EUROPEAN SPALLATION SOURCE

The European Spallation Source

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e-Infrastructure Reflection Group, November 10th 2014

Outline

- (Very brief) What is neutron scattering?
- Context for the ESS project + (very brief) why is ESS brighter
- ESS Partnership + Organization
- DMSC – Data Management and Software Centre
  – Mission & scope for ESS + other projects
- Where could e-Infrastructures help ESS ??

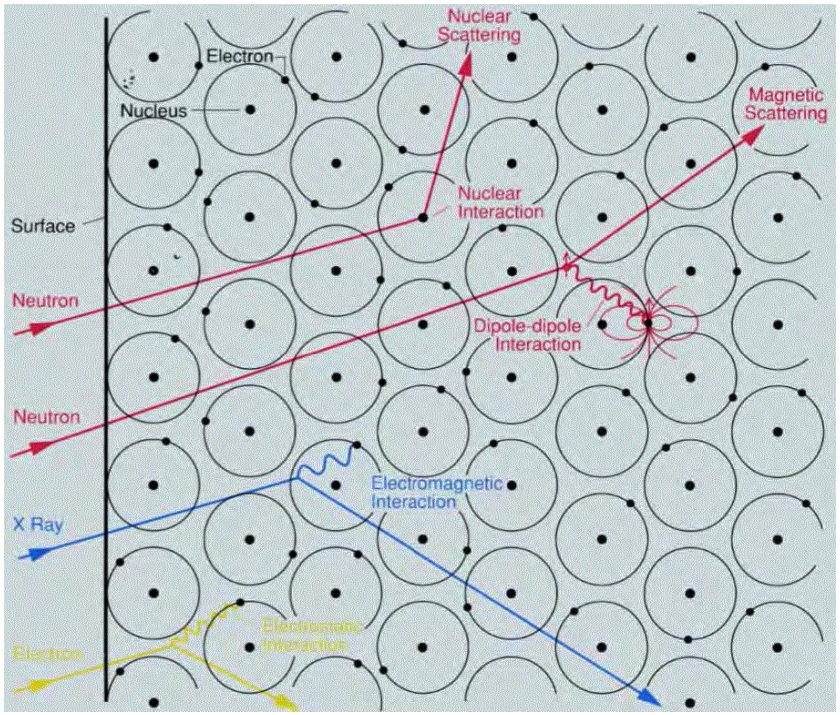
Timeline:

- ESS accelerator & target produce first neutrons – 2019
- ESS (first 16) instrument construction completes – 2019 to 2025
- ESS User research program begins in 2023

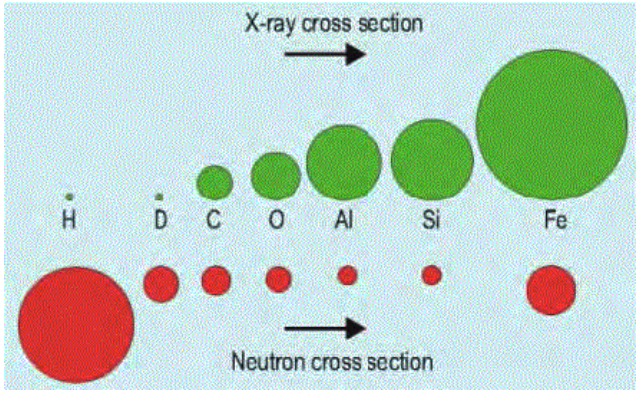
Thermal Neutron Scattering

Charge neutral
Deeply penetrating

Thermal neutrons
Wavelengths and energies comparable to the inter-atomic spacings and lattice dynamical energies in materials



Nuclear scattering
Sensitive to light elements and isotopes



S=1/2 spin
probe directly magnetism

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}(\gamma r_0)^2 \left|\frac{g}{2}F(\vec{\kappa})\right|^2 e^{-2W(\vec{\kappa})} \sum_{\alpha\beta}\left(\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta\right) \times \int dt\, e^{-i\omega t} \sum_{ll'} e^{i\vec{\kappa}\cdot(\mathbf{r}_l - \mathbf{r}_{l'})} \left\langle \mathbf{S}_l^\alpha(0)\mathbf{S}_{l'}^\beta(t)\right\rangle$$

Thermal Neutron Scattering

Neutron scattering as a technique can be used in the study of a wide variety of materials,

- Soft Condensed Matter
  - Self-assembled colloids
  - Polymers
  - Thin film devices
- Life Sciences
  - Macromolecular structures
  - Solution of macromolecular complexes
  - Bio-molecules
- Magnetic phenomena
  - High temperature superconductivity
  - Quantum phenomena
  - Molecular magnets
- Chemistry
  - In-Situ processing
  - Catalysis
  - Waste management
- Energy research
  - Fuel cells
  - Gas storage materials
  - New battery materials
- Engineering sciences, environmental sciences & culture
  - In-situ welding
  - Cultural heritage
- Fundamental physics
  - Lifetime of the neutron
  - Decay mechanisms

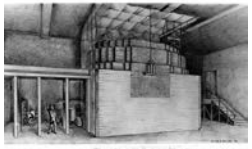
Global context for ESS Project

- 1996 – OECD setup a Neutron Sources Working Group as part of its Megascience forum
- 1998 OECD report – 3 major economic areas, USA, Japan, Europe should build new next generation neutron sources both for capacity & to replace older sources
- 2006 ESFRI (European Strategy Forum on Research Infrastructures) priority for ESS/neutrons 2010 roadmap update, 2014 priority to move forward
- Part of a suite of neutron and x-ray facilities for materials research

	USA	Japan	Europe
High intensity x-ray synchrotron	Advanced Photon Source	Spring-8	European Synchrotron Radiation Facility(1)
Free Electron Laser pulsed x-rays	Linac Coherent Light Source	SACLA (FEL)	European XFEL (1,2)
High flux reactor neutron source	HFIR reactor	JRR3M reactor	Institut Laue Langevin (1)
High intensity spallation neutron source	Spallation Neutron Source	J-PARC (JSNS)	European Spallation Source (1,2)

