 EUROPEAN
SPALLATION
SOURCE

ESS – Opportunities for the Life Sciences

Sindra Petersson Årsköld
Ass. Prof, Senior Advisor

www.europeanspallationsource.se
19-03-12

Neutron science: Fundamental science
with applications

 EUROPEAN
SPALLATION
SOURCE

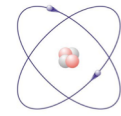


Energy Environment and climate Medicine and health Electronics and IT Manufacturing and industry Natural world Heritage science

Hydrogen-fuelled society Sub-zero survival Superconductors Disease resistant crops Tackling chemical waste in the pharmaceutical industry

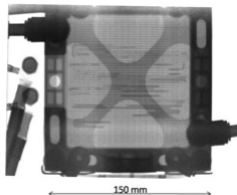
Flexible plastic solar cells Tracking cholesterol Enhanced oil recovery Infection sensors Stress relief in the air

Neutrons are special



SCIENCEPHOTOLIBRARY

Charge neutral
Deeply penetrating

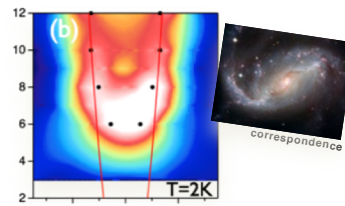


Li motion in fuel cells



Improve electric cars

Magnetic moment (spin)
Probe of magnetism

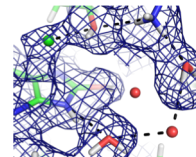


Solve the high-temperature
Superconductivity puzzle

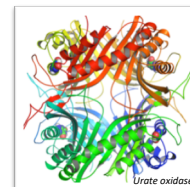


Efficient high-speed trains

Nuclear scattering
Sensitive to light
elements and isotopes



Active sites in proteins

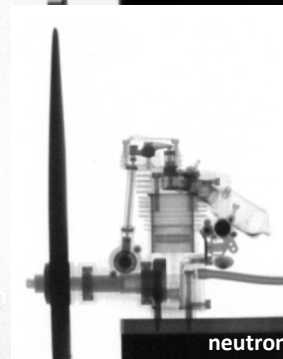
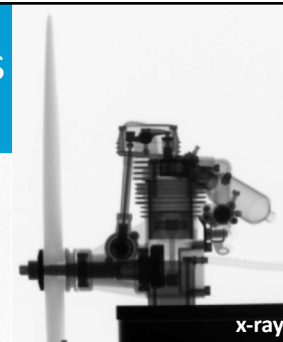


Better drugs

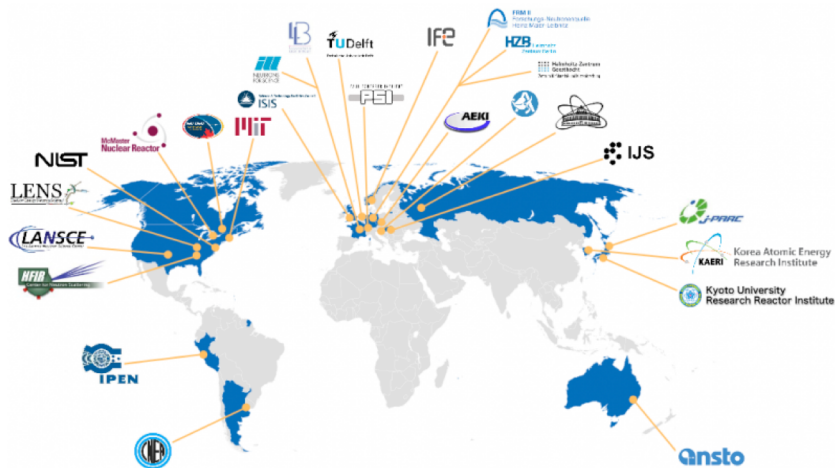
Neutrons See the Light Elements



Courtesy of the NIAG group, PSI,
Switzerland.

