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SPALLATION  
SOURCE

# ESS: An Introduction

Dimitri Argyriou  
Director for Science

SAC Orientation  
4 February 2014

# What is ESS ?



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**ESS-AÉG**  
Engineering Students' Society  
Association des Étudiant(e)s en Génie





# What is ESS ?



Packaging Ltd



## ESS-AÉG

Engineering Students' Society  
Association des Étudiant(e)s en Génie



# Welcome !





# Road to realising the world's leading facility for research using neutrons



**2007**

ESS secretariat was set up in Lund

**2009**  
Decision: ESS will be built in Lund

**2013**

ESS enter construction phase of the project

**2014**

Construction work starts on the site

**2019**

First neutrons on instruments

**2023**

ESS starts user program

**2025**  
ESS construction complete



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Joint Nordic Focus on Research Infrastructure  
James Yeck



# Design update delivered 2012





# The ESS Project



**Proton Accelerator**  
Energy: 2.5 GeV  
Frequency: 14 Hz  
Current: 50 mA

**Target Station**  
Solid Rotating W  
He or Water Cooled  
5MW average power  
>22 beam ports

**Instruments**  
22 Instruments in  
construction  
budget

5 times brighter than SNS  
30 times brighter than ILL

**Total Cost of Project**  
1843 (2013) Mil €



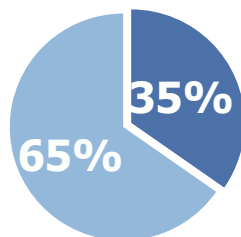
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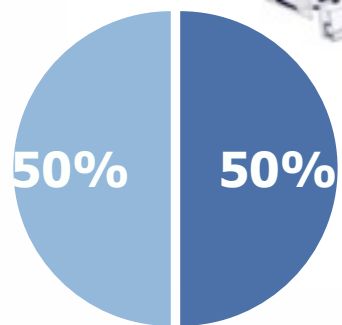
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James Yeck

# ESS In-kind contributions potential

Total construction cost:  
€ 1,84 billion

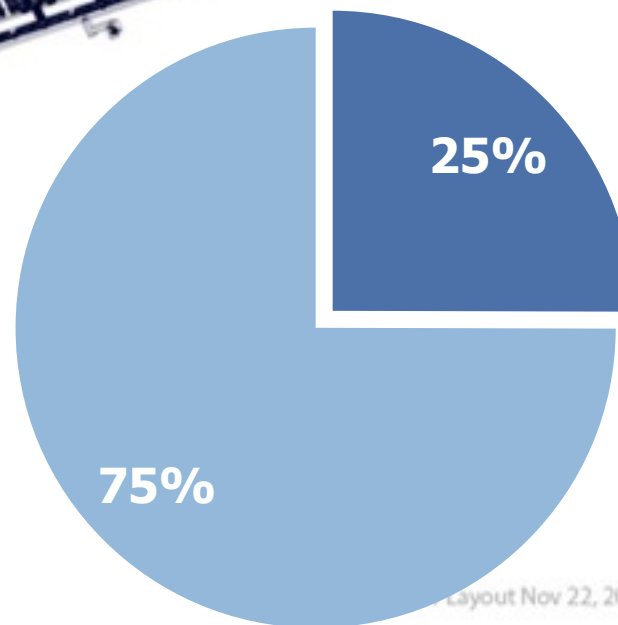


Target station  
€ 154M



NSS/Instruments  
€ 350M

Accelerator  
€ 522M



- <http://europeanspallationsource.se/eoi>
- 683 Proposals from 115 Respondents
- 52% Companies
- 48% Organisations

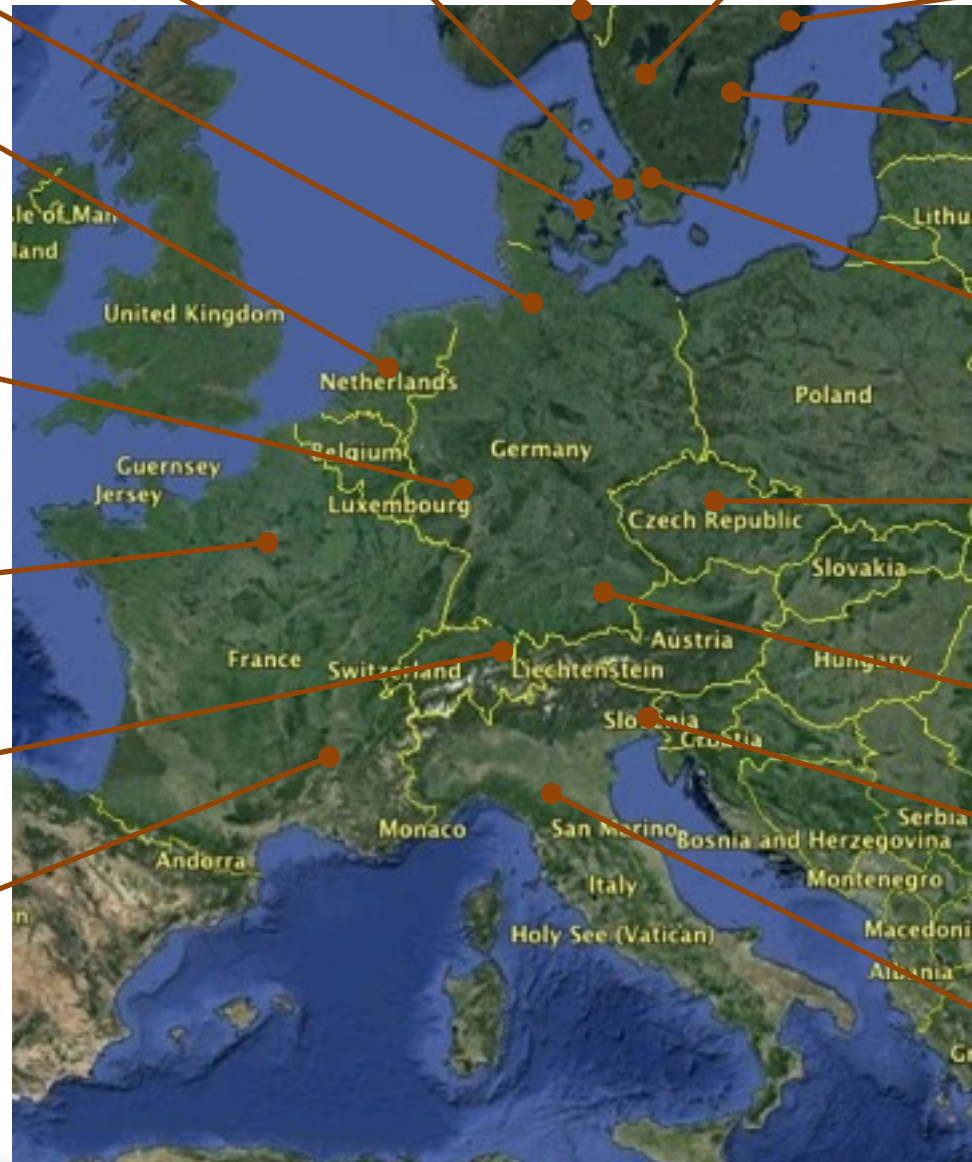


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Joint Nordic Focus on Research Infrastructure  
James Yeck





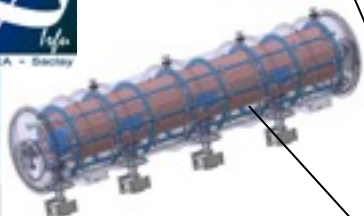
# Prototyping the ESS accelerator



Sebastien Bousson



Pierre Bosland



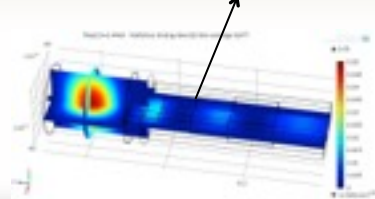
CERN



Roger Barlow



Ibon Bustinduy



Santo Gammino



Søren Pape Møller



Roger Ruber



Anders J Johansson



The National Center for Nuclear Research, Swierk



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Workshop on Nordic Neutron Science Collaboration

Dimitri Argyriou

# Short Update on the Politics

- **ESS continues to enjoy wide support from Science Community and European Nations.**
- **France recently announced that it will participate in the construction and operation of ESS.**
  - Support from French Science Community important !
  - ESS seen as an important infra-structure for France after finding from recent review.
  - Positive decisions in Switzerland and Czech Republic made already !
- **Numerous interactions on details of commitments between various countries and Host states;**
  - Germany, Spain Italy, UK, Switzerland, Poland, Baltic Countries and Holland.
  - Positive interactions with European Investment Bank
- **Host countries and management feel optimistic that we will be able to reach 85% threshold for commitments in order to begin construction in**

# Organisation



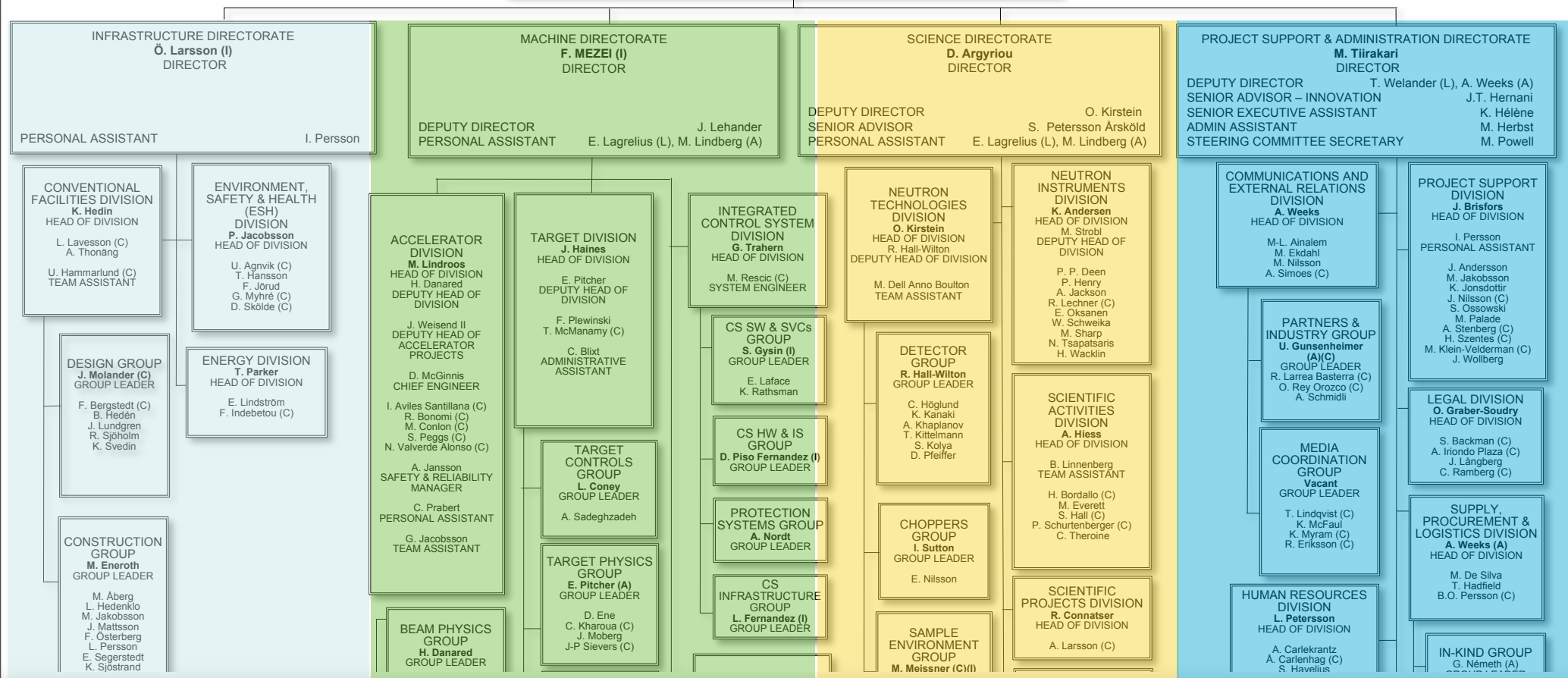
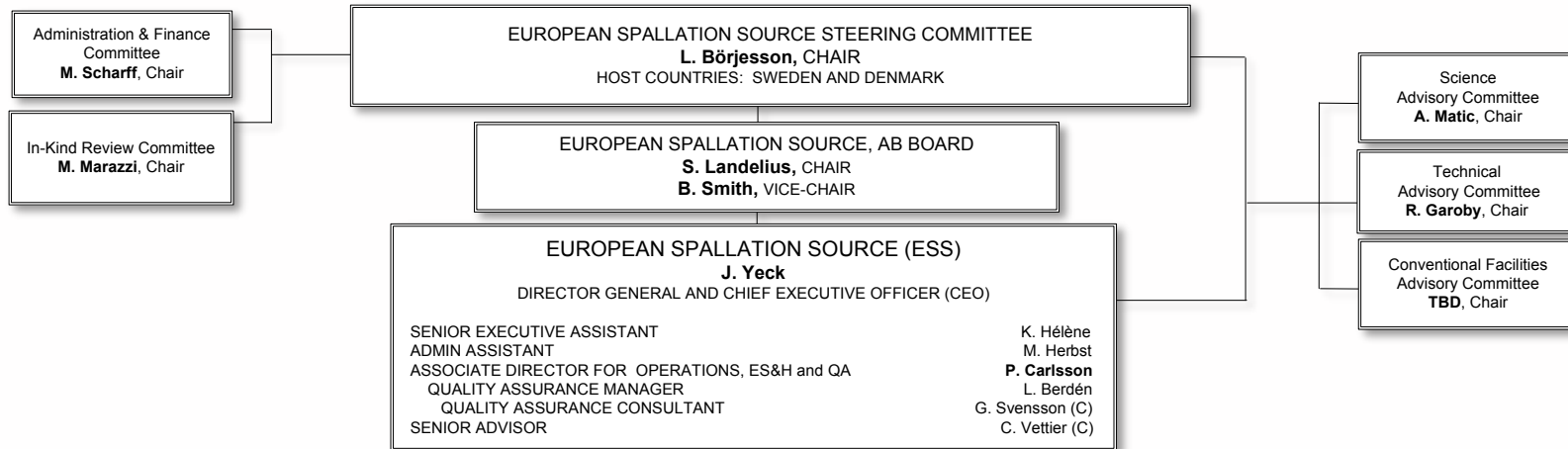
# Largest European science project



**Sweden,  
Denmark and Norway:  
50% of construction  
15-20% of operations**

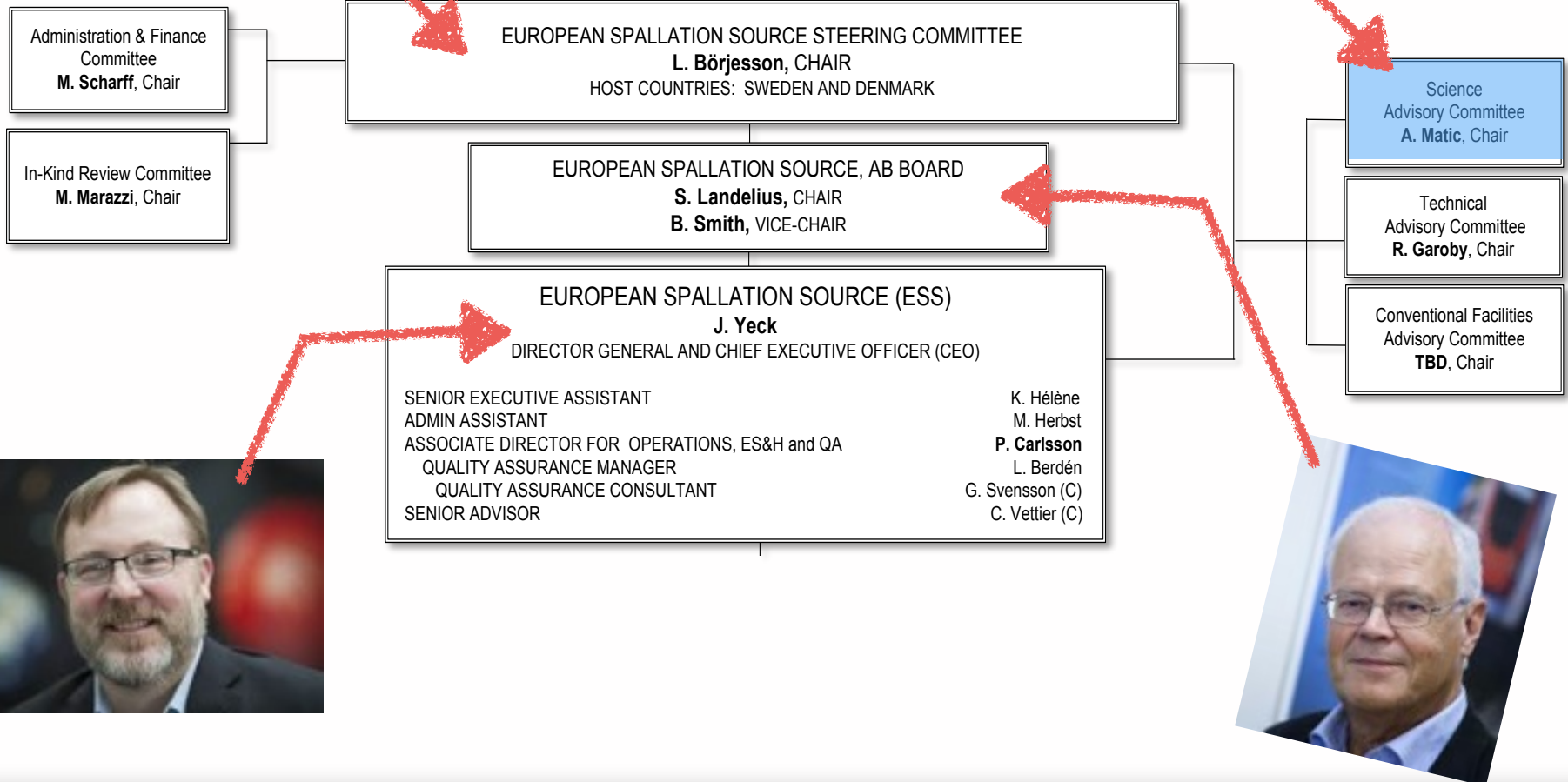


**European partners:  
50% of construction**

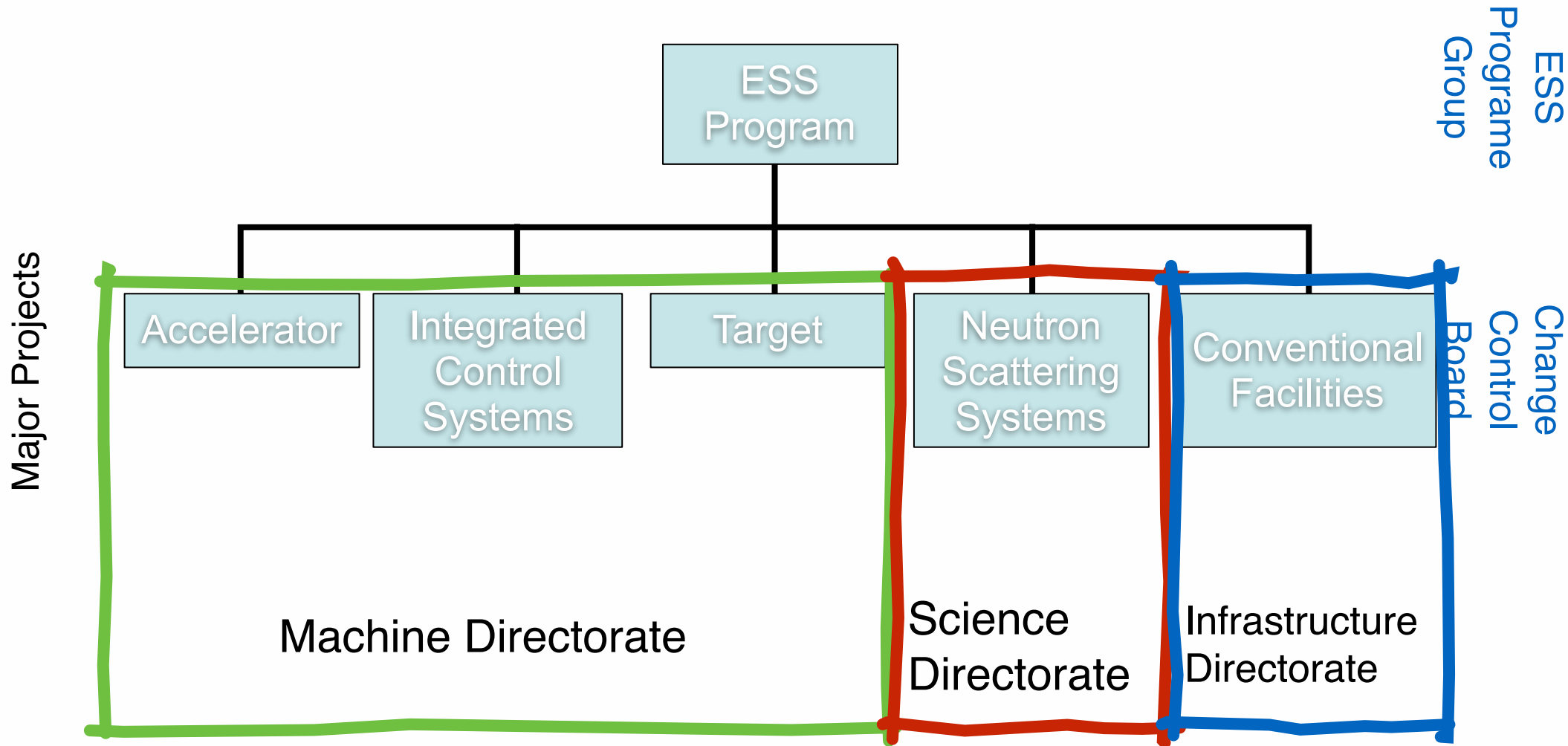




You are  
here !



# ESS Project Structure



# Charge to Science Advisory Council

## Terms of reference of the European Spallation Source Science Advisory Committee

### Committee Charge

The Scientific Advisory Committee (SAC) will independently assess the scientific goals and the overall layout of the ESS as presented by ESS AB. The Science Advisory Committee (SAC) will advise on the scientific objectives and ensure that they are adhered to. It will provide independent advice, in particular, on all relevant scientific and technical issues related to the instrument suite and the desired characteristics of the neutron beams and the accelerator performance, as well as facilities for scientific support and the scientific operation of the facility.

SAC will monitor the costs for the construction and operation of ESS within its area of expertise.

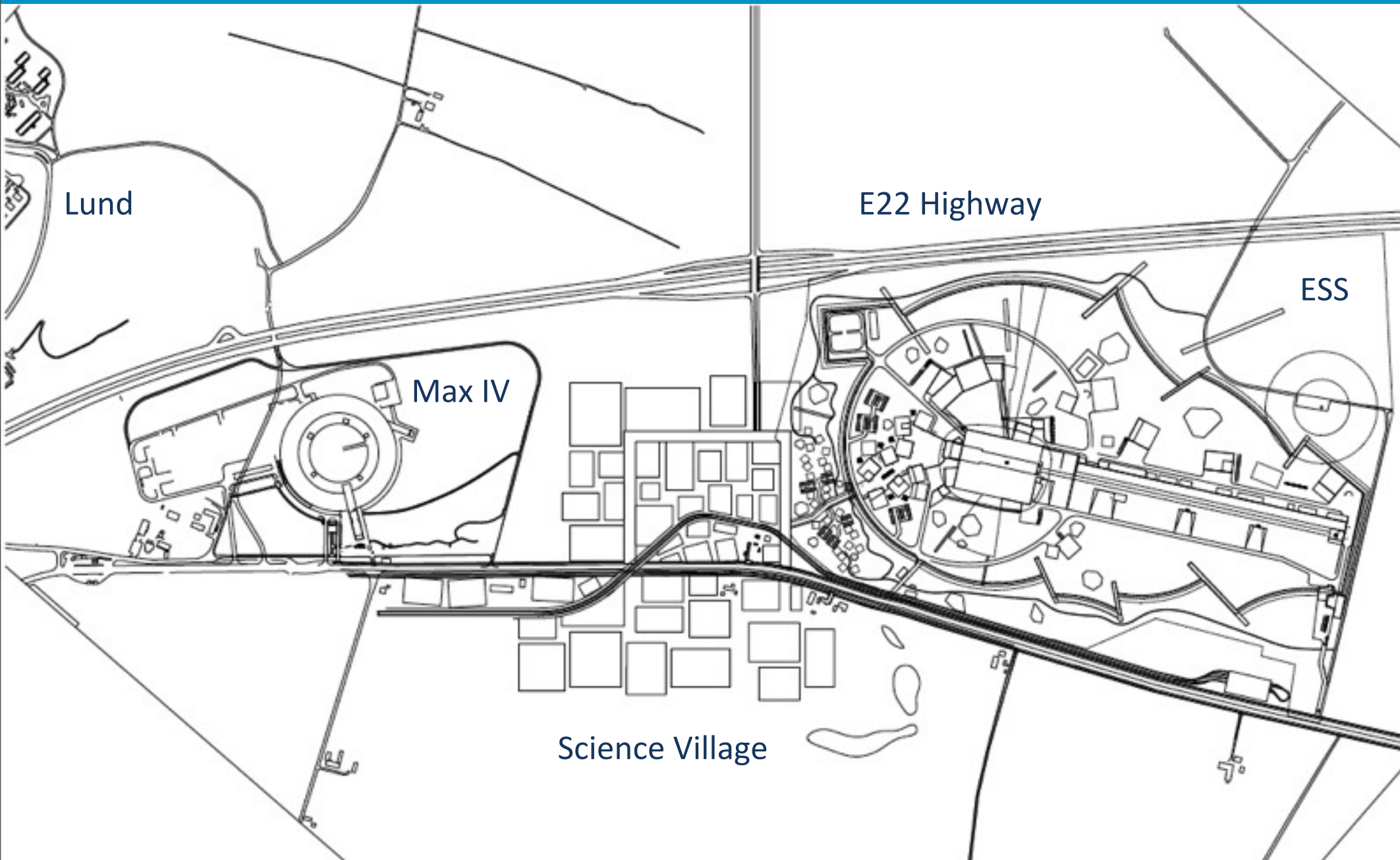
The SAC will advise ESS AB and report its advice to the Steering Committee (STC).

