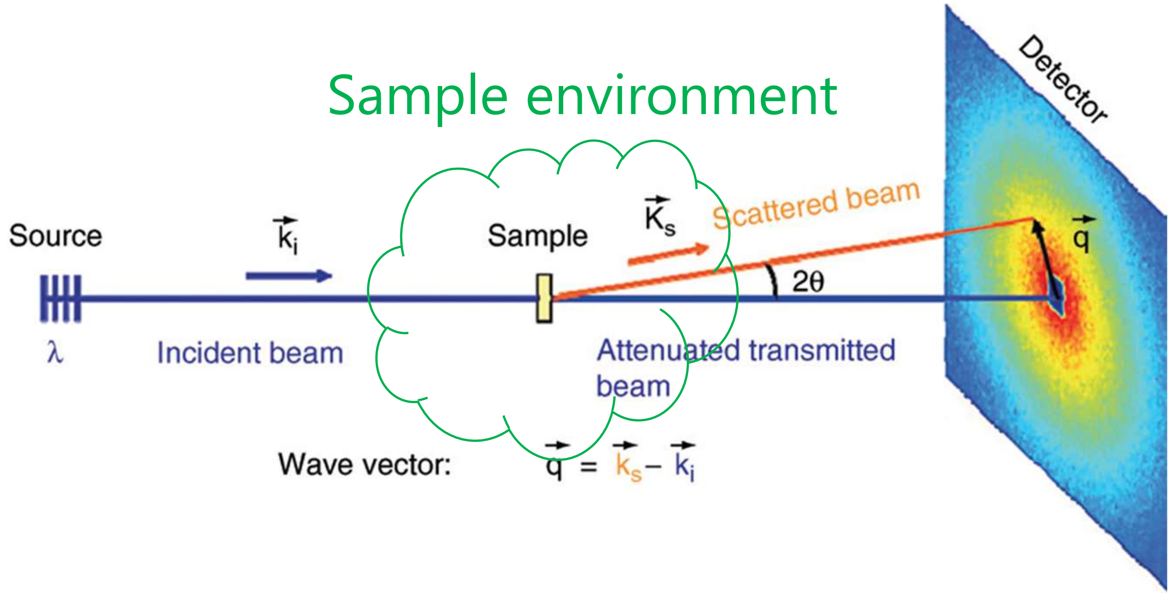
Sample Environment at ESS and beyond

ALEXANDER T HOLMES, ESS

2020-02-06

Neutron (and x-ray) scattering gives information on the molecular and atomic level

The wavelength of a neutron = the distance between atoms in a material
=> diffraction pattern



Neutrons tell us: Where are the atoms, and what are they doing?

Anatomy of a scattering experiment

Users

Scientific question

- What is going on inside a high temperature superconductor?
- How do self assembled lipid structures react to shear stress?
- What happens in a battery during a charging cycle?

Facility

Scattering technique

- Neutrons/X-rays
- Small angle scattering
- Polarised neutrons
- Inelastic scattering

Sample Environment

User/Facility

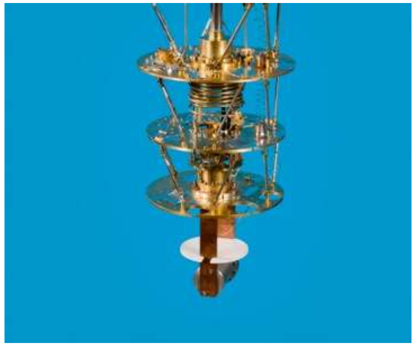
Control parameters

- Temperature
- Pressure
- Magnetic Field
- Electric field
- Flow
- pH
- Gas concentration