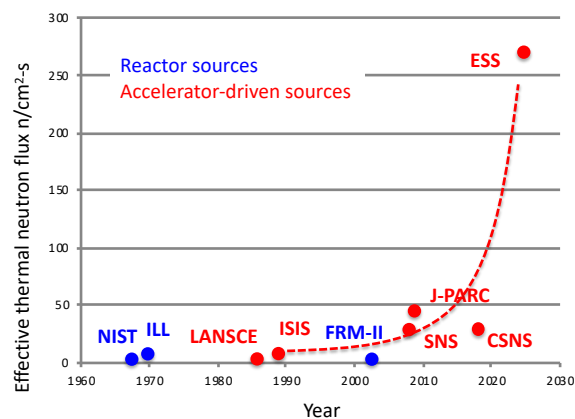


Neutron facilities today

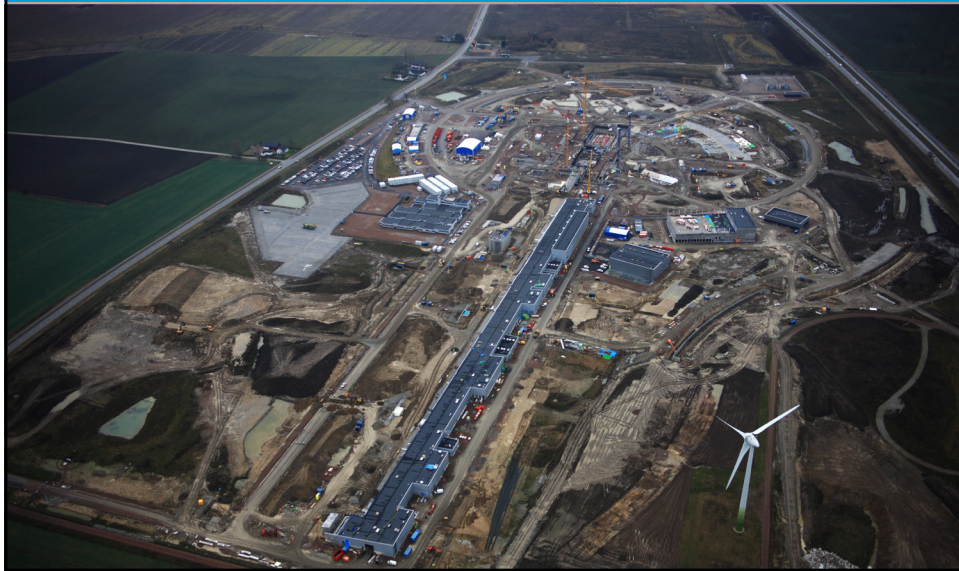


Sindra Petersson Årsköld

Higher neutron flux gives more experimental possibilities



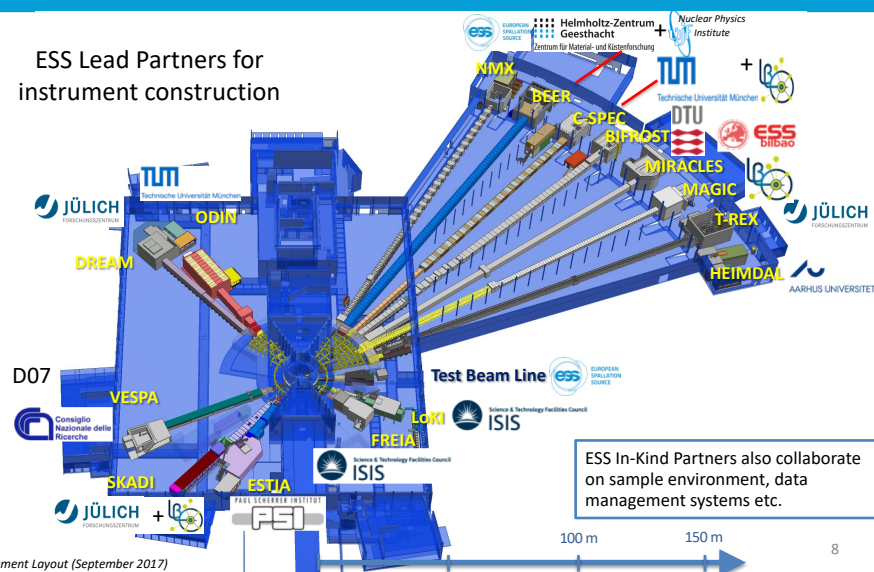
ESS: Accelerator, target, and instruments for science