# Conventional Facilities



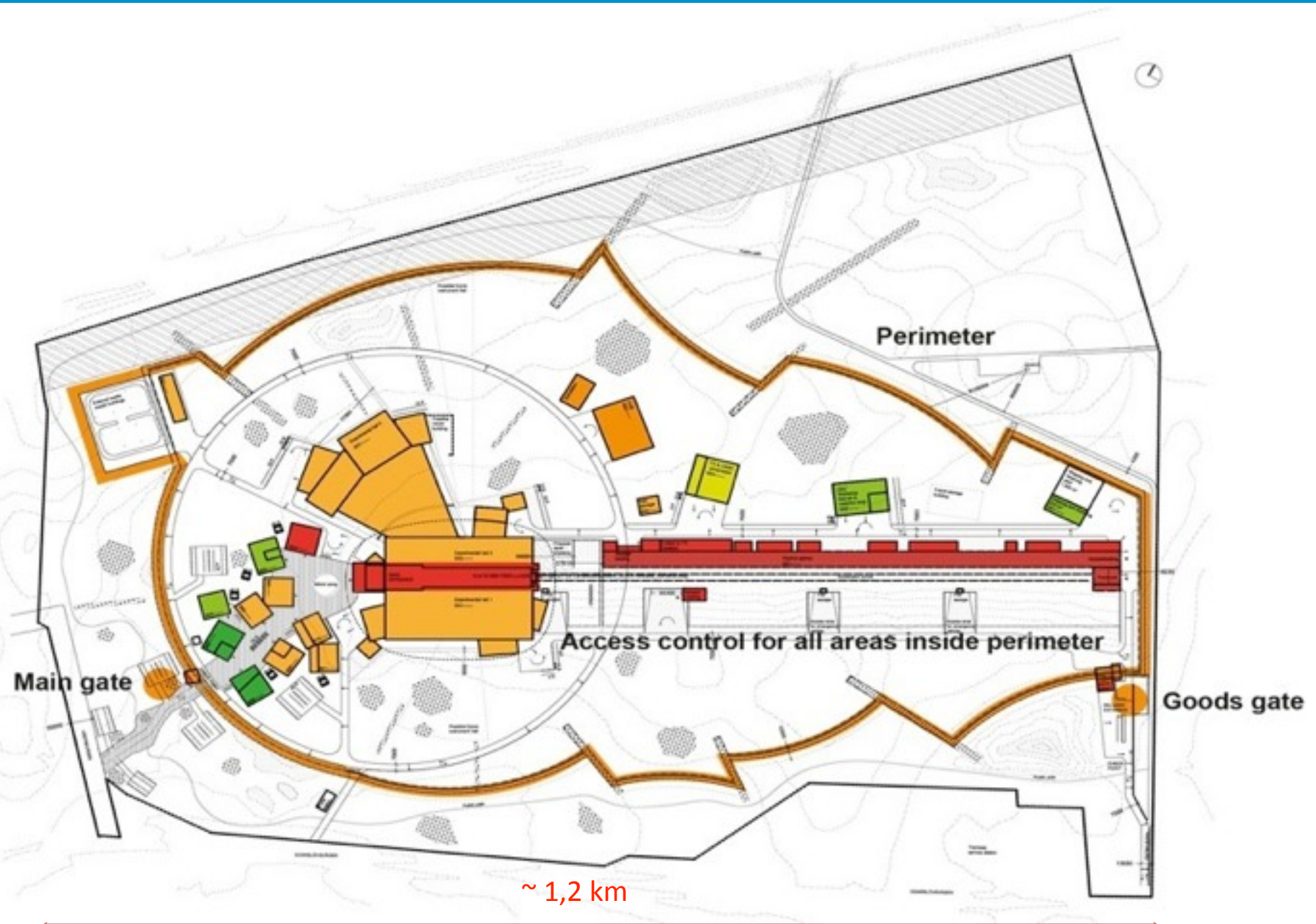


# ESS is co-located with Max IV and Science Village in close proximity to Lund



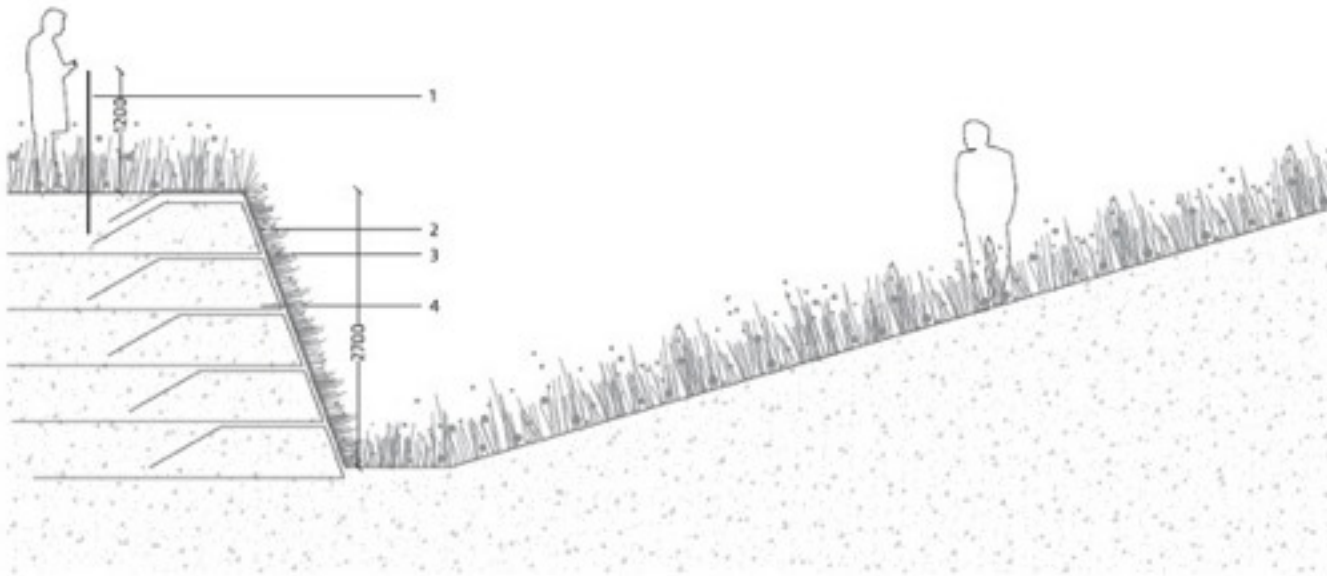


# The ESS Site covers 75 hectares

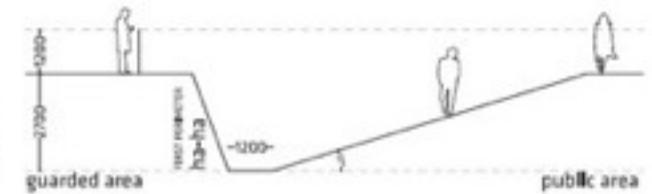


## Perimeter detail 2013-10-25

### C) 3.42 perimeter ha-ha detail

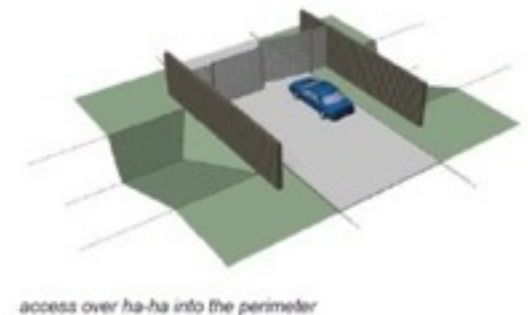
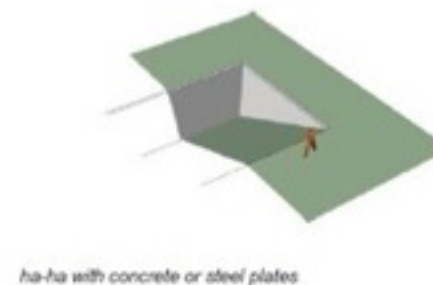
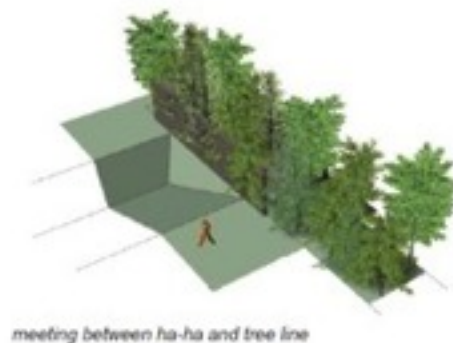
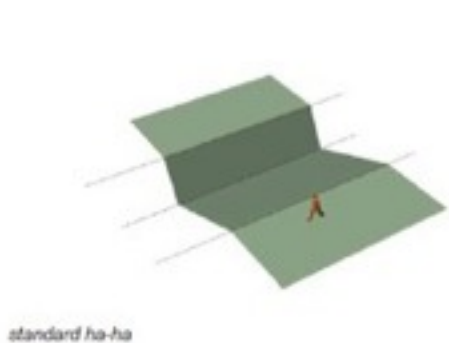


Ha-ha with green retaining wall  
height: 2,7 m  
wall slope: 70-80°



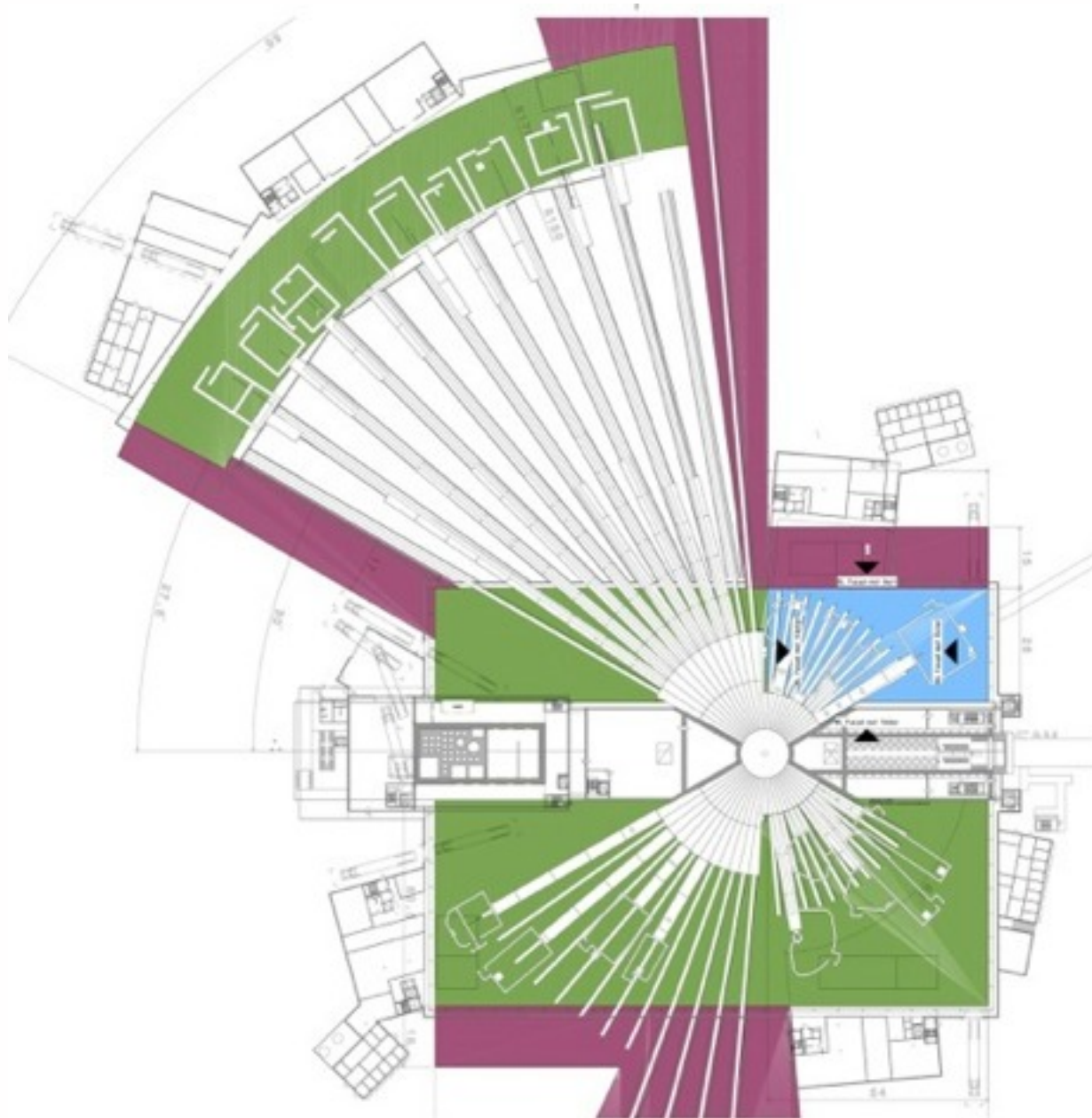
- 1 animal fence
- 2 erosion protection mat
- 3 geogrid
- 4 filled ground

cross section 1:50

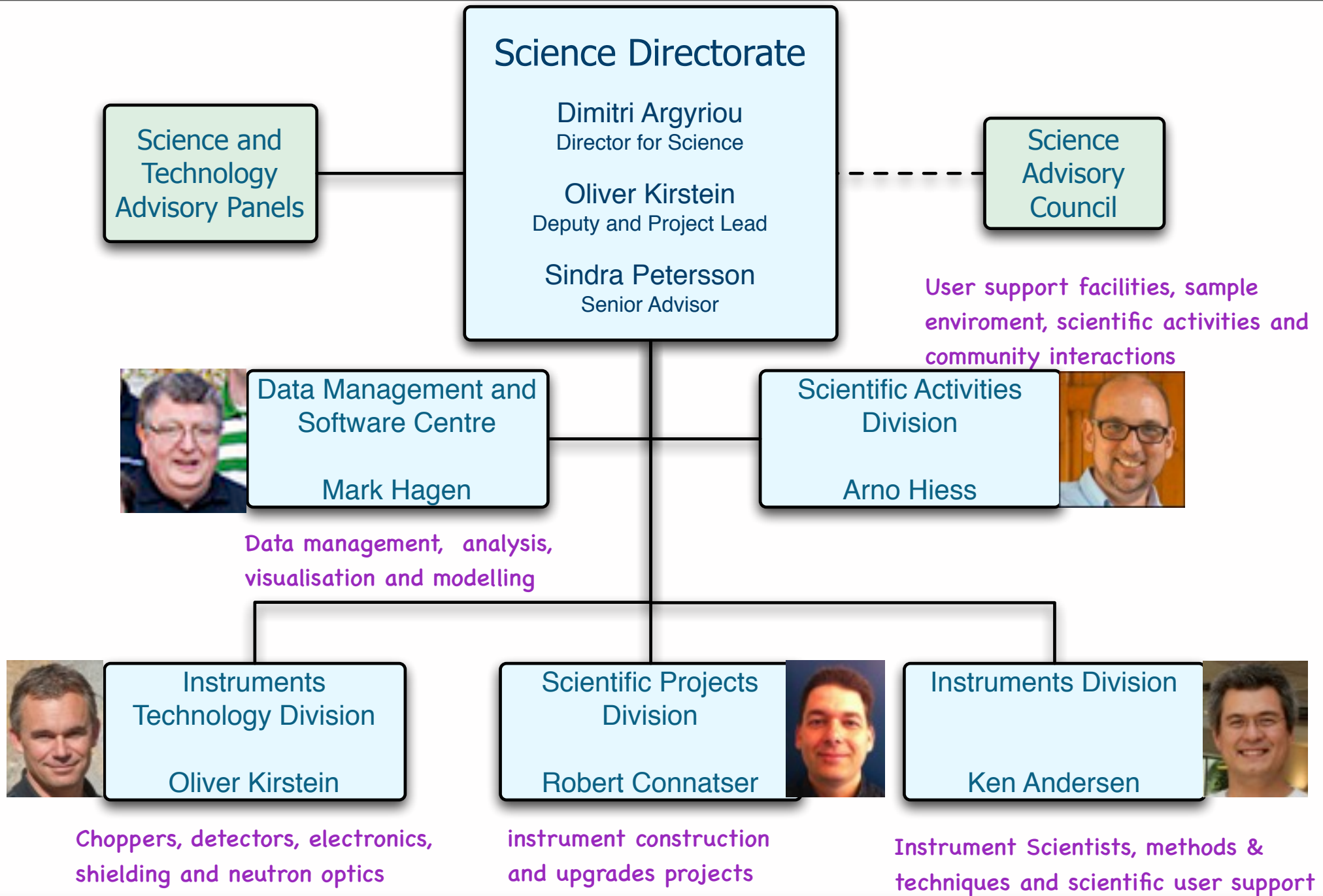




# Target and Instruments



# Introduction to Science Directorate



# Neutron Scattering Systems Project Scope

## The scope:

Construct the 22 “public” instrument suite of ESS together with a technical and scientific support infrastructure that enables scientific excellence and high quality scientific user service with reliable and sustainable operations.



22 Instruments



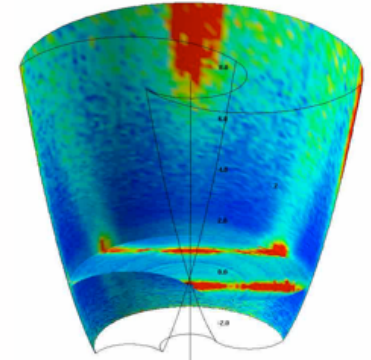
Sample Environment



Science Support Laboratories



Analysis and Visualisation Software



# Pre-Construction Phase

## Teams Around Europe are Exploring Novel Instrument Concepts for ESS

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	Small- sample SANS Full DU SANS, SD004DE/c	Reflectometer for magnetic layers Full DU, focus, pol., SD003DE/b		Single Crystal Mag. Diffraction. Full DU French collaboration	Multi Purp. Extreme Environ.Diffr. Full DU, tests, SD008DE	CEED Full DU, tests, PH, SD033CZ	Larmor Label. Full DU, TOF DF imaging SD056AL	Bispectral Chopper Spectrometer Full DU, RRM pol., SD003DE/b	CAMEA Full DU plus tests and prototyping, SD018DC	Wide Angle NSE Full DU, SD003DE/b	UCN Full DU Not covered
	Pol. SANS Full DU, incl. SE devices SD054NL	Vertical focusing reflectometer Full DU, SILENE plus prototype tests, design full instrument, SD017DC/a			Hybrid Diffraction potent. including SANS and imaging Full DU, SD018DC	Hi Flex. Mat. & Engin. Diff. Full DU, WPM, flex. res., SPEED, Fourier, POLDI SD039ESS	Multi-Purpose High-Res Imaging Full DU in close collab. GER, phase, fast, high res., SD029CH	Thermal Chopper Spectrometer Full DU, RRM and pol. cap. SD038ESS/a	Backscatt. Spectrometer Full DU, variable 1 to 20 micro eV resolution SD039ESS Danish In-kind	NRSE Resonant NSE, SD007DE/b	
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	Broadband SANS Full DU, SD063ESS	Freia Reflectometer Full DU, broad simultaneous q-ranges, SD039ESS			Pulsed Monochr. Powder Diffr. multi monochromators or chop.; concept, design SD037ESS			Crystal Monochr. Spectrometer Full DU Italian collaboration	Q – TAS Farm Full DU, SD043ESS Not covered		
	VSANS/ GSANS Full DU French collaboration	Spin-Echo label. in Pol. Reflectom. SD055NL			Larmor label. in diffr. (TOFLAR) SD057NL						
Simulation software development, general simulations, supporting GER simulations, VITESS SD041DE											
General simulations, in-house supporting simulations, interface moderator-beam extraction, McStas SD022DK											



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# Pre-Construction Phase

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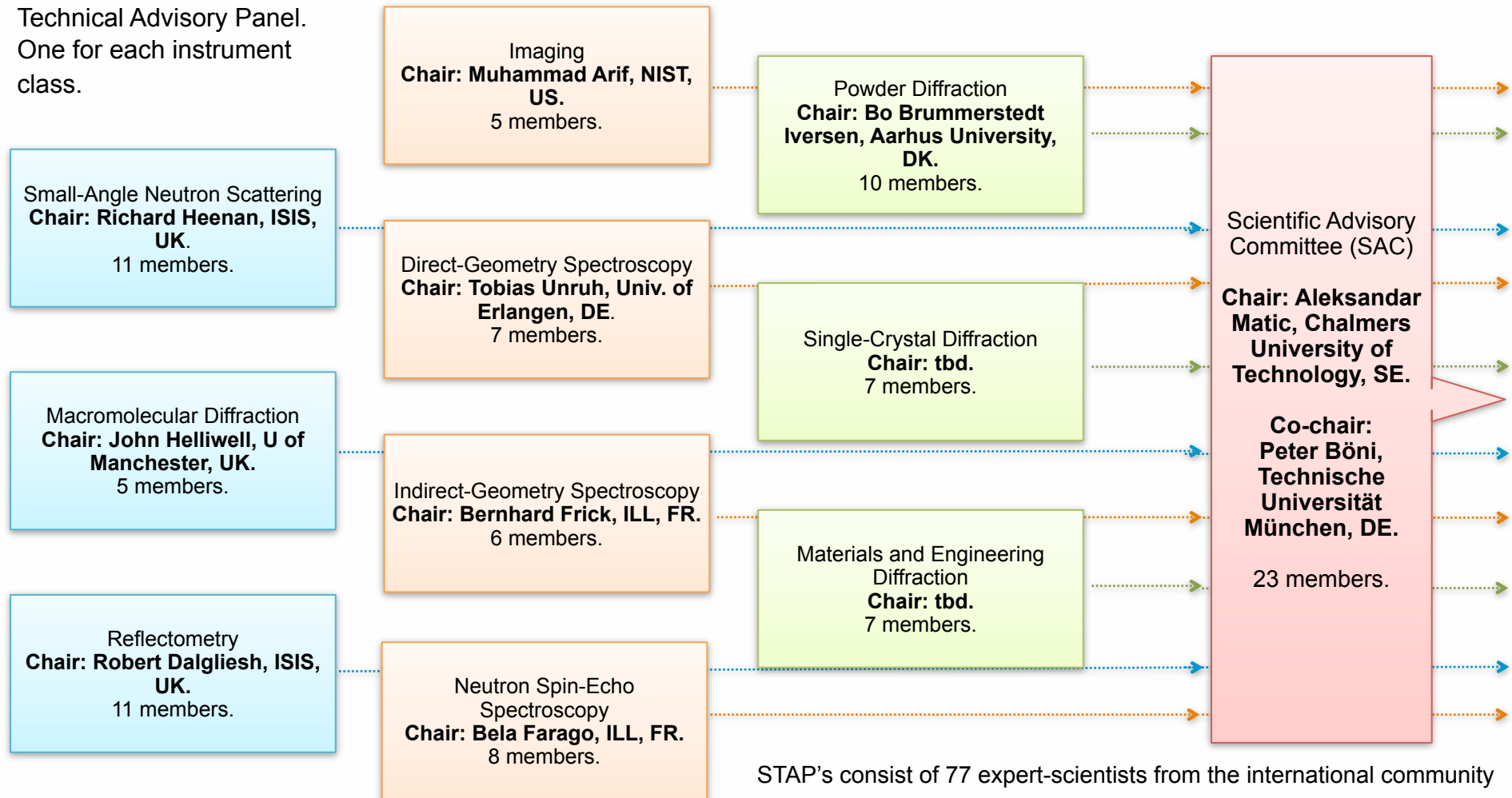


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# The Community Advises ESS on Instruments through the STAPs and SAC

**STAP:** Scientific and Technical Advisory Panel.  
One for each instrument class.

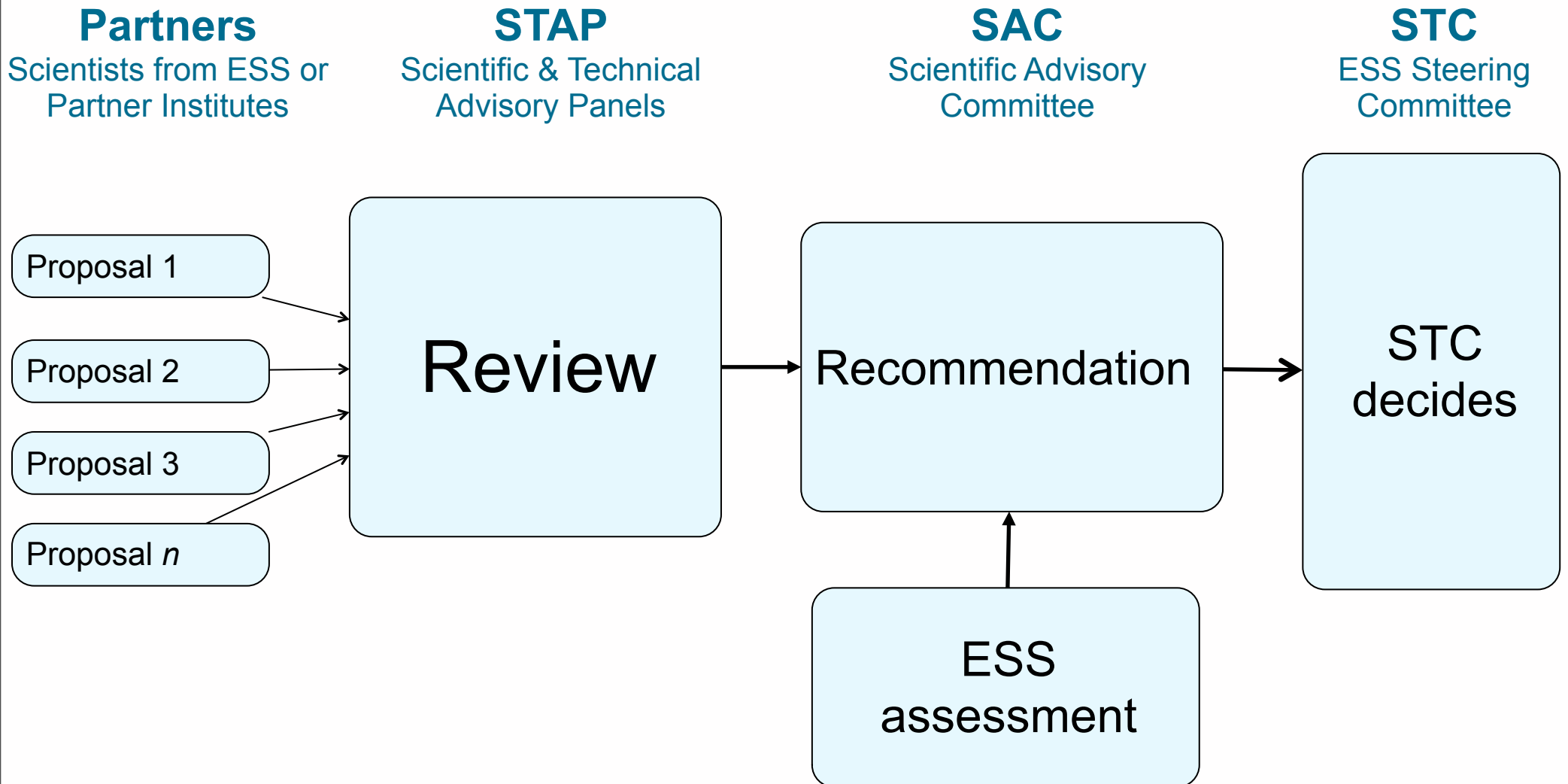


STAP's consist of 77 expert-scientists from the international community  
STAP advises ESS management and informs SAC.  
SAC advises ESS management, who proposes to STC.

