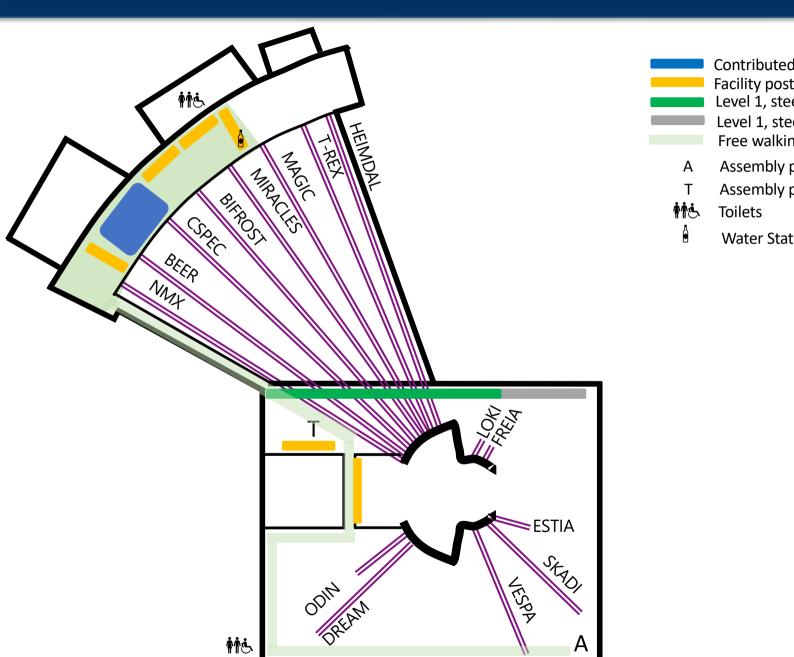


### AF Borgen Room Guide





### ESS Site Plan



Contributed posters Facility posters Level 1, steel walkway (open) Level 1, steel walkway (closed) Free walking area

Assembly point for accelerator tours

Assembly point for target tours

**Water Station** 

### Programme Overview

| 09:00<br>09:10<br>09:30<br>09:50<br>10:00 | Opening remarks ESS facility update ILL facility update Practical Information Autonomous neutron e | experiments  | Helmut Schober<br>Andreas Schreyer<br>Jacques Jestin<br>Andreas Schreyer<br>Martin Boehm | Stora Salen<br>Stora Salen<br>Stora Salen<br>Stora Salen<br>Stora Salen        | Chair: H. Schober  |
|---|--|--|--|--|--|
| 10:30                                     | Coffee   |  |  |  |  |
| 11:00                                     | Neutrons and Current H   | lealth Challenges  | Marianna Yanez Arteta<br>Lukas Gajdos<br>Andrey Kovalevsky<br>Garry Laverty              | Stora Salen  | Chair: Z. Fisher, M. Blakeley  |
| 12:30                                     | Lunch  |  |  |  |  |
| 13:30                                     | Fundamental and<br>Particle Physics<br>Stora Salen   | <b>Diffraction and Applied Materials</b> <i>Gustafscenen</i>     | Imaging and Energy<br>Materials<br>Sångsalen   | Large Scale Structure<br>and the Life Sciences<br>Lilla Salen                  |  |
|   | Marcus Scheck<br>Anastasio Fratangelo<br>Kazimierez Bodek  | Peter Hedström<br>Zifan Wang<br>Wen Cui<br>Stavros Samothrakitis | Ralf Ziesche<br>Erik Lübke<br>Estrid Naver<br>Alex Backs<br>Domenico Battaglia           | Petri Kursula<br>Sophie Ayscough<br>Ben Humphreys<br>Naved Malek<br>Joao Ramos | Tobias Weber<br>Romain Sibille<br>Abhijit Kademane<br>Astrid Schneidewind<br>Siobhan Tobin |
| 15:00                                     |  | sses to site visit and pos                                       | ter  |  |  |
| 19:00                                     |  | session<br>from site visit                                       |  |  |  |