Sample environment turns a measurement into an experiment

Ultra Low Temperature

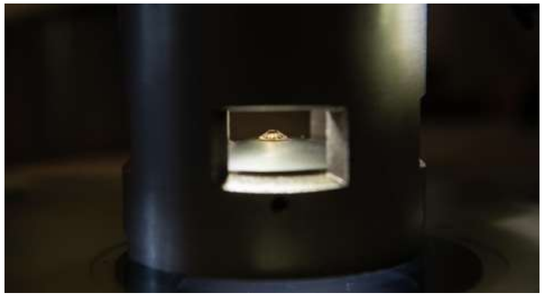
T < 50mK



Magnetic field

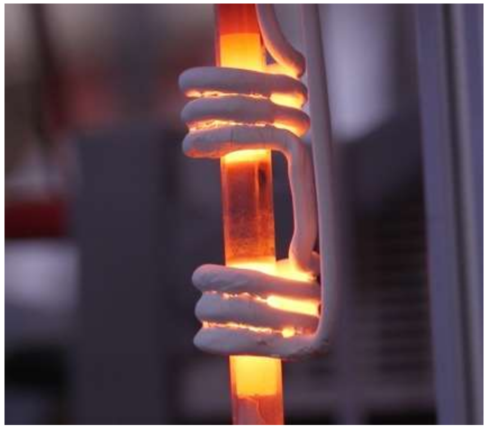
B > 16 T

Pressure



P > 100 GPa

High temperature



T > 1000°C

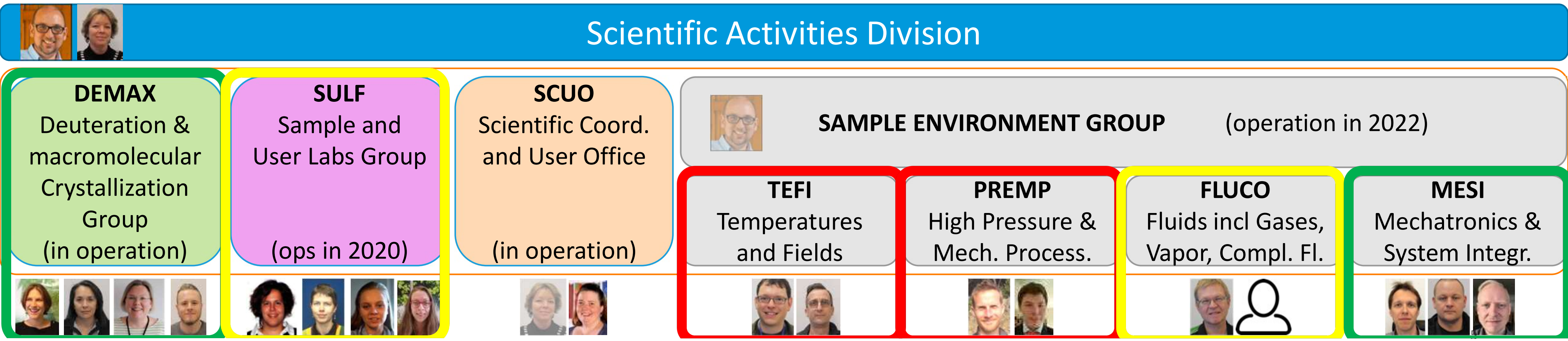
Soft matter

Complex fluids, colloids, interface

The Scientific Activities Division delivers Science Support Systems:

Sample Environment, Scientific Laboratory and Sample Services, Scientific Coordination and User Office

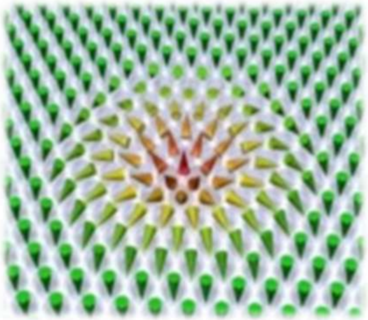
*for **first 8 instruments** as part of **NSS construction budget***

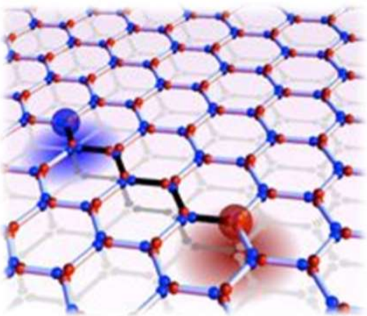


Neutrons for magnetic and electronic phenomena

Hunting for materials that make our tec[illegible] sm[illegible]

Understanding quantum phenomena and novel states of matter in detail



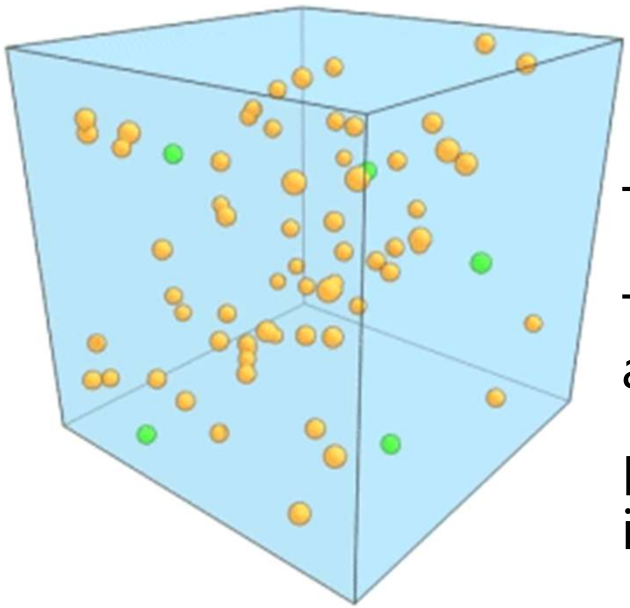


Improving electronic properties and exploiting quantum phenomena

The sensitivity of neutrons to magnetism and the unique ESS neutron flux makes it possible to study quantum materials 'in-operandi' to understand them at a microscopic level.

Cryogenics is [illegible]

Cryogenics - Why do we want to cool things?



Translational motion
Credit: Sean Kelley/NIST

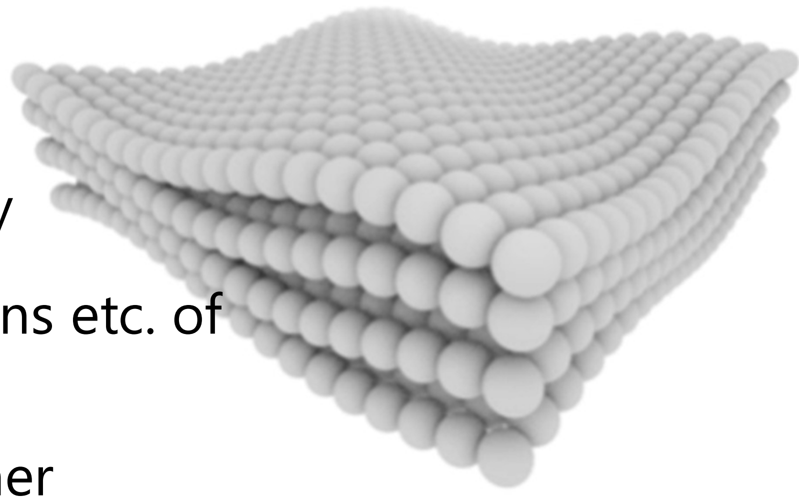
Temperature ⇔ kinetic energy

Translation, vibrations, rotations etc. of atoms, molecules, electrons…

Lower temperature allows other interactions to take over ⇒

Phase transitions:

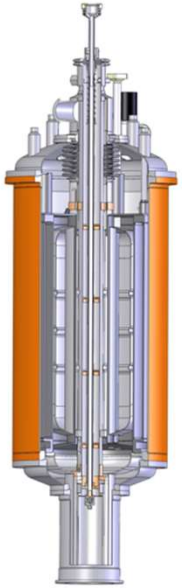
Classical (e.g.crystallisation)
or
Quantum (magnetism, superconductivity)

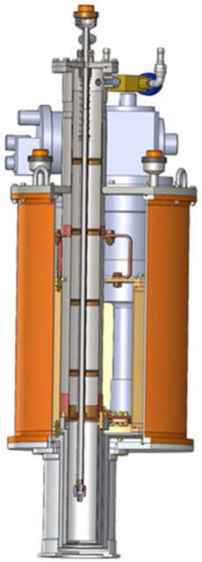


Collective motions (phonons).
Credit: Sean Kelley/NIST

Neutron energies match well with phonons and other excitations

Typical cryogenic sample environment planned for ESS





Wet, dry, dilution, He3,
Flow cryostats (not shown)

Typically Variable Temperature Insert into outer cryostat/cryomagnet
To allow rapid sample changeover

Pictures: ILL, HZB, STFC, other manufacturers are available…

Delivering High pressure at the ESS

- Full suite of ‘conventional’ equipment (gas, clamp and PE)

gas cells Left to right: TiZr; Al; ISIS website

Left to right: NiCrAl Bezaeva et al Geophys Res Lett (2007). ; Al clamp and TiZr Clamps R.A. Sadykov (ILL website)

Sine2020 website

- Designs optimized for ESS instruments (sample volumes, cell materials, collimation)
- Benefit from strong collaboration with STFC, CSEC
- IK proposal with LLB
- Indirectly supported by activities such as Sine2020

Delivering High pressure at the ESS

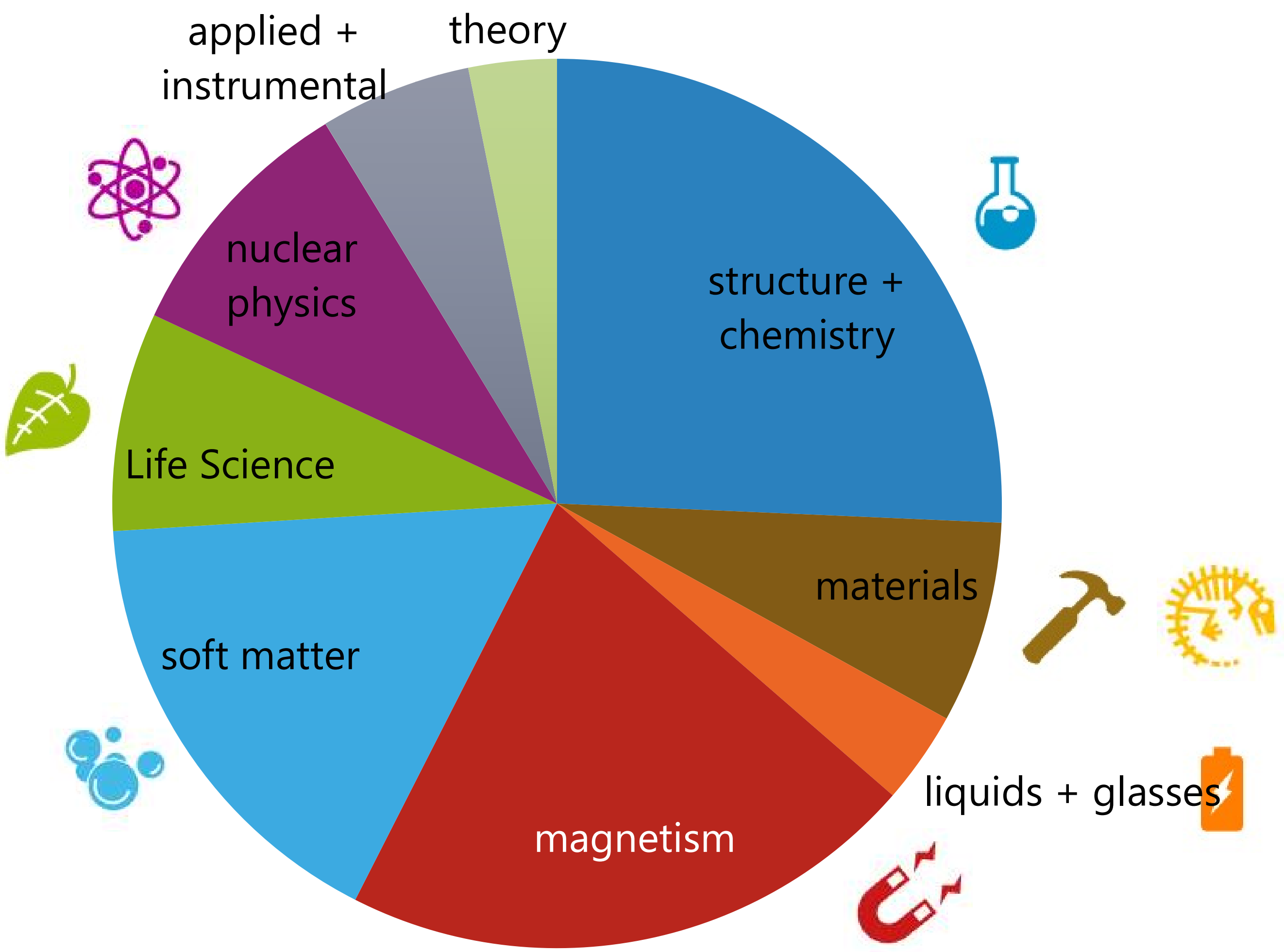
- State-of-the-art new cells (ultra-high pressure, ultra-low temperature)