Europe's Spallation Source

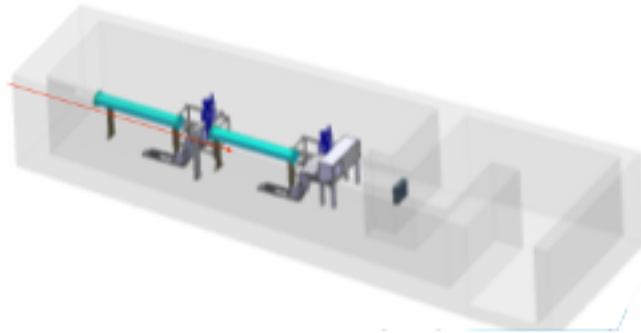


# From Idea to Construction via an Open Process

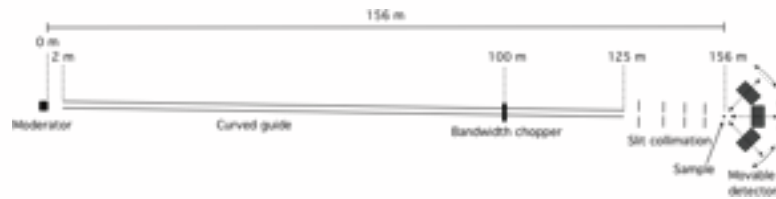


# First Instruments Selected

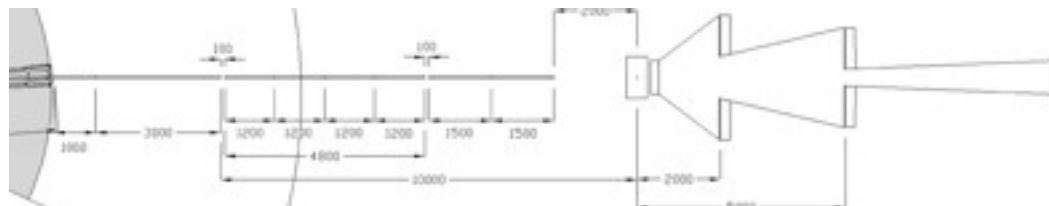
## ODIN - Optical and Diffraction Imaging with Neutrons



## NMX Macromolecular Diffractometer



## LoKI - A Broad-Band SANS Instrument



Geo & engineering  
Heritage



Magnetism  
Soft matter

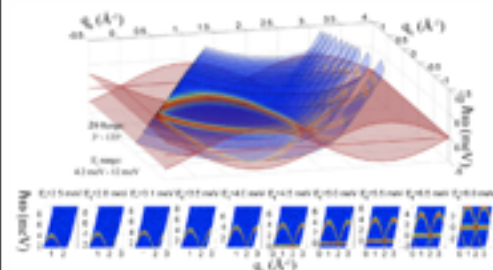


Life science  
Chemistry



# 16 Instrument Concepts were Presented at IKON5

## Spectroscopy

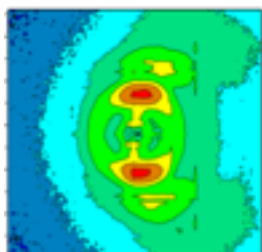


VOR  
T-REX  
ESS-CCS  
Tempus Fugit  
CAMEA  
ESS-NSE



Wide Bandwidth Spectrometer  
Bi-Spectral Spectrometer  
Cold Chopper Spectrometer  
Time-Focusing Spectrometer  
Indirect Geometry Spectrometer  
Spin Echo Spectrometer

## SANS

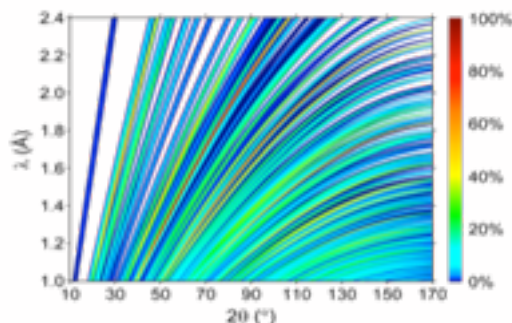


SKADI  
Compact-SANS



High Intensity SANS  
SANS Biology & Materials Science

## Diffraction

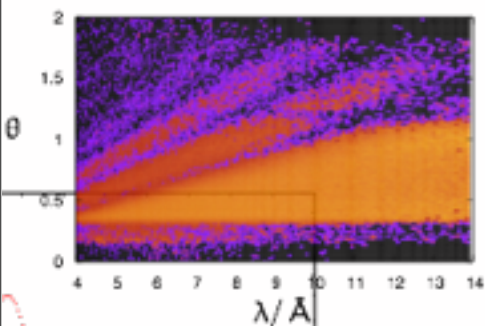


ESS-ENG  
MODI  
HEIMDAL  
POWHOW



Engineering Diffractometer  
Monochromatic Diffractometer  
Thermal Powder Diffractometer  
Bi-Spectral Powder Diffractometer

## Reflectometry



FREIA  
THOR  
ESS-PAREF  
ESTIA



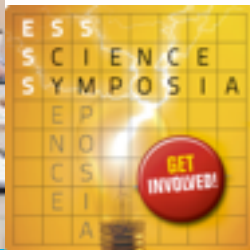
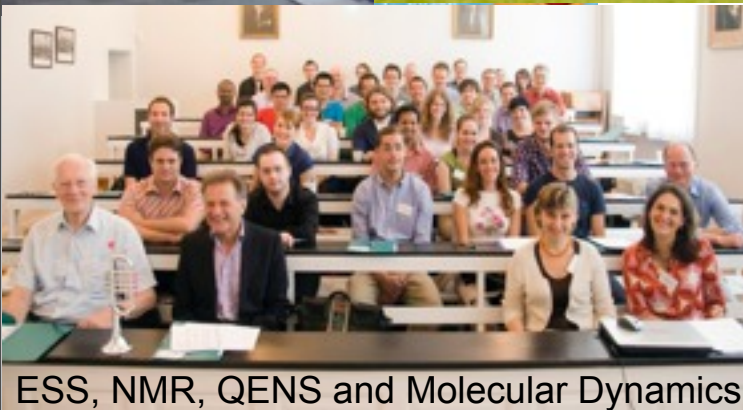
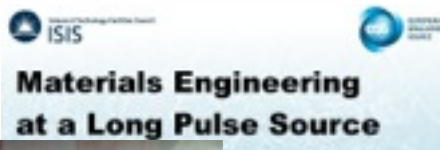
Reflectometer for liquid interfaces  
Horizontal Reflectometer  
Polarised Reflectometer  
Focusing Reflectometer

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# Active Engagement with Community and Partners

## Science

- 20 **Science Symposia** proposed by the community
- More than 400 people participating
- Real Input into the planning of ESS

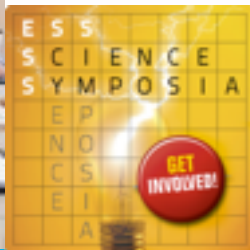
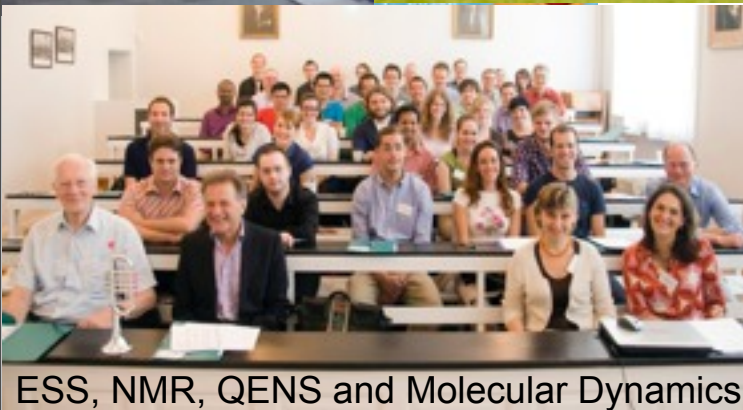




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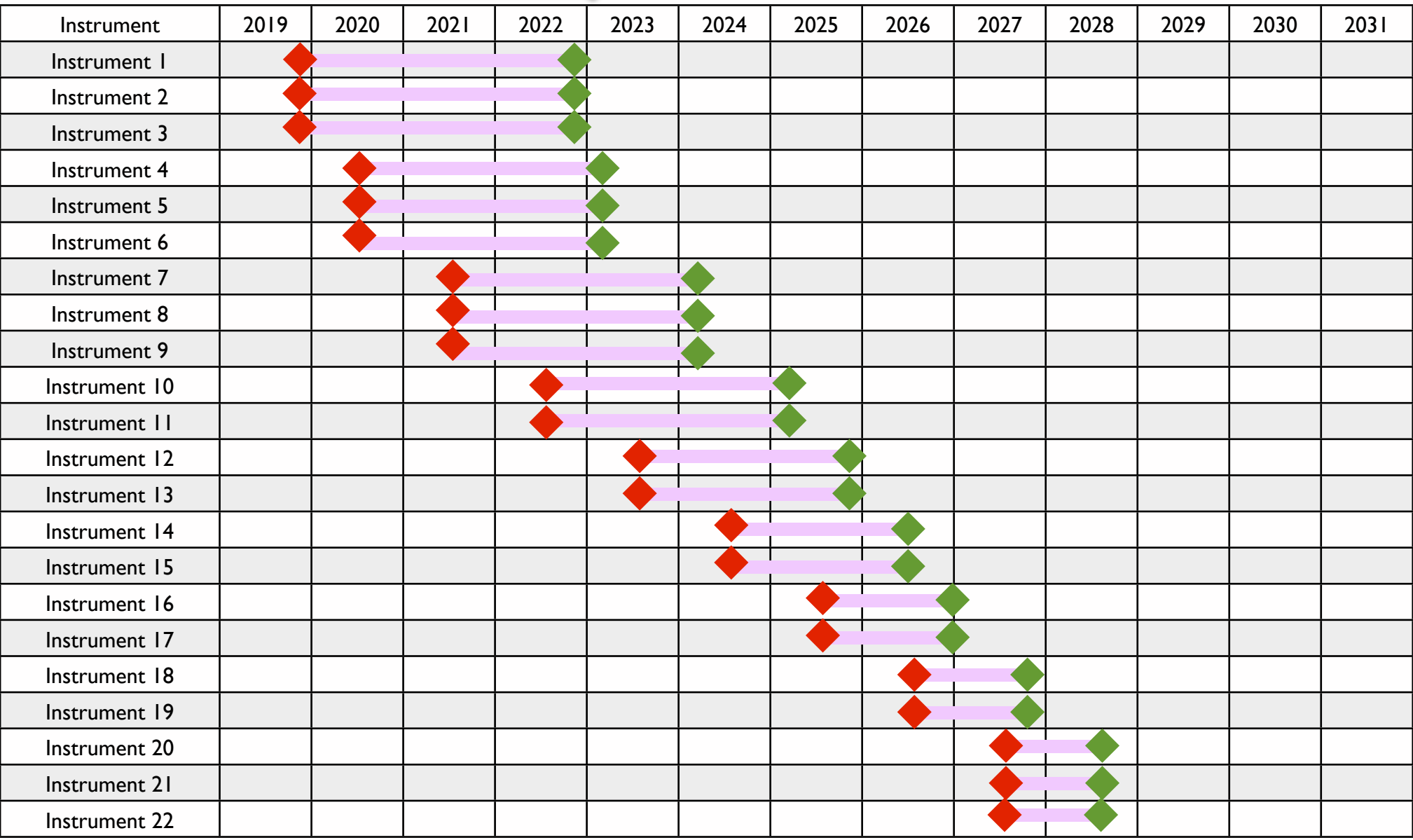


## Instruments

- 5 **IKON** Collaboration meetings
- Regular attendance by as much as 160 partners every six months
- Instrument concepts, technologies, STAP meetings



# Scenario for Transition of Instruments into User Program



- ◆ Start of Hot Commissioning/instrument
- ◆ Start of Scientific User Program/instrument
- Hot Commissioning/ Demonstration Experiments/Friendly Users

# An Early Success Strategy for ESS Prioritisation

- ESS will be judged as a success or failure **early** !
- The first instruments need to:
  - Attract a wide user community.
  - Provide scientific impact.
  - Work as expected
  - High quality user service (Software, sample environment, science support)
- Prioritise the right instruments
- Prioritise the support for those instruments



# Key Assumptions

- The NSS construction budget is set to 350 Mil €(2013-2025).
  - Budget is ring fenced
  - Inflation corrections will be applied through the construction phase
  - The construction budget is consistent with 16 instruments
- The NSS construction budget alone will not deliver the scope of 22 instruments.
  - Additional support and strategies to supplement the NSS construction investment that extended beyond the boundaries of the capped ESS construction budget.
- The average cost-book value of a “bare” instrument is 12.5 Mil Euro.
  - This price is an explicit price and does not include the additional value that ESS adds on each instruments. Eg. common shielding, ICS, software, instrument technology standards and support.



# NSS budget allocation of 350M€

Instrument projects 188.7 M€  
**Number of instruments** 15 (16)  
 Average cost (\*) 10.5 M€

## Instrument-build programme

Common bunker / shielding for up to 32 instruments

Management & Administration 7.1 M€  
 Instrument Concepts 8.8 M€  
 Science Support Systems 24.3M€

Administration, concept developments,  
and supporting scientific infrastructure

DMSC 26.2 M€  
 Detector systems 39 M€  
 Chopper systems 12.1 M€  
 Neutron Optics & Shielding 8.7 M€  
 Electrical Engineering 11.4 M€

Technical platforms that provide  
added value to instruments by  
suite wide solutions,  
standardisation and support

Contingency 15.7M€  
 Budget plug 2013 8M€

## NSS Contingency

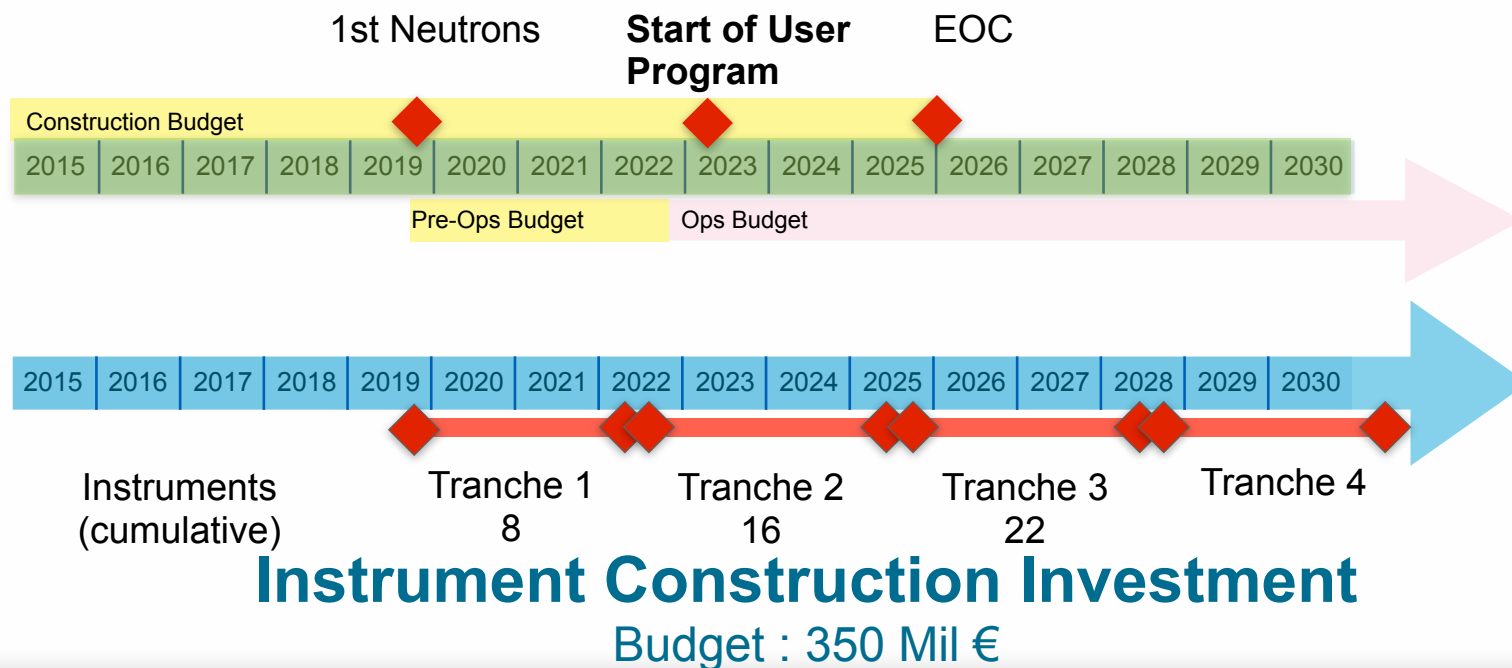
**Total 350 M€**

137,6 M€

# Strategies to meet the NSS Scope and Goals

In order to deliver project scope NSS will need to;

- Draw from pre- and steady state operations funding.
  - Implies in-kind contributions into the operations phase of ESS
- Encourage and support community-lead funding initiatives to supplement instrument budgets.
  - Leveraging can provide conservatively up to 15% of the instrument cost.
- Interact with in-kind partners to devise plans to maximise the value that is obtained from their contributions



# Key Risks and Mitigations for Science Programme

- Failure to engage or align the priorities of ESS with the priorities and needs of the user community
  - Extensive engagement programme bringing in community and partners in the design and choice of instruments and support facilities
- Construction partners disengagement / Construction partner focus on own interests and priorities / Partner Interfaces
  - Construct a framework of shared ownership of the science programme and bring partners as close as possible into the process of ESS
  - Establish “Resource Board” like structures to manage in-kind contribution between ESS, partners and funders.
  - Establish remote “Competency Centers” to ensure technical integration of partners
- Interfaces with Target and other parts of ESS are vital for Scientific Success
  - Improve and build better inter-directorate relationships and establish better management of interface-controls

# Summary

- We are engaging with the community
  - IKON, Science Symposia, STAPs, Science and Scientists Meetings
  - Facility has wide support and interacts broadly with the community
  - Will offer quantum leap in performance opening up scientific new horizons
- We have a plan that delivers the TDR scope of 22 public instruments
  - Construction investments will deliver world-class instrument program
  - Additional investments, leveraged during construction and initial operations, will be used to realise the TDR scope
- We are positioning ESS to deliver the instrument program
  - Community is expecting ESS to lead and direct
  - Continuous engagement with the science community
  - Success is assured by working with our partners using the in-kind framework





EUROPEAN  
SPALLATION  
SOURCE

# Instrument Concepts WP

Ken Andersen

Head of Neutron Instruments Division

SAC Orientation Day  
4 February 2014

# Introduction

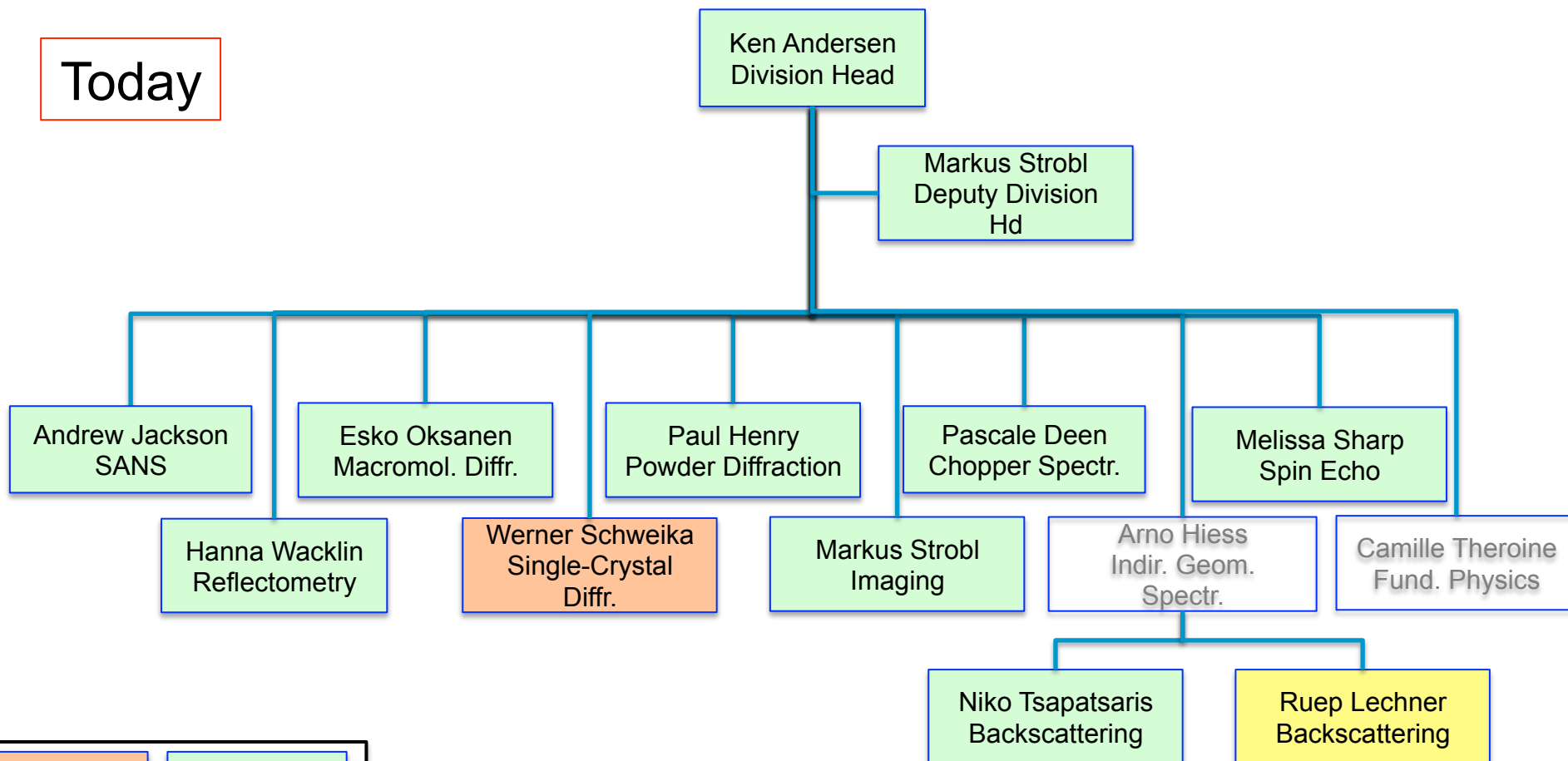
## Ken Andersen



- ▶ 1988-1992 PhD in Physics on elementary excitations in superfluid  $^4\text{He}$  from Keele University (UK) with ILL studentship
- ▶ 1992-1994 Post-doc at KENS (Japan) on percolating antiferromagnets
- ▶ 1995-1999 ILL Instrument Scientist for D7 diffuse-scattering diffractometer with polarisation analysis
- ▶ 1999-2002 ISIS Instrument Scientist for OSIRIS backscattering spectrometer with powder diffraction
- ▶ 2002-2010 ILL Head of Neutron Optics Lab
- ▶ 2010: ESS Neutron Instruments Division Head, WP leader for the Instrument Concepts WP

# Neutron Instruments Division Organization

Today



seconded  
staff

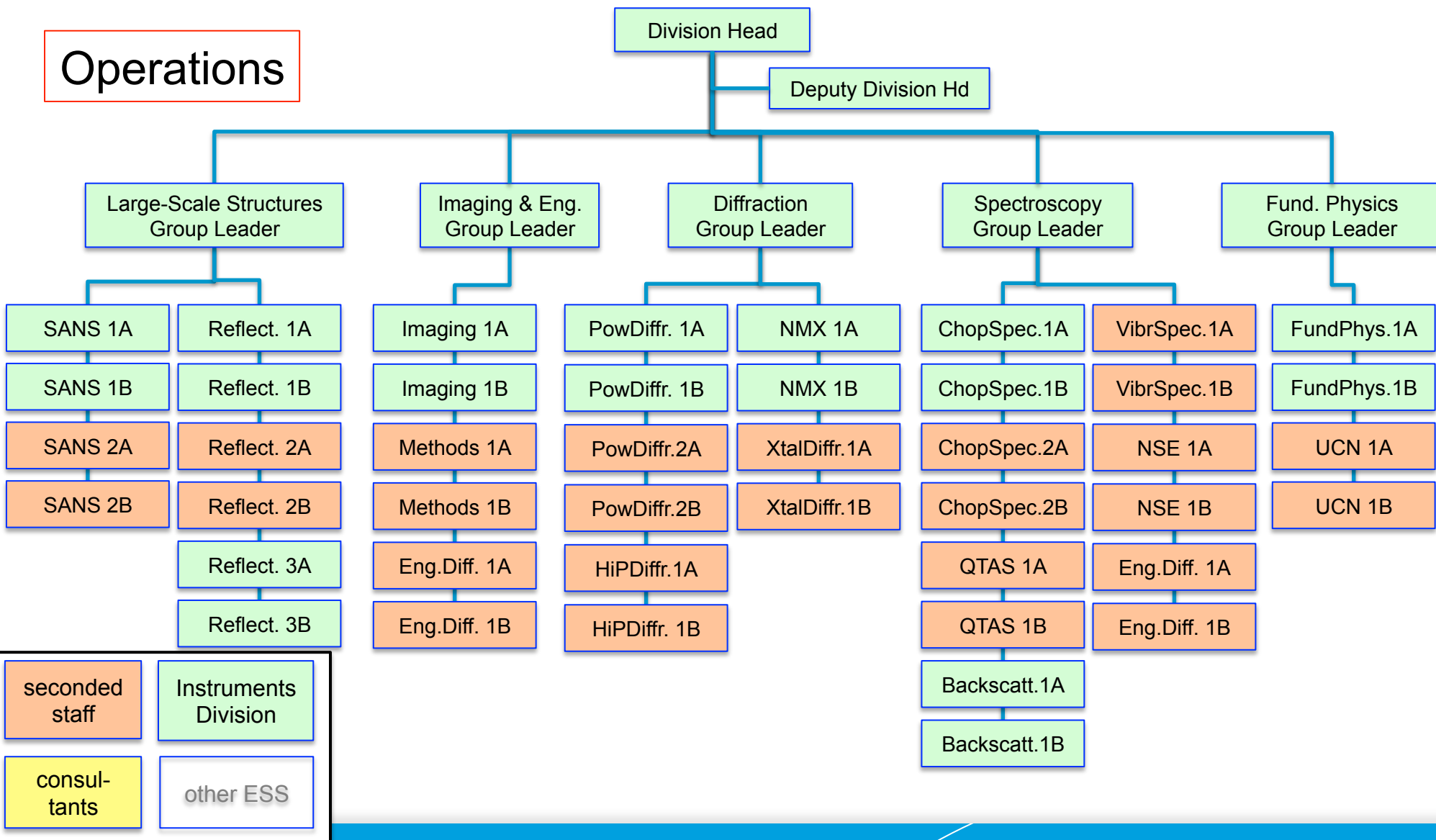
Instruments  
Division

consul-  
tants

other ESS

# Neutron Instruments Division Organization

Operations





# Scope of Instrument Concepts Work Package

Top-level requirement:

