Science at ESS and MAX-IV

Ken Andersen

International Beam Instrumentation Conference IBIC 2019

Malmö, 9th September 2019

ESS & MAX-IV

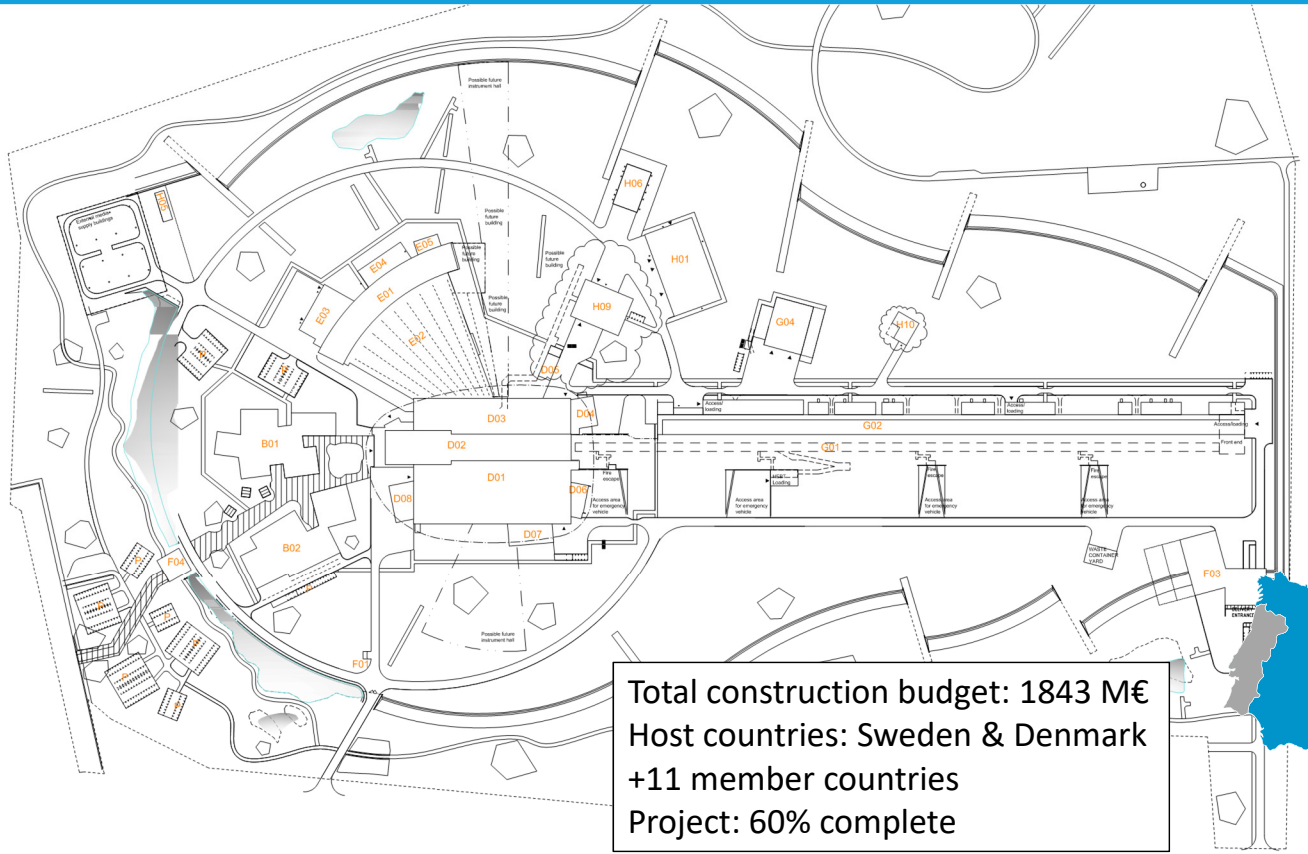
both views

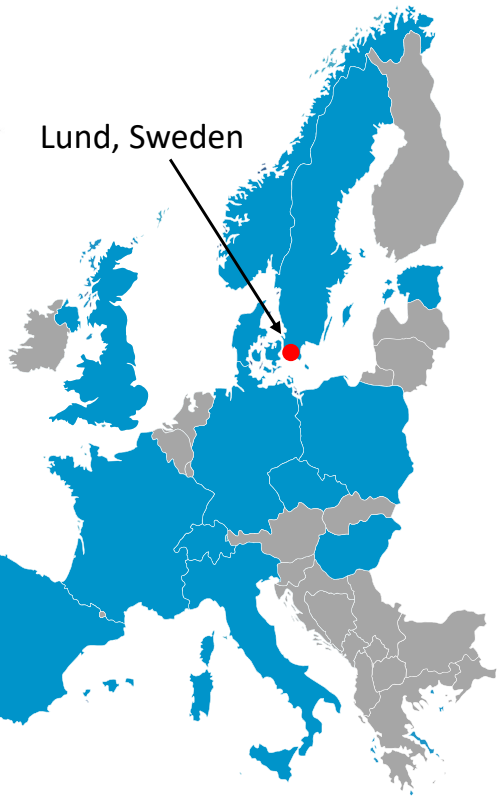
ESS & MAX-IV

both views

EUROPEAN SPALLATION SOURCE

ESS: The Next-Generation Neutron Source

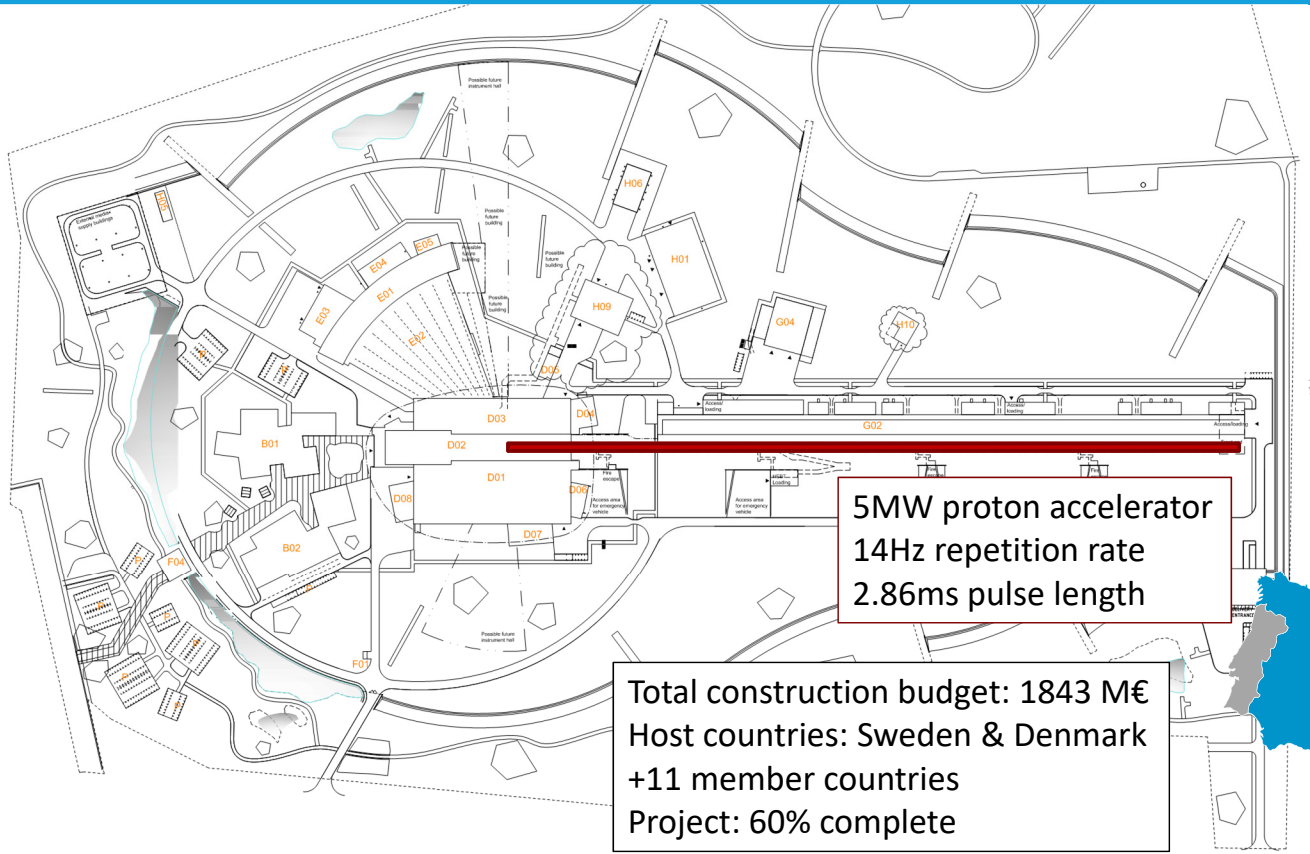




Total construction budget: 1843 M€
Host countries: Sweden & Denmark
+11 member countries
Project: 60% complete