Oak Ridge DACs
(collaboration with R. Boehler, B. Haberl, ORNL)

Low T Uniaxial clamp
(collaboration with P. Deen)

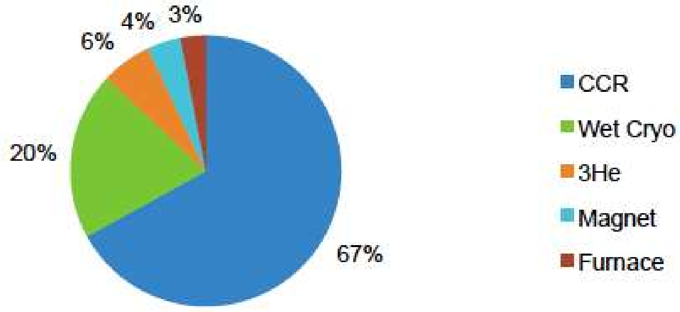
ESS DAC
(collaboration with J. Loveday University of Edinburgh)

Neutron use per science topic

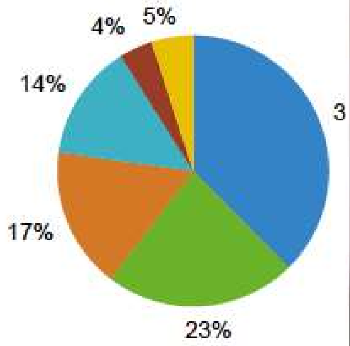


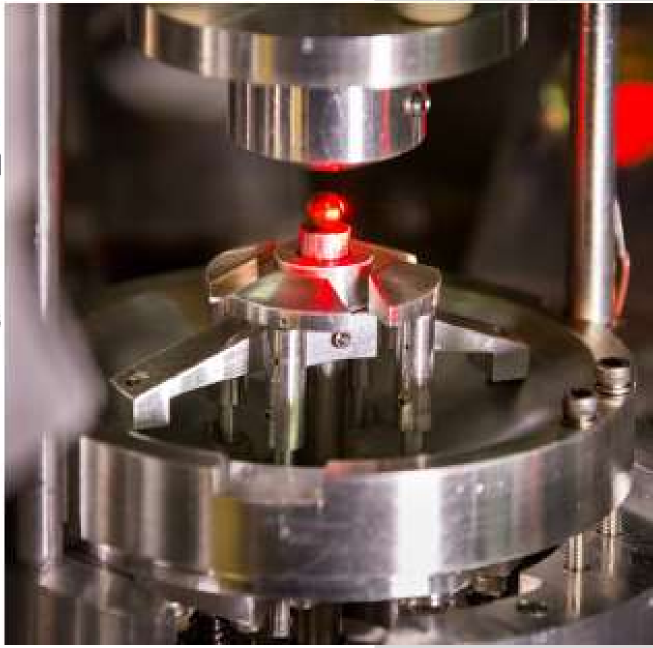