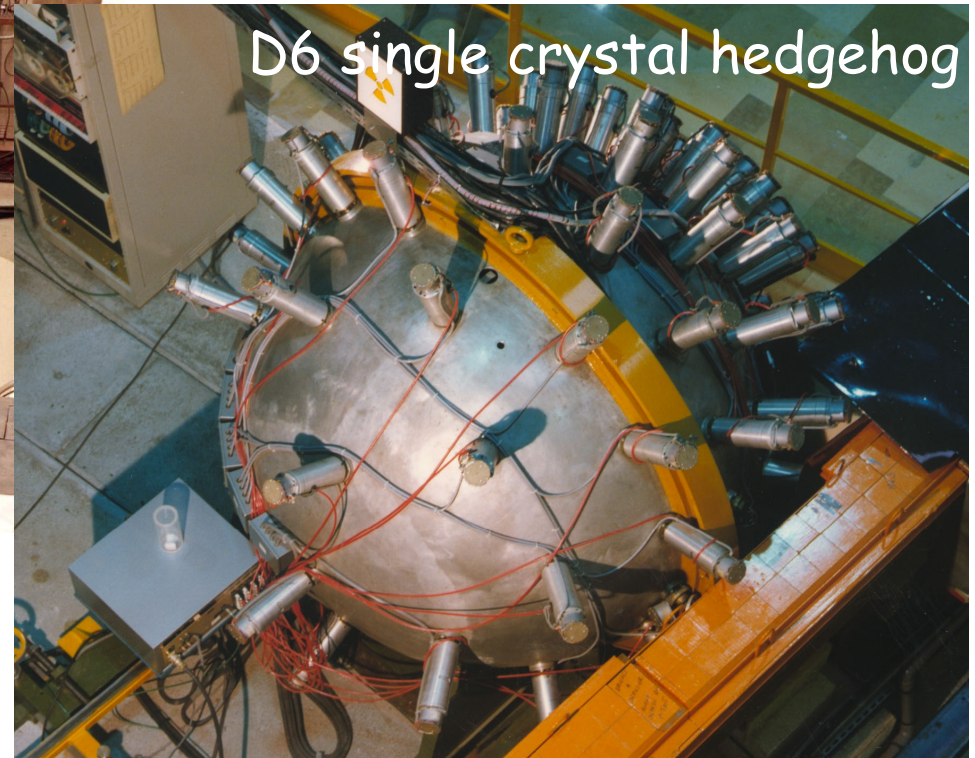
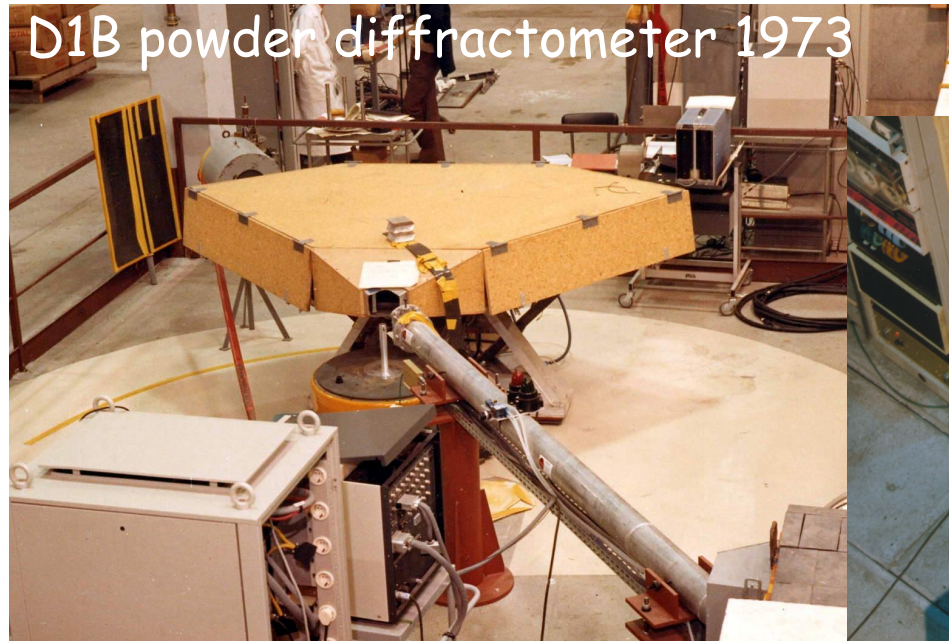
Deliver 22 instrument concepts, ready for construction

- Ensure the ESS instruments can deliver the science programme
  - optimized to provide world-leading performance
  - delivering instrument capabilities for a broad and topical science programme
  - taking full advantage of the long-pulse performance
- Develop and evaluate concepts
  - develop science case, concept and methods
  - management and coordination, e.g. IKON meetings
  - identify instrument opportunities and gaps in scientific capabilities
  - peer-review by Scientific and Technical Advisory Panels (STAPs)
  - annual submission of instrument construction proposals

# Workhorses vs Hedgehogs



# Workhorses vs Hedgehogs



# Scope of Instrument Concepts WP

- Develop instrument concepts for 22 instruments
  - adapt present-day concepts to the ESS long pulse
  - evaluate crazy ideas
  - manage peer-review selection process
- Instrument Concepts WP
  - includes exploration of science cases
  - includes method development & instrument-specific prototyping
  - has sufficient resources to allow some concept developments to fail
  - minimise risks for instrument construction projects



# Instrument Concepts Overview

SANS

Reflectometry

Macromolecular  
Crystallography

Single Crystal  
Diffraction

Powder  
Diffraction

Mat. & Engin.  
Diffraction

Imaging

Direct Geometry  
Spectroscopy

Indirect Geometry  
Spectroscopy

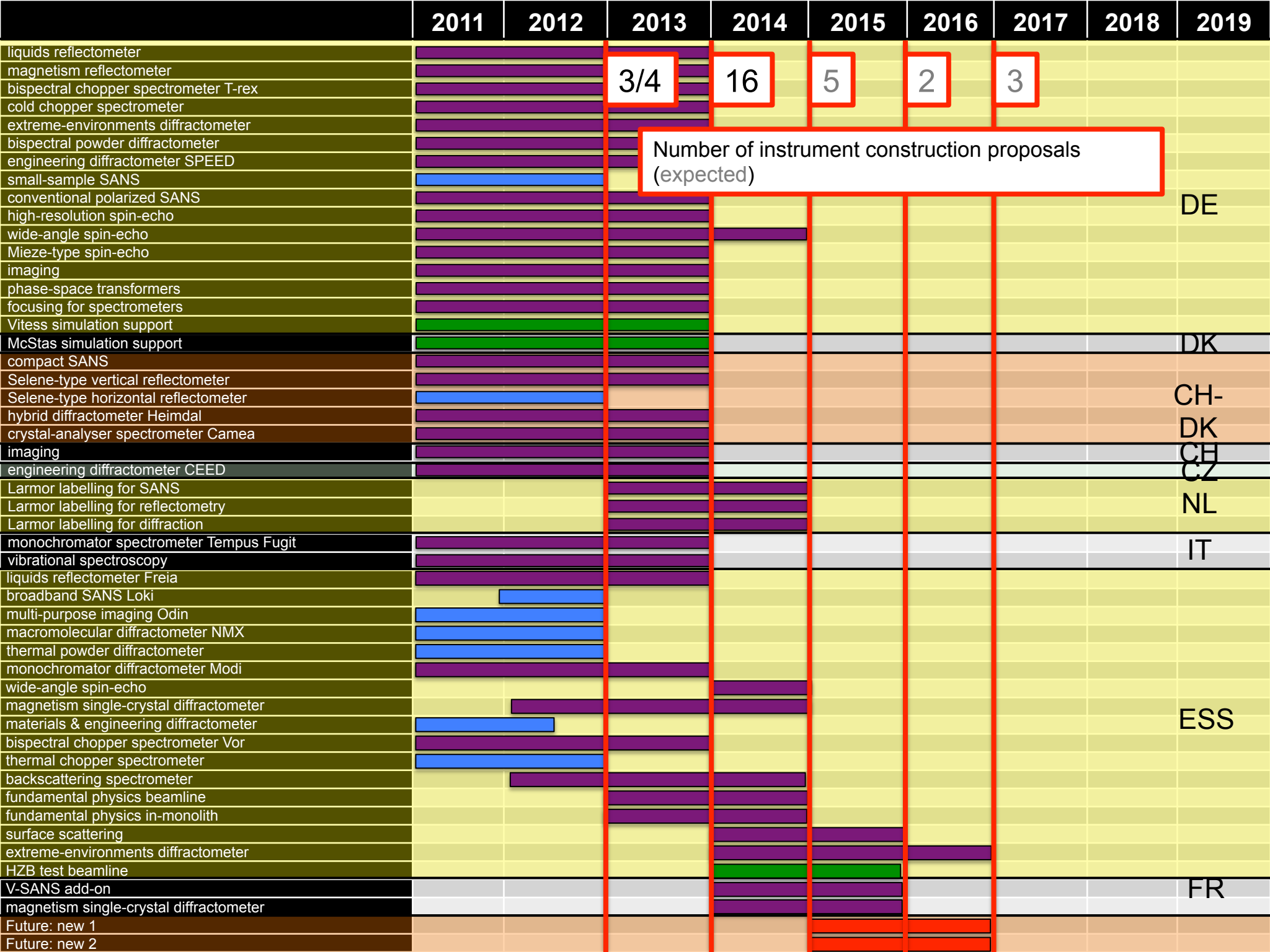
Spin Echo  
Spectroscopy

Fundamental &  
Particle Physics

Conventional SANS Skadi Full Instrument Design SD004DE/ab	Reflectometer for Liquid Surfaces and Soft Matter Thor Full Instrument Design SD003DE/a	Macromolecular Diffractometer Full Instrument Design SD036ESS	Magnetism Single Crystal Diffractom. Half Instrument Design SD060ESS	Bi-spectr. Powder Diffractometer PowHow Full Instrument Design SD003DE/b	Engineering Diffraction Half Instrument Design SD005DE/a	Multi Purp. HR Imaging 1/3 Instrument Design SD006DE	Cold Chopper Spectrom. C-SPEC Full Instrument Design SD001DE/a	Phase Space Transformers Instrument Add-on SD007DE/a	High Resolution Spin-Echo Essense Full Instrument Design SD002DE/a	Fundamental Physics Beamline Full Instrument Design SD069ESS
Small-sample SANS Design stopped SD004DE/c	Reflectometer for Magnetic Layers Full Instrument Design SD003DE/b		Magnetism Single Crystal Diffractom. Half Instrument Design SD066FR	Multi-Purpose Extreme Environ. Diffractometer Full Instrument Design SD008DE	CEED Half Instrument Design SD033CZ	Larmor Labelling in Imaging Instrument Add-on SD056NL	Bispectral Chopper Spectrometer VOR Full Instrument Design SD001DE/b	Crystal-Analys. Spectrometer CAMEA Full Instrument Design SD016DC	Wide Angle Spin-Echo Full Instrument Design SD002DE/b	Fundamental Physics In-Monolith Full Instrument Design SD069ESS
Larmor labelling in SANS Instrument Add-on SD054NL	Selene-Focusing Vertical Reflectom. Estia Full Instrument Design SD017DC/a			Hybrid Diffract. Heimdal Full Instrument Design SD019DC	Hi Flex. Mat. & Engin. Diff. Full Instrument Design SD059ESS	Multi Purp. HR Imaging 1/3 Instrument Design SD028CH	Bispectral Chopper Spectrom. T-REX Full Instrument Design SD064ESS	Backscattering Spectrometer Half Instrument Design SD039ESS	NRSE Full Instrument Design SD007DE/b	N-Nbar Oscillation Beamline Not covered
Compact SANS Full Instrument Design SD018DC	Selene-Focusing Horiz. Reflectom. Design stopped SD017DC/b			Thermal Powder Diffractometer Design stopped SD035ESS	Irradiation Beamline Not covered	Multi Purp. HR Imaging 1/3 Instrument Design SD040ESS	Crystal Monochrom. Spectrometer Tempus Fugit Full Instrument Design SD001DE	Backscattering Spectrometer Half Instrument Design SD068DK	Focusing Optics Instrument Add-on Full DU, SD007DE/c	Neutrino Physics Beamline Not covered
Broadband SANS Loki Full Instrument Design SD062ESS	Freia Horizontal Reflectometer Full Instrument Design SD034ESS			Pulsed Monochr. Powder Diffract. Modi Full Instrument Design SD037ESS			Versatile Multispectral TOF Spectrometer Full Instrument Design SD001DE	Vibrational Spectrometer Full Instrument Design SD061TT		
VSANS/GISANS Instrument Add-on SD065FR	Larmor Labelling in Reflectometry Instrument Add-on SD055NL			Larmor Label. in Diff. (TOFLAR) Instrument Add-on SD057NL			Thermal Chopper Spectrometer Full Instrument Design SD038ESS/a	Q -- TAS Farm Full Instrument Design SD062ESS Not covered		
Simulation software development, general simulations, supporting GER simulations, VITESS SD015DE										
General simulations, in-house supporting simulations, interface moderator-beam extraction, McStas SD022DK										

Blue = Stopped  
Red = Not Covered

Yellow = Proposed 2013-14



# Science Support Systems

Arno Hiess  
Head of Scientific Activities Division

[www.europeanspallationsource.se](http://www.europeanspallationsource.se)

Update January 2014

# Scope and Requirements

## Science Support Systems

Management  
Administration

Science Coord.  
& User Office

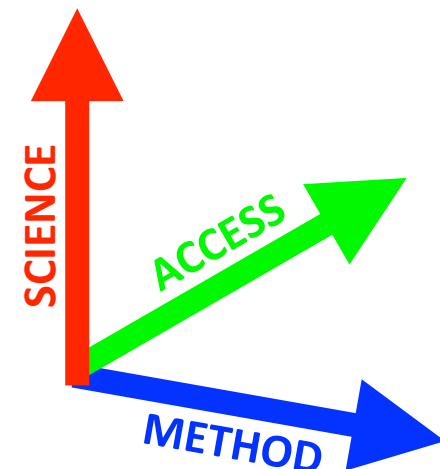
Sample  
Environment

Laboratories  
and Facilities

ESS will provide experimental possibilities for **research** using **neutrons** to **users** from both academia and industry.

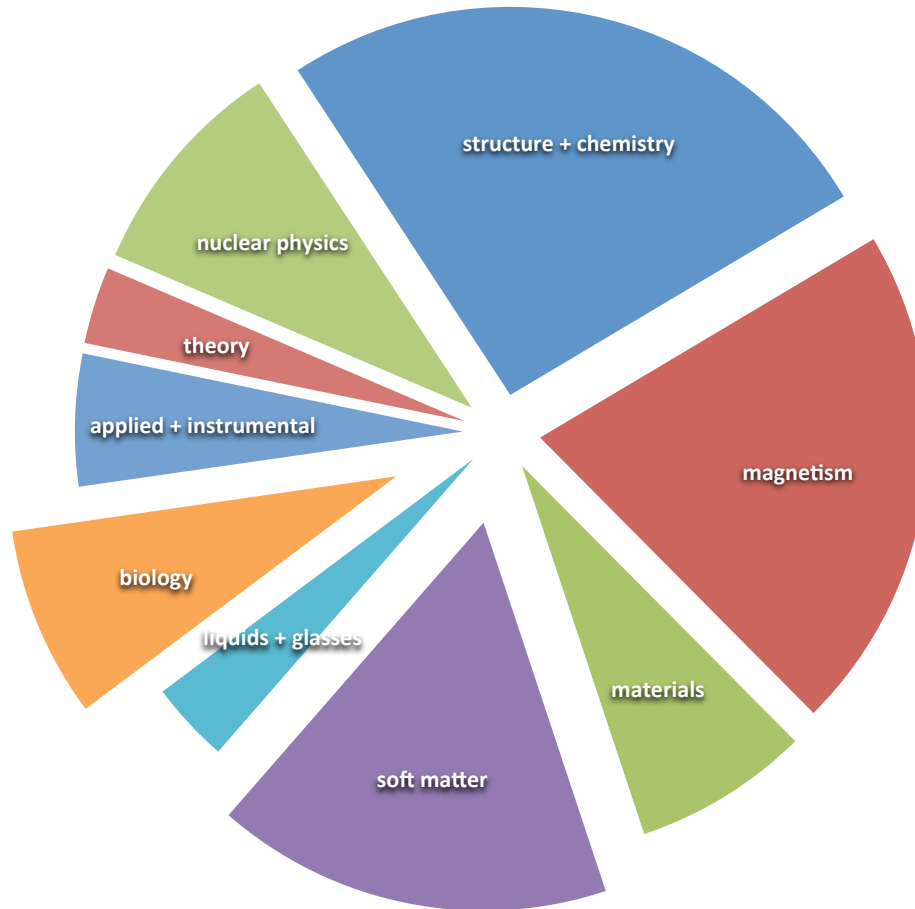
**‘Scientific Support Systems’** will deliver the scientific and technical environment supporting the **needs for the user program**. Enabling **research** using **neutrons** adds value to the facility by providing

- **‘scientific coordination & user office’**
- **‘sample environment’** and
- **‘support laboratories’.**



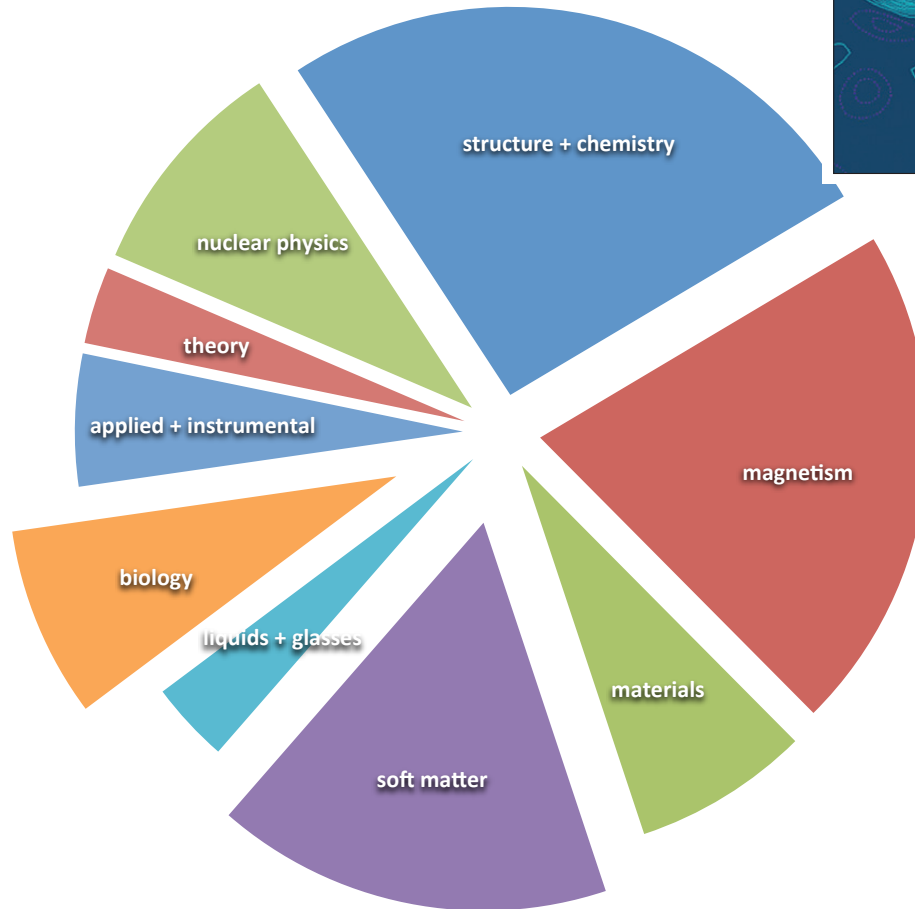
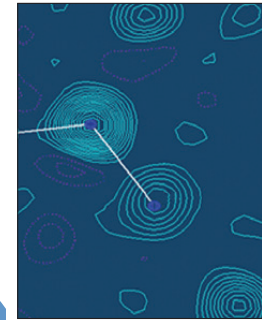


# Science Topics Today



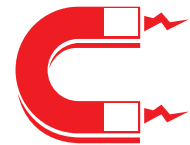
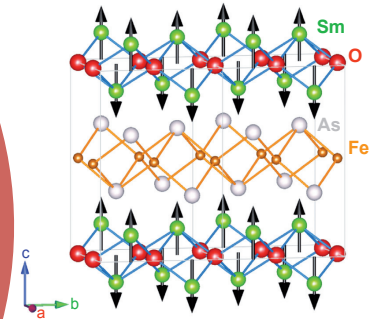
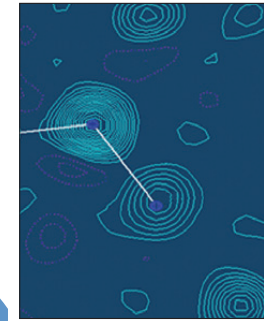
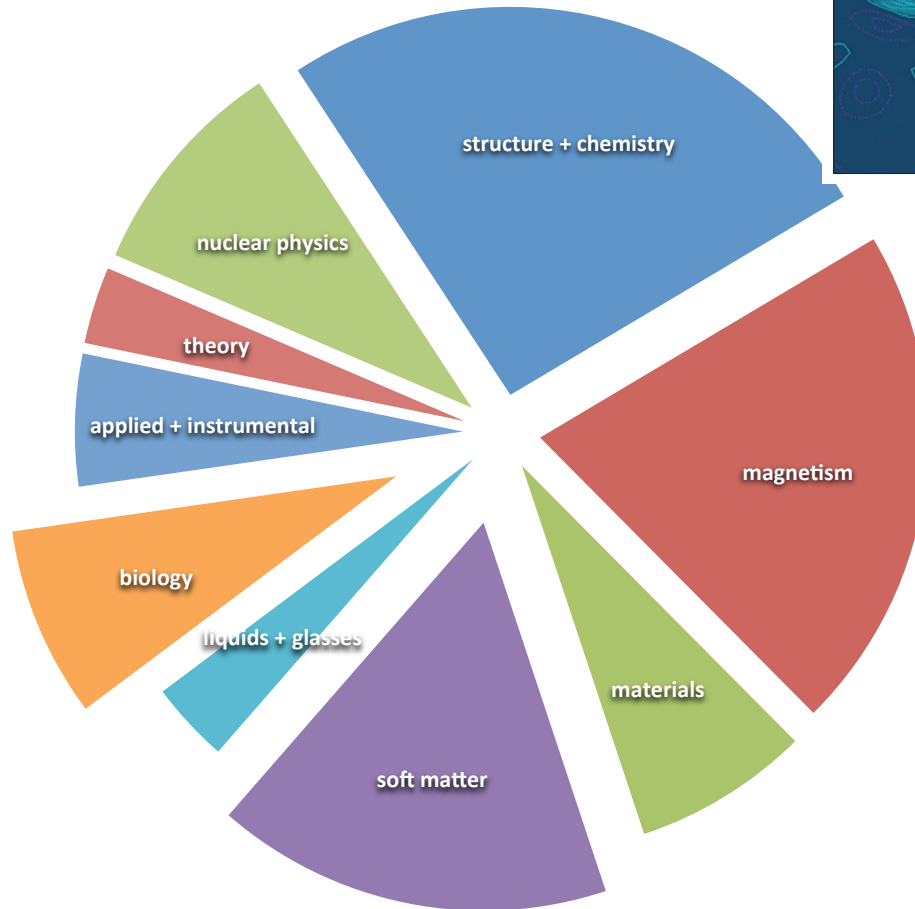
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# Science Topics Today