(1) On the ESFRI roadmap, (2) Under construction

Historical context for ESS Project



Reactors

Spallation

Steady State Sources

Pulsed Sources

NRX

X-10

CP-2

CP-1

Berkeley 37-inch cyclotron

350 mCi Ra-Be source

Chadwick

MTR

NRU

HFIR

HFBR

ILL

ZINP-P/

WNR

ZINP-P

LANSCE

ISIS

IPNS

KENS

SNS

ISIS-TS2

J-PARC (1MW)

J-PARC

SINQ

FRM-II

OPAL

PIK

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Effective thermal neutron flux n/cm^2-s

10^{20}

10^{15}

10^{10}

10^{5}

1

1930 1940 1950 1960 1970 1980 1990 2000 2010 2020

ESS, SNS and MLF/J-PARC

- **Things that are the same:**
  - Use protons to create neutrons via Spallation

- **Things that are different:**
  - SNS uses H- and a ring to produce p
  - ESS will produce p from a plasma & only a Linac
  - SNS & MLF/J-PARC use Liq-Hg target
  - ESS will use rotating W wheel

  - J-PARC & SNS have short p & n pulses
  - ESS will have a long pulse structure

- **Things that are the same:**
  - Time of flight neutron scattering instruments
  - “Materials and Life Sciences” Research