HFIR and SNS Experiment Profiles

HFIR FY 2012, 7 Cycles, 267 Total Experiments

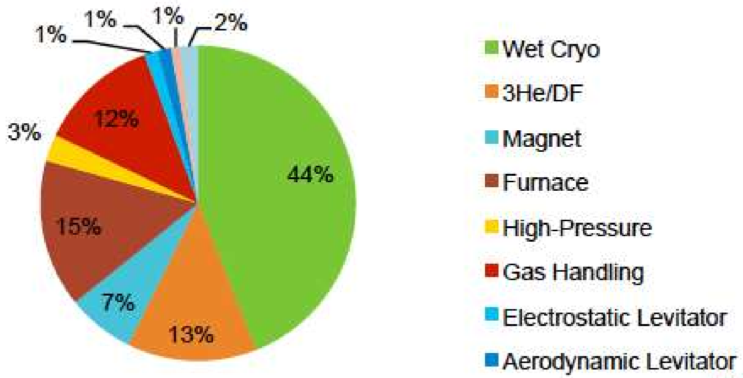


HFIR FY 2015, 6 Experim

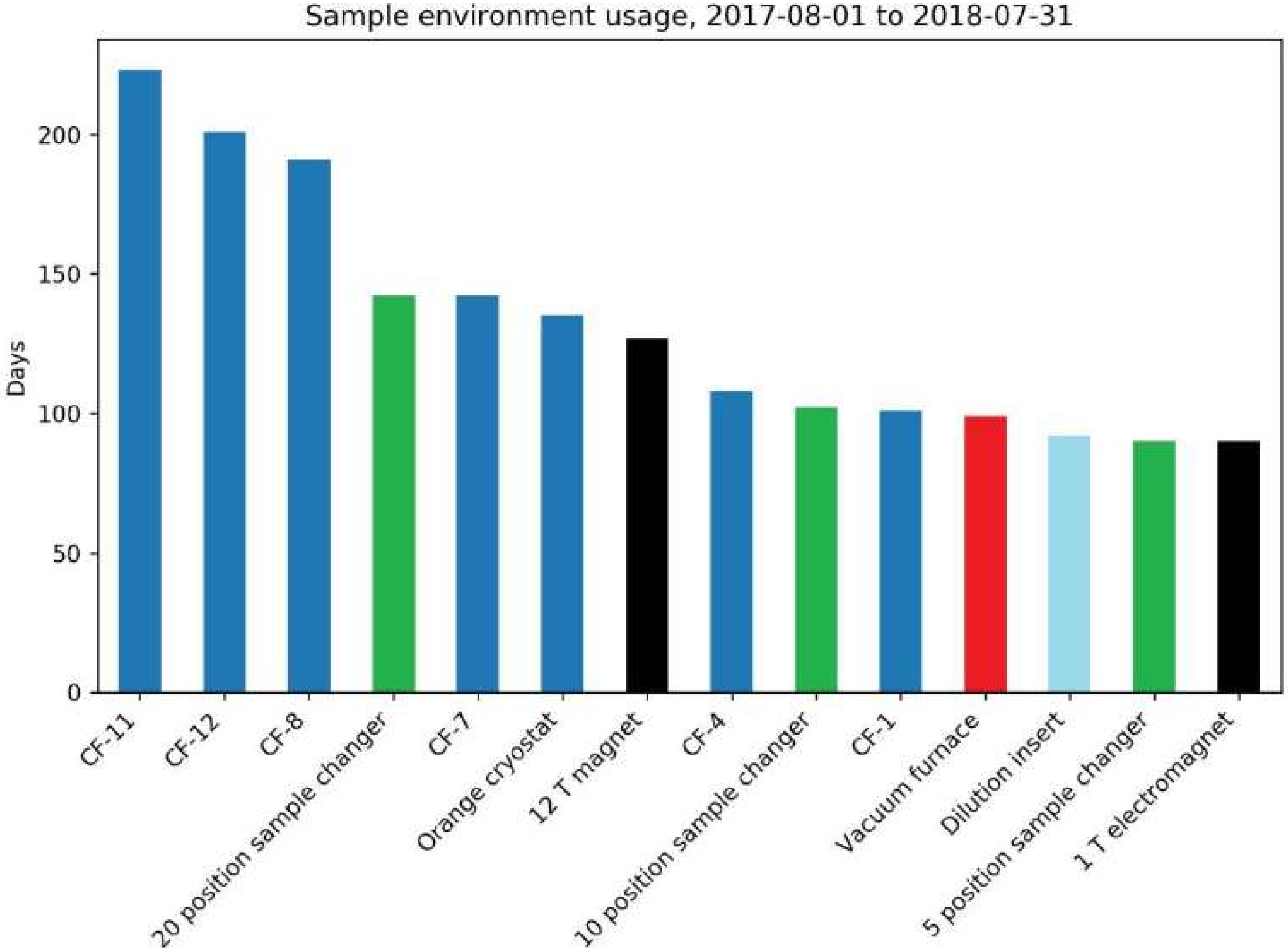


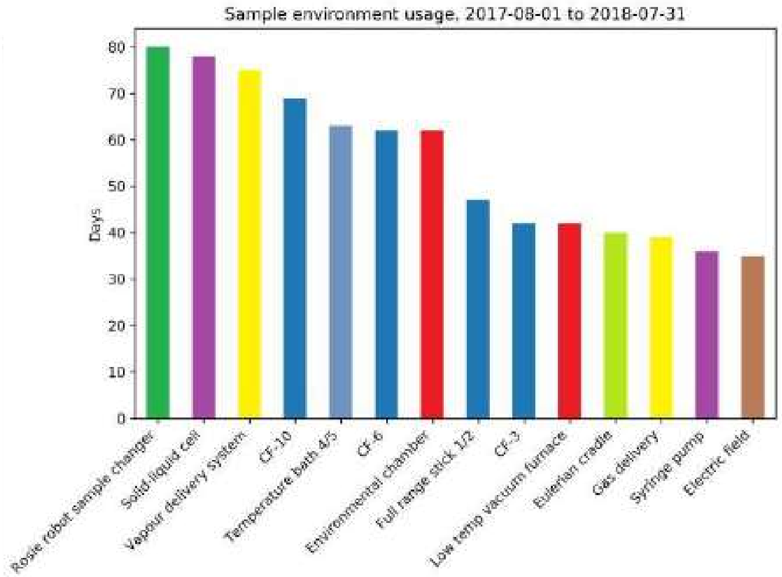


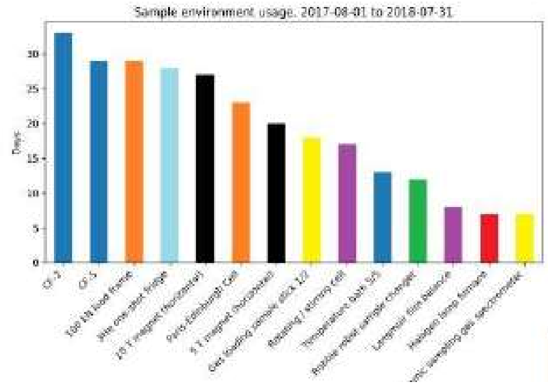
SNS FY 2015, 218 Experiments



What Do Our Users Want To Use?