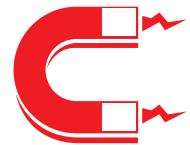
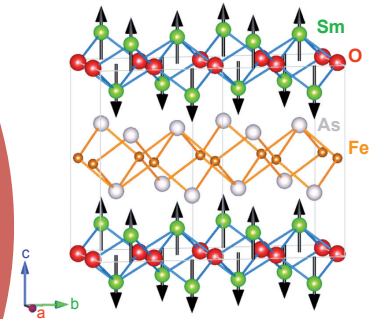
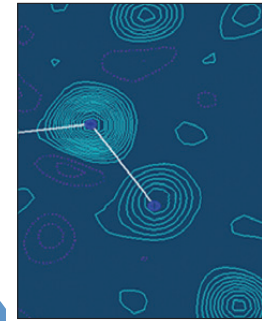
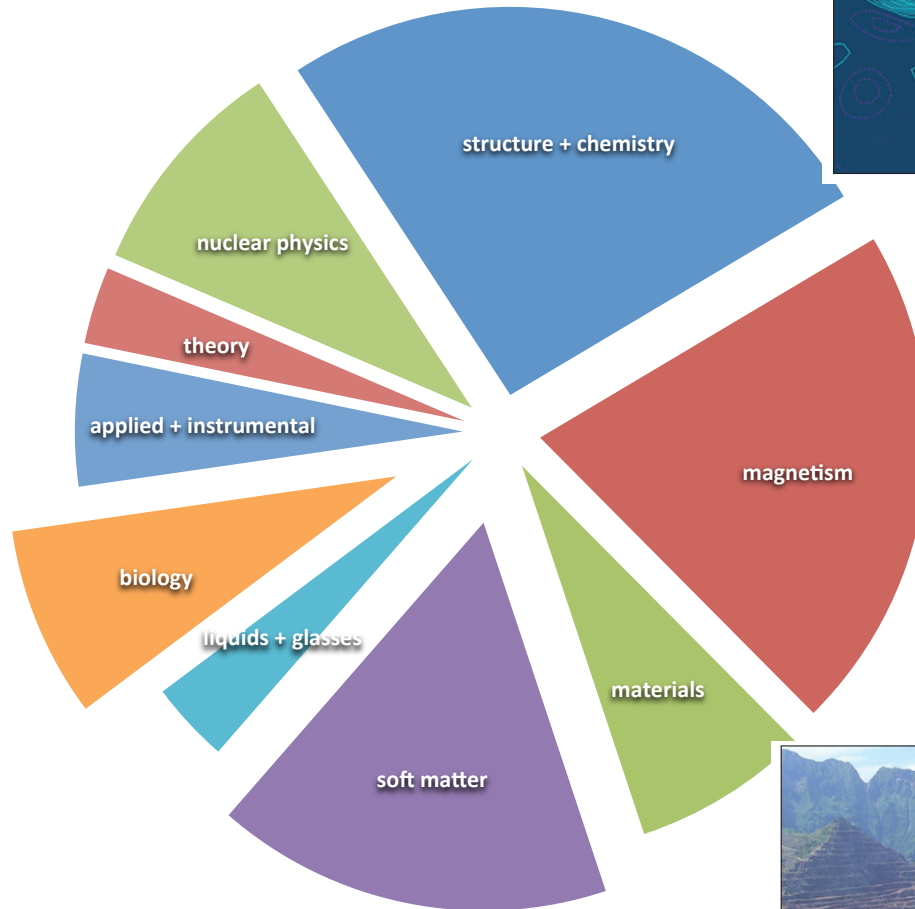
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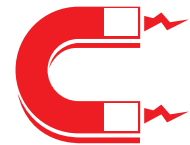
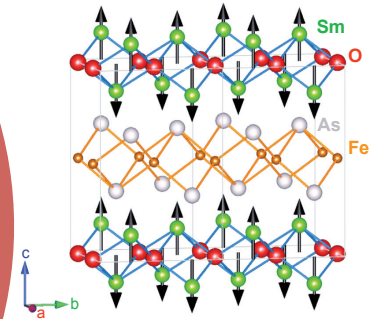
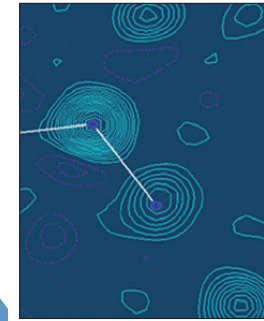
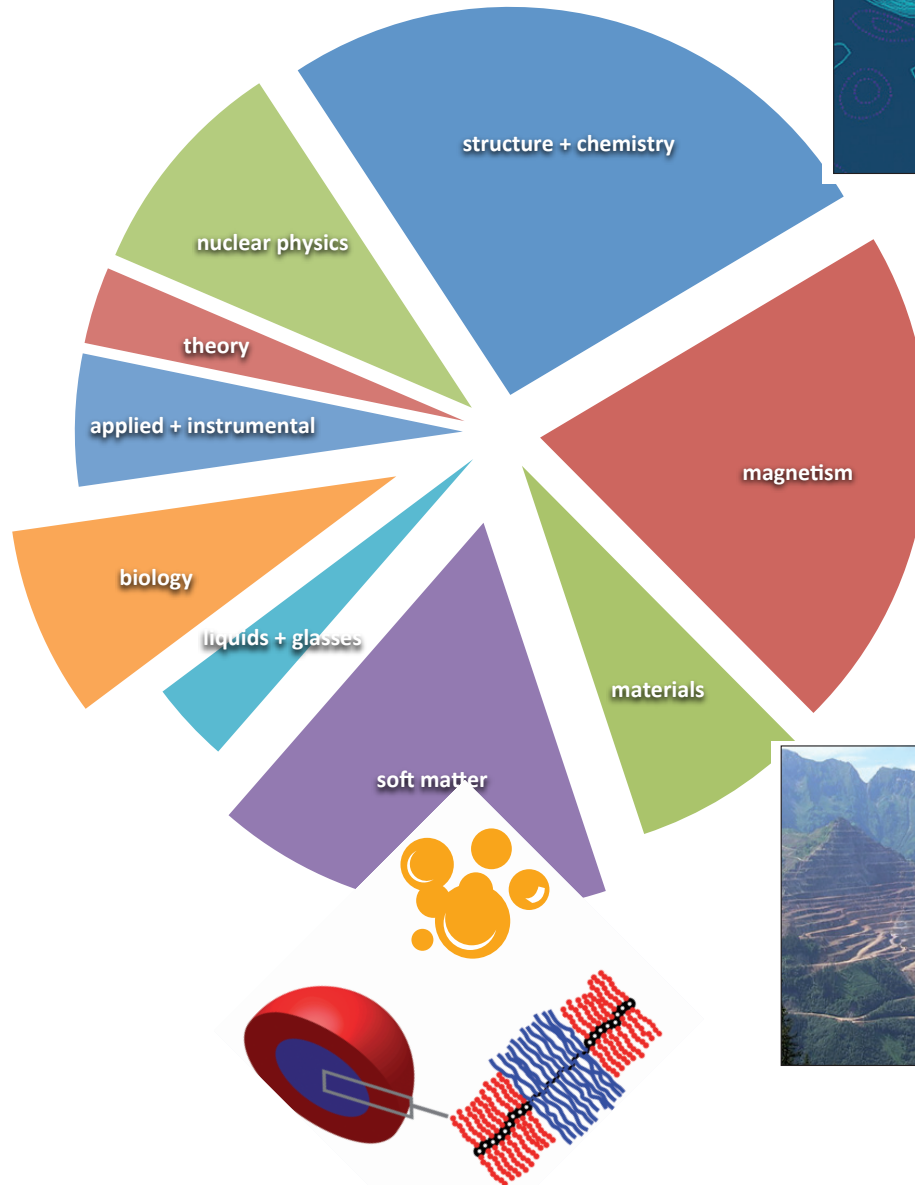
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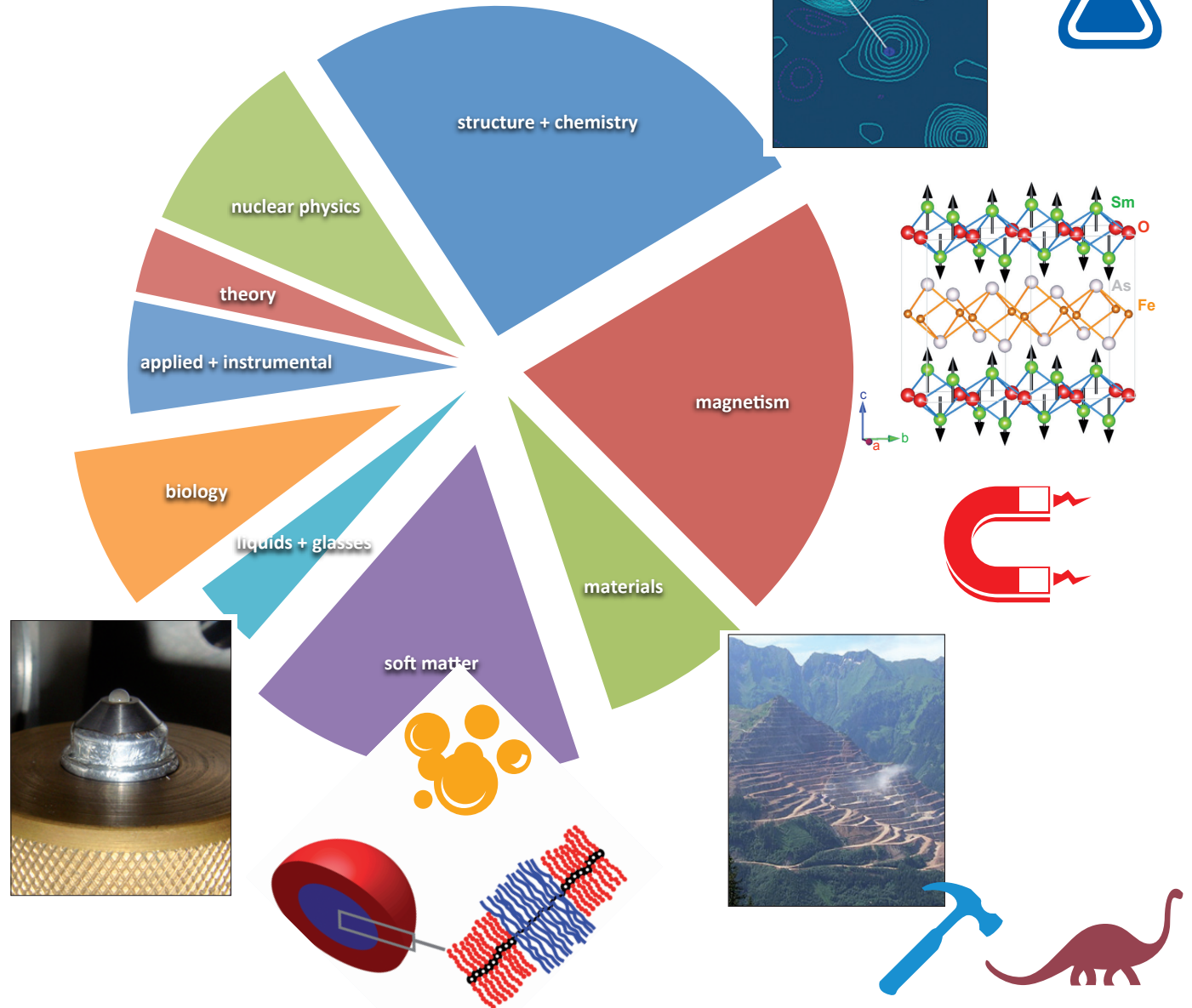


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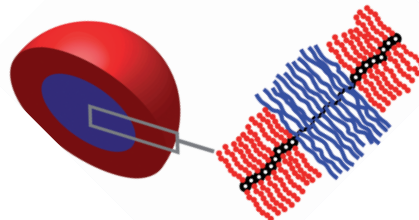
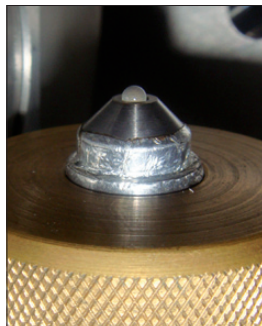
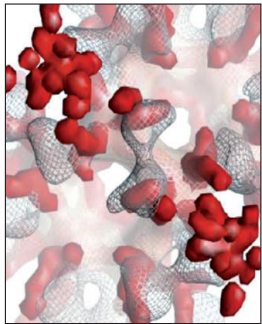
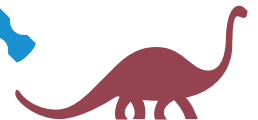
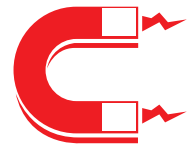
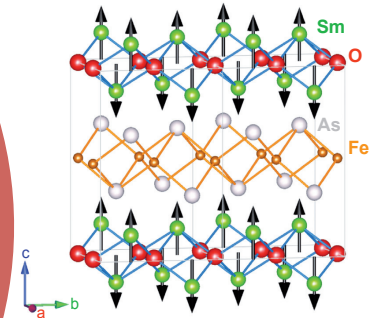
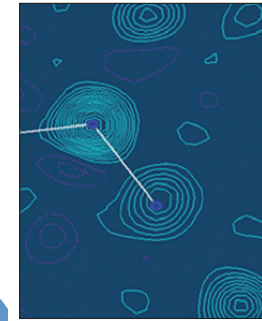
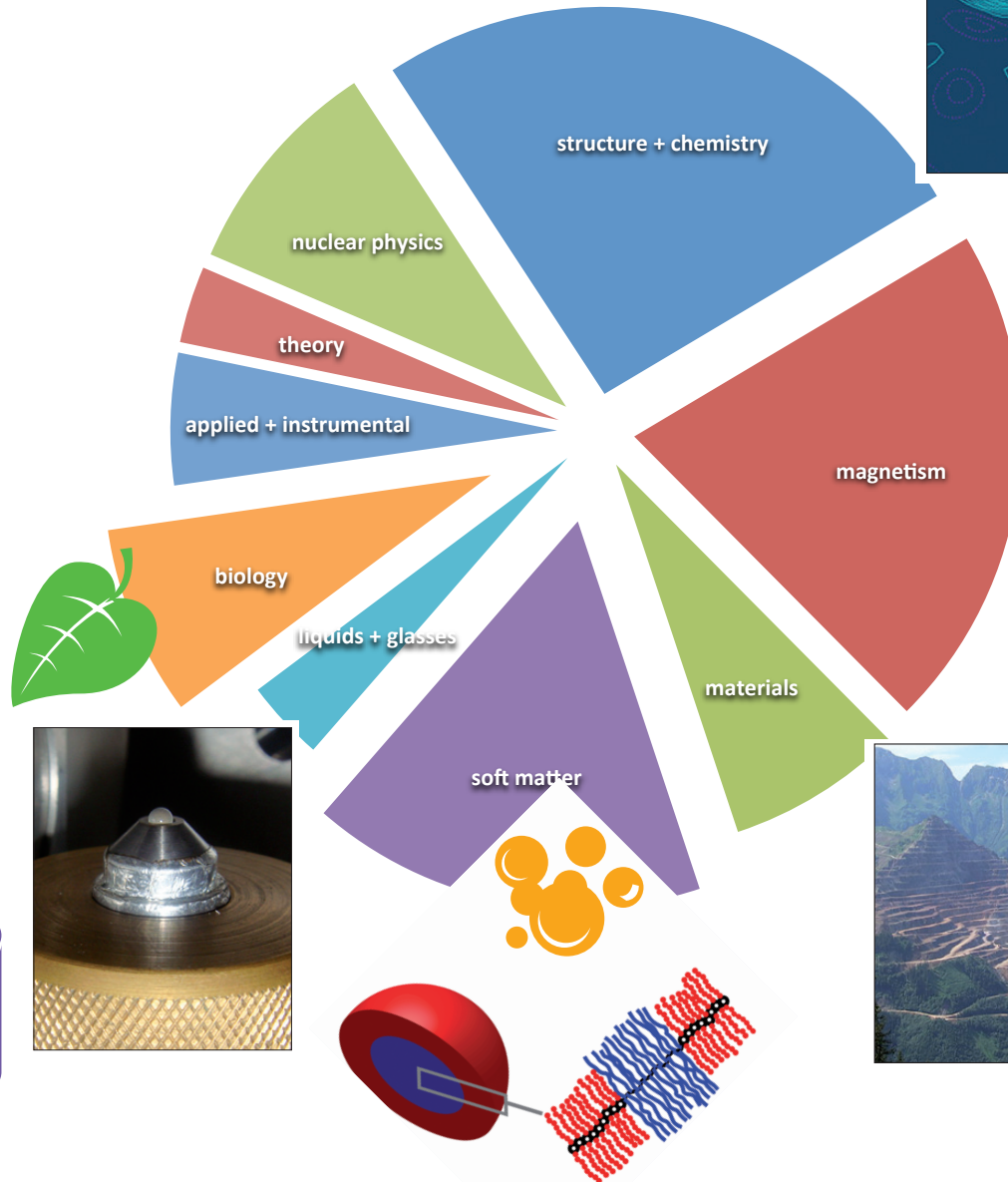


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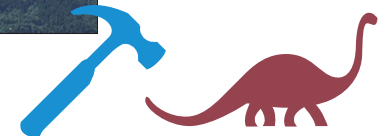
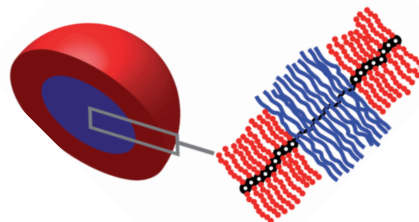
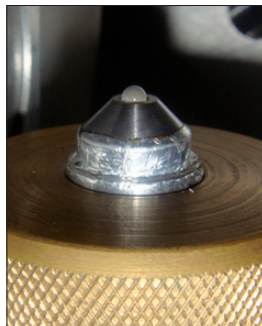
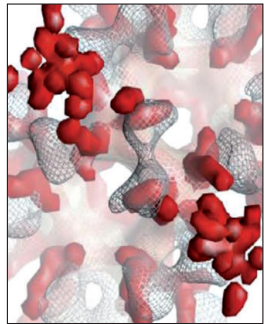
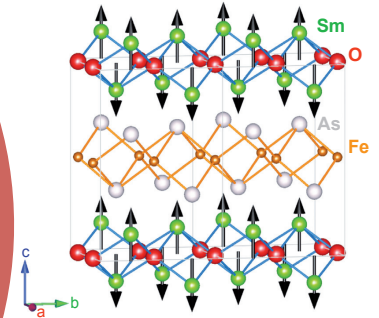
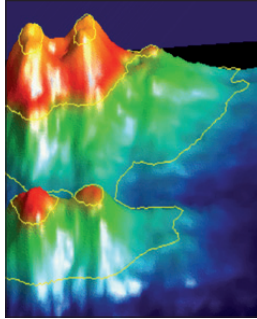
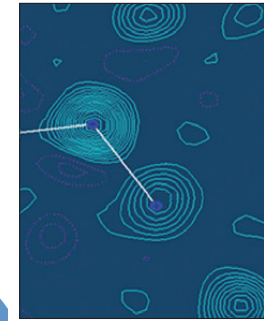
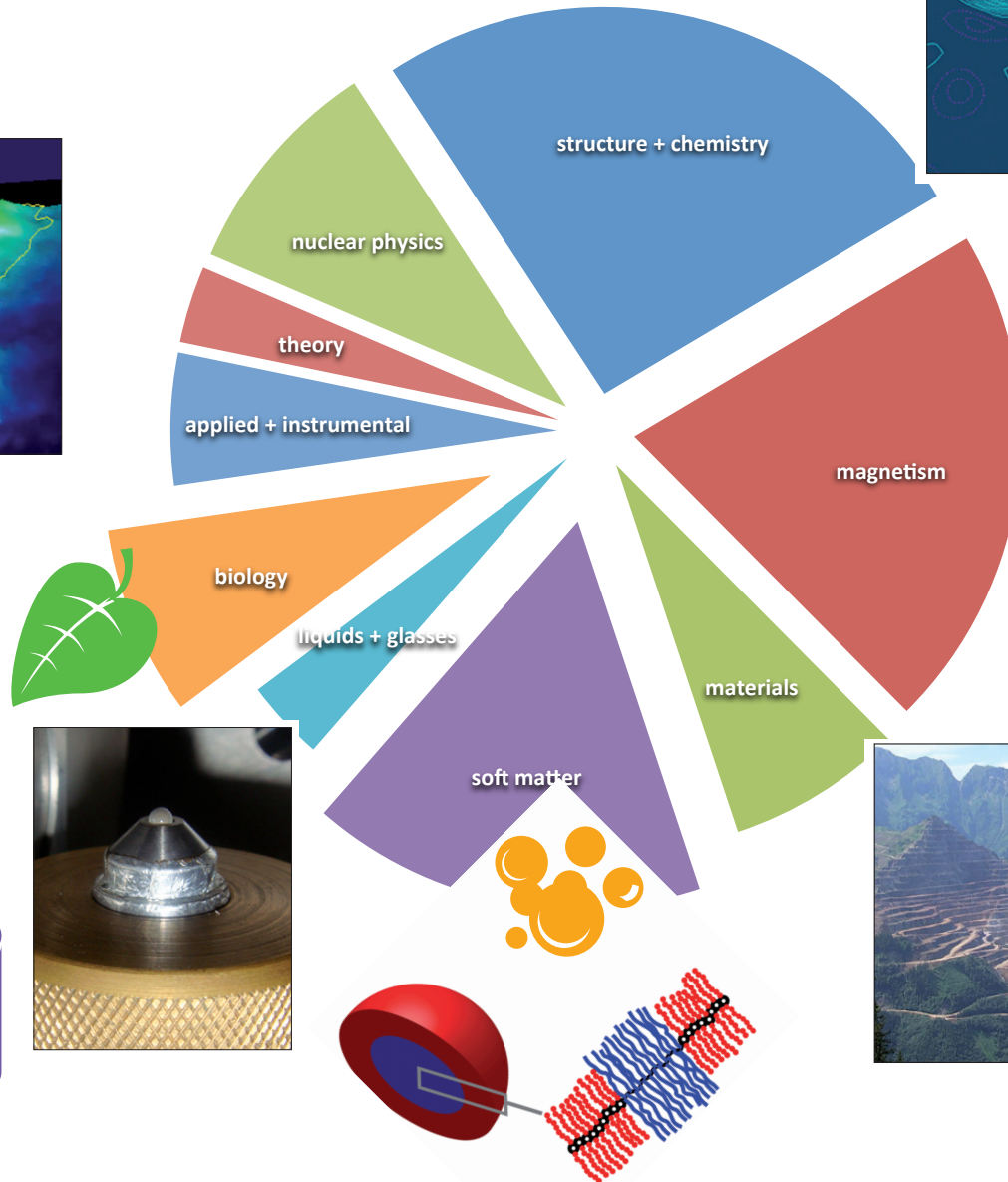


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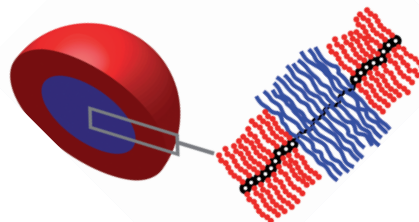
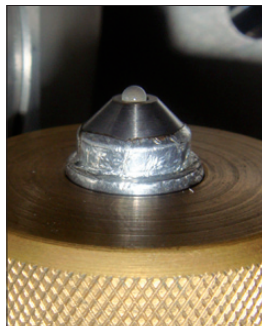
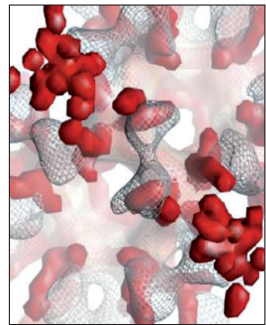
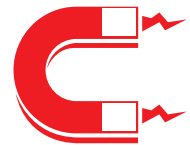
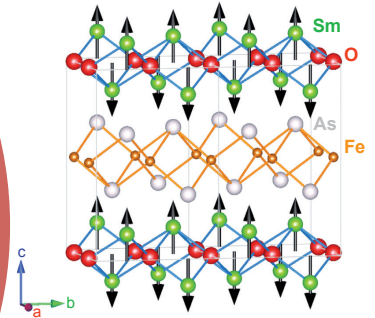
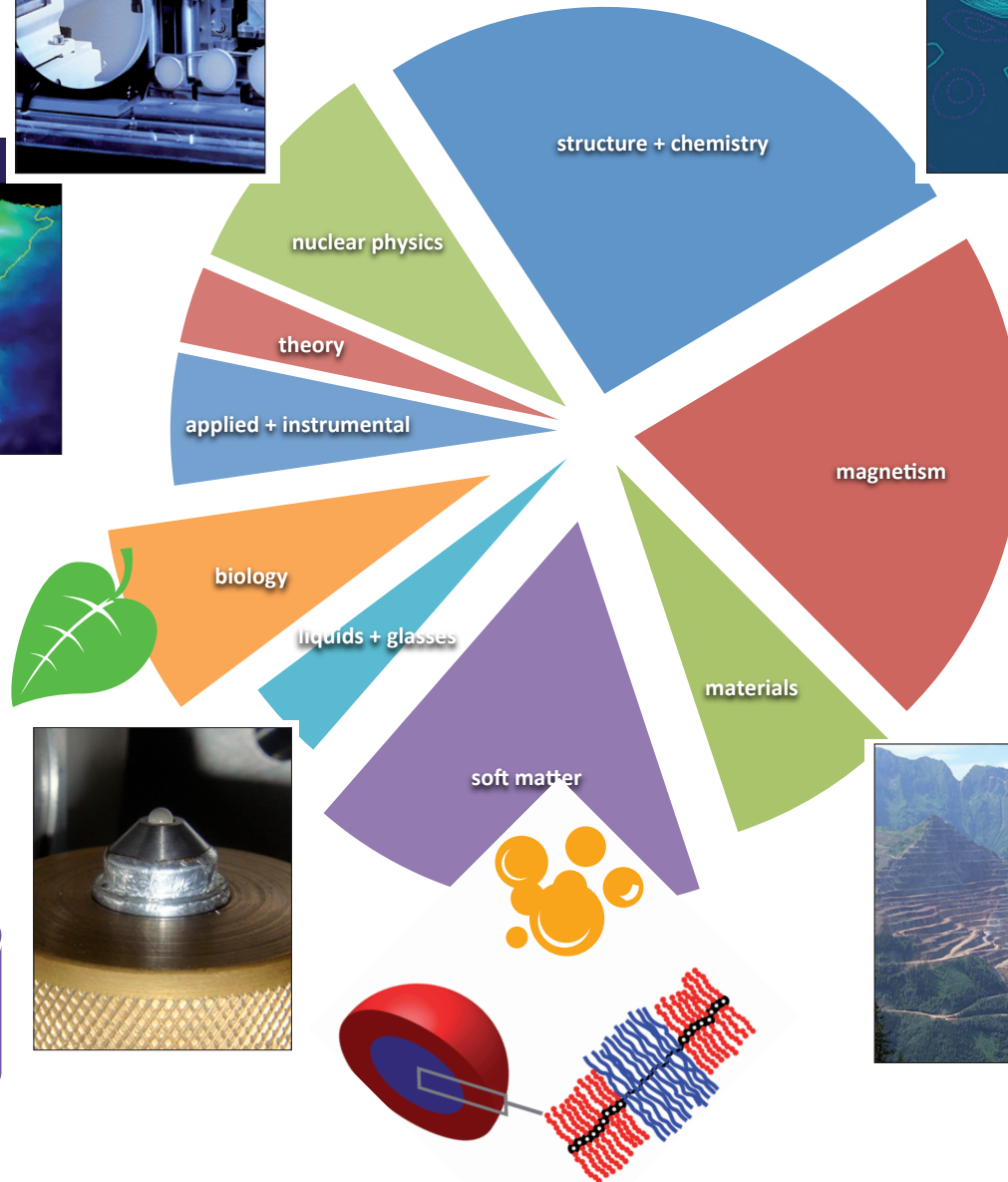
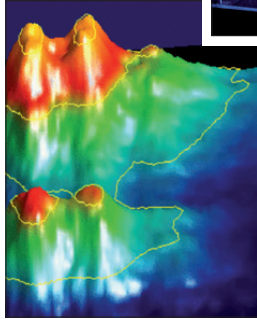
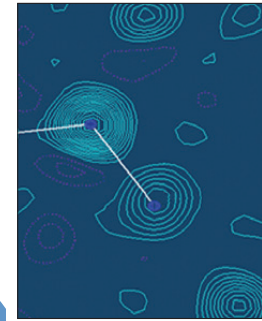
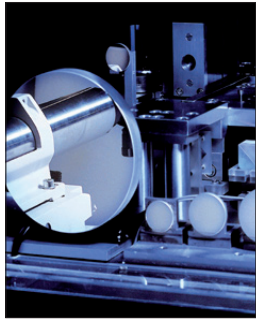
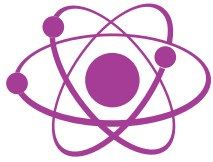
# Science Topics Today