ESS: The Next-Generation Neutron Source

EUROPEAN SPALLATION SOURCE



5MW proton accelerator
14Hz repetition rate
2.86ms pulse length

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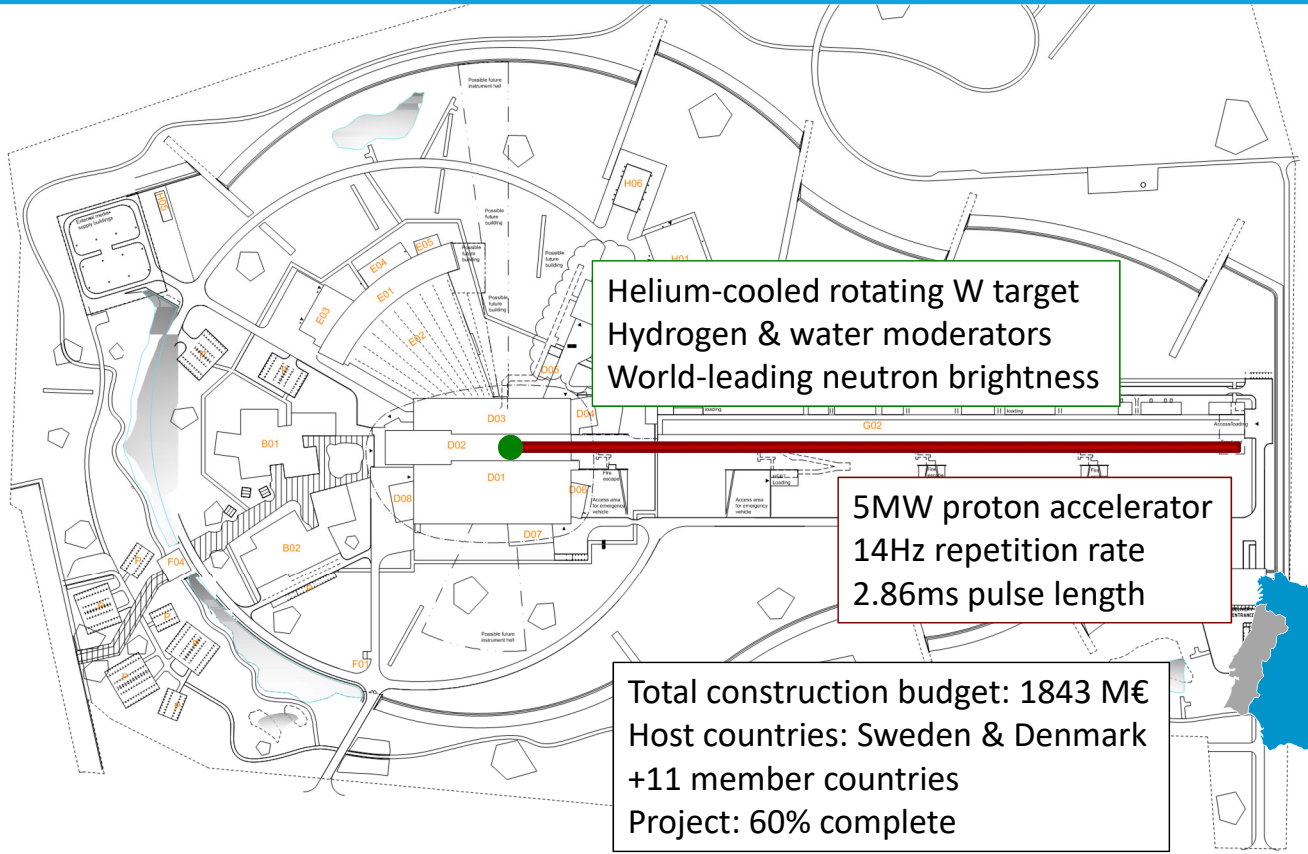
ESS: The Next-Generation Neutron Source



Helium-cooled rotating W target
Hydrogen & water moderators
World-leading neutron brightness

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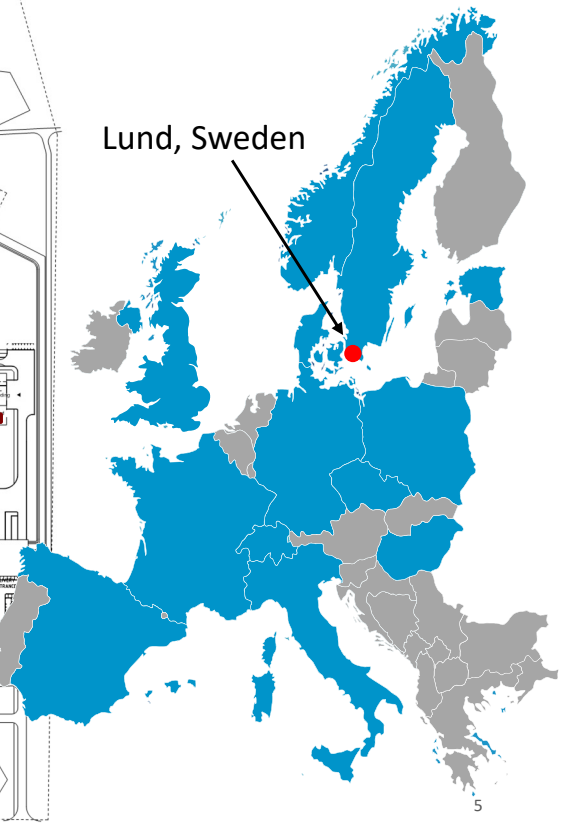
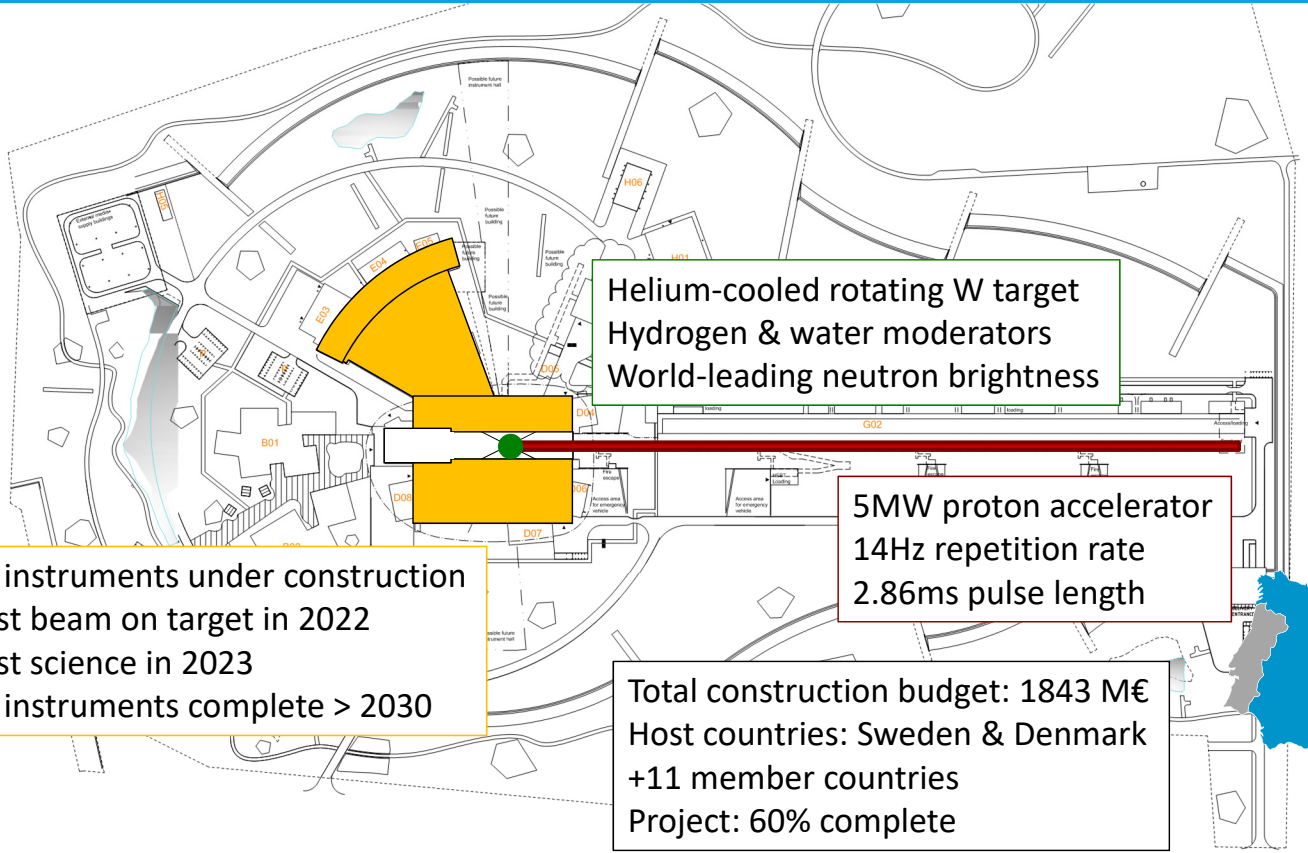


ESS: The Next-Generation Neutron Source

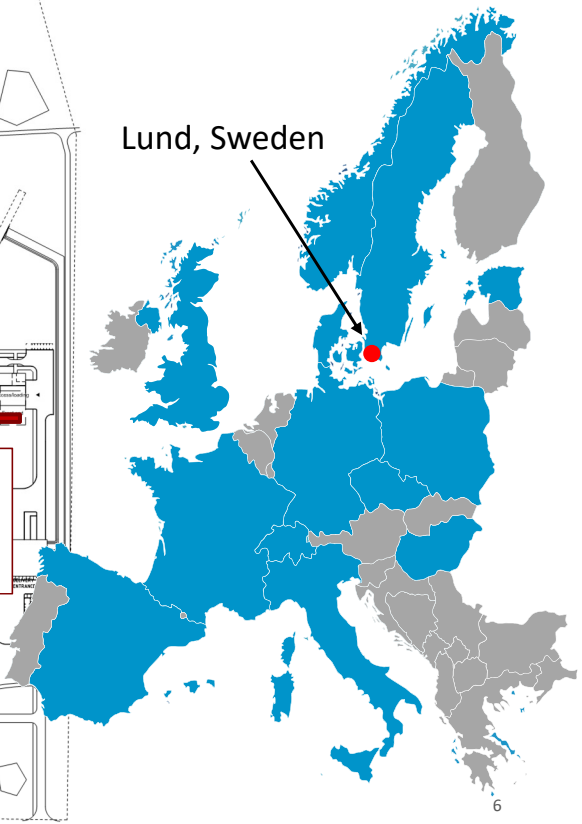


Helium-cooled rotating W target
Hydrogen & water moderators
World-leading neutron brightness

5MW proton accelerator
14Hz repetition rate
2.86ms pulse length

15 instruments under construction
First beam on target in 2022
First science in 2023
22 instruments complete > 2030

Total construction budget: 1843 M€
Host countries: Sweden & Denmark
+11 member countries
Project: 60% complete