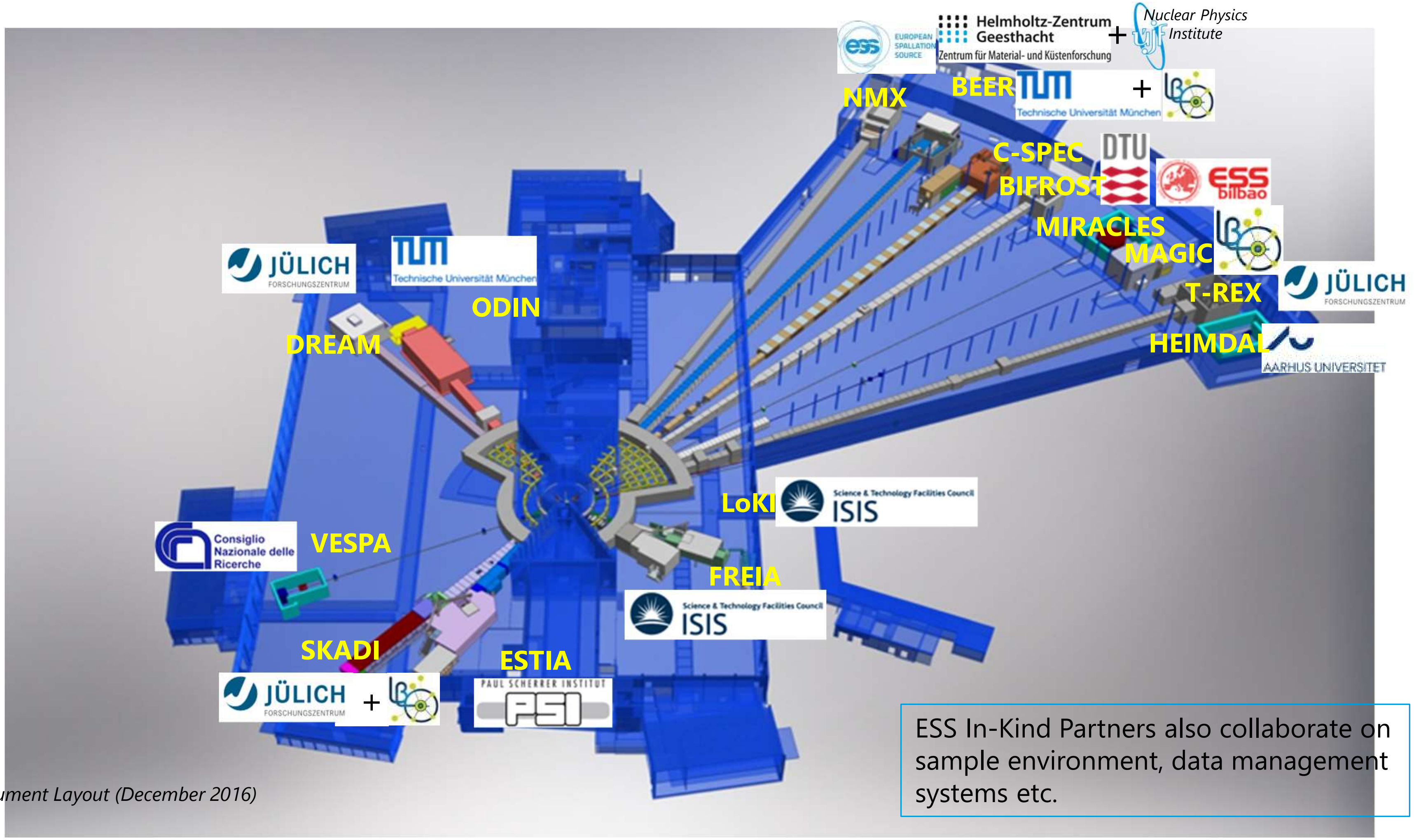






NSS Neutron Instruments

ESS Lead Partners for instrument construction



ESS Instrument Layout (December 2016)

ESS In-Kind Partners also collaborate on sample environment, data management systems etc.

ESS instruments cater to many science topics

EUROPEAN SPALLATION SOURCE

Version 2/11/2017

Large-Scale Structures

- ODIN Imaging Instrument
- SKADI General Purpose SANS
- LOKI Broadband SANS
- Surface Scattering
- FREIA Horizontal Reflectom.
- ESTIA Vertical Reflectom.

Diffraction

- HEIMDAL Powder Diffract.
- DREAM Powder Diffract.
- Monochromatic Powder Diffract.
- BEER Engineering Diffract.
- Extreme Conditions Diffract.
- MAGIC Magnetism Diffract.
- NMX Macromolecular Diffract.