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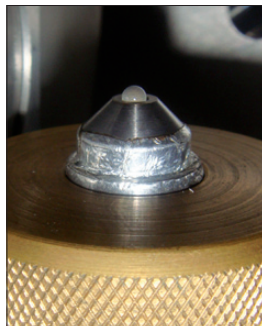
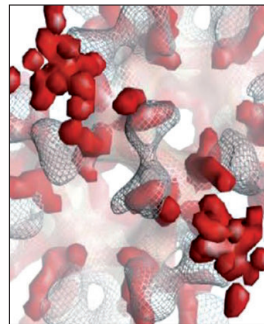
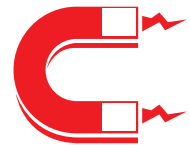
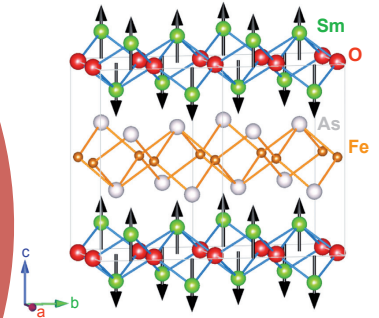
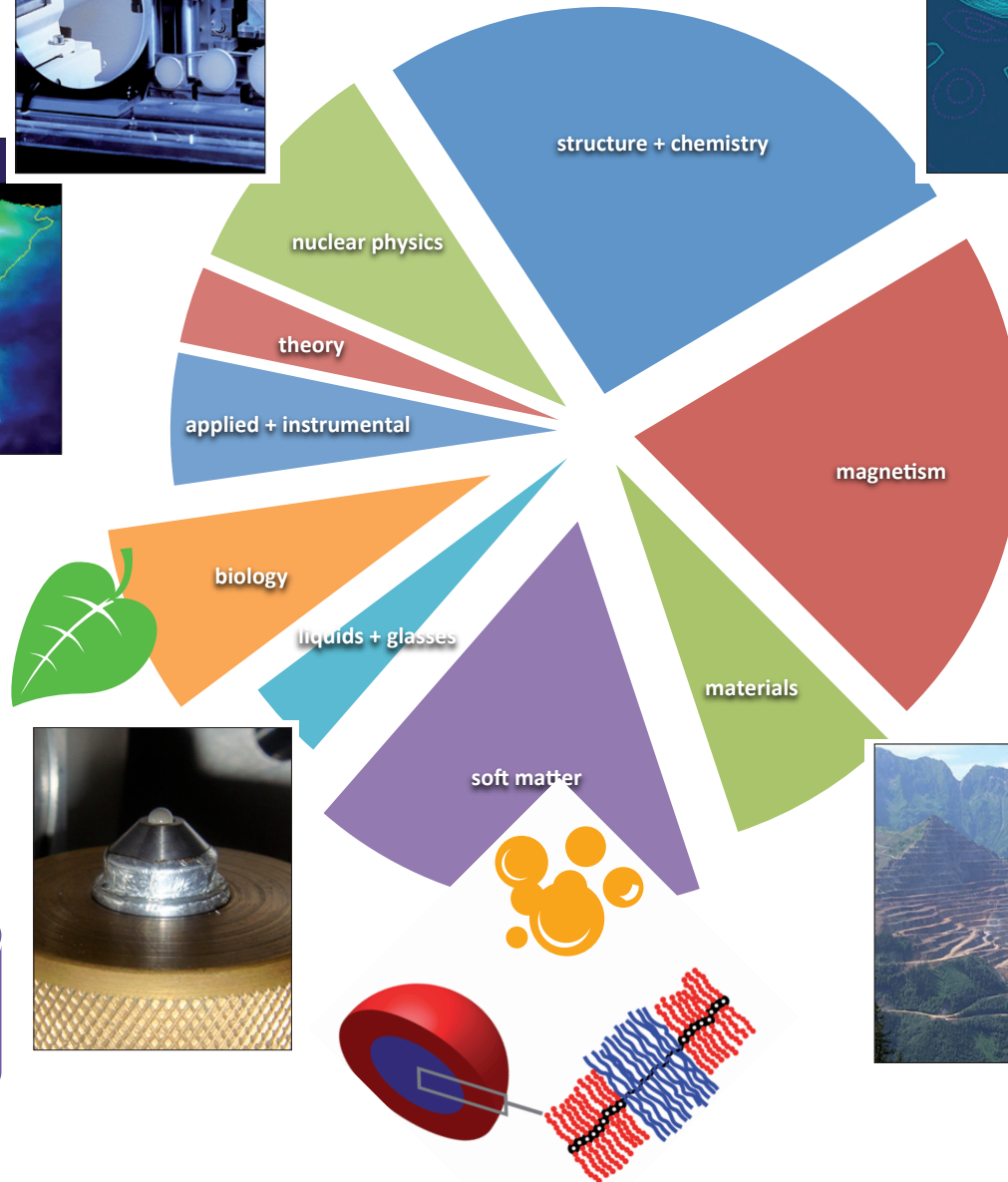
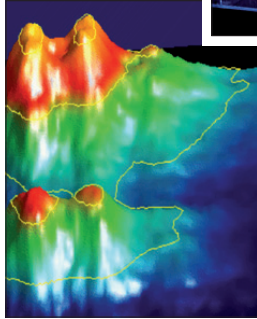
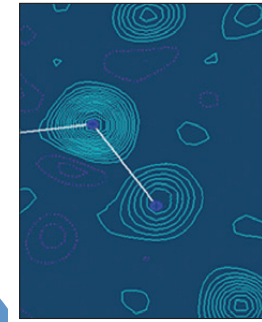
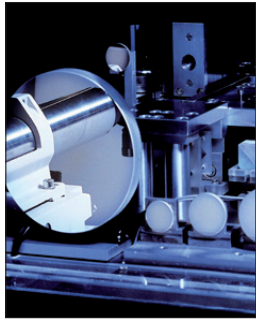
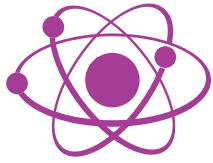


# Science Topics Today



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# Science Topics Today



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# Reference Instrument Suite: Science Drivers

Multi-Purpose Imaging



General-Purpose SANS



Broadband SANS



Surface Scattering



Horizontal Reflectometer



Vertical Reflectometer

Thermal Powder  
DiffractometerBispectral Power  
DiffractometerPulsed Monochromatic  
Powder DiffractometerMaterials Science  
DiffractometerExtreme Conditions  
InstrumentSingle-Crystal Magnetism  
DiffractometerMacromolecular  
Diffractometer

Cold Chopper Spectrometer

Bispectral Chopper  
SpectrometerThermal Chopper  
SpectrometerCold Crystal-Analyser  
Spectrometer

Vibrational Spectroscopy

Backscattering  
Spectrometer

High-Resolution Spin-Echo



Wide-Angle Spin-Echo

Fundamental & Particle  
Physics

life sciences



soft condensed matter



chemistry of materials



energy research

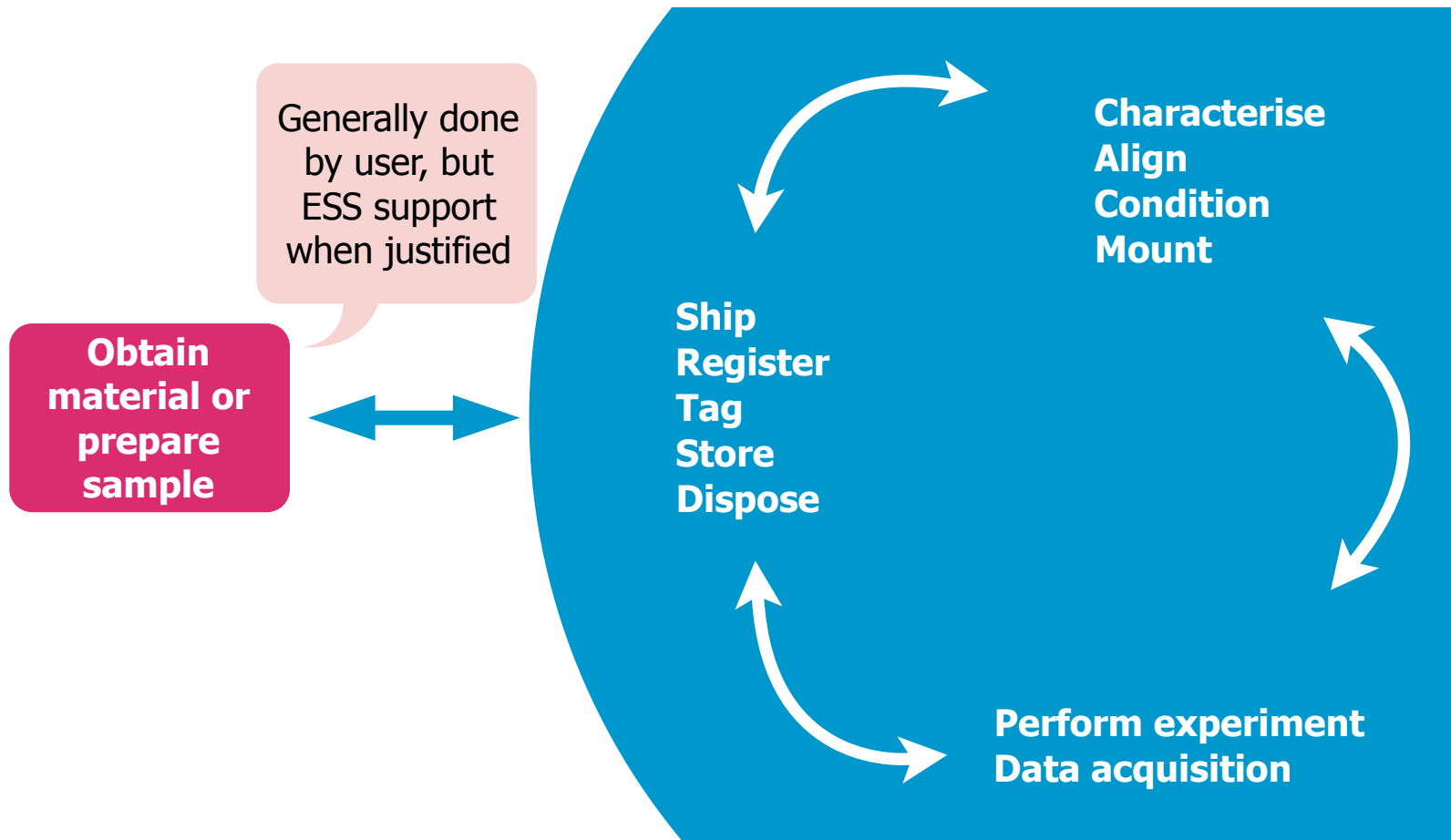
magnetism &  
superconductivity

engineering &amp; geo-sciences

archeology & heritage  
conservationfundamental & particle  
physics

# Sample Flow for Successful Experiments

Set-up common support platforms (laboratories and sample environment) to meet the needs for successful experiments. Enable users to perform their science.





# Organisation and Staffing (2014)

## Science Support Systems

### Management Administration

details	Management and administrative support
staff	A. Hiess (HoD), B. Linnenberg (Assist.), <i>advisors</i>
timeline	started; to ops in 2020









### Science Coord. & User Office

TDR2.6.1	Science focus areas, community, user office,
staff	C. Theroine (PD Fund), ' <i>scientist basket</i> ', PhD
timeline	started; to ops in 2020

### Sample Environment

TDR2.7.4	temp, fields, pressure, gas, changer, atm, surf
staff	NNEngineer(mechatronics); NNScientist(T,B)
timeline	start 2014, Phase1 to 2019, Phase2 to 2023

### Laboratories and Facilities

TDR2.6.ff	labs        
staff	M. Everett (Lab), Z. Fisher (xtalo), NN (hi-p)
timeline	start 2014, Phase1 to 2019, Phase2 to 2023

# Details Science Coordination and User Office

**Science  
Support  
Systems**

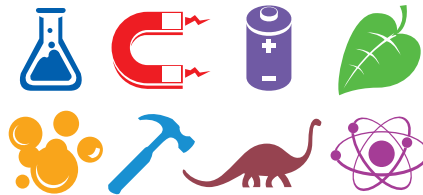
**Management  
Administration**

**Science Coord.  
& User Office**

**Sample  
Environment**

**Laboratories  
and Facilities**

**Science Focus  
Areas**



**Community  
Interaction &  
industrial R&D**


**User Office**


details	environment for ESS scientists local seminars, lectures incl. fund physics with target / acc.
strategy	invited scientists, attract speaker
interface	all Science, Target/Acc (fund)
details	symposia, conferences, seminars schools, lectures, partner days
strategy	exchange ESS scientists, partners
interface	Communications
details	set-up user office, on-site visits
strategy	standardise with other facilities
interface	software by DMSC, Admin.

# seminars, workshops, symposia

- IKON: meetings of in-kind collaboration on Instrument Construction
- Science Symposia: 16 symposia exploring the ESS scientific possibilities
- ESS - SFT seminars: internal ESS seminars covering various science topics
- NewScience Seminars: topical seminars organised jointly with LU and MaxIV.







Seminar series on New Science  
Research Opportunities with Neutrons  
and Synchrotron X-Ray Radiation

**Understanding the anisotropic water dynamics  
in clays by coupling QENS and MD**

The study of the anisotropic transport properties in clays, which are a main component of soils, is crucial for environment and industry. Indeed clays are used as barriers for radioactive waste and CO<sub>2</sub> storage in aquifers. The analysis of the dynamics of water in these materials is of crucial importance, and has been determined by means of Quasi Elastic Neutron Scattering (QENS) in several clay systems. The analysis of the experimental results, however, are often done without accounting for the distinctive features of transport in these lamellar negatively charged aluminosilicates (anisotropy, complex diffusion processes, etc.), and the choice of an irrelevant model of analysis can lead to erroneous interpretations. With the help of molecular dynamics simulations, which allow a description of the water-clay system at the same space and time scale (nm and ns) accessed by the neutron experiments, we show how to choose the adequate model for the relevant analysis of the experiments. The limits of this model will also be discussed in this talk.

Seminar with:  
**Prof. Virginie Marry**  
Université  
Pierre et Marie Curie, Paris

**DATE:** 24 October 2013  
**TIME:** 14h15  
**PLACE:** Chem. Dept. Lecture Hall B



Professor Virginie Marry works at the University Pierre et Marie Curie in Paris, France. She is a member of the group "Multiscale Modelling and Dynamics" of the laboratory PECSA. She studies the structure and transport properties of fluids in porous media using molecular simulations and neutron scattering.

**Hosts:** Heloisa Bordallo and Arno Hess ESS,  
Ulf Olsson LTH

# Details Sample Environment

**Science  
Support  
Systems**

**Temperature  
& Fields**

details low & high T, magn. & other fields

strategy phase 1: dry systems, std. magnet

**Management  
Administration**

**High Pressure  
& Gas handling**

details pressure cells, gas handling syst.

strategy phase 1: clamp cells, link to labs

**Science Coord.  
& User Office**

**SE Systems**



details changers, gas-vap-liquid, surface...

strategy link to Instruments; nmx, loki ...

**Sample  
Environment**

**SE Systems**



details geo science, cultural heritage

strategy link to Instruments; odin

**Laboratories  
and Facilities**

**Workshop  
Development**

details workshops, maintenance equip.

strategy link Instrument Technology team

# Sample Environment - Temperatures and Fields

- ‘Cryogen-free’ systems for low temperatures and magnetic fields
  - PTR or GMR from industrial suppliers for  $T = 2.5\text{K} - 600\text{K}$  (phase 1)
  - Re-condensing systems for  $T < 2.5\text{ K}$  and  $B > 10\text{T}$  (phase 2)
- Small devices for temperature control ( $T = 30\text{ K} - 800\text{ K}$ ) using Peltier coolers, Stirling CCR or gas flow devices integrated and adapted from suppliers. collaborations within SE@NSF FP7 network. (phase 2)
- Follow closely and collaborate for development of pulsed magnets (phase 2) and superconducting hybrids (phase 3)
- Vacuum furnaces (phase 1)  
mirror and levitation furnaces (phase 2)



# Sample Environment - Pressure

- Designs for pressure cells for gases, liquids and solids are available.
  - isostatic clamp pressure cells ( $p < 20$  kbar) (phase 1)
  - uni-axial pressure ( $p > 1$  kbar) (phase 2)
  - gas pressure (several kbar) (phase 2)
- Gas handling including Hydrogen (phase 1)
- High pressure cells (PE) require collaboration with expert groups (phase 2)
- Multi-anvil systems (phase 3)

# Sample Environment - In-situ equip, Automatisation, Life Science / Soft Matter

- In-house development of liquid handling, robotic and linear changers, surface preparation and growth, humidity control (phase 1)
- Gas/Vapor/Liquid interfaces, chemical reactions, stress strain analysis, pump-probe, kinetics, shear (phase 2)
- Load frame for engineering and geosciences with geo lab (phase 2)
- Requires integration of commercial components and SE data acquisition and processing within Instrument Control; collaboration DMSC and ICS.

# Details Laboratories and Facilities

**Science  
Support  
Systems**

**Sample Handl.  
Lab Coord.**

details coordinate MV, define on-site lab

strategy health & safety, facilities, MAX IV

**Management  
Administration**

**Deuteration  
Crystallisation**

details process macromolecular xtalo

strategy link to LU deuteration platform

**Science Coord.  
& User Office**

**Labs**



details changers, gas-vap-liquid, surface...

strategy link to instr., std. lab fitting only ...

**Sample  
Environment**

**Labs**



details charact. & pressure platf.; powder

strategy link to instr., std. lab fitting only ...

**Laboratories  
and Facilities**

**Labs**



details metrology, cultural heritage

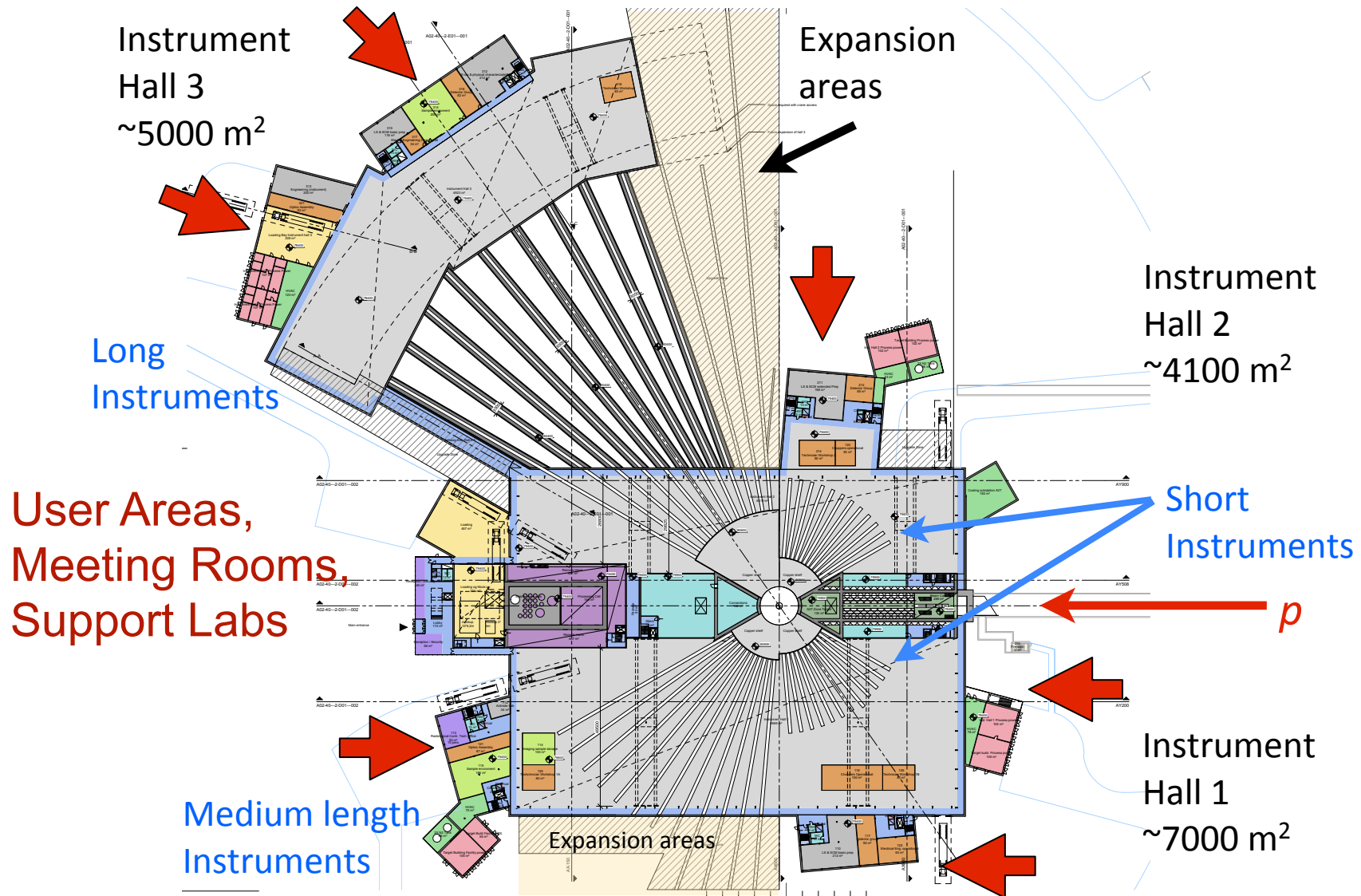
strategy link Instrument Technology team

# User Laboratories and Facilities around Experimental Halls



- 3 Life Science and Soft Condensed Matter Labs
- 3 Basic Chemistry Labs
- Extended Chemistry including glass sealing, furnaces, and thin film prep
- Engineering
- Imaging
- X-ray and Physical Characterization
- Actinide
- Coffee rooms and user lounges in each quadrant

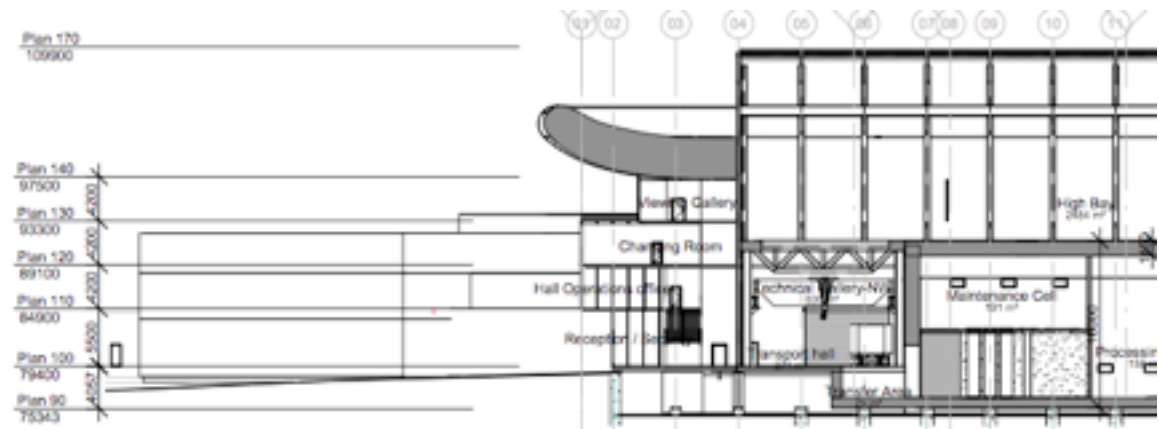
# User Areas and Support Labs in the Experimental Halls





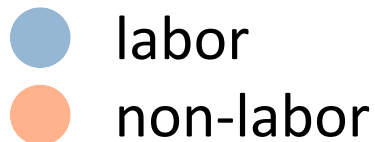
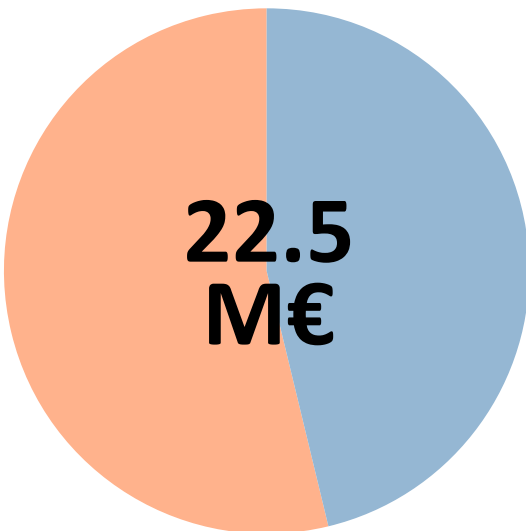
# A few construction facts

- Level 100 throughout has 5.5 m of total space leaving ~4 m of free space
- All other levels have 4.2 m of total space
- Instrument hall floor in Halls 1 and 2 is 2 m below target center line
- Instrument hall floor in Hall 3 is 3 m below target center line where most of our top loaders will be
- Crane hook height is planned to be 8.9 m in Halls 1 and 2
- Crane hook height is planned to be 6.5 m in Hall 3



# Cost Estimate

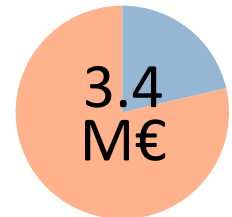
## Science Support Systems



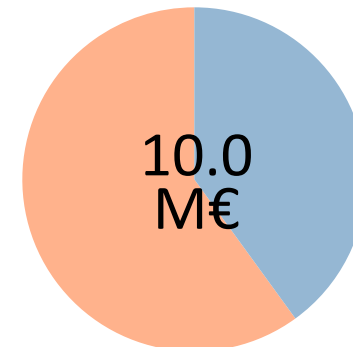
## Management Administration



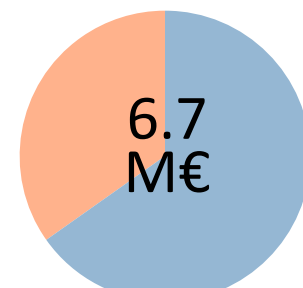
## Science Coord. & User Office



## Sample Environment

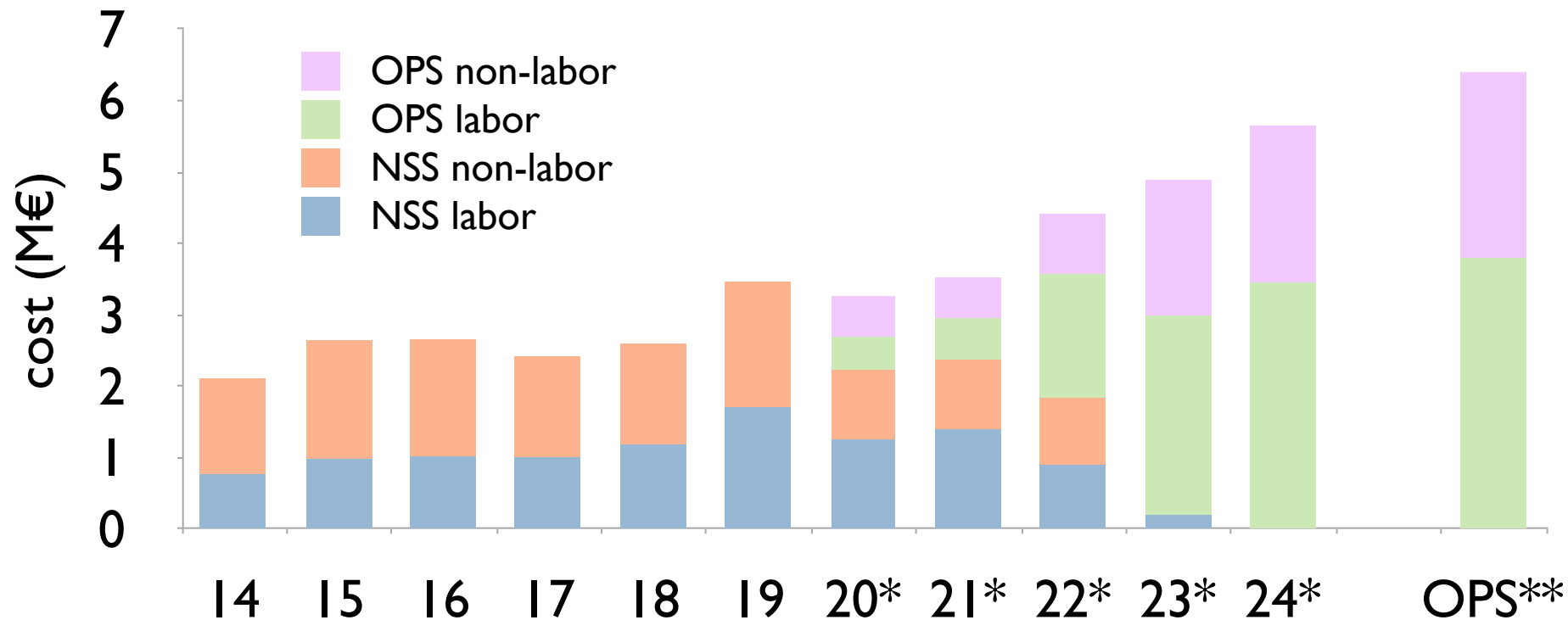


## Laboratories and Facilities



# Cost Estimate and Schedule

- Only core functionalities for first neutrons ensured by construction budget.
- Ramp up follows selected instrument (nmx, loki, odin) construction schedule.
- Additional functions for operation require external funding sources.



\* requires operational funds

\*\* without user reimbursement and PhD prg (~ 5 M€/y)

# Strategy for in-kind and additional funding



SAC February 2014

- Only core functionalities ensured by ESS NSS construction budget.
- Standard sample environment equipment and laboratory fitting potentially provided in-kind. Could involve university partners with restricted budget.
- Additional functionalities require funding outside in-kind framework. Permits leverage of budget risks during construction and operation.
- Added value for instruments and user programme by enabling users to come with their resources during operation phase.