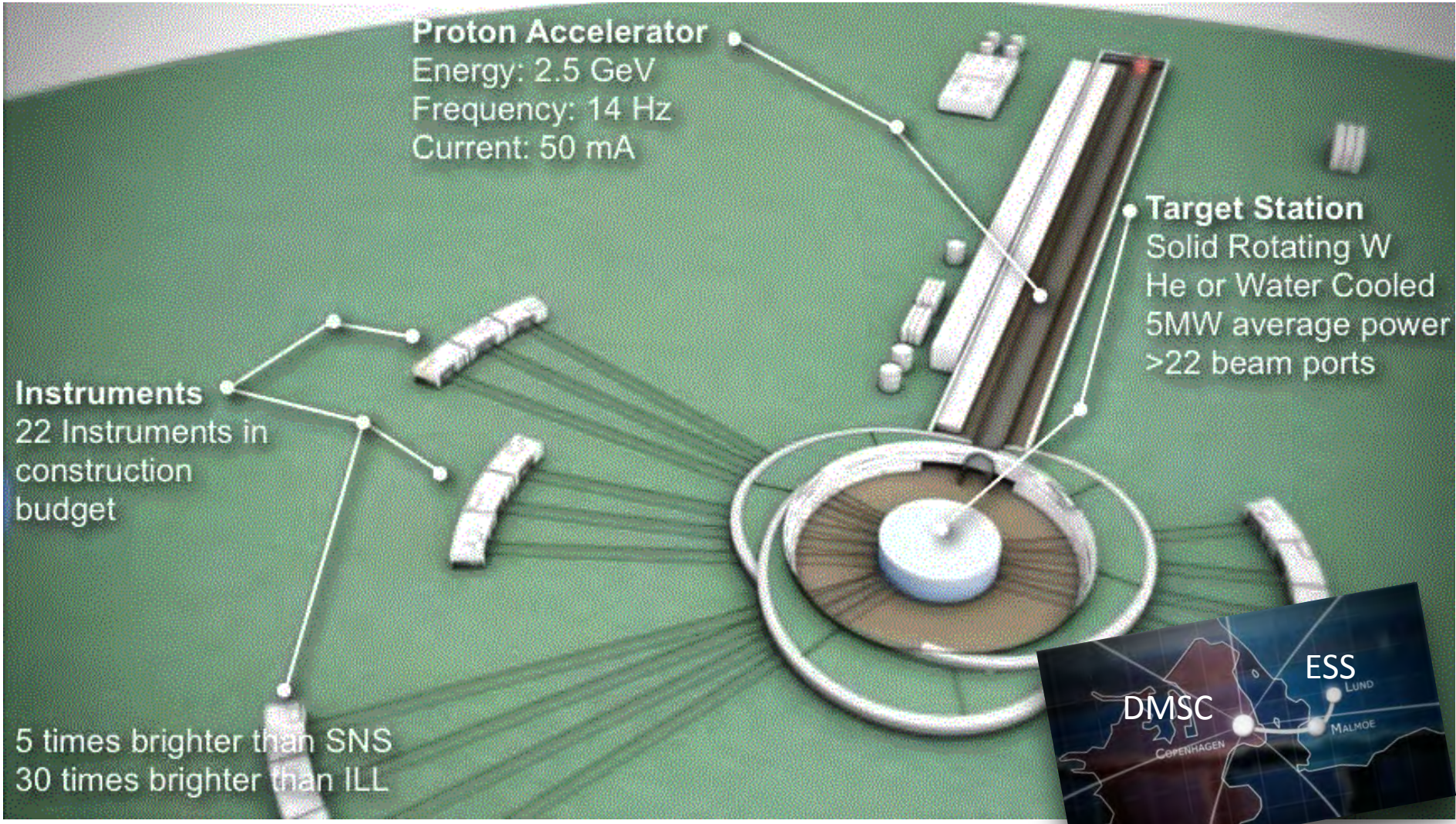
Europe is in a good position

Materials Structure Facilities

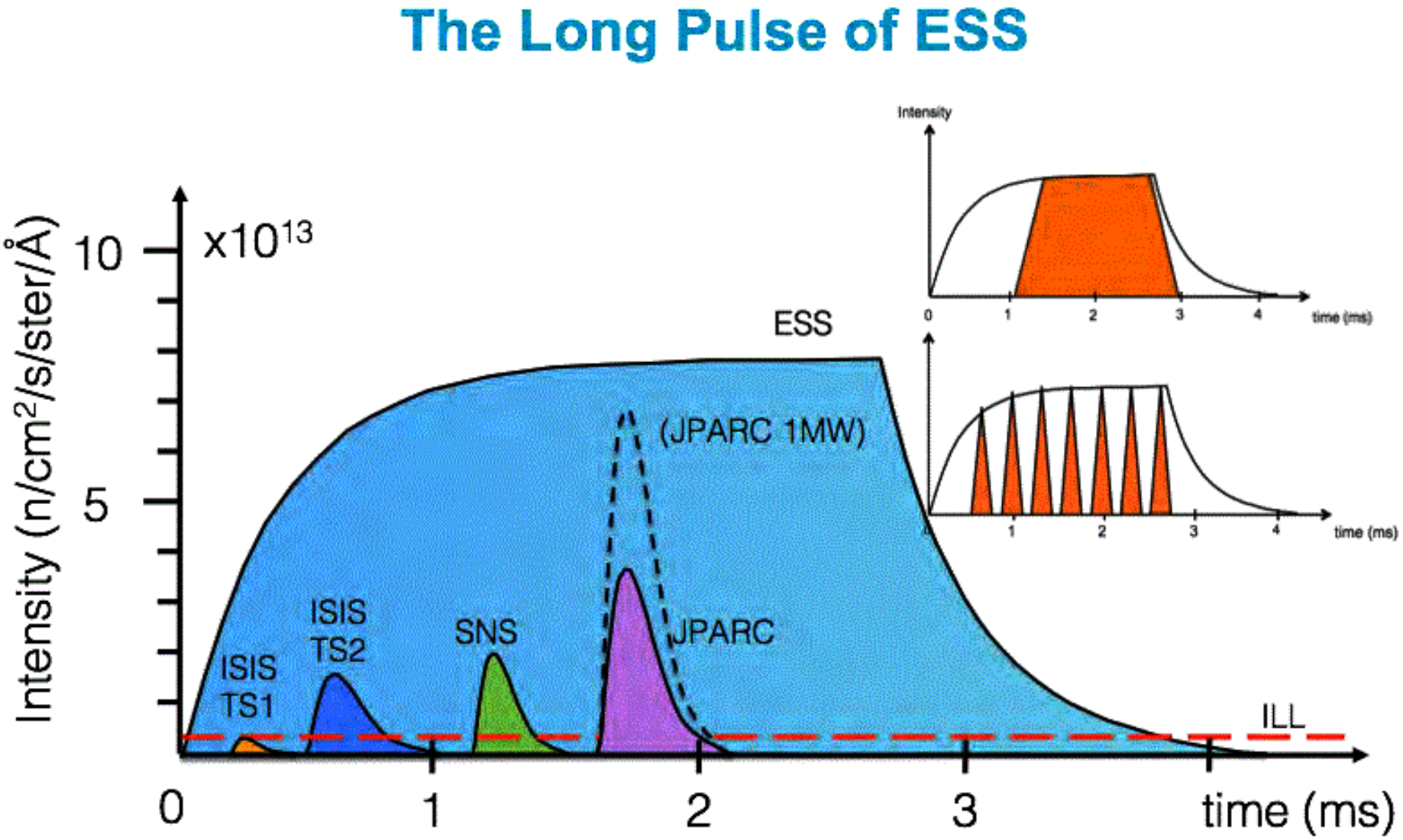
Two best facilities in world:
Reactor: I.L.L.
X-ray synchrotron: ESRF

Under construction 2 best facilities in world:
XFEL: European XFEL
Spallation: E.S.S.

How will the ESS work?