Spectroscopy

- CSPEC Cold Chopper Spec.
- Broadband Spectrometer
- T-REX Thermal Chopper Spec.
- BIFROST Xtal Analyser Spec.
- VESPA Vibrational Spec.
- MIRACLES Backscatt. Spec.
- High-Resolution Spin-Echo
- Wide-Angle Spin-Echo
- Particle Physics Instrument

life sciences

soft condensed matter

chemistry of materials

energy research

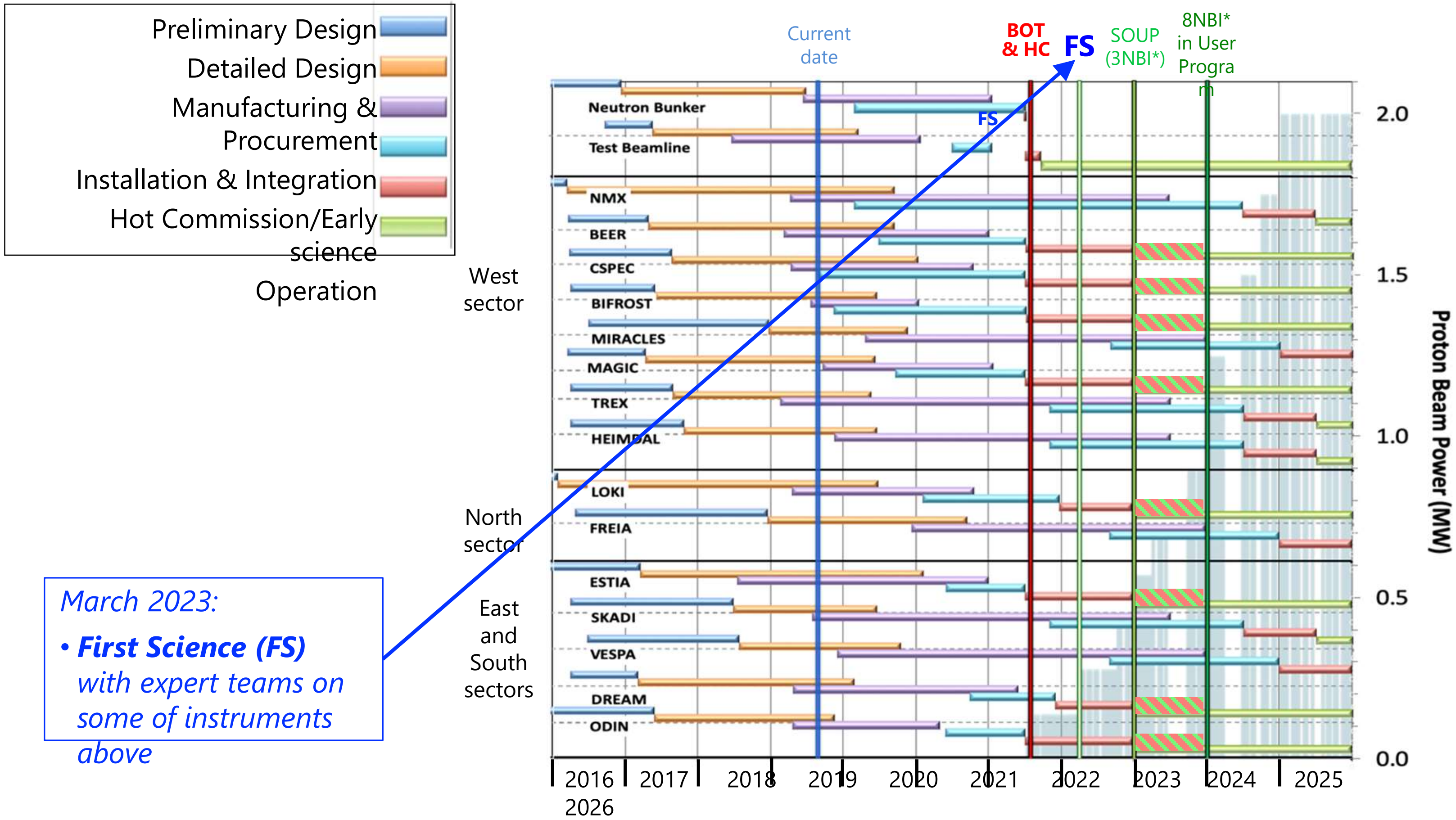
magnetism & superconductivity

engineering & geo-sciences

archeology & heritage conservation

particle physics

Baseline schedule for Neutron Beam Instruments
(NSS MS V4.2)



March 2023:

- ***First Science (FS)*** *with expert teams on some of instruments above*

* NBI = Neutron Beam Instrument

Special requirements for scattering experiments

What do we need beyond usual laboratory type equipment

Reliability

- Beamtime 50k€/day
- Possibility for in-house repair

Connectivity

- Remote monitoring
- Remote control
- SECOP (see later)

Interfaces

- Mechanical mounts
- Standard connectors
- Vacuum
- Motion control

Materials

- Activation
- Transmission
- Background scattering
- Magnetism

Portability

- Wheels
- Crane

Timing

- Fast sample change
- Time dependent properties

Geometry

- Shape & Size
- Detector coverage

SECOP

The Sample Environment Communication Protocol

Journal of Neutron Research -1 (2019) 1–15 1
DOI 10.3233/JNR-190143
IOS Press

An introduction to SECoP – the sample environment communication protocol

Klaus Kiefer [a,*], Lutz Rossa [a], Frank Wutzler [a], Niklas Ektröm [b], Anders Pettersson [b], Enrico Faulhaber [c] and Markus Zolliker [d]