| Programme | Overview |
|-----------|----------|
|           |          |

| 09:00 | Neutrons and Current                                    | Climate Challenges   | Wiebke Lohstroh<br>Konstantinos Stefanopoulo<br>Luis Barbosa<br>Philip Yang                              | <i>Stora Salen</i><br>s   | Chair: M. Feygenson<br>P. Fouquet  |
|-------|---|--|--|---|--|
| 10:30 | Coffee  |  | Timp rang  |   |  |
| 11:00 | The magnetic flux line – a exploring unconventional     |  | Elizabeth Blackburn  | Stora Salen   | Chair: A. Hiess  |
| 11:30 | Gas hydrates: from their n<br>environment to energy inr |  | Arnaud Desmedt   | Stora Salen   |  |
| 12:00 | Development of an Ultra (<br>Cold Neutron Source at th  | ,  | Valentina Santoro  | Stora Salen   |  |
| 12:30 | Lunch   |  |  |   |  |
| 14:00 | Molecular insights into prointeractions: endocytosis,   |  | Nathan Zaccai  | Stora Salen   | Chair: J. Jestin   |
| 14:30 | Connecting protein struct dynamics: the neutron per     |  | Frank Schreiber  | Stora Salen   |  |
| 15:00 | Coffee  |  |  |   |  |
| 15:30 | Industrial Applications of<br>Neutrons<br>Stora Salen   | <b>Diffraction and Magnetism</b> <i>Gustafscenen</i>                               | Imaging and La<br>Engineering Materials<br>Sångsalen   | arge Scale Structures<br>and Soft Matter<br>Lilla Salen                             | Spectroscopy and Functional Materials  Nya Fest  |
|       | Peter Dowding<br>Hanna Leemreize<br>Ilaria Mosca        | Oksana Zaharko<br>Ellen Fogh<br>Werner Schweika<br>Jennifer Graham<br>Jian Rui Soh | Josefin Martell<br>Fernando Vieira Lima<br>E Tobias Wrammerfors<br>Robert Cubitt<br>Alessnadr Tengattini | Andrea Scotti<br>Annekatrin Sill<br>Paavo Pentitilä<br>Wenke Mueller<br>Karin Edler | Fabrizia Foglia<br>Bettina Schwaighofer<br>Mohamed Aouane<br>Peter Fouquet<br>Rasmus Lavén |

## Programme Overview

| 09:00 | Imaging for<br>Archeology and<br>Material Science<br>Stora Salen             | Diffraction for Energy<br>and Sustainability<br>Gustafscenen            | Fundamental and<br>Particle Physics<br>Sångsalen  | Large Scale Structures<br>and Hard Matter<br>Lilla Salen                         | Spectroscopy and<br>Soft Matter<br>Nya Fest  |
|-------|--|---|---|--|--|
|       | Stephen Hall<br>Hanna Isaksson<br>Camilla Larsen & Stavros<br>Samothrakitits | Anatoliy Senyshyn<br>Neelima Paul<br>Ida Nielsen<br>François Goutenoire | Francesc Morabal Capilla<br>Karina Bernert<br>Michael Jentschel<br>Richard Wagner<br>Hanno Filter | Grace Causer<br>Emma Campillo<br>Xaver Brems<br>Sebastian Stock<br>Ahmed Alshemi | Stephane Longville<br>Maria Rescigno<br>Michaela Zamponi<br>Maria Paula Marques<br>Peter Falus |
| 10:30 | Coffee   |   |   |  |  |
| 11:00 | Advancing electrochem with neutron radiograp                                 |   | Antoni Forner-Cuenca  | Stora Salen  | Chair: A. Schreyer   |
| 11:30 | ENSA Update  | · · · y   | Henrik Rønnow   | Stora Salen  |  |
| 12:00 | Q&A Panel  |   | TBA   | Stora Salen  |  |
| 12:30 | Closing Remarks  |   | Paul Langan   | Stora Salen  |  |