Site Photos

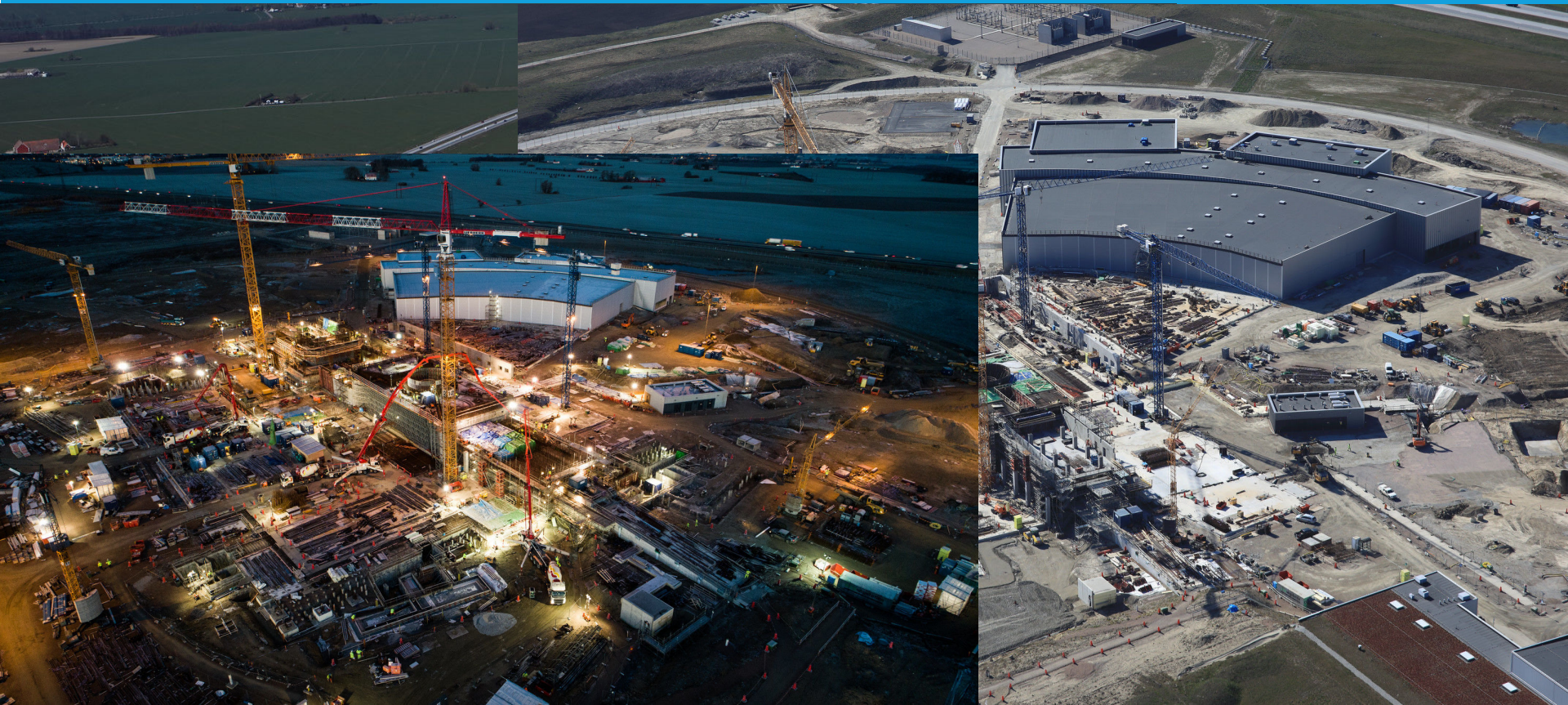
April-May 2019

Site Photos

April-May 2019

Site Photos

April-May 2019



Site Photos

April-May 2019

https://europeanspallationsource.se/site-weekly-updates

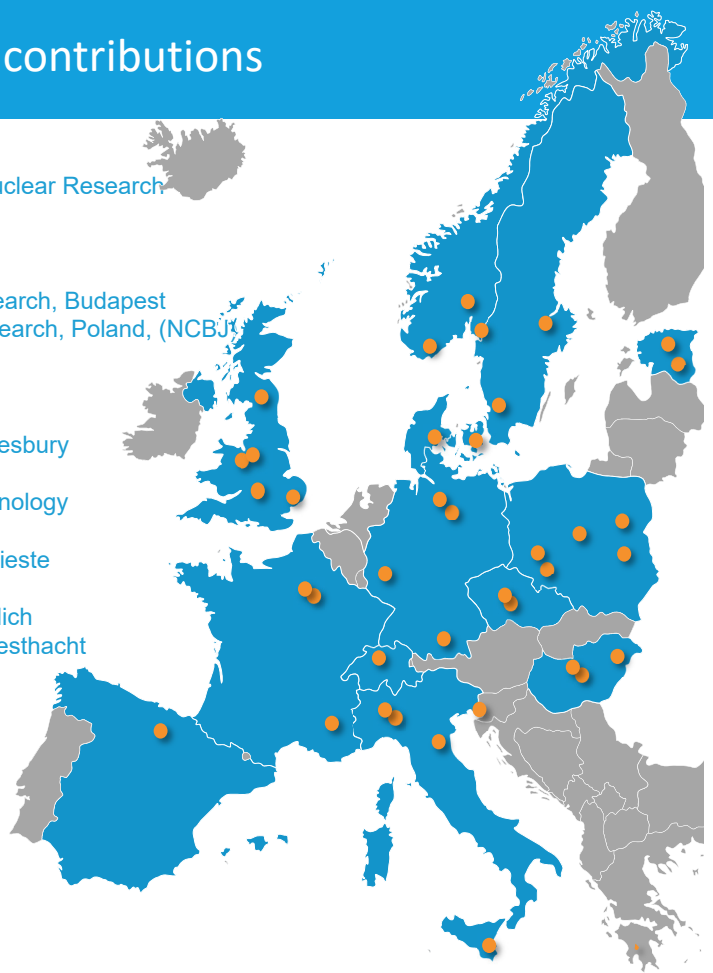
The ESS Project

Countries and Partners for in-kind contributions

Sweden and Denmark:
47,5% Construction
15-20% Operations
Cash ~100%

Partner Countries:
52,5% Construction
80-85% Operations
IKC/Cash ~ 70% / 30%

Aarhus University
Atomki - Institute for Nuclear Research
Agder University
Bergen University
CEA Saclay, Paris
Centre for Energy Research, Budapest
Centre for Nuclear Research, Poland, (NCBJ)
CERN, Geneva
CNR, Rome
CNRS Orsay, Paris
Cockcroft Institute, Daresbury
DESY, Hamburg
Delft University of Technology
Edinburgh University
Elettra – Sincrotrone Trieste
ESS Bilbao
Forschungszentrum Jülich
Helmholtz-Zentrum Geesthacht
Huddersfield University
IFJ PAN, Krakow
INFN, Catania
INFN, Legnaro
INFN, Milan



Institute for Energy Research (IFE)
Institut Laue-Langevin (ILL)
Rutherford-Appleton Laboratory, Oxford(ISIS)
Copenhagen University
Laboratoire Léon Brilouin (LLB)
Lodz University of Technology
Lund University
Nuclear Physics Institute of the ASCR
Oslo University
Paul Scherrer Institute
Roskilde University
Tallinn Technical Univesrsity
Technical University of Chemnitz
Technical University of Denmark
Technical University Munich
Science and Technology Facilities Council
University of Tartu
Uppsala University
WIGNER Research Centre for Physics
Wroclaw Univesrity of technology
Warsaw University of Technology
Zurich University of Applied Sciences (ZHAW)

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Rome
Orsay, Paris
Institute, Daresbury
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University
ncrotrone Trieste
gszentrum Jülich
z-Zentrum Geesthacht
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AN, Krakow
NFN, Catania
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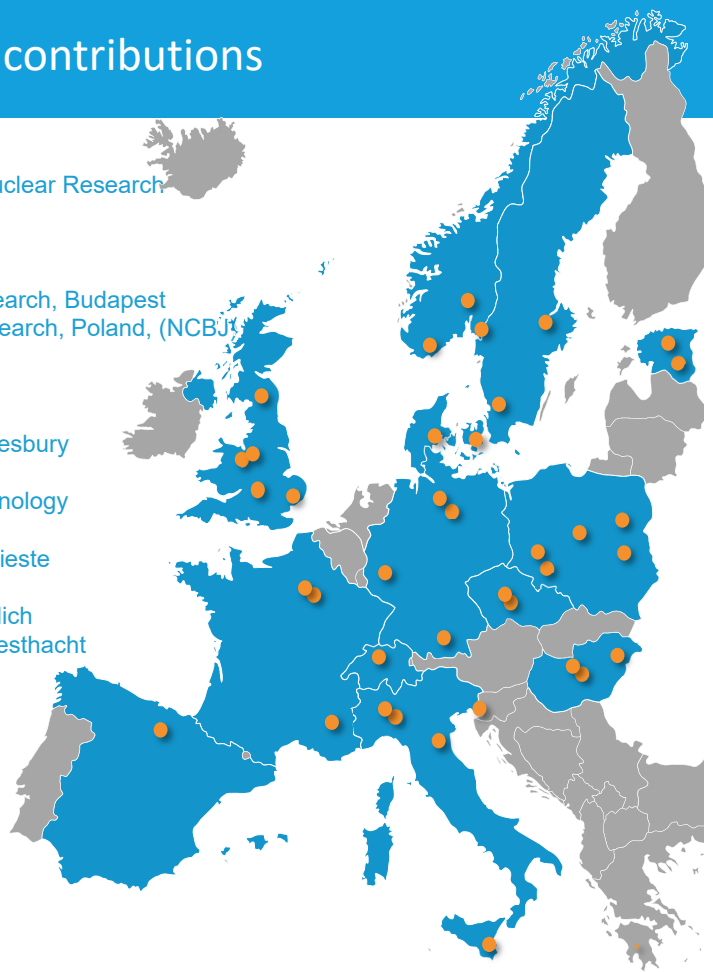