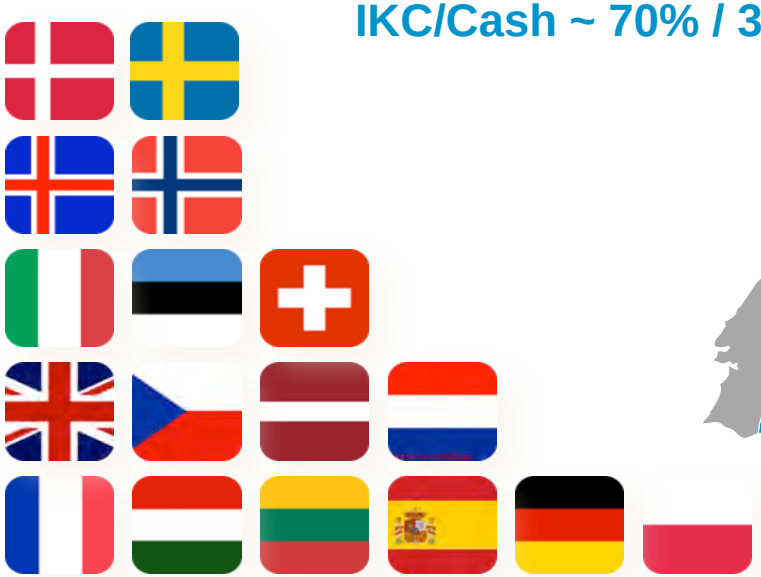
ESS and the Long Pulse

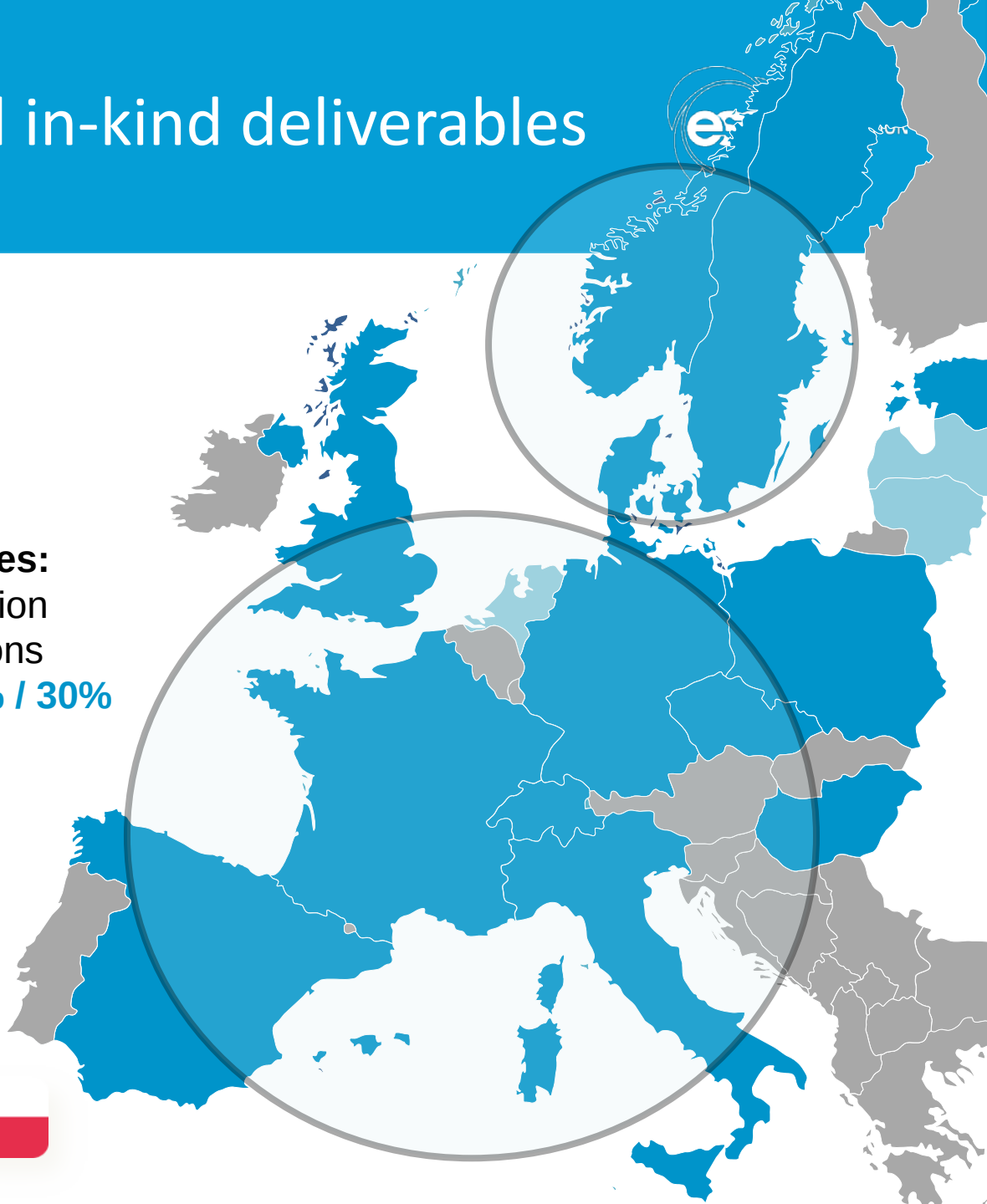


Funding is cash and in-kind deliverables

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

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





ESS construction funding status

Contributions by Member Country (August 2014)	
Country	**Percentage**
Sweden	35.0%
Denmark	12.5%
Germany	11.0%
United Kingdom	10.0%
France	8.0%
Italy	6.0%
Spain	5.0%
Switzerland*	3.5%
Norway	2.5%
Poland	2.0%
Hungary	1.5%
Czech	0.3%
Estonia	0.25%
To Be Determined **	2.5%
Total	100%

* 3.5% planned share. 1.4% adopted for the period 2014-2019.

** Discussion ongoing with the Netherlands, Latvia, Lithuania and Iceland.

ESS Cost Baseline

ESS Construction Budget	**M€[1)]**
Conventional Facilities, Energy, and Infrastructure Support	531.9
Accelerator Systems	510.0
Target Systems	155.3
Neutron Scattering Systems	350.0
Integrated Control System	72.9
Design & Engineering	33.7
Project Support & Administration and Licensing[2)]	123.7
Contingency	158.5
Conventional Facilities Funded by Host Countries[3)]	-93.0
Total Construction Budget and ESS Cost Book Value	**1843.0**

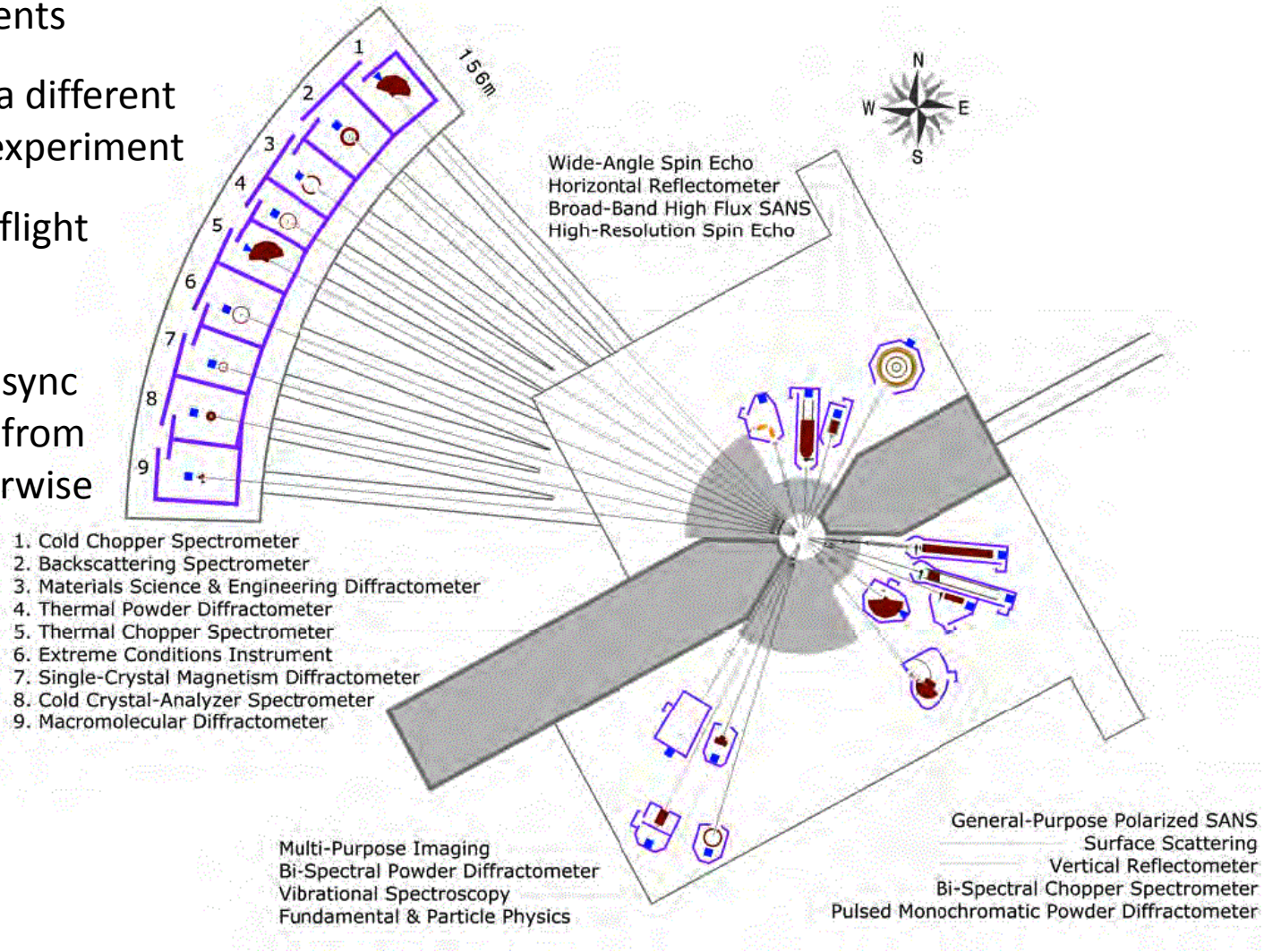
[1)] All costs are stated in January 2013 pricing