ESS Neutron Instruments 1-15 + test beamline



ESS Lead Partners for instrument construction




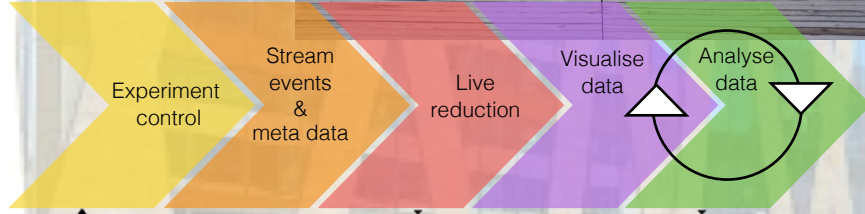
The ESS Data Management and Software Centre is located in Copenhagen

Provide world leading scientific software and scientific computing support for neutron scattering at ESS

Scientific Software development.
 Experiment control
 Data acquisition system
 Data reduction, analysis & modelling

Data centre operations.
 Dual location - Lund & Copenhagen
 Data management and curation

User programme support
 Data scientists
 User office software
 Remote access to data and software tools

Experiment control → Stream events & meta data → Live reduction → Visualise data → Analyse data



Financing includes cash and deliverables



Construction investment 1 843 M€₍₂₀₁₃₎

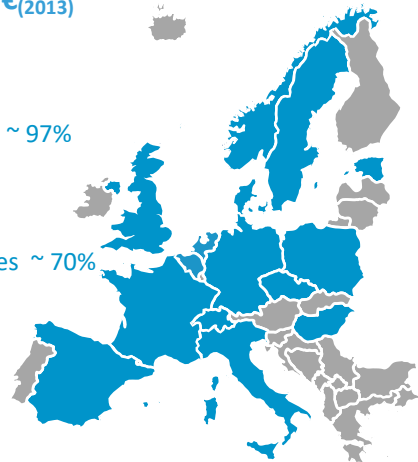
Operations cost ~150 M€/yr

Host Countries Sweden and Denmark

Construction 47.5% **Cash Investment ~ 97%**
Operations 15%

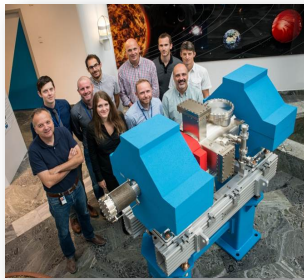
Non-host Member Countries

Construction 52.5% **In-kind Deliverables ~ 70%**
Operations 85%



11

ESS In-kind Partners



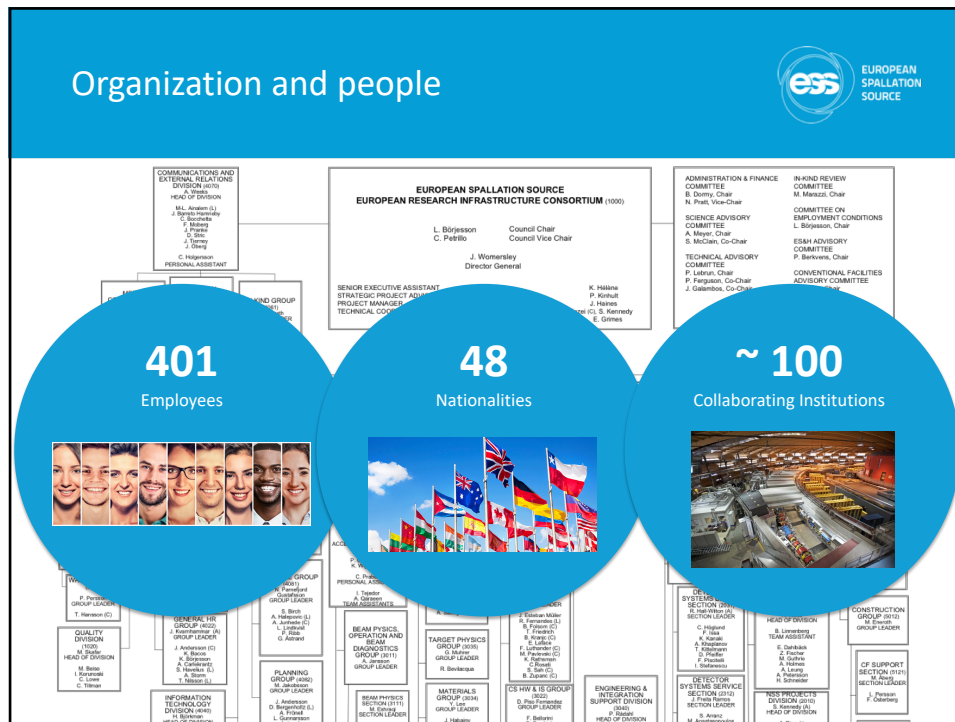
Elettra – Sincrotrone Trieste
ESS Bilbao
Forschungszentrum Jülich
Helmholtz-Zentrum Geesthacht
Huddersfield University
IFJ PAN, Krakow
INFN, Catania
INFN, Legnaro
INFN, Milan
Institute for Energy
Research (IFE)