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niversity of Denmark
niversity Munich
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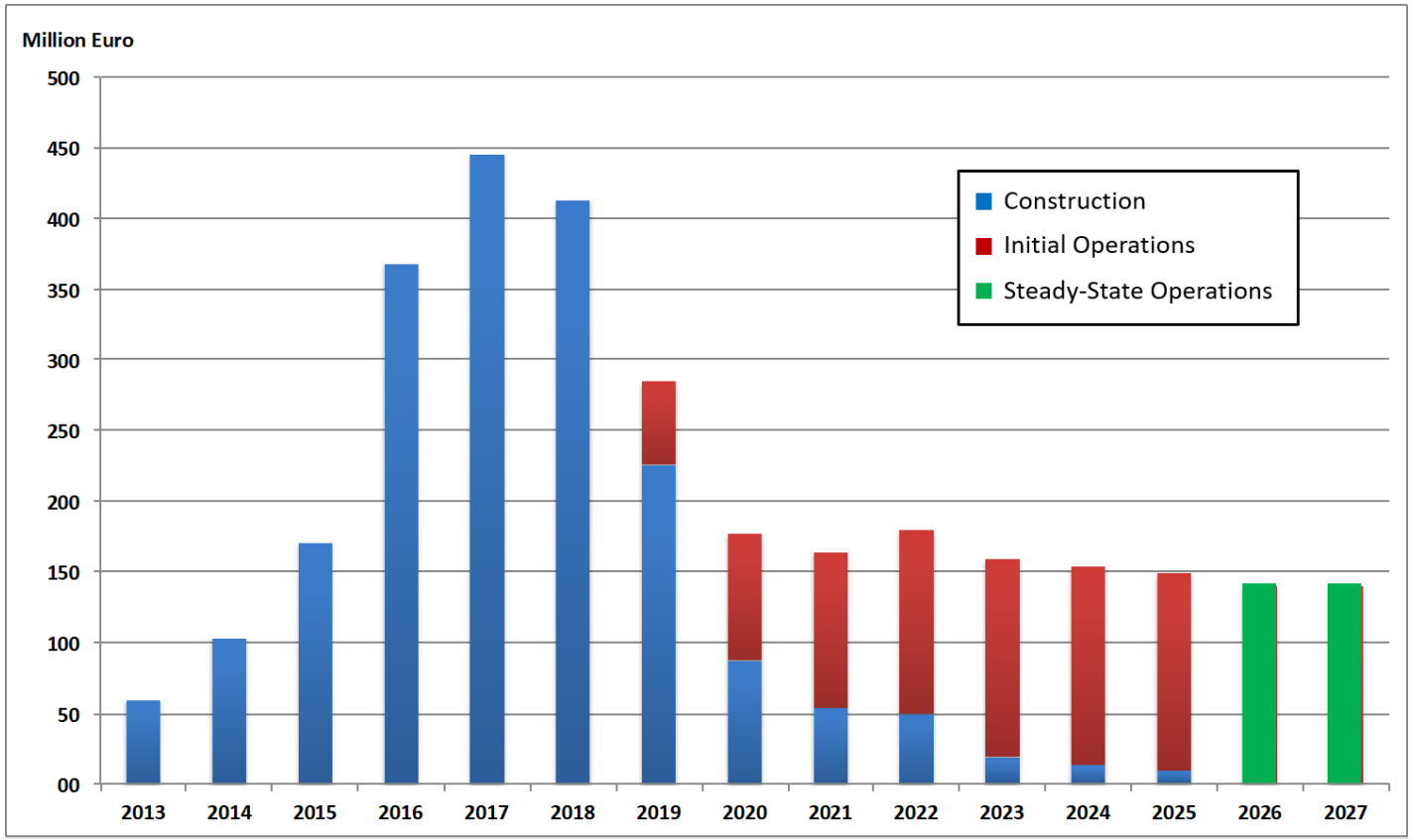
Warsaw University of Technology
Zurich University of Applied Sciences (ZHAW)

The ESS Project

Construction and Operations Budgets



15 Instruments under Construction

First Science on 3 instruments, 8 instruments to be in user operation by 2024

EUROPEAN SPALLATION SOURCE

Large-Scale Structures

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

Diffraction

- HEIMDAL Powder Diffractometer
- DREAM Powder Diffractometer
- Monochromatic Powder Diffractometer
- BEER Engineering Diffractometer
- Extreme Conditions Diffractometer
- MAGiC Magnetism Diffractometer
- NMX Macromolecular Diffractometer

Spectroscopy

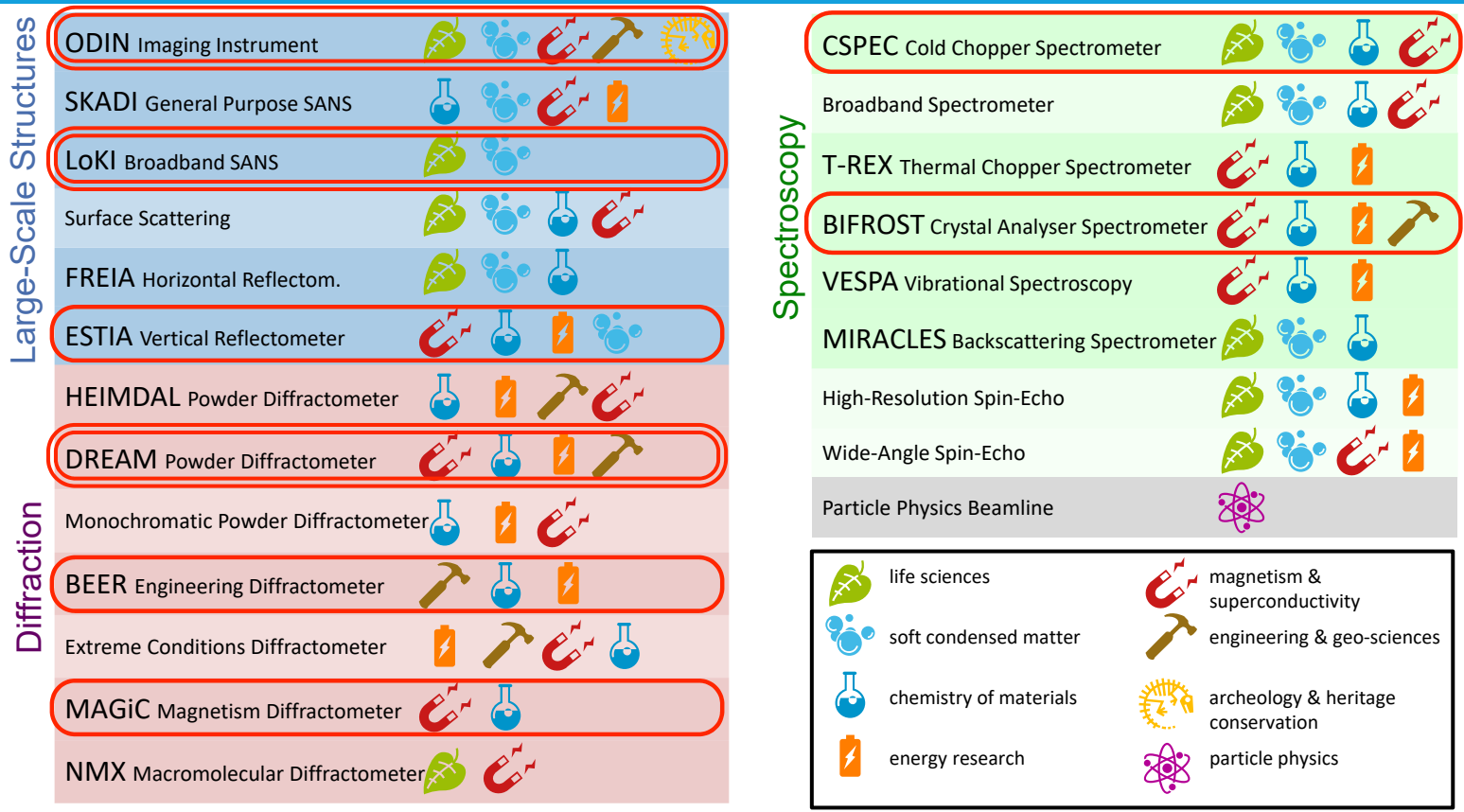
- CSPEC Cold Chopper Spectrometer
- Broadband Spectrometer
- T-REX Thermal Chopper Spectrometer
- BIFROST Crystal Analyser Spectrometer
- VESPA Vibrational Spectroscopy
- MIRACLES Backscattering Spectrometer
- High-Resolution Spin-Echo
- Wide-Angle Spin-Echo
- Particle Physics Beamline

- life sciences
- soft condensed matter
- chemistry of materials
- energy research
- magnetism & superconductivity
- engineering & geo-sciences
- archeology & heritage conservation
- particle physics

15 Instruments under Construction

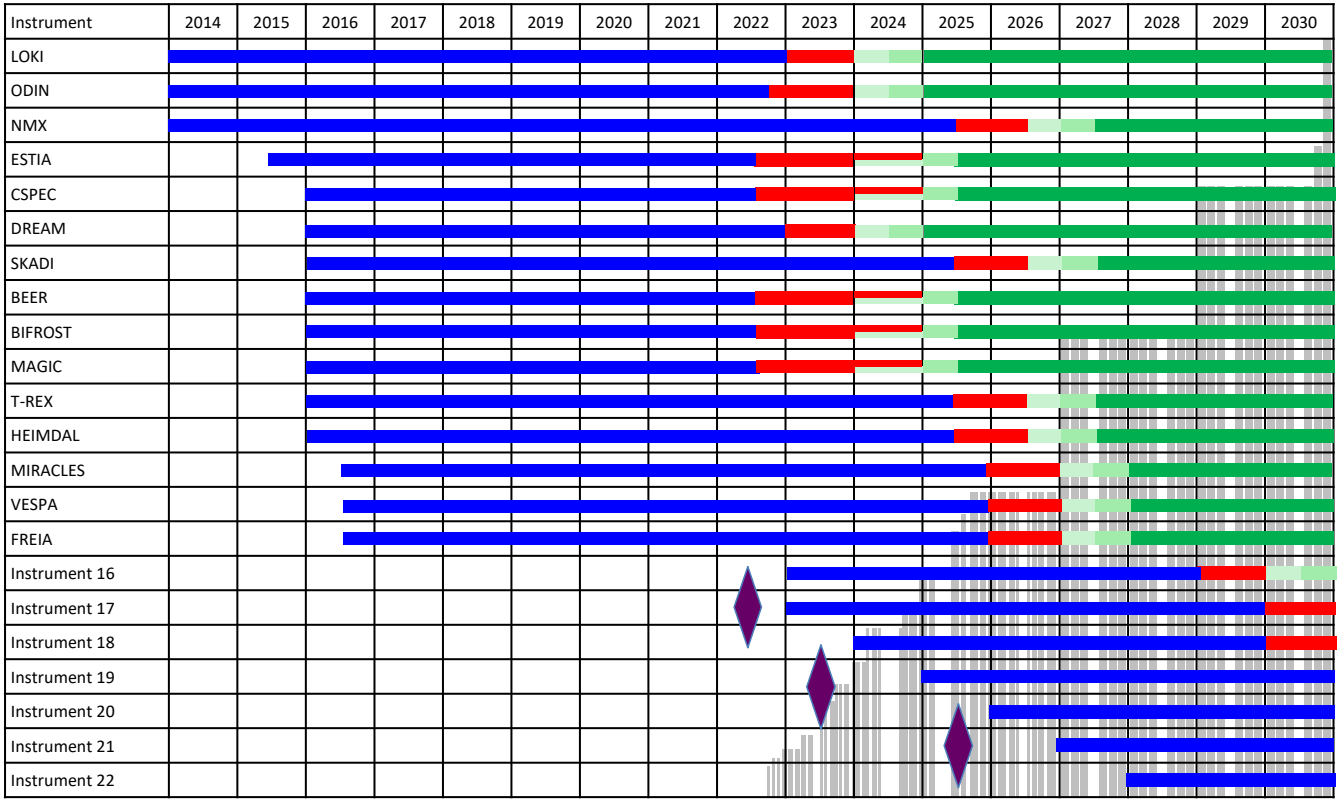
First Science on 3 instruments, 8 instruments to be in user operation by 2024