[2)] Project Support & Administration includes the DG Office and AD for Operations, ES&H and QA

[3)] Conventional Facilities construction budget assumes Host Countries will cover costs and risk above the 423 M€ value described in the ESS Cost Report, dated December 2012.

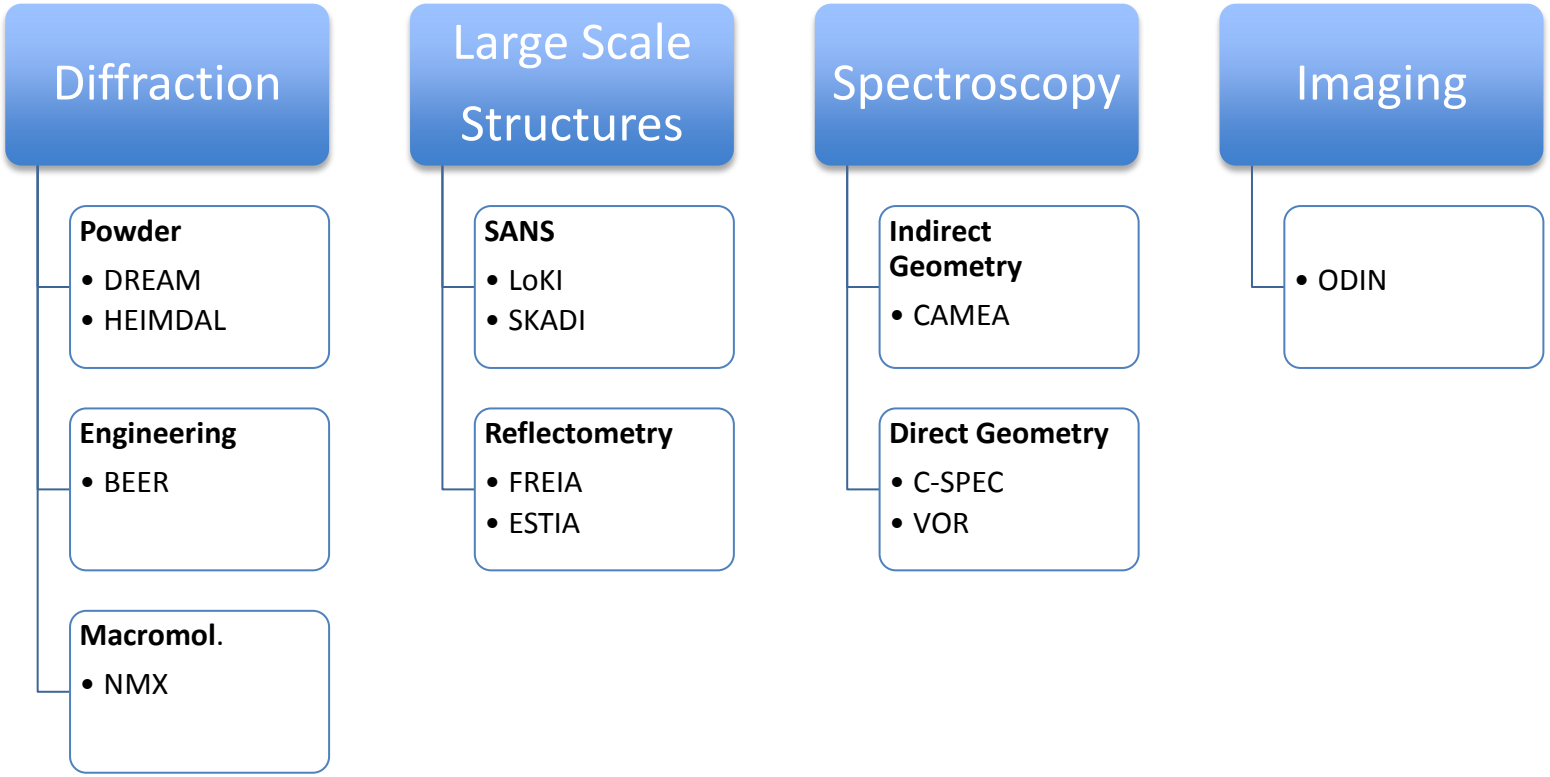
Science Research Program

- Suite of 16 instruments
- Each optimized for a different class of scattering experiment
- Operate by time of flight neutron scattering
- All receive a timing sync pulse and neutrons from the source but otherwise operate independently.