# Summary

- Illustrated path to adequate science support during operations adding value to the instruments and ESS as a (materials) science-driven facility.
- Priorities ensuring core functionality in-line with instrument construction.
- Current team covers scientific coordination (science focus areas, community interaction and lab coordination).
- Build up core team for sample environment and support platforms to timely start in-kind partner involvement and additional funding.
- Refine interfaces to profit from opportunities.



# Data Management and Software Centre

Mark Hagen  
Head of DMSC

[www.europeanspallationsource.se](http://www.europeanspallationsource.se)

SAC Orientation February 4<sup>th</sup> 2014

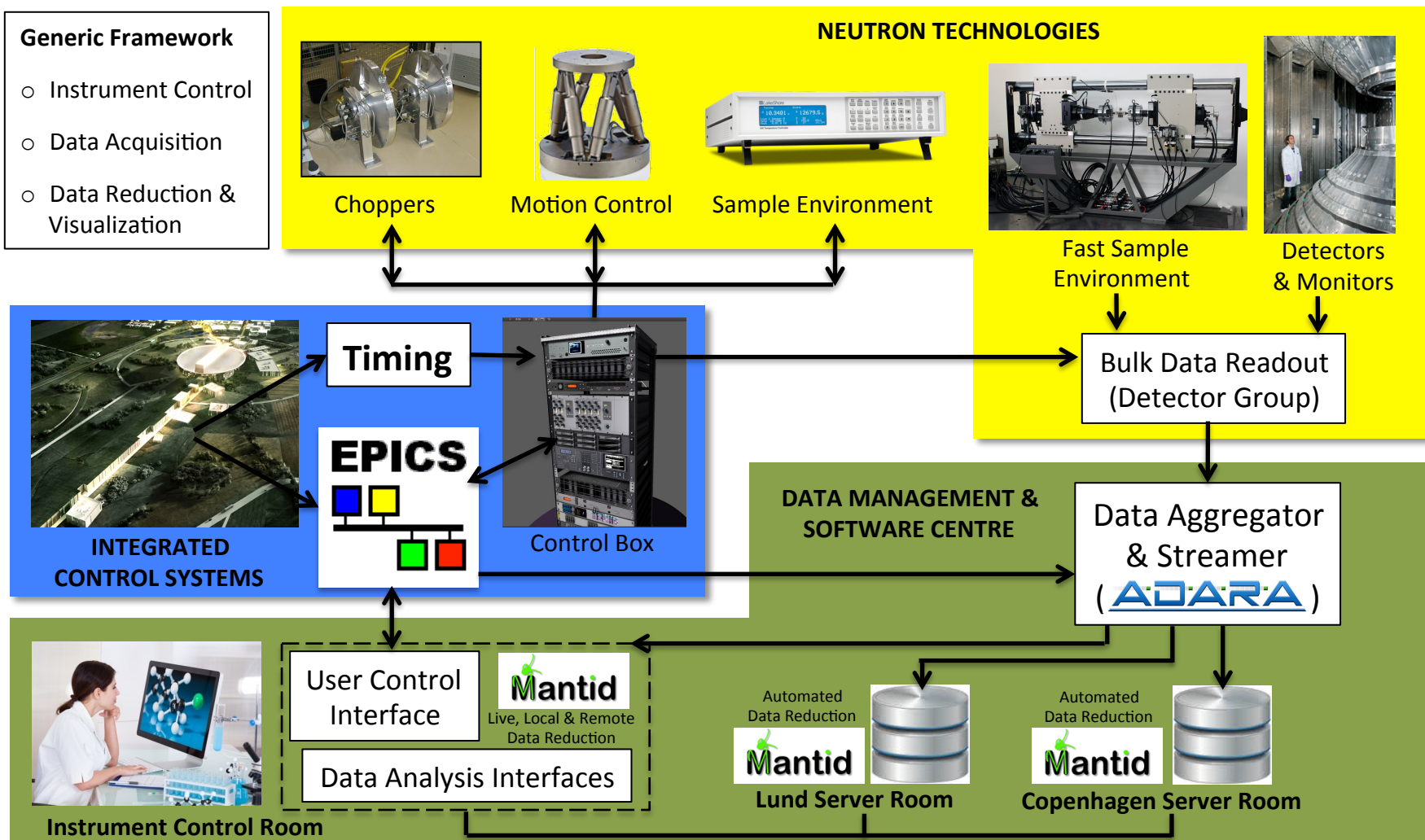
# What is DMSC ?

- Data Management and Software Centre (DMSC)
- A Division of ESS Science Directorate...
  - Just like Instrument Technologies, Neutron Instruments etc.
  - Two campuses: ESS Lund & ESS Copenhagen  
(Universitetsparken, Københavns Universitet)
  - DMSC building to be constructed in Copenhagen
- Responsibility: design, develop & implement for the ESS instruments:
  - Software (user control interfaces, data acquisition, reduction & analysis)
  - Hardware (servers, networks, workstations, clusters, disks, pfs etc.)

# Data Acquisition, Reduction & Control

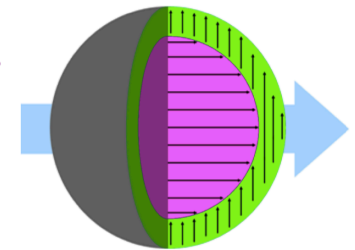
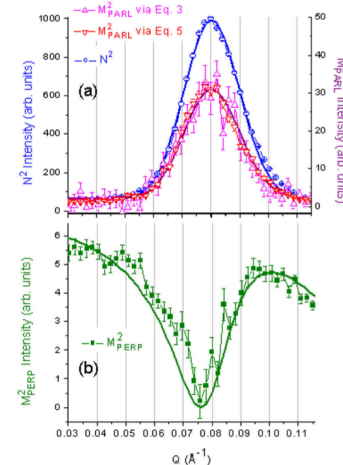
## Generic Framework

- Instrument Control
- Data Acquisition
- Data Reduction & Visualization



- Data on disk is useless!
  - It is published *results* from the data that makes progress
- Need to ensure that ESS users have access to
  - appropriate software packages for data analysis
  - the necessary computational resources to exploit the software to obtain those results
  - analysis software during experiment to influence the data taking strategies
- Roll out in-sync with instruments

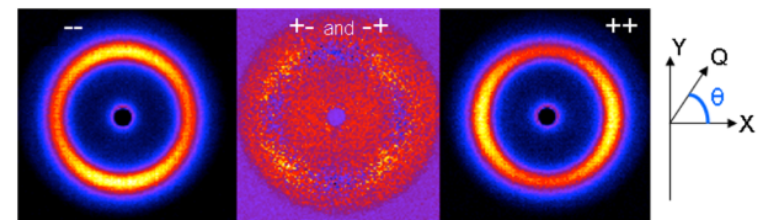
## Structure of Nanomaterials



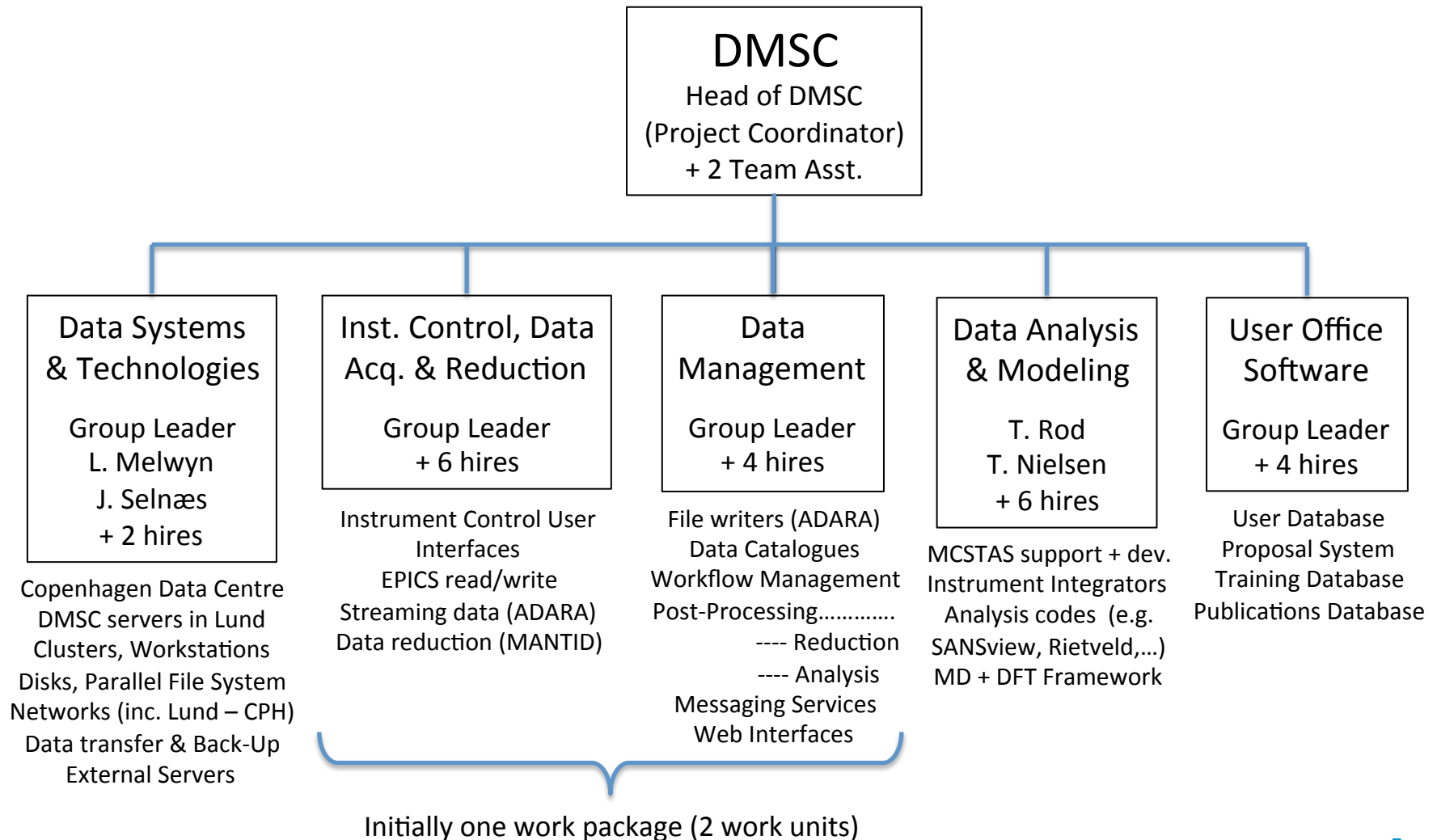
K. L. Krycka et al. **Core Shell Magnetic Morphology of Structurally Uniform Magnetite Nanoparticles**  
*PRL* **104**, 207203 (2010)

Polarized SANS demonstrated that these nanoparticles have uniform nuclear structure but core-shell magnetic structure.

Required development of both data reduction and data analysis methods and tools.



# Organization





## **Head of DMSC since Oct. 21 2013**

### **Spallation Neutron Source, USA (2004 – 2013)**

HYSPEC Inst. Scientist/Project Manager (2004 – 2011)

Inelastic Group Leader (2007 – 2011)

Data Analysis Group Leader (2010 – 2013)

### **ANSTO, Australia (2002 – 2004)**

Wombat High Intensity Powder Diff. Inst. Scientist/Project Manager  
(Echidna High Res. Pow. Diff., Taipan TAS)

### **ISIS Spallation Neutron Source & Keele Univ., U.K. (1987 – 2001)**

Physics Dept. Staff at Keele

PRISMA instrument scientist at ISIS

### **Ph.D & Post-doc**

Ph.D – University of Edinburgh (1980 – 83)

Post-docs – ILL (1984) HFIR, ORNL, USA (1985-86)



# QUESTIONS

# Instrument Technologies Division

Oliver Kirstein

[www.europeanspallationsource.se](http://www.europeanspallationsource.se)

February 4, 2014

# Who am I?

## ***Education***

- 1997 - PhD in Physics from Kiel University, Germany
- 2007 - Diploma of Business/Frontline Management, Swinburne University, Australia
- 2012 - Guest researcher at Uppsala University, Sweden
- 2013 - C/Prof at School of Engineering, Univ. Newcastle, Australia



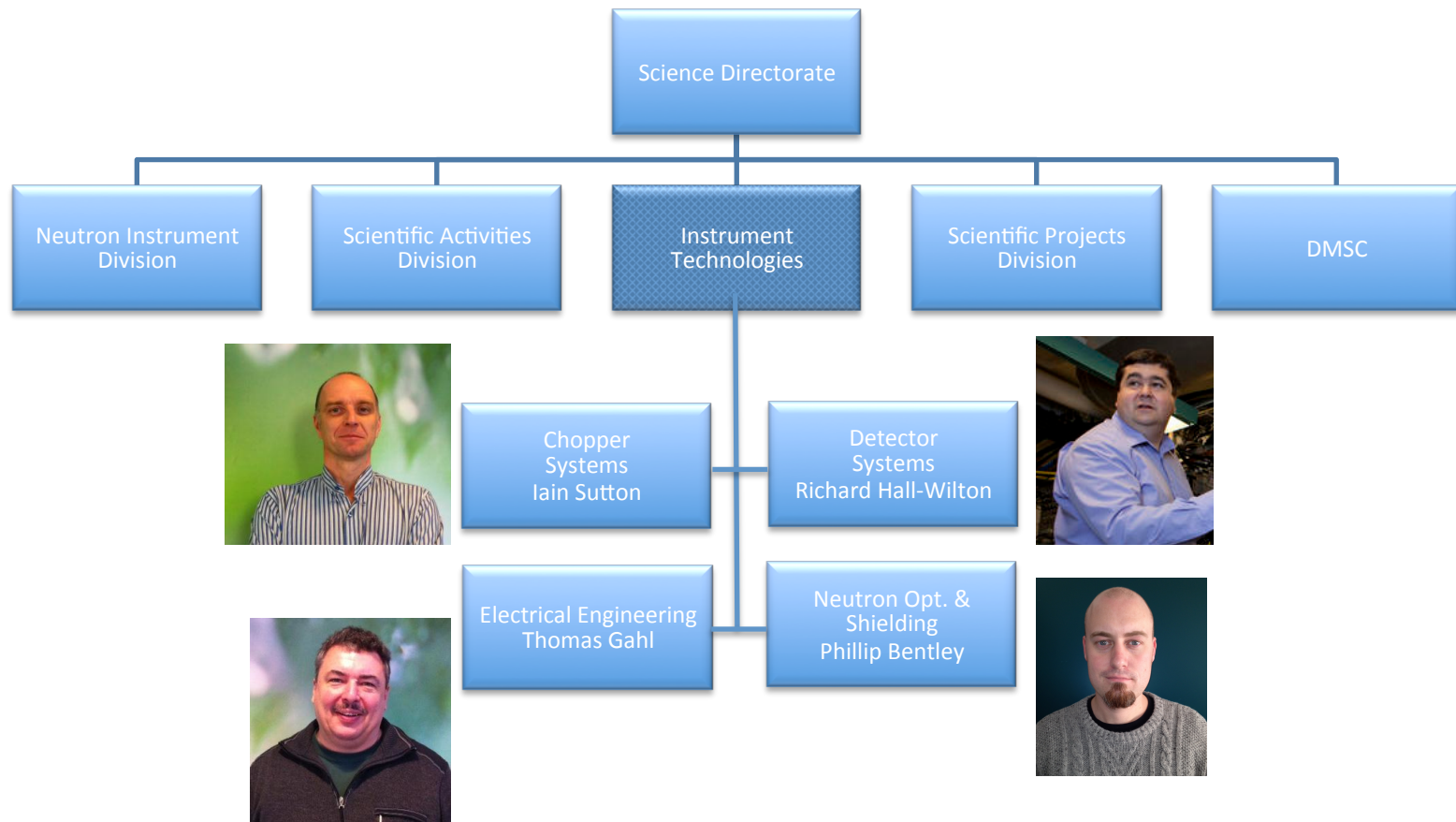
## ***Scientific projects; user operation***

- 1998 - Instrument scientist & project leader for SPHERES backscattering spectrometer at FRM-II reactor, Garching, Germany
- 2002 - Instrument scientist and project leader for the residual stress diffractometer KOWARI at the OPAL reactor at ANSTO, Sydney, Australia

## ***European Spallation Source***

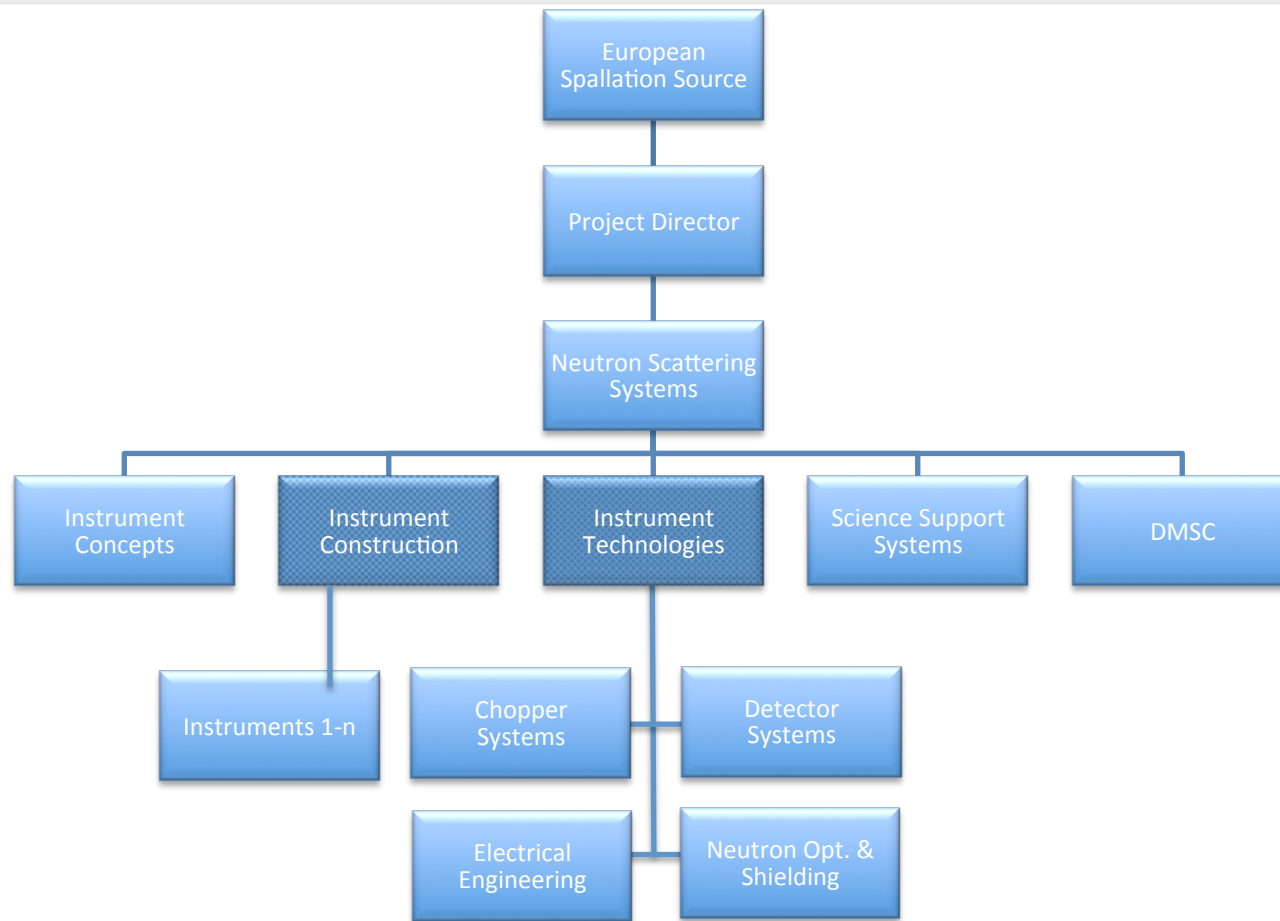
- 2002 - Member of ESS 'Indirect Geometry Instruments Group'
- 2011 - May; Head of Instrument Technologies Division - Science Directorate  
*Detector systems, Chopper systems, Neutron Optics & shielding, Electrical Engineering*
- 2012 - April; Project leader of Neutron Scattering Systems (NSS)

# Organisation - Line





# Organisation - Project

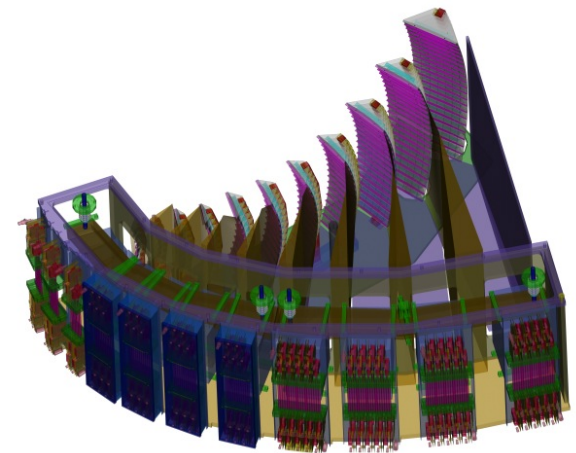
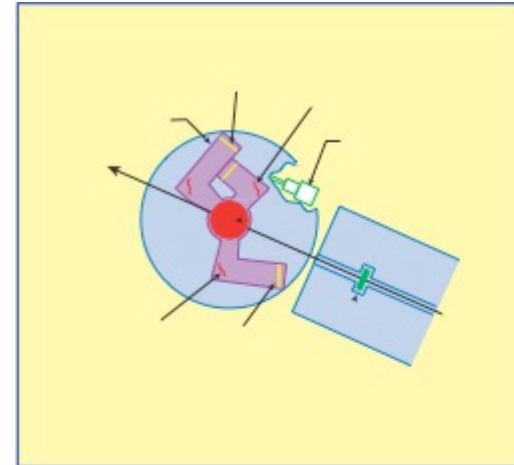


# Instrument Construction

Rob Connatser  
Head, Scientific Projects Division

# Background, Intense Pulsed Neutron Source

- Neutrons since 1998
  - Scientific Assistant on QENS at IPNS
- Managed the QENS Upgrade project
  - From three rotating analyzer arms to 22 stationary arms
- Supported users & experiments



# Background, Spallation Neutron Source



- 2004-2012
- Instrument Construction & Installation

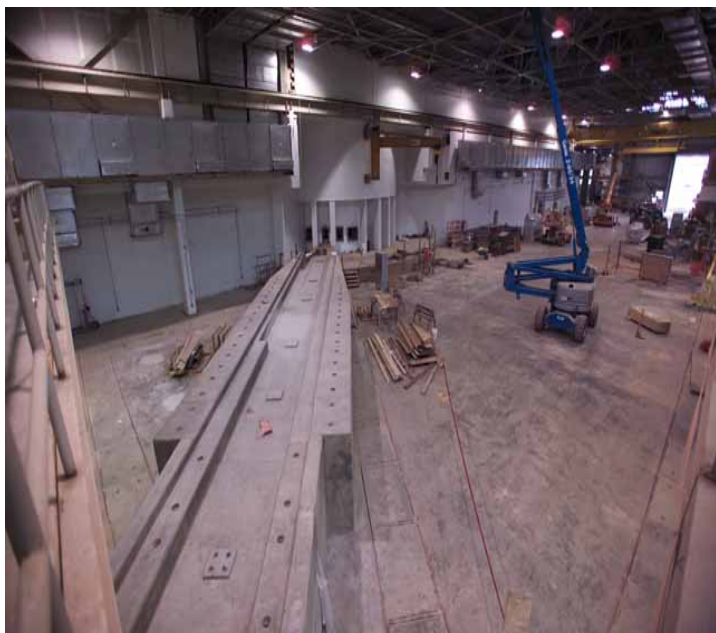
# Background, Spallation Neutron Source

- 2004-2012
- Instrument Construction & Installation



# Background, Spallation Neutron Source

- 2004-2012
- Instrument Construction & Installation



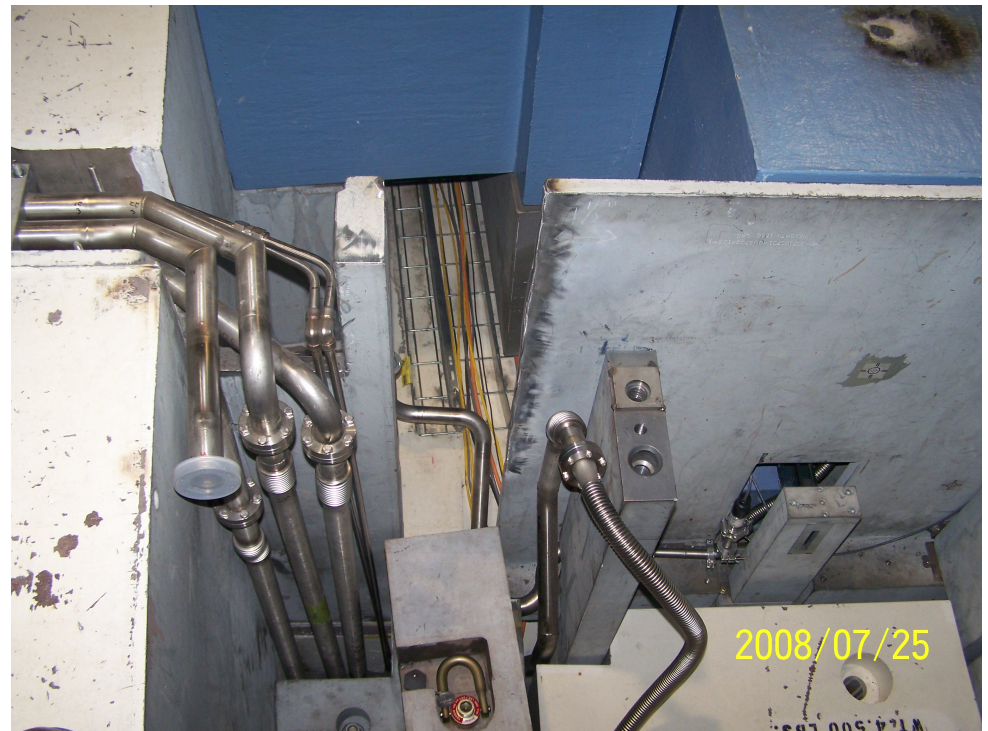


# Action

- Developed reality based installation schedules, working with scientists and engineers.
- Integrated schedule of all beamline installation and construction activities.
- Learned the mechanics and organization of the T&M installation contract used for technical installation activities at SNS.
- Worked with instrument teams and technical teams to install the instruments.

# Practical Lessons

- The majority of the “installation” activities more closely resemble a slightly non-standard civil construction effort.



# Practical Lessons

- Close coordination is required not just within the different projects but also among all of the parties working in the experiment hall.