EUROPEAN SPALLATION SOURCE



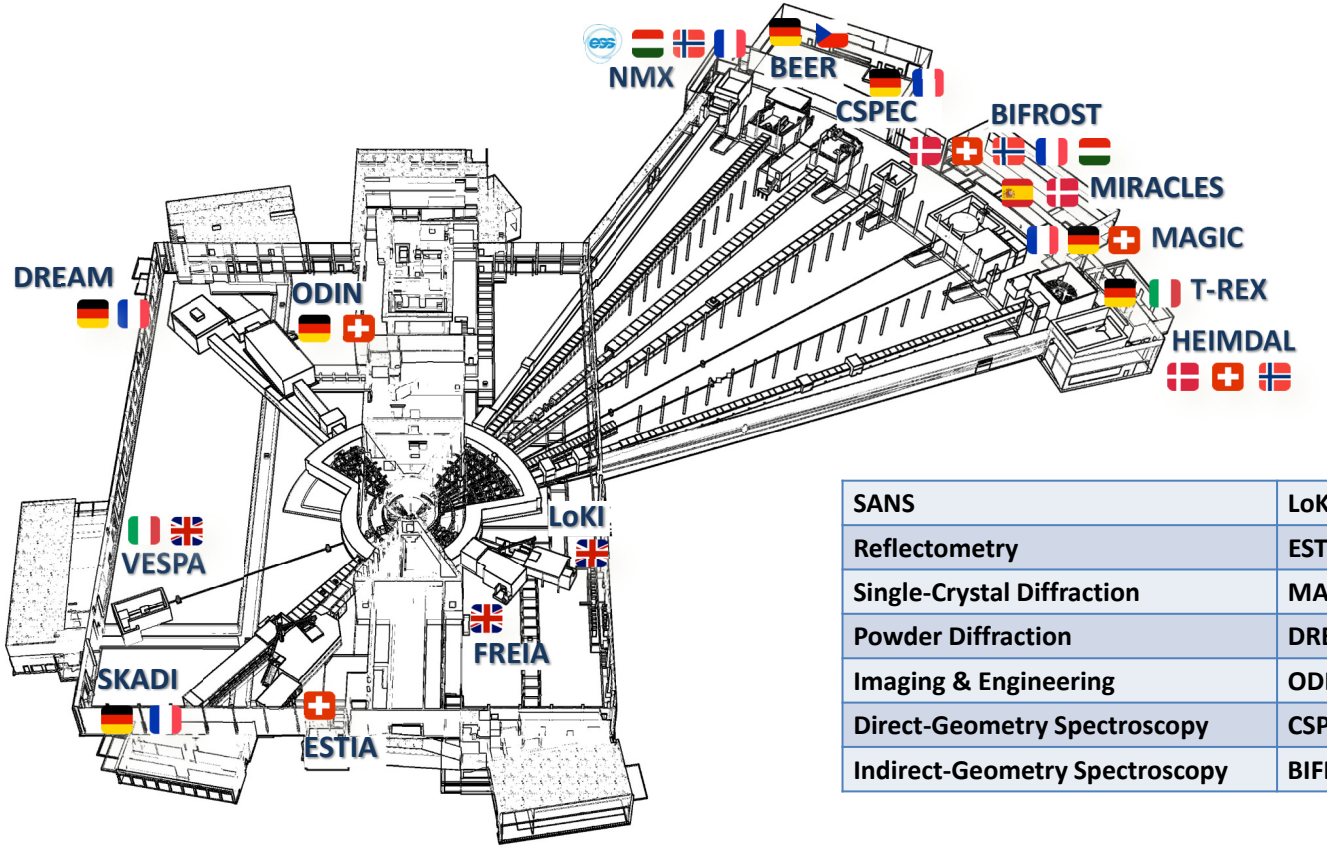
Tentative Instrument Ramp-up

Version 28/6/2019, based on Instrument Construction Working Schedule V4.1



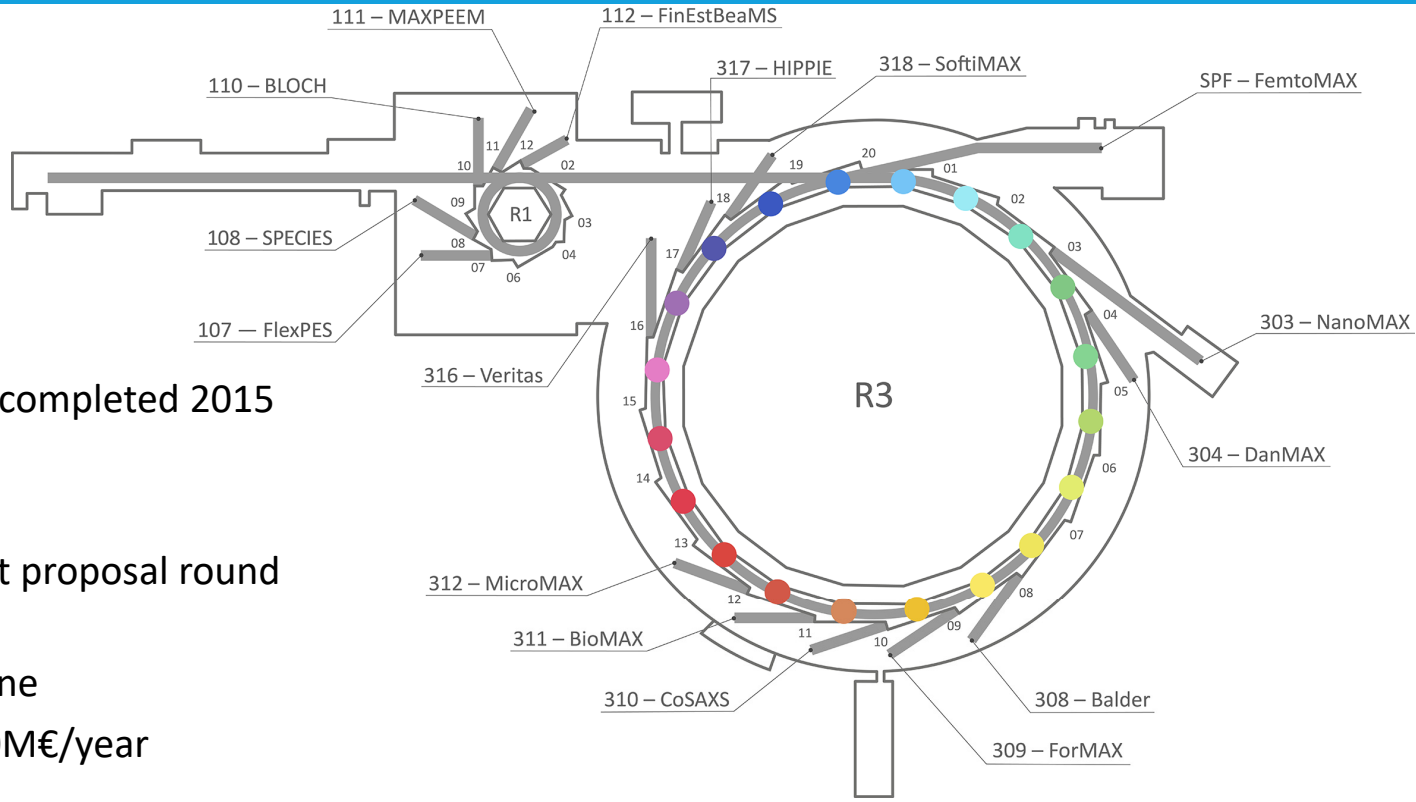
- Instruments 1-15:
  - 2023: First science on 3 instruments
  - 2024: >3 instruments in user programme
  - 2025: 8 instruments in user programme
  - 2027: 15 instruments in user programme
- Instruments 16-22:
  - concept development to start in 2020
  - select first two in 2022
  - Council approval needed

Instrument Suite



SANS	**LoKI,** *SKADI*
Reflectometry	**ESTIA**, FREIA
Single-Crystal Diffraction	**MAGiC**, *NMX*
Powder Diffraction	**DREAM**, HEIMDAL
Imaging & Engineering	**ODIN**, **BEER**
Direct-Geometry Spectroscopy	**CSPEC**, *T-REX*
Indirect-Geometry Spectroscopy	**BIFROST**, MIRACLES, VESPA

MAX-IV Instrument Suite



- Construction project completed 2015
  - 190 M€ budget
- 16 beamlines funded
- 10 beamlines in latest proposal round
  - 22nd August 2019
- 10-15 M€ per beamline
- Operating budget: 50M€/year
  - with 25 beamlines