ESS Neutron Instrument Suite

- Process: Proposals → Scientific & Tech. Advisory Panels → Science Advisory Council (SAC)
- ESS Steering Committee (STC) has approved 12 instruments for suite
- This leaves 4 instruments still to choose out of funding for 16 instruments



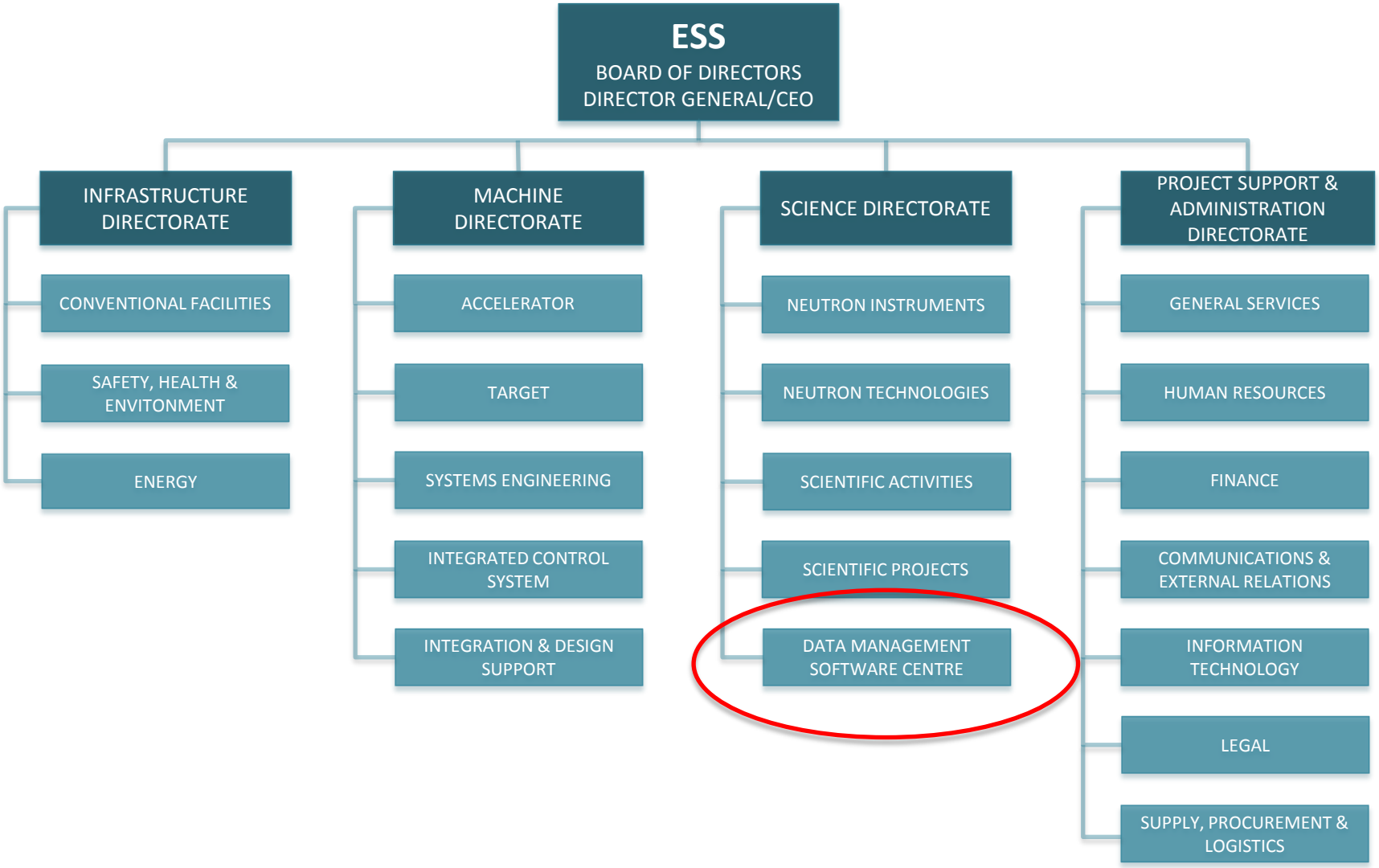
User Research Program (Operations)

User Facility

- 1947: First neutron scattering experiments
- Nobel Laureate – Cliff Shull
- 1950/60's – neutron scattering done in small groups
- 1970's: new model ➔ "User" Facility
- "Open Access" model now used by "all" facilities
- Model required to be an ESFRI
- Competitive and responsive

- 6 monthly call for proposals to use instruments (advertised, web submission)
- Open to anyone: academia, research institutes, companies, etc.
- Peer review of proposals done by external (non-ESS) panels
- ESS provides staff to:
  - Operate the instruments with the users
  - Operate the sample environment equipment
  - Provide data analysis support to users
  - Schedule the scientific user program (proposals, travel, training…)

ESS Organization



Science Directorate/NSS Project

Science Directorate is responsible for the scientific research program at ESS

- During the construction phase for the process of selecting & constructing the instruments for the research
- During operations for the operation of the user facility research program

Neutron Instruments Division: The scientists involved in the conceptual design in construction and who work with the users to perform the experiments in operations

Neutron Technologies Division: Responsible for the specialized instrument components, choppers, guides, detectors.

Scientific Activities Division: Responsible for the scientific coordination of the user scientific research program and the scientific support facilities – sample environment, chemistry & biology laboratories.

Data Management and Software Centre: Responsible for instrument control, data acquisition/reduction/analysis software and making data/software available to users.

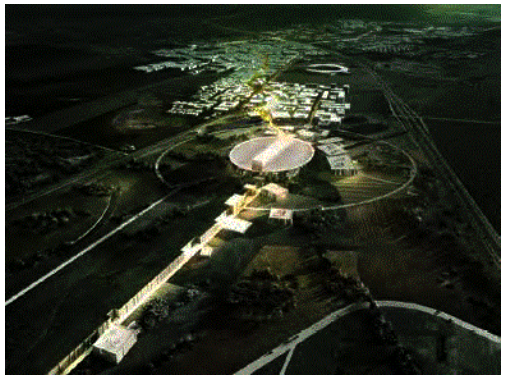
Scientific Projects Division: During construction for coordinating the engineering and construction of the instruments.

What is DMSC ?

- Data Management and Software Centre (DMSC)
- A Division of ESS Science Directorate…
  … just like Neutron Technologies,
  Neutron Instruments etc.
- Mission:

  To use the techniques and methods of scientific computing to facilitate, enable and advance the scientific research to be carried out using the neutron beam instruments at the European Spallation Source.