Rutherford-Appleton Laboratory,
Oxford(ISIS)
Kopenhagen University
Laboratoire Léon Brillouin (LLB)
Lund University
Nuclear Physics Institute of the ASCR
Oslo University
Paul Scherrer Institute (PSI)
Polska Grupa Energetyczna - PGE
Roskilde University
Tallinn Technical University




12



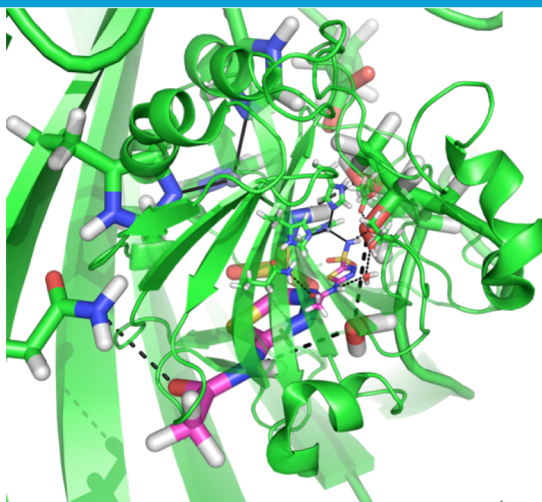
ESS is a user facility


**EUROPEAN
SPALLATION
SOURCE**

- Researchers who need neutron beams for their experiments.
- From universities, institutes, industry.
- ESS provides tools & support; the users bring their projects and perform the experiments.
- 2000-3000 visiting users/year. A stay can be days or weeks.
- Many different disciplines: materials research, physics, chemistry, life science...
- Access modes vary: from open and free-of-charge to proprietary pay-for-beamtime.



Neutrons reveal how drugs interact with drug targets

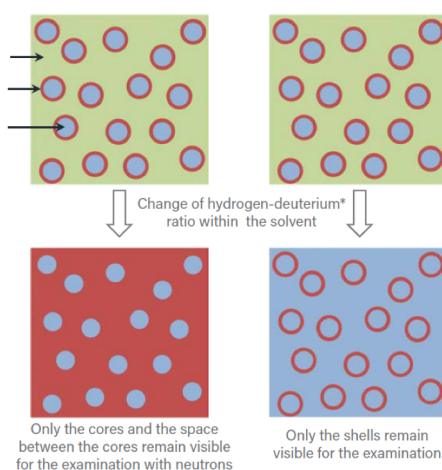


The enzyme carbonic anhydrase transports CO_2 and regulates blood acidity. It is a major player in some cancers, glaucoma, obesity and high blood pressure

Neutron crystallography pinpoints protons and waters in the active site, showing how the drug Acetazolamide binds

Image: Fisher, S. Z. *et al.* 2012 JACS

Selective deuteration and neutrons lets us unravel information on complex samples



*When the monster came,
Lola remained undetected.*

*Harold, of course, was
immediately devoured.*

Selective deuteration in combination with neutrons lets us investigate selected parts of complex assemblies.

I. Grillo, ILL

Neutrons Make Pregnancy Tests More Sensitive and Cheaper



With neutron reflectometry experiments, scientists can investigate the interaction between antibody and antigens and the importance of a blocking protein, present in home pregnancy tests.

They found that it is not worth to increase the quantity of antibodies above a certain level for an optimal performance. Thus, neutron studies can help to not only control the quality but also reduce cost considerably, as antibodies are very expensive.

Case: J.R. Lu et. al, University of Manchester, UK

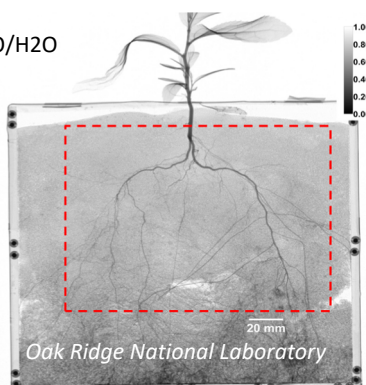
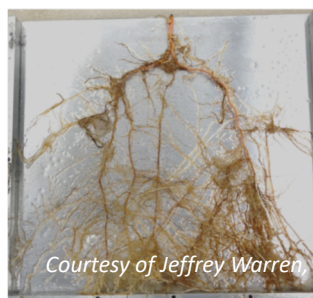
Bioimaging with neutrons



Neutron imaging is very successful in engineering science.
The ODIN instrument at ESS will be world-leading in neutron imaging.