MAX-IV Inauguration 2016

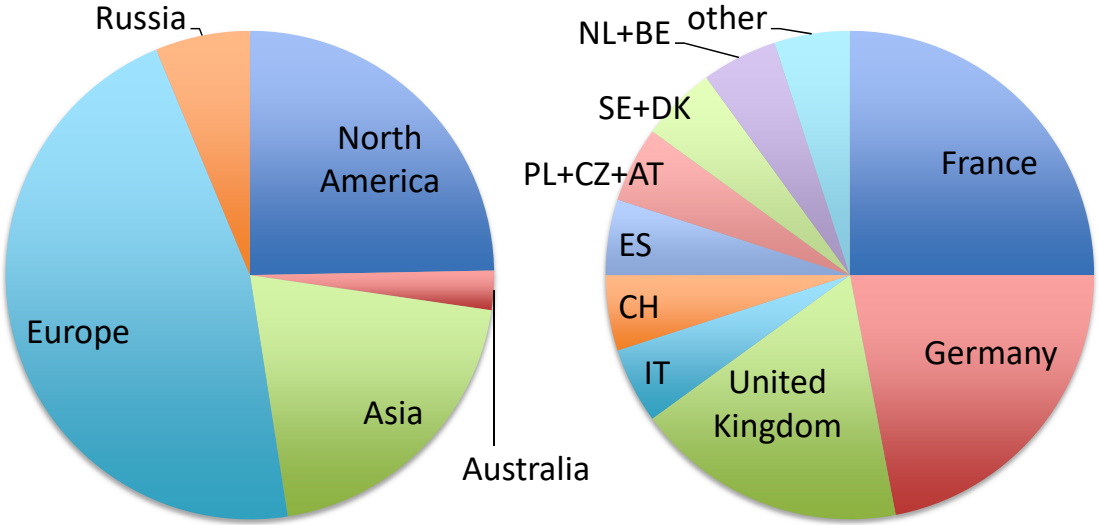
- Inauguration 21st June 2016
  - Director Christoph Quitmann
  - Prime Minister Stefan Löfven
  - King of Sweden Carl XVI Gustaf
- Technical progression
  - MAX-I 1987
  - MAX-II 1995
  - MAX-III 2007
  - MAX-IV 2016
- Swedish national facility
  - located at Lund University

ESS Installation of Ion Source and LEBT

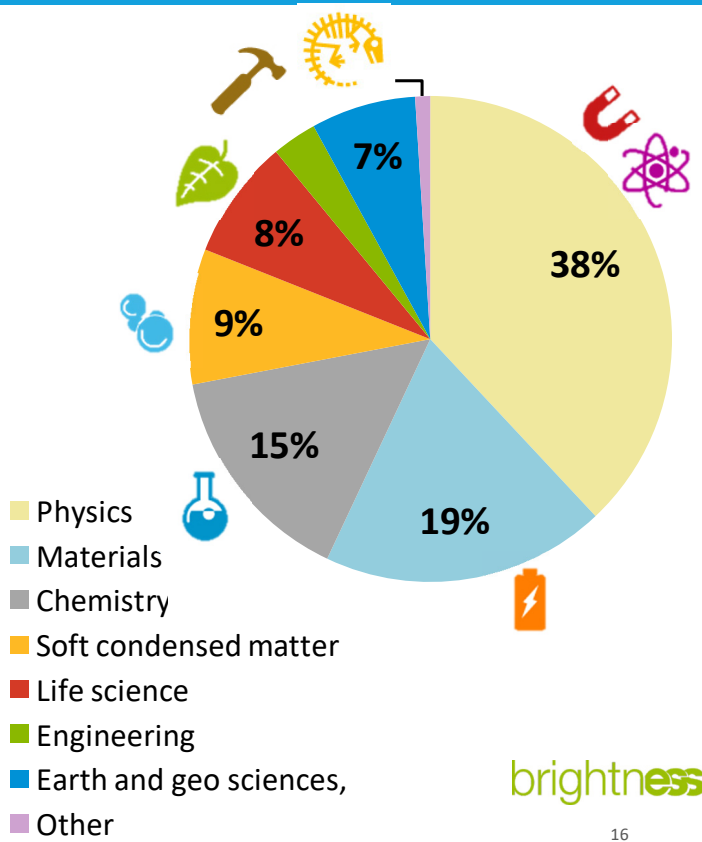
Italian state visit 2018

- Machine inauguration 15th November 2018
  - Director John Womersley
  - King of Sweden Carl XVI Gustaf
  - President of Italy Sergio Mattarella

Neutron User Community



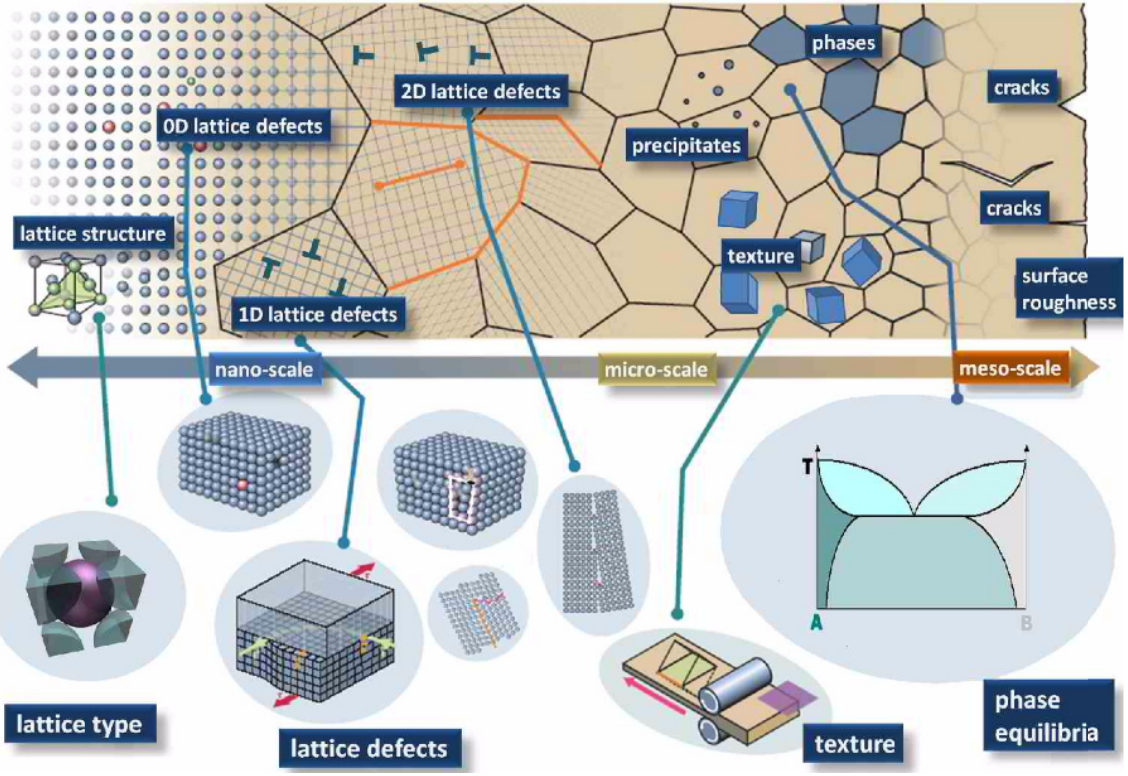
European Community
5000 - 6000 researchers
2000 publications per year