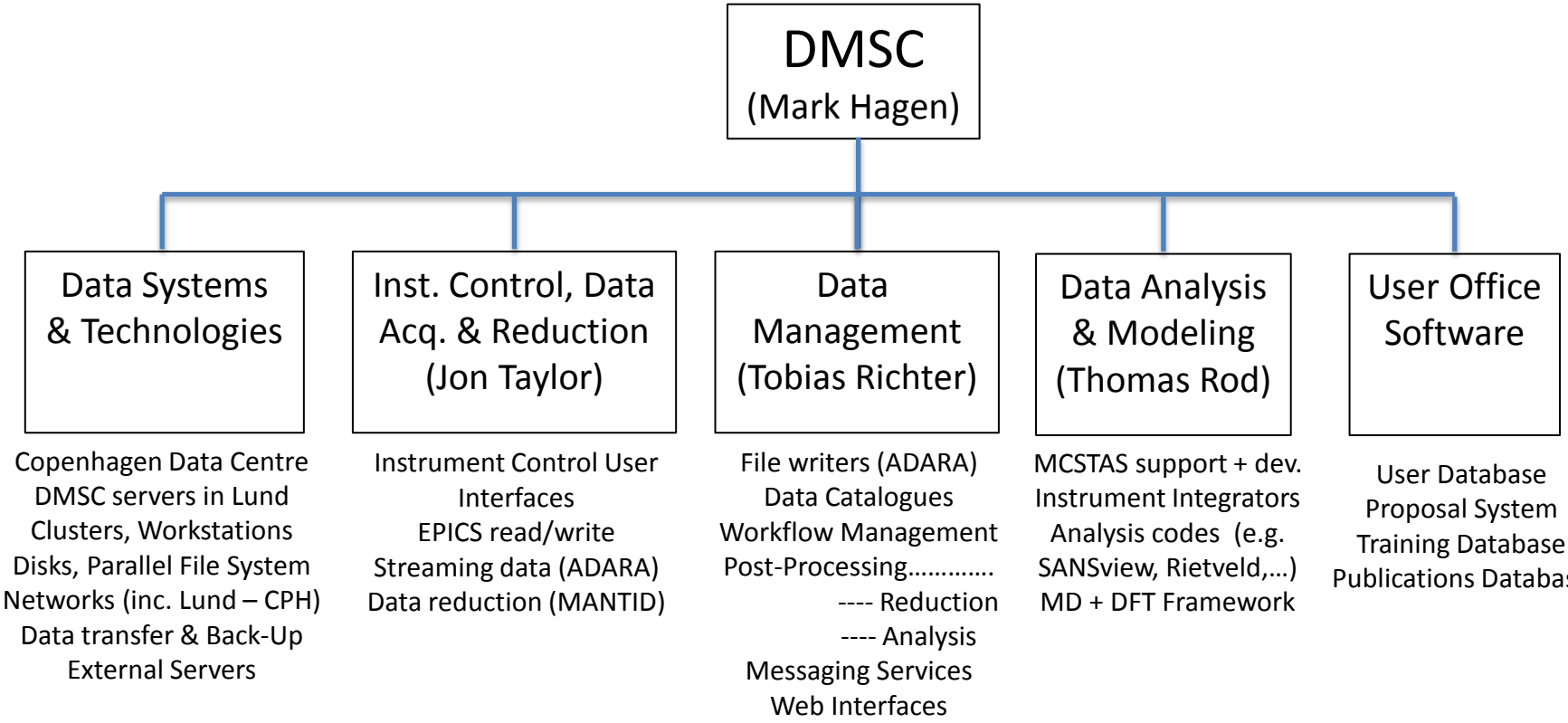
- Two campuses: ESS Lund & ESS Copenhagen
  (Universitetparken, Københavns Universitet)
- DMSC building to be constructed in Copenhagen



What is DMSC's scope?

- Construction Phase of ESS (2014 – 2019) & Neutron Beam Instruments (2014 – 2025)
  - Software for the Inst. Control & Data Management (Acq., Reduction, etc.)
  - Software for Data Analysis
  - Software framework to do Live and Automated Data Reduction/Analysis
  - Software for managing the scientific user program
  - Hardware for data storage and data reduction/analysis (inc. remote)
- Operations Phase of ESS & Neutron Beam Instruments (2019 – 2067)
  - Maintenance and development of all of the above software
  - Emphasis on Data Analysis, Modeling & Simulation for ESS Users/Science
    - Supporting ESS Users with Data Analysis, Modeling & Simulation
    - Integration of simulation/modeling techniques (e.g. Molecular Dynamics and Density Functional Theory) into calculation of neutron scattering cross sections & data analysis