#### **Neutrons and Current Health Challenges**

| 11:00   | Marianna Yanez Arteta Structural investigation of lipid nanoparticles is key for successful mRNA delivery                                       |  |  |  |
|---|---|--|--|--|
| 11:30   | Lukas Gajdos<br>Neutrons for structural glycobiology: lectin-carbohydrate recognition in host-pathogen interactions                             |  |  |  |
| 12:00   | Andrey Kovalevsky   |  |  |  |
| 12:15   | Neutron crystallography to uncover SARS-CoV-2 main protease function and design potent inhibitors  Garry Laverty                                |  |  |  |
|   | Understanding the microscopic properties and drug diffusion kinetics in long-acting peptide hydrogel drug delivery implants for HIV/AIDs        |  |  |  |
|   | Fundamental and Particle Physics (Chair: C. Michelagnoli)   |  |  |  |
| 13:30   | Marcus Scheck<br>Nuclear Physics Research at ILL – an overview  |  |  |  |
| 14:00   | (WITHDRAWN) Stephan Sponar  |  |  |  |
| 4400  | (WITHDRAWN) Weak and which-way measurements in neutron interferometry Anastasio Fratangelo  |  |  |  |
| 14:30   | BeamEDM - A beam experiment to search for the neutron electric dipole moment  |  |  |  |
| 14:45   | Kazimierez Bodek  |  |  |  |
| 3   | BRAND – search for exotic couplings in weak interactions using the transverse electron polarization in the decay of free neutrons               |  |  |  |
| Diffraction and Applied Materials (Chair: P. Beran, Th. Hansen) |   |  |  |  |
| 13:30   | Peter Hedström  |  |  |  |
| 13.33   | In-situ neutron diffraction studies of phase separation in mixed carbides Zifan Wang  |  |  |  |
| 14:00   | In situ neutron diffraction investigation of grain boundary effect on degradation of Superelasticity in near equiatomic NiTi alloy              |  |  |  |
| 14:15   | Wen Cui   |  |  |  |
|   | Standardization of industrial residual stress measurement for metallic components: diffraction and destructive techniques Stavros Samothrakitis |  |  |  |
| 14:30   | Considering instrumentation for a high intensity moderator at the European spallation source  |  |  |  |

|       | Imaging and Energy Materials (Chair: Lukas Helfen, Søren Schmidt)   |
|-------|---|
| 13:30 | Ralf Ziesche  |
| 13.50 | 4D neutron imaging of lithium batteries and fuel cells  |
| 14:00 | Erik Lübke  |
|       | Investigation of silicon-based anodes for Li-ion batteries using X-ray and Neutron 3D/4D imaging techniques             |
| 14:15 | Estrid Naver  |
|       | Phase contrast neutron imaging of solid oxide electrochemical cells   |
| 14:30 | Alex Backs  |
|       | Magnetic bulk properties of ferromagnetic metal sheets  |
| 14:45 | Domenico Battaglia  |
|       | Operando multimodal study of degradation and sodium storage processes in sodium-ion batteries                           |
|       | Large Scale Structures and the Life Sciences (Chair: Giovanna Fragneto)   |
| 13:30 | Petri Kursula The myelin membrane visualised using photons, neutrons, and electrons                                     |
|       | Sophie Ayscough   |
| 14:00 | The role of hydrocarbons in cyanobacterial membranes  |
| 14.15 | Ben Humphreys   |
| 14:15 | Lipolysis of a Thin Triolein Film   |
| 14:30 | Navéd Malek   |
| 14.50 | Multi responsive, self-healable and injectable ionic liquid based polymeric hydrogel for the treatment of breast cancer |
| 14:45 | Joao Ramos  |
| 17.75 | A clear picture of the active site of hen egg-white lysozyme from atomic resolution neutron crystallography             |
|       | Spectroscopy and Magnetism (Chair: P. Deen, U. Bengaard Hansen)   |
| 13:30 | Tobias Weber  |
| 15.50 | Topological magnon band structure of emergent Landau levels in a skyrmion lattice                                       |
| 14:00 | Romain Sibille  |
| 14.00 | High-resolution spectrum of fractional excitations in Ce <sub>2</sub> Sn <sub>2</sub> O <sub>7</sub>                    |
| 14:15 | Abhijit Kademane  |
|       | Singlet magnetism in SrTm₂O₄  |
| 14:30 | Astrid Schneidewind   |
|       | Al-assisted neutron spectroscopy – Log-Gaussian processes for TAS<br>Siobhan Tobin                                      |
| 14:45 | Magnetic structure and spin waves of the doped cobalt oxide La2-xBaxCoO4  |
|       | magnetic structure and spiri waves of the doped cobait onlide Laz-AbaxCOO4  |