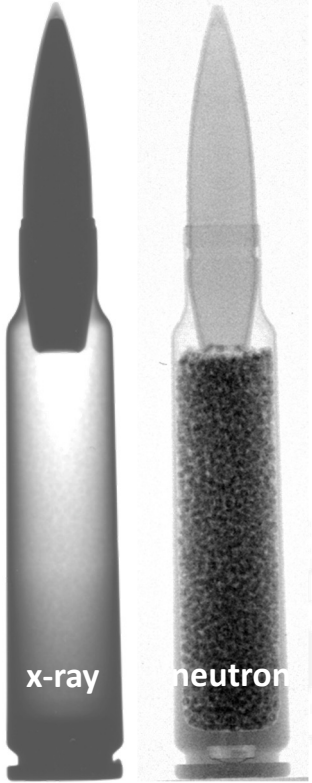


data: ESFRI, KFN

Materials science at many length scales

Neutrons and X-rays are complementary

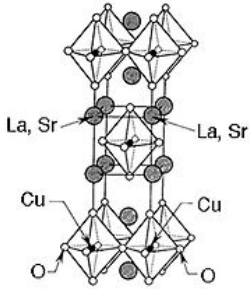


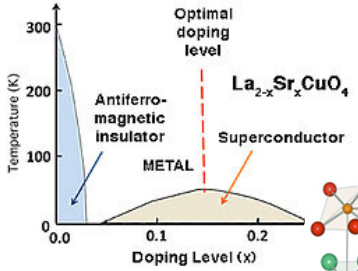


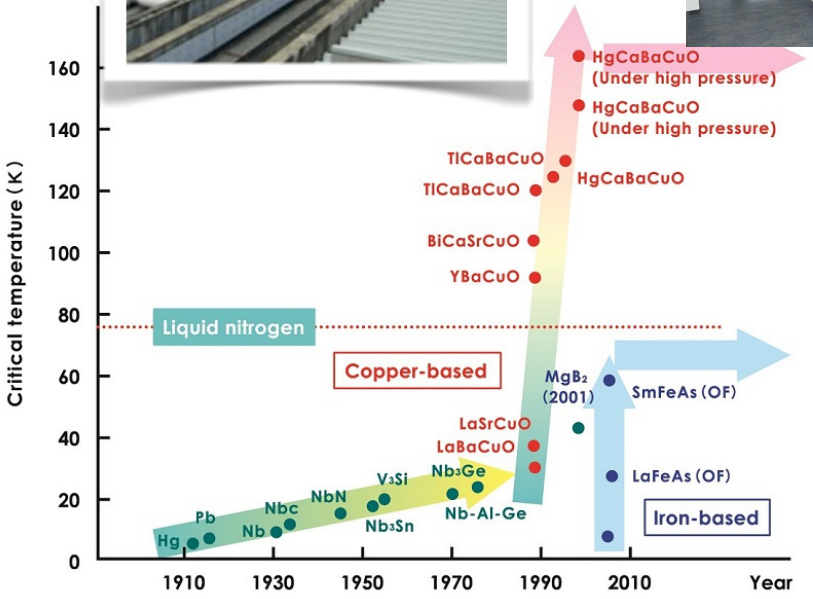
Source: http://www.dierk-raabe.com/

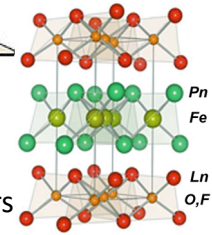
Magnetism and Superconductivity

closely linked phenomena





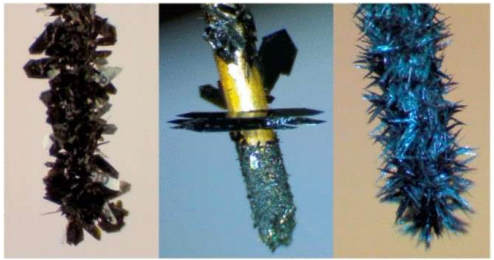


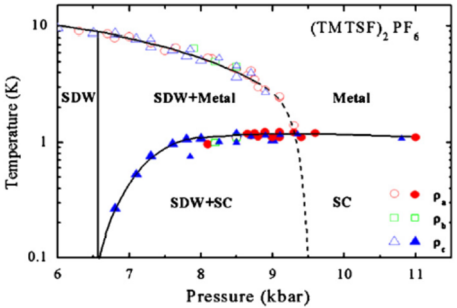


2-dimensional cuprate superconductors

2-dimensional Fe-pnictide superconductors

1-dimensional organic superconductors, needing high pressure



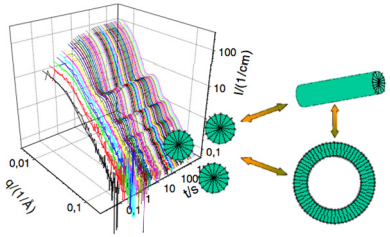


Soft Matter and Life Science Challenges

Complexity and Heterogeneity

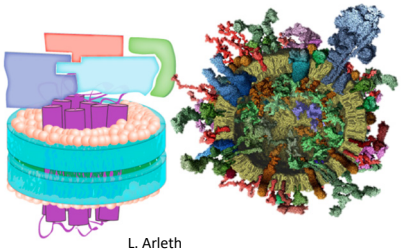
EUROPEAN SPALLATION SOURCE

Kinetics



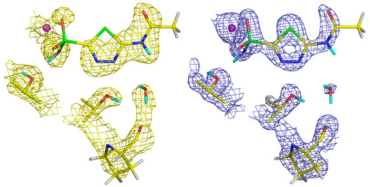
Bressel et al. (2010) Coll. and Polym. Sci. 288, 827

Bio-molecular Complexes



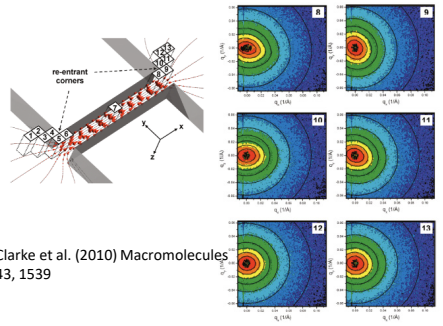
L. Arleth

Rational Drug Design



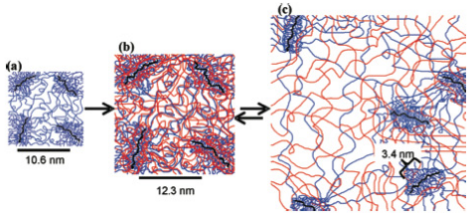
Fisher et al. (2012) JACS 134, p.14726.

Flow Mapping



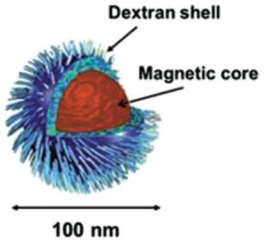
Clarke et al. (2010) Macromolecules 43, 1539

Hierarchical Structures



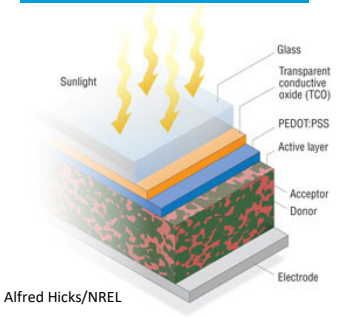
Waters et. al (2011) Macromolecules 44 5776

Hybrid Soft-Hard



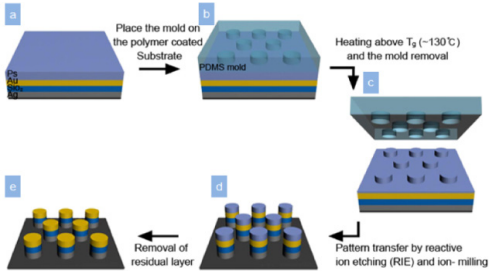
Krycka, K. L., et al. *J. Appl. Phys.* **2011**, *09*, 07B513

Operating Devices



Alfred Hicks/NREL

Patterned Materials

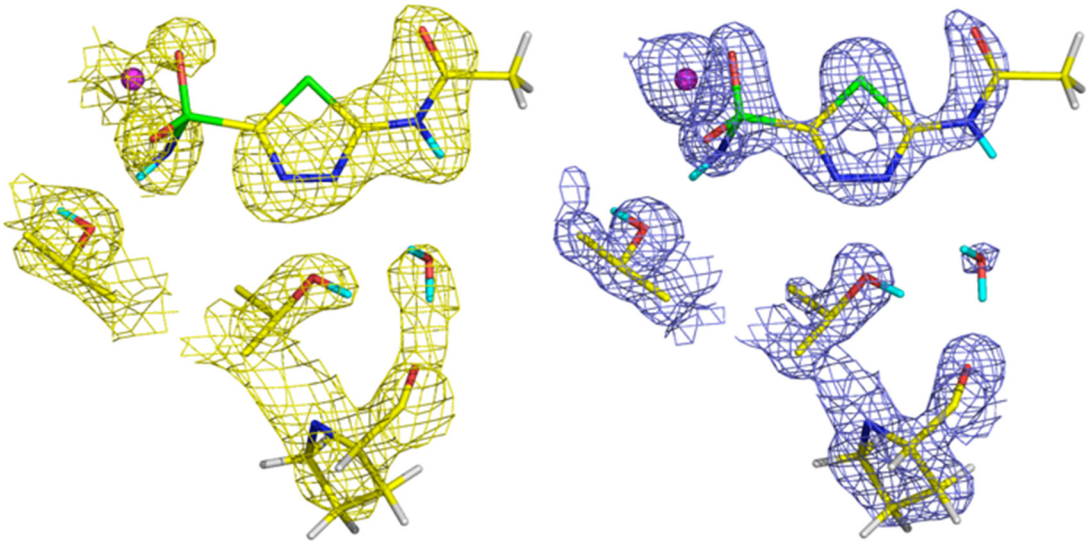


Kim et al. (2012) Nanotechnology **23** 315302

Drug-Target Binding

Macromolecular Crystallography: “go-to” technique for rational drug design

X-rays and neutrons combined can elucidate specific binding interactions between drug and disease target.
Data can reveal protonation state of ligands.
Can determine the atomic details of drug binding as mediated by hydrogen bonding, solvent-mediated interactions, and which groups of the protein and/or drug are directly involved.
** Get clues about which parts of the drug to target for modification.



Neutrons X-rays

Clinically used drug (acetazolamide – commonly used diuretic) in complex with human drug target, carbonic anhydrase.

Yellow: nuclear density maps reveal H atoms

Blue: electron density maps reveal positions of heavier atoms

Joint X-ray & neutron studies reveal the “full” details of drug binding (water-mediated, H-bonds). Complementary!
Fisher et al. (2012) JACS 134, p.14726.

Where is the world heading?

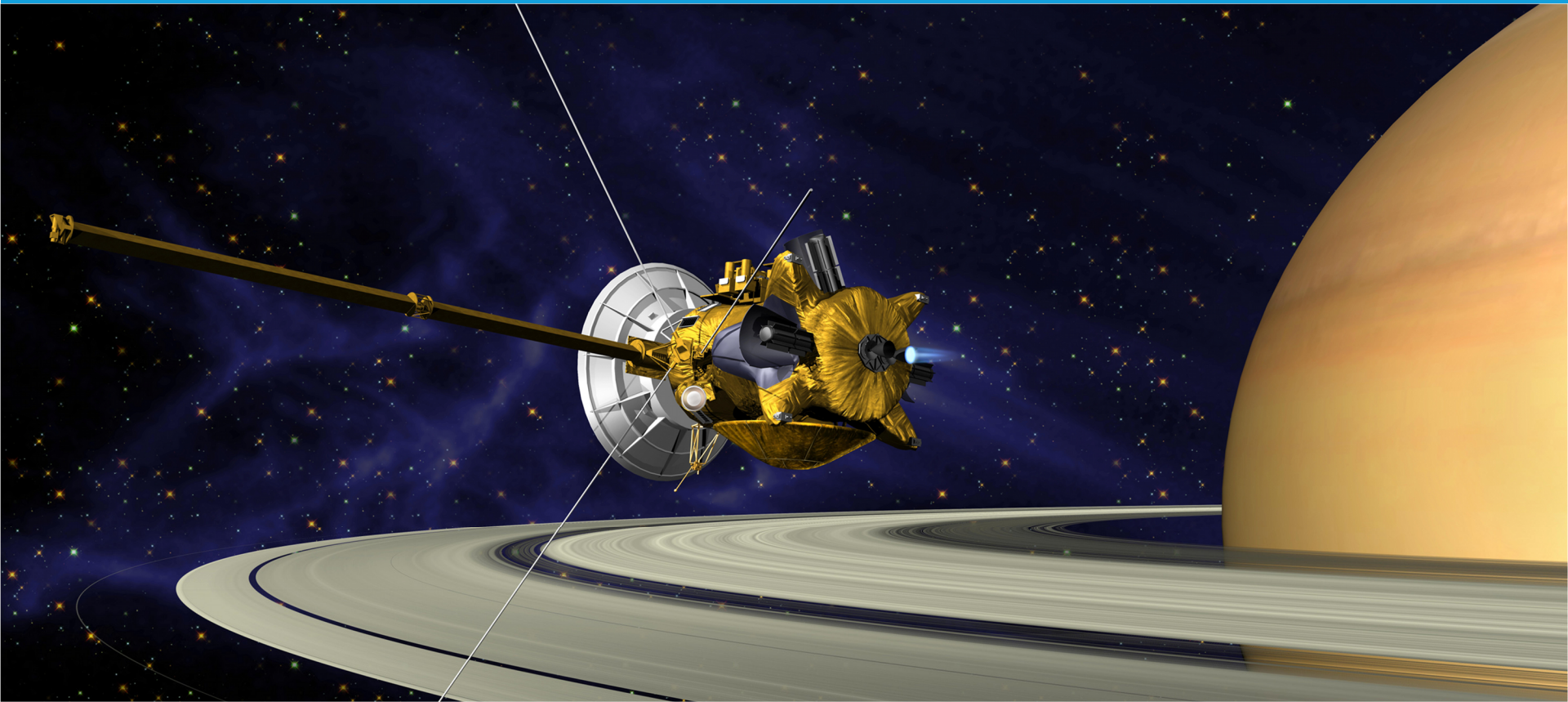
where is science going?