[a] *Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany*
E-mails: klaus.kiefer@helmholtz-berlin.de, rossa@helmholtz-berlin.de, frank.wutzler@helmholtz-berlin.de
[b] *European Spallation Source ERIC, SE-224 84 Lund, Sweden*
E-mails: niklas.ekstrom@esss.se, Anders.Pettersson@esss.se
[c] *Technische Universität München, Heinz Maier-Leibnitz Zentrum, D-85747 Garching, Germany*
E-mail: Enrico.Faulhaber@frm2.tum.de
[d] *Paul Scherrer Institut, CH-5232 Villigen, Switzerland*
E-mail: markus.zolliker@psi.ch

Abstract. The Sample Environment Communication Protocol (SECoP) serves as an international standard for the communication between sample environment equipment and the experiment control software at neutron and photon sources. It eases the integration of sample environment equipment supplied by external research groups and by industrial manufacturers. SECoP is designed to be simple, inclusive and self-describing. SECoP facilitates and structures the provision of metadata which is associated with sample environment equipment. Several existing implementations of SECoP support the development of SECoP-compatible sample environment control software. This article introduces SECoP Version 1.0, the first official version of SECoP published in September 2019. It was developed during the SINE2020 project in close cooperation with the International Society for Sample Environment. The complete specifications of SECoP Version 1.0 are available on GitHub.

Keywords: Sample environment, software, neutron, photon

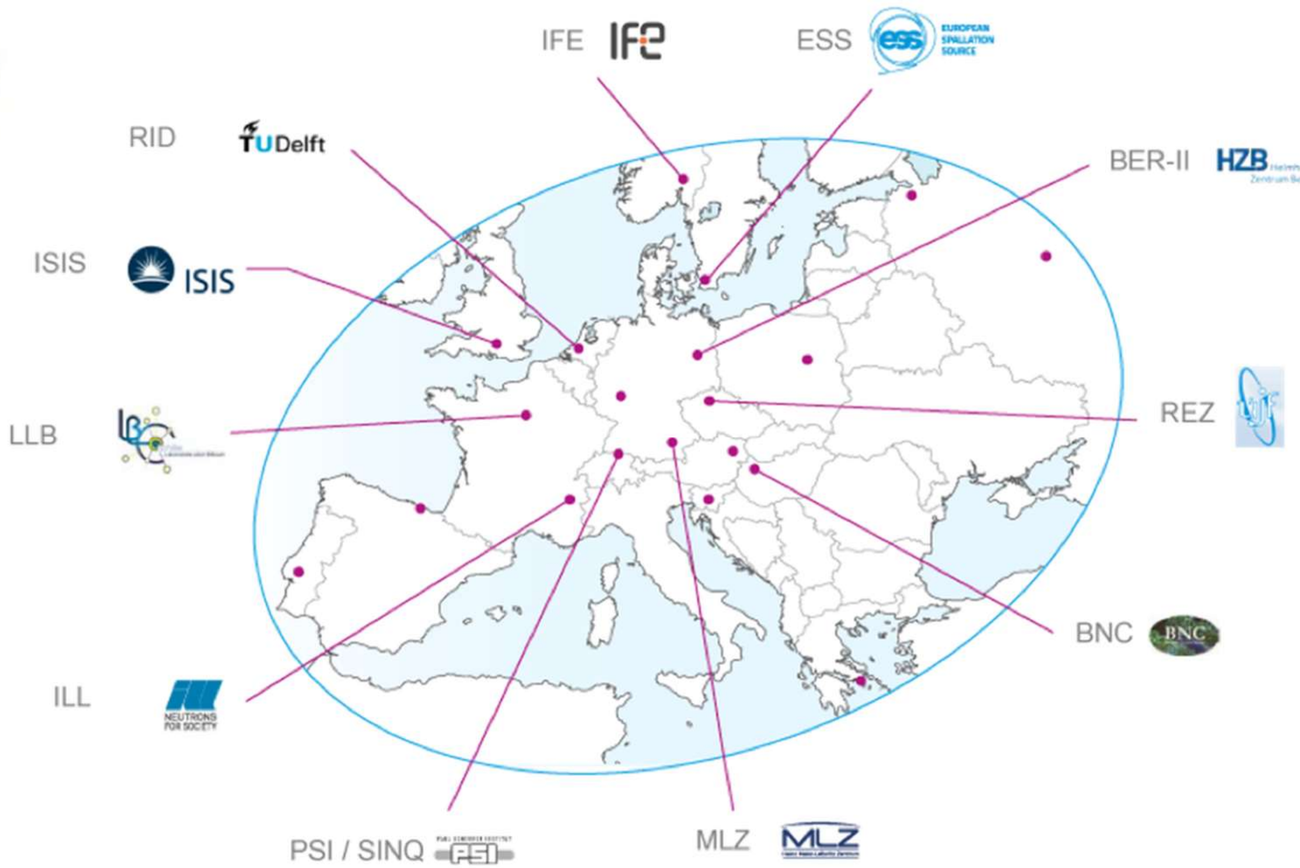
https://doi.org/10.3233/JNR-190143

Synchrotron and XFEL facilities

ISSE

http://www.sampleenvironment.org/

Neutron facilities



Conclusions

Routes into the sample environment business

- High quality components
- Esoteric specialisation – e.g. superconducting magnets
- Close links with user groups (universities, industry, not just facilities)
- Turn a prototype into a “few-off”
- Don’t lose sight of the

Future opportunities for ESS and elsewhere

- Rapid automation
- Fast parameter control
- In-situ complex measurements