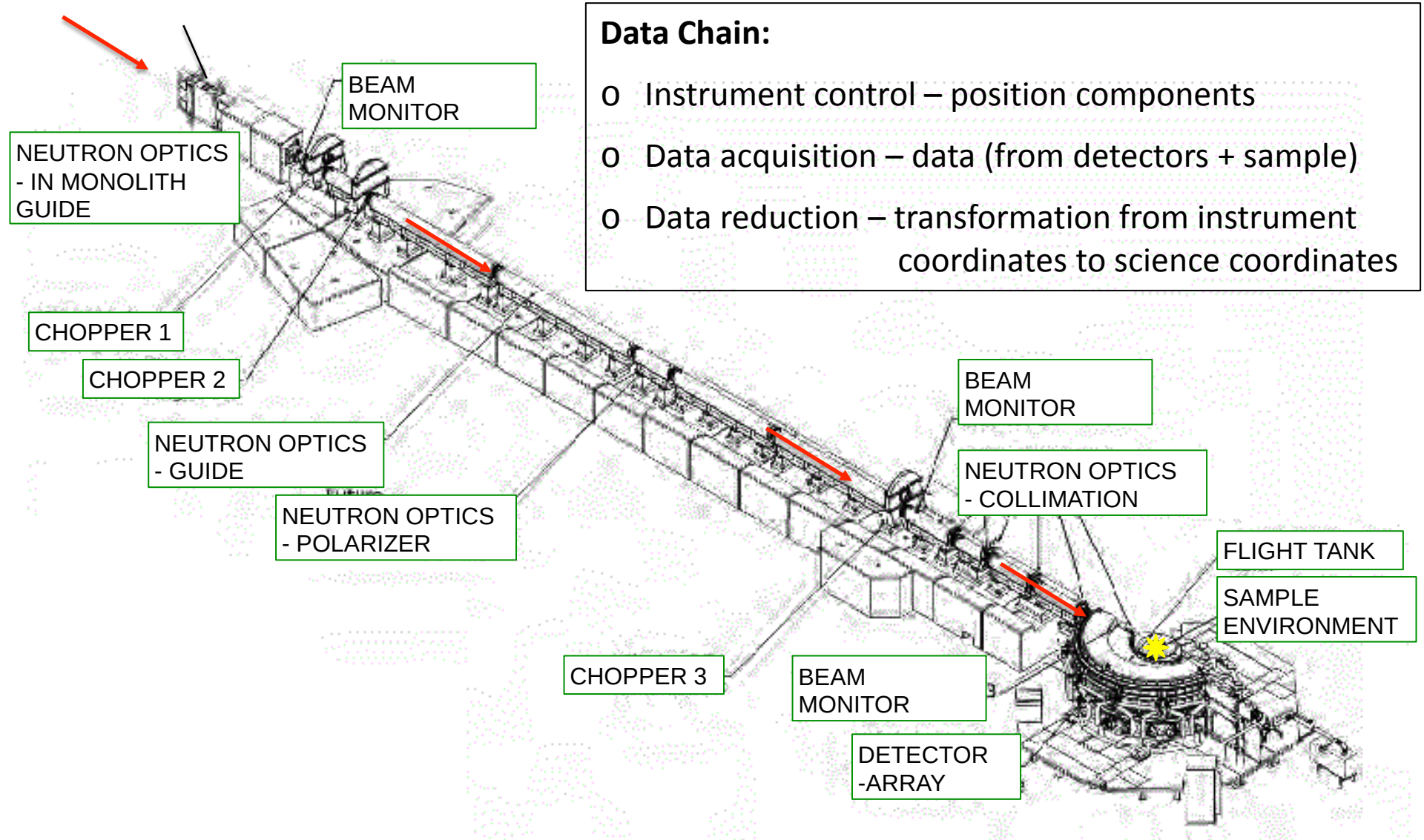
DMSC's Organization



Time of Flight Neutron Instruments

Data Chain:

- Instrument control – position components
- Data acquisition – data (from detectors + sample)
- Data reduction – transformation from instrument coordinates to science coordinates



DMSC's Priorities

During the construction phase:

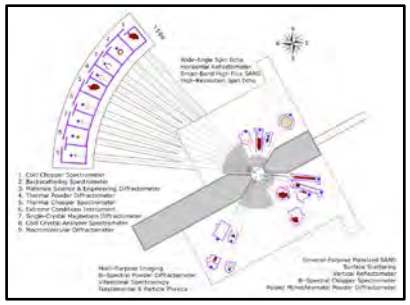
1. The *highest priority* for DMSC must be that the instrument control software and data management infrastructure and software are *ready, tested and working* when the first ESS instruments come online.

2. The *second highest priority* for DMSC should be that basic data analysis and modelling software is also available for those instruments.

3. The software for the business management of the scientific research program must be ready, tested and working for the start of the scientific user research program in 2023.

4. The data analysis and modelling work must be ramped up during construction in order to be ready to meet this need in ~2023 onwards.

Data Acquisition, Reduction & Control

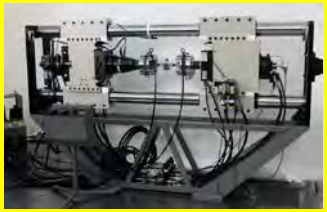


NEUTRON TECHNOLOGIES

Motion Control

Sample Environment

Choppers



Fast Sample Environment

Detectors & Monitors

Timing

Fast Data Readout

EPICS

INTEGRATED CONTROL SYSTEMS

Control Box

DATA MANAGEMENT & SOFTWARE CENTRE

Data Aggregator & Streamer (ADARA)

User Control Interface

Mantid

Live, Local & Remote Data Reduction

Data Analysis Interfaces

Automated Data Reduction

Mantid

Lund Server Room

Instrument Control Room

Data Acquisition, Reduction & Control

Data Acquisition, Streaming & Reduction

EPICS

Used by ESS accelerator/target, SLS, Diamond, US light sources, to be used by ISIS & SNS

ISIS

ADARA

Publish/subscribe software & protocol for streaming data (neutron + meta)

SNS SPALLATION NEUTRON SOURCE

Mantid

Data reduction framework in Python & C++ developed by ISIS & SNS

Data Management

pandata

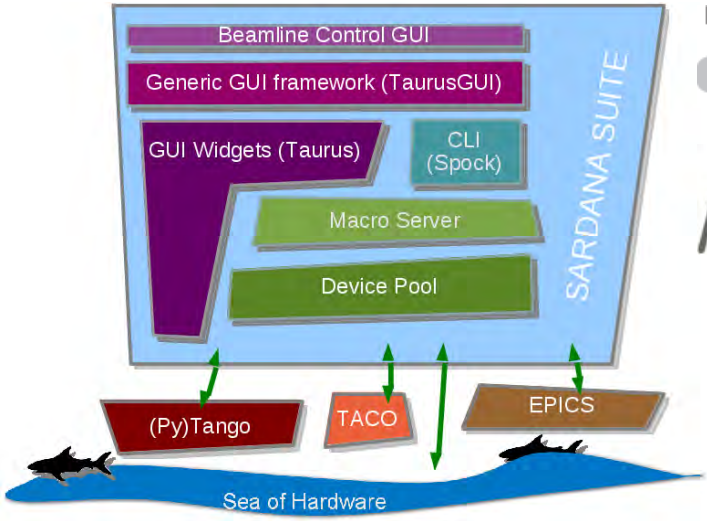
ICAT data cataloguing software developed under NMI3 by PanData collaboration of