- Societal grand challenges
  - energy: generation, distribution, storage, sustainability
  - environment: climate change, pollution, desertification
  - health: antibiotic resistance, cancer, ageing, infectious diseases
  - transport: electrification, self-driving
  - manufacturing: additive manufacturing, strain, microstructure
  - economic competitiveness: knowledge-based, technology, artificial intelligence, machine learning
- All these areas require improvements in materials
  - basic research underpins all commercial materials R&D
  - timescale from basic research to market is too long for most industry funding
- Current trends in materials research:
  - targeted materials discovery requires much better microscopic understanding
  - functional biological molecules
  - high-pressure environments for planetary sciences and geology
  - real materials are heterogeneous – needs understanding on many length scales
- Neutron and x-ray scattering provide unique insights in all these areas!

Are large science facilities good value for money?

astronomy versus materials science

EUROPEAN SPALLATION SOURCE



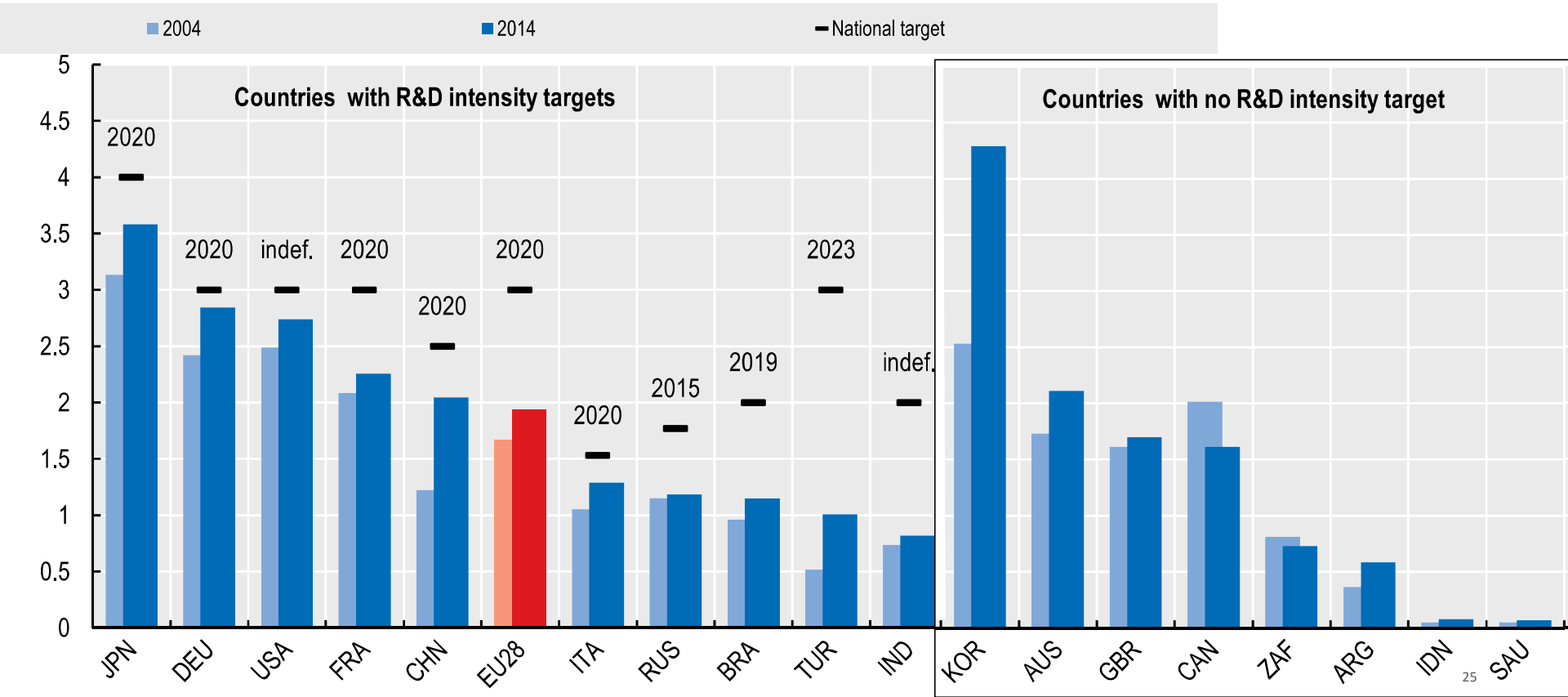
Are large science facilities good value for money?

astronomy versus materials science

- Cassini-Huygens mission
  - total cost: 3.9 G$ over 20 years
  - 3948 science papers
- MAX-IV: 1.2 G€ over 20 years (2012-2031), including 15 years of operations
- ESS: 3.8 G€ over 20 years (2013-2032), including 10 years of operations
- Each will deliver ~ 3000 papers during that period
- Each will deliver primarily societally-relevant materials research
- Each will operate for way more than 20 years

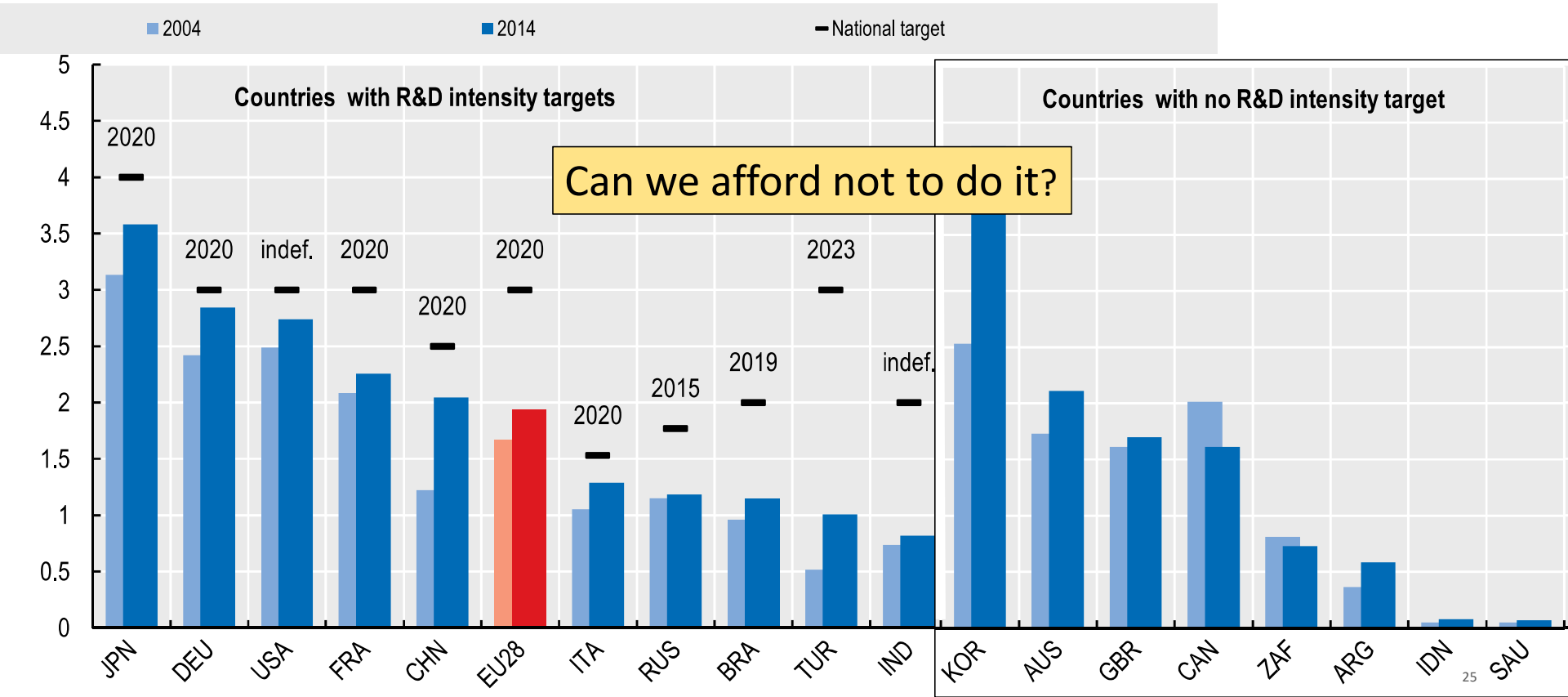
Can we afford materials science research?

G20 Innovation Report 2016



Can we afford materials science research?

G20 Innovation Report 2016



Final words…

- ESS and MAX-IV will both be world-leading in their field
  - unique assets for scientists locally, regionally, world-wide
- Large-scale research infrastructure investments
  - neutrons and x-rays are central to materials R&D
  - especially in wealthy countries
  - self-interest: economic competitiveness
  - globally: addressing the most important societal challenges
- Lund is uniquely placed as a materials science hub

Thank you!