#### **Neutrons and Current Climate Challenges**

|       | Neutrons and Current Climate Challenges  |
|-------|--|
| 09:00 | Wiebke Lohstroh<br>Complex hydrides for energy applications  |
| 09:30 | Konstantinos Stefanopoulos Neutron scattering studies on CO2 confined in nanoporous mate-rials: Applications to CO2 sequestration and oil recovery |
| 10:00 | Luis Barbosa  In situ flow exchange experiments between macropore and soil matrix combining Neutron and X-ray tomographies                         |
| 10:15 | Philip Yang Investigating the physical behaviour of novel cyclic poly(lactone)s using SANS   |
|       | Industrial Applications of Neutrons (Chair: C. Boudou)   |
| 15:30 | Peter Dowding Using neutrons to unlock the properties of commercial oil additives  |
| 16:00 | Hanna Leemreize<br>Making neutron characterization tools available to industry   |
| 16:15 | Ilaria Mosca<br>Dynamic cluster formation, viscosity and diffusion in monoclonal antibody solutions  |
|       | <b>Diffraction and Magnetism</b> (Chair, W. Schweika, P. Beran)  |
| 15:30 | Oksana Zaharko Exotic spin states in frustrated antiferromagnet MnSc <sub>2</sub> S <sub>4</sub>   |
| 16:00 | Ellen Fogh Randomness and frustration in a $S = 1/2$ square-lattice Heisenberg antiferromagnet   |
| 16:15 | Werner Schweika<br>Chiral spin liquid ground state in YBaCo₃FeO <sub>7</sub>   |
| 16:30 | Jennifer Graham  Co-existing long- and short-range magnetic order in the frustrated diamond antiferromagnet, LiYbO <sub>2</sub>                    |
| 16:45 | Jian Rui Soh<br>Detection of Magneto-electric Multipoles   |

| 15:30 | Josefin Martell   |
|-------|---|
| 13.30 | Insights into martian meteorites and other planetary materials from X-ray and neutron tomography  |
| 15:45 | Fernando Viera Lima   |
| 13.73 | Characterization of triaxial deformation and hydraulic behavior of sandstones through in-situ testing with x-ray and neutron tomography |
| 16:00 | Edvin Wrammerfors   |
| 10.00 | Exploratory neutron tomography of human articular cartilage   |
| 16:15 | Robert Cubitt   |
| 10.15 | Quantitative measurement of boron-10 using ToF transmission   |
| 16:30 | Ilija Vego  |
|       | 5D tomography of couscous particles exposed to high relative humidity   |
| 16:45 | Open discussion   |

### Large Scale Structures and Soft Matter (Chair: Trevor Forsyth)

| 15:30 | Andrea Scotti   |
|-------|---|
|       | Small-angle scattering and neutron reflectometry investigation of ultra-soft colloids in two and three dimensions       |
| 16:00 | Annekatrin Sill   |
|       | In situ neutron reflectivity studies of vertical polyelectrolyte diffusion in layer-by-layer films in aqueous solutions |
| 16:15 | Paavo Penttilä  |
|       | Nanoscale wood-water interactions studied with small-angle neutron scattering   |
| 16:30 | Wenke Mueller   |
|       | Localization of dye molecules in surfactant assemblies via SANS contrast variation                                      |
| 16:45 | Karin Edler   |
|       | Nanostructure in amphiphile-based deep eutectic solvents  |