Bioimaging with neutrons

- With ODIN, resolution down to $\sim 10 \mu\text{m}$, $\sim 1 \text{ s}$.
- Contrast in biological samples can be challenging.
- Following liquids is often a successful approach. D₂O/H₂O exchange.
- Most mature bioimaging science area now: plant roots.
- Neutrons don't see all roots, but they see all H₂O.

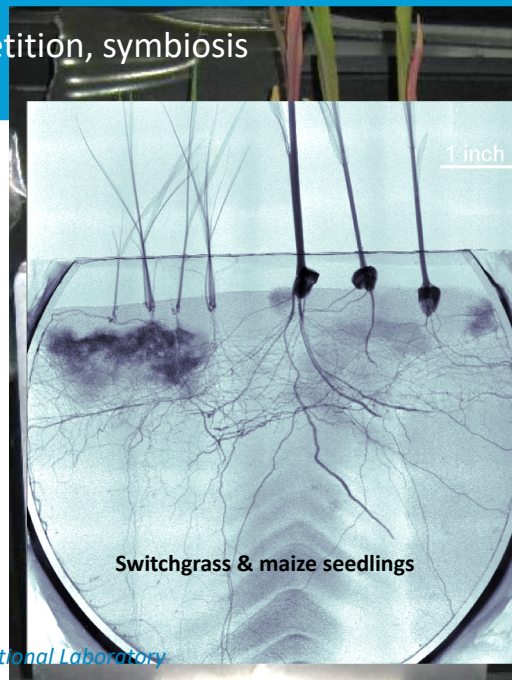


Root distribution, competition, symbiosis

Coarse and fine root morphology and distribution readily visible.

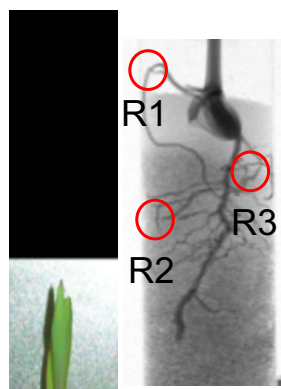
Fungal hyphal mass visible near roots of switchgrass, revealing substantial hydration of the rhizosphere.

Triangular pattern in soil indicates varying water content & porosity due to separation of particle sizes as chamber was filled with sand.



Courtesy of Jeffrey Warren, Oak Ridge National Laboratory


3D tomography of 10 day old maize seedling



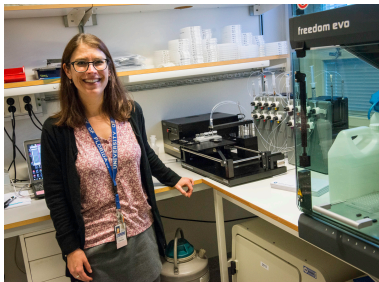
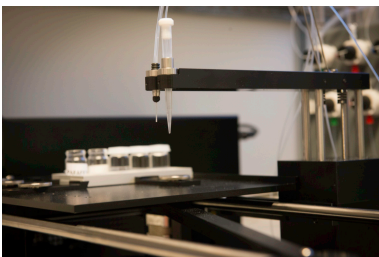
- Neutron radiograph at 100 μm pixel resolution illustrating root distribution (0.2-1.6 mm)
- Track water flow through three roots

Courtesy of Jeffrey Warren, Oak Ridge National Laboratory

DEMAX: Supporting life science users of ESS



EUROPEAN
SPALLATION
SOURCE





Collaborative service

- Crystallization
- Biological deuteration
- Chemical deuteration (DEUNET)

A knowledge hub

- Lund University collaboration: Synergies in staffing, equipment and space. **Critical intellectual mass.**
- Similar support for other methods, such as MS and NMR.
- A hub for training and meetings, a natural meeting place in the global neutron structural biology community.



European Molecular
Biology Laboratory

EMBL: “ESS could be a game changer for our use of neutrons.”

Thank you!



February 2017







DMSC August 2016