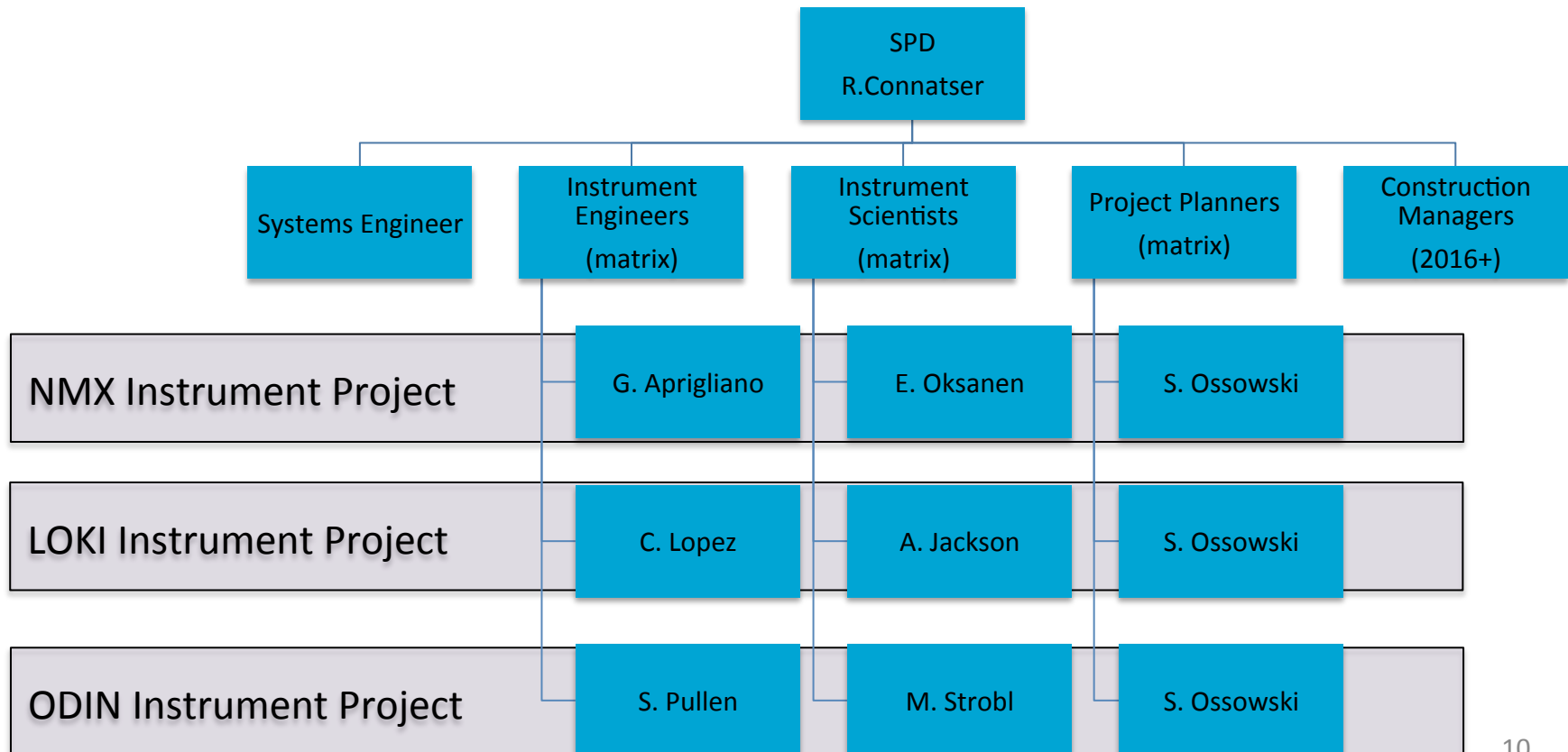
INSTALLATION	8/10	8/11	8/12	8/13	8/14	8/15	8/16	TARGET FACILITY	8/10	8/11	8/12	8/13	8/14	8/15	8/16	8/17	8/18
SAFETY TOPIC	Porting change	LADDER SAFETY	DISCUSS THIS (W/ H/ OTHERS)		Paper cuts			FIRE PROTECTION SYSTEM	ON	ON	ON	ON					
LOTO								BEAM STATUS	Outage	Outage	Outage	Outage					
SURVEY & ALIGNMENT	BL12 change BL12	→	→	BL12 BL14	Chopper cage			CRANES	South Ins Full choppers	South Ins	NI	NI					
MEZZANINE	BL11 BL12	→	→	BL12 BL14	Chopper cage			SAMPLE ENVIRONMENT	cool work 4th floor	→	→	→					
NORTH HALL	BL11 Z.C.1	→	→	BL12 BL14	Chopper cage			OPERATIONS	POD	POD	POD	POD					
SOUTH HALL	BL11	→	→	BL12 BL14	Chopper cage			REMOTE HANDLING	POD	POD							
HIGH BAY								FACILITY MAINTENANCE	POD PM'S	POD PM'S	POD PM'S	POD water room					
4th FLOOR								RAD PROTECTION	Support	Support	Support	Support					
BASEMENT								INSTR. HALL COORDINATOR	Inst Support	Inst Support	2TV Power out PPS TST	Norths: de Elec outage 6am →					
BL11 BL12	→	→	→	→	→			Instrument Support Group	BL5 BL6	BL5 BL6 BL7, 13	BL5, 6, 17, 18, 11						

# ESS Responsibilities

- Responsible for the budget of the instrument projects
  - Sub-project manager for Instrument Construction within the Neutron Scattering Systems Project

# ESS Responsibilities

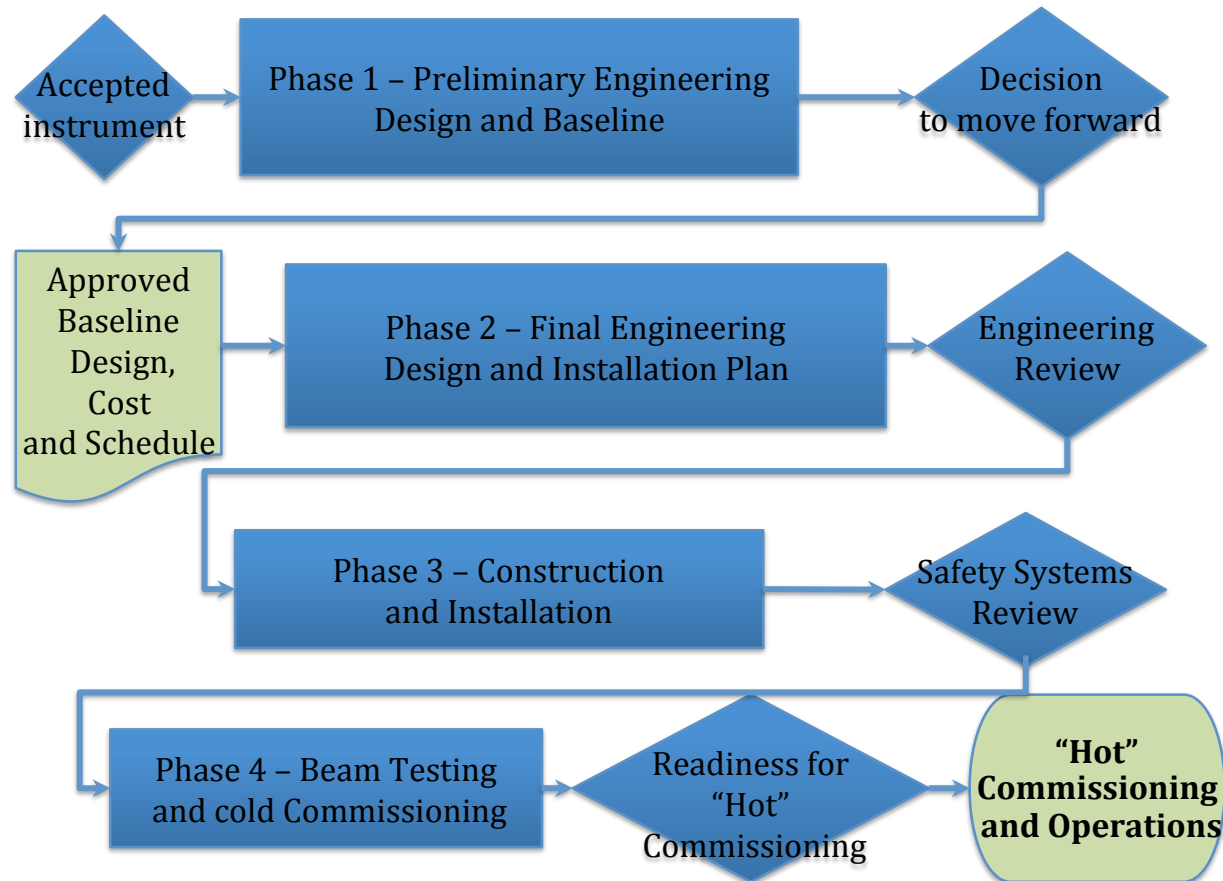
- Organize and develop the resources (people, tools, & space)





# ESS Responsibilities

- Develop processes and make the plans needed

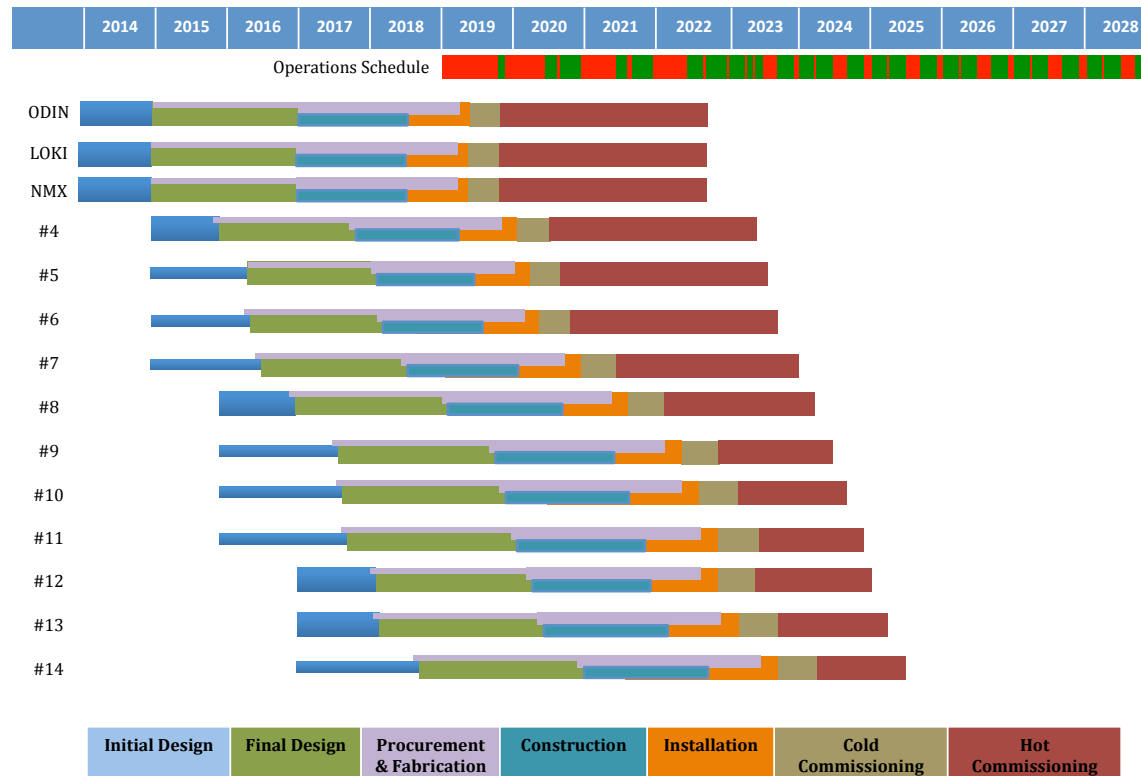




# ESS Responsibilities

- Develop processes and make the plans needed

## Instrument Installation



# ESS Responsibilities

- Coordinate with partners
- Manage and track the work being performed



EUROPEAN  
SPALLATION  
SOURCE

# Community Interactions

ESS SAC Orientation Day

Sindra Petersson Årsköld

[www.europeanspallationsource.se](http://www.europeanspallationsource.se)

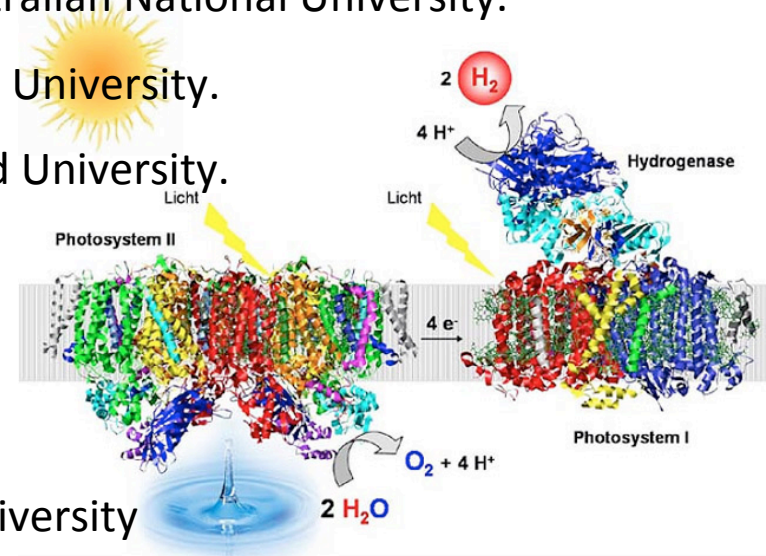
February 4, 2014

# Introduction

## Sindra Petersson Årsköld



- 1996 M.Sc. Physics, Stockholm University.
- 2000 Ph.D. Biochemistry, Lund University.
- 2001-2003 Postdoctoral Research Fellow, The Australian National University.
- 2003-2010 Assistant Professor, Biochemistry, Lund University.
- 2010-2011 Associate Professor, Biochemistry, Lund University.
- Now** **Senior Advisor, ESS**  
**Science strategy**  
**Policy**  
**Outreach & community interactions**
- Also** Vice Chairman of the Board, Malmö University  
Board member & co-founder, Probation Labs AB.



# Built by the Community, for the Community



## Exploring the scientific potential of ESS together

*ESS Science Symposia*

*Science & Scientists at ESS*

## Expanding the science case and the user base

*Scientific outreach*

*Conference participation*

## Developing the facility together: instruments, neutron technologies, support facilities, sample environment, data management & analysis

*NSS Project Collaborations*

*IKON meetings*

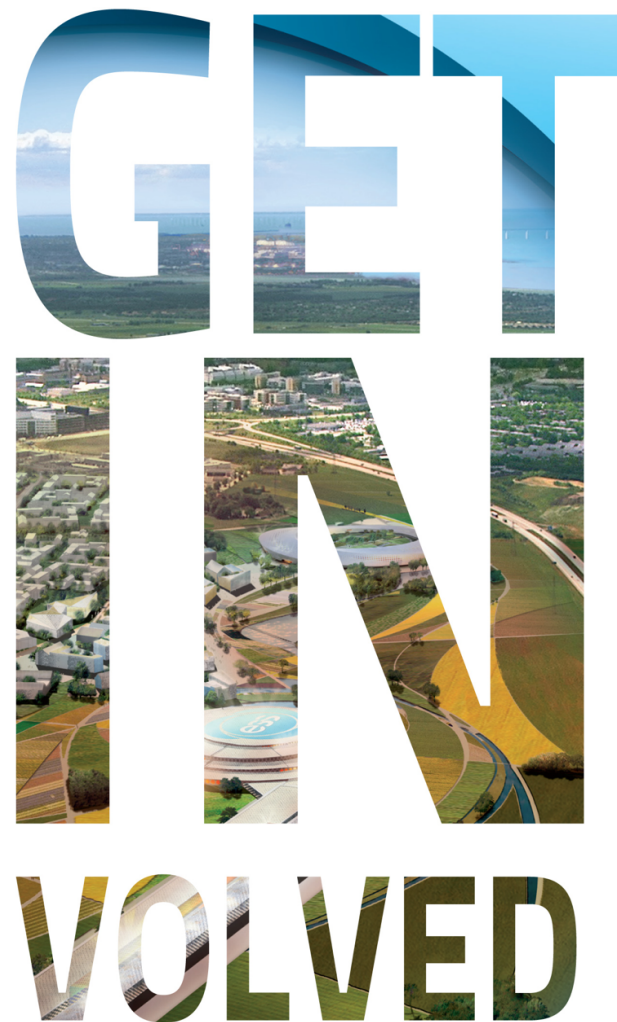
## Advice on the scientific and technical development

*Scientific and Technical Advisory Panels*

*Scientific Advisory Committee*

## Governance

*Steering Committee*



# Collaboration is Key to Success

- Competence & experience
- Technology transfer between labs
- Training of the next generation
- Community engagement & buy-in
- Third-party funding opportunities, **H2020**

# BUY-IN

- Seconded personnel
- Joint postdocs & PhD students
- Technical & scientific collaborations



FEED-BACK  
EXPERIENCE  
SKILLS  
COMMITMENT  
RECRUITMENT  
USERS  
PARTNERING  
COMPETENCE  
COLLABORATIONS  
OWNERSHIP  
ENGAGEMENT  
FUTURE  
VISION  
COLLECTIVE  
SUPPORT  
INPUT



# Exploring Scientific Potential at the *ESS Science Symposia*

**Organized by scientists on their topic of choice.**

**Sponsored by ESS.**

Attended by ESS staff.

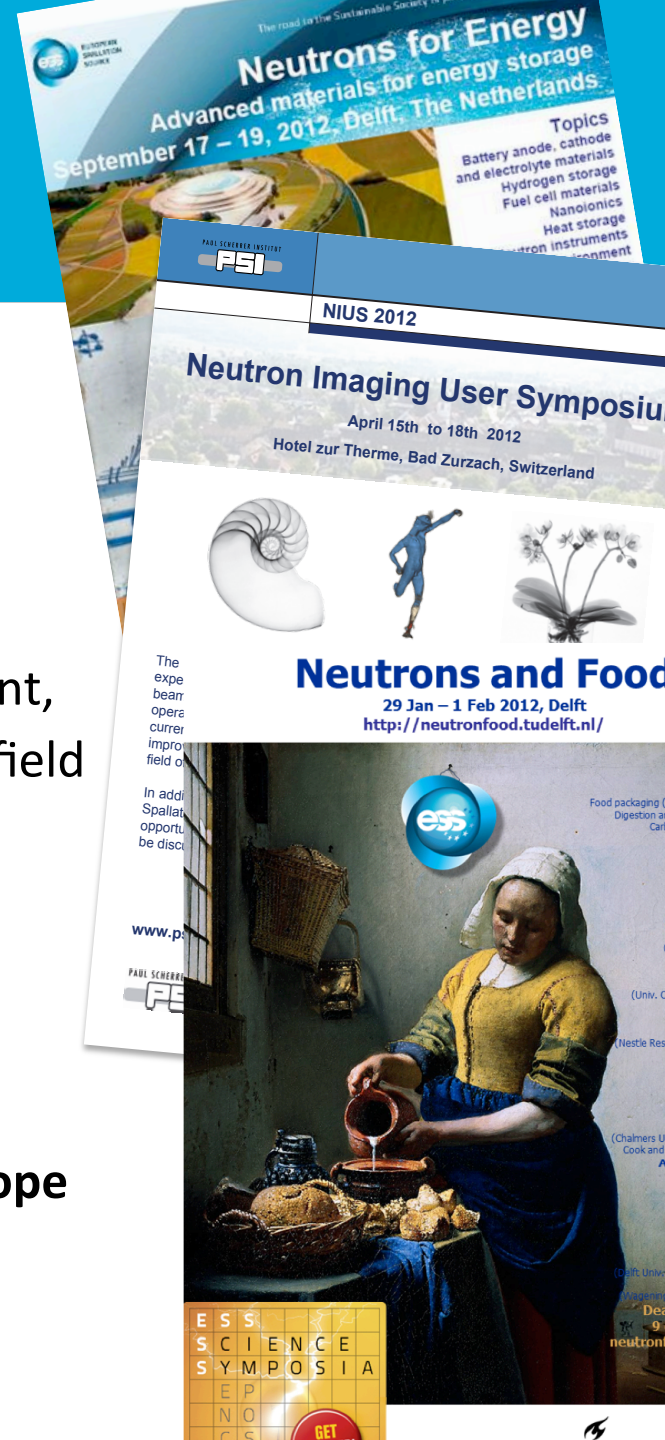
Aim of each symposium: To discuss future development, neutron possibilities and challenges in that particular field of science.

Report to us afterwards: requirements on the next-generation neutron source, “wish list”.

**These reports feed our science strategy.**

**18 ESS Science Symposia have been held around Europe since 2011.**

The call is open for more.



# Exploring Scientific Potential at the *ESS Science Symposia*



Surface and Interface Reconstruction, TUM 2014	In-situ Chemistry, 2012 Gothenburg
Neutrons for future energy strategies, 2013 PSI	NUIS, 2012 PSI
New Generation Green Construction Materials, 2013 Stockholm	Correlated Electron Systems, 2012 UK
NS at Extreme Conditions, 2013 Edinburgh	The Future of Soft-Matter SANS, 2012 Lund
Neutron Particle Physics at LPS, 2013 Grenoble	Neutrons and Food, 2012 Delft
Protein Crystallography, 2013 Aarhus	Off-Specular NS workshop, 2012 Brussels
Neutrons and Life Sciences, 2013 Lund	NBI ESS Symposium, 2011 Nils Bohr Institute
Phys. Sim. of Processes in Engineering Materials, 2012 Prague	Topological Materials, 2011 ILL
Materials for Energy Storage, 2012 Delft	Materials Engineering at a Long-Pulse Source, 2011 UK

**Reports from each symposium at [esss.se](http://esss.se)!**

# Science & Scientists at ESS and IKON



## IKON meetings

For discussing the development of instruments, technologies and support facilities in the NSS project.

Every 6 months in Lund.

Up to 160 participants from all partner countries.



IKON1 Sep 2011

IKON2 Feb 2012

IKON3 Sep 2012

IKON4 Feb 2013

IKON5 Sep 2013

IKON6 Feb 2014

## Science & Scientists at ESS meetings

For discussing the science to be enabled by ESS, across the various scientific disciplines.

2011 in Prague (ECNS satellite)

2012 in Berlin

*336 participants from 19 countries*

2013 in Edinburgh (ICNS satellite)

*130 participants from 17 countries*



# Regional Rooting for a Vibrant Scientific Environment



## Why is this Important?

A prerequisite for a thriving, resilient science facility.

An academic home for ESS staff.

Enhanced user experience through a strong local environment.

Added value in support facilities through collaborations.

## Adjunct Positions for ESS Science Staff

Lund University: Chemistry, Physics, LTH

Copenhagen University: Niels Bohr Institute

Chalmers Institute of Technology

Uppsala University

Mid-Sweden University

## Joint Senior Positions/Advisors

Lund University, Copenhagen University

## Activities

Seminar Series with MAX IV & LU

Exhibition at LTH Science Centre

## Collaborations

MAX IV: joint detector lab and much more

Linköping University: detectors

Lund Protein Production Platform

LTH: Accelerator

## Other Bridges

Lund University: Legal, Astronomy,

Pufendorf Institute of Advanced Studies

Copenhagen University: Legal



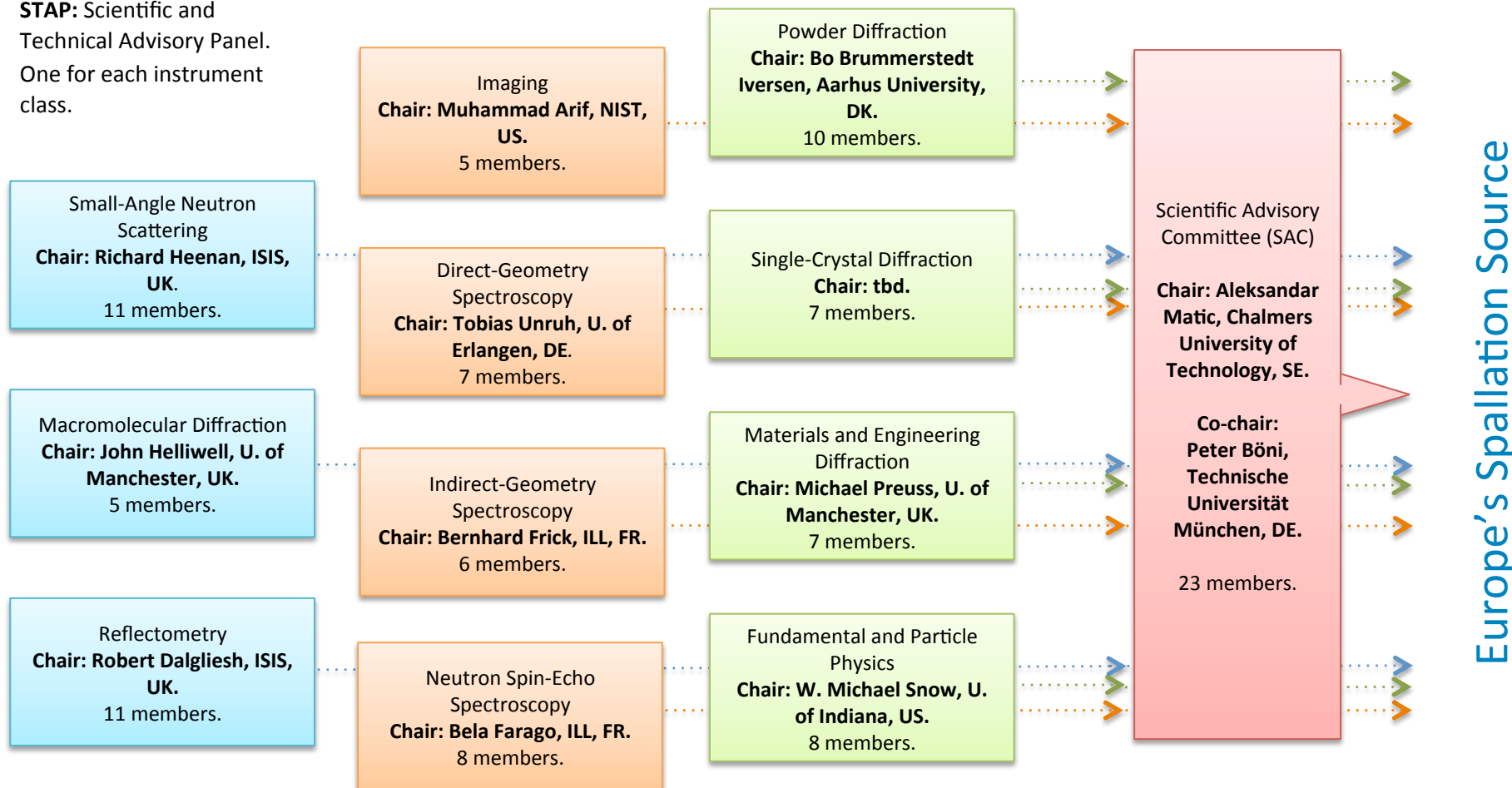
# Communications at ESS

Target group	Subgroup	Main responsibility
Scientific community	<i>European &amp; regional</i>	Science Dir.
	<i>Current &amp; potential neutron users</i>	Science Dir.
Funding bodies	<i>Science &amp; facility</i>	Communications Div.
Decision makers	<i>European &amp; regional</i>	Communications Div.
Regional actors	<i>Scientific &amp; societal</i>	Science Dir. & Communications Div.
General public	<i>European &amp; regional</i>	Communications Div.



# >100 External Experts Have Advisory Roles in the Development of ESS

**STAP:** Scientific and Technical Advisory Panel.  
One for each instrument class.



The STAPs consist of 85 expert scientists from the international community  
Each STAP advises ESS management and informs SAC.  
SAC advises ESS management, who proposes to STC.



# Welcome to the ESS team!