### **Spectroscopy and Functional Materials** (Chair: J. Ollivier)

| 15:30   | Fabrizia Foglia  |
|---------|--|
| . 5.5 5 | Anionic exchange membranes for fuel cells: insight into ion, polymer, and water dynamics from neutron spectroscopy |
| 16:00   | Bettina Schwaighofer   |
|         | A combined experimental and computational study of oxide ion conductors  |
| 16:15   | Mohamed Aouane   |
| . 0 5   | Endofullerenes: dynamics in confinement - CH <sub>4</sub> @C <sub>60</sub> study                                   |
| 16:30   | Peter Fouquet  |
| . 0.00  | Hydrogen mobility and reactivity in MoS <sub>2</sub> catalyst  |
| 16:45   | Rasmus Lavén   |
| 10.15   | Vibrational properties of APbl₃: from harmonic vibrations to a phonon liquid                                       |

| Imaging for Archeology and Material Science | (Chair: Alessandro | Tengattini, Robin Woracek) |
|---|--------------------|----------------------------|
|---|--------------------|----------------------------|

| 09:00 | Stephen Hall  |
|-------|---|
| 09.00 | Using neutrons to explore processes in geomaterials   |
| 09:30 | Hanna Isaksson  |
| 09.30 | Dual modality neutron and X-ray tomography data from skeletal tissues   |
| 10:00 | Camilla Larsen & Stavros Samothrakitits   |
|       | Laue and time-of-flight neutron diffractive imaging methods for 3D grain mapping of polycrystalline materials |

#### **Diffraction for Energy and Sustainability** (Chair: Th. Hansen, W. Schweika)

| 00.00 | Anatoliy Senyshyn   |
|-------|---|
| 09:00 | Quantification of operation-driven active material losses in Li-ion batteries using neutron diffraction |
| 09:30 | Neelima Paul  |
|       | Neutrons to understand improvement in battery performance on electrode modification                     |
| 09:45 | Ida Nielsen   |
|       | The first neutron investigation of multiple phase transitions in Prussian White                         |
| 10:00 | François Goutenoire   |
|       | Exploring phase diagrams with neutron powder diffraction  |

#### Fundamental and Particle Physics: Experiment Highlight (Chair: V. Santoro)

| 00.00 | Francesc Morabal Capilla   |
|-------|--|
| 09:00 | Neutrino-Nucleus Coherent Scattering, ESS Research Program Status    |
| 00.20 | Karina Bernert   |
| 09:30 | Measurement of the Fierz interference term with PERKEO III           |
|       | Michael Jentschel  |
| 09:45 | Diffraction enhanced experiments for particle physics                |
|       | Richard Wagner   |
| 10:00 | The Neutron - anti-neutron oscillation (NNBAR) experiment at the ESS |
|       | Hanno Filter   |
| 10:15 | Status of the PanEDM neutron electric dipole moment experiment       |
|       | ·  |

### Large Scale Structures and Hard Matter (Chair: Björgvin Hjörvarsson)

| 09:00          | Grace Causer  |
|----------------|---|
| 00.20          | Topological non-collinear magnetism: from skyrmions to solitons<br>Emma Campillo  |
| 09:30          | Analysis of time-of-flight SANS data on mesoscopic crystals such as flux line lattices  |
| 09:45          | Xaver Brems   |
| 10:00          | Vortex matter transport phenomena of the IMS<br>Sebastian Stock   |
| 10.00          | In situ small-angle neutron scattering study of hydrogen physisorption in nanoporous carbons  |
| 10:15          | Ahmed Alshemi Investigating the superconducting state of 2H-NbS2  |
|                | investigating the superconducting state of 211-Nb32   |
|                |   |
|                | Spectroscopy and Soft Matter (Chair: D. Noferini, O. Czakkel)   |
| 00.00          | <b>Spectroscopy and Soft Matter</b> (Chair: D. Noferini, O. Czakkel) Stephane Longeville  |
| 09:00          | Stephane Longeville Hemoglobin S polymerization and diffusion in hemoglobin mixtures HbF <sub>x</sub> HbS <sub>(1-x)</sub> and implication to Sickle cell disease   |
| 09:00<br>09:30 | Stephane Longeville Hemoglobin S polymerization and diffusion in hemoglobin mixtures HbF <sub>x</sub> HbS <sub>(1-x)</sub> and implication to Sickle cell disease Maria Rescigno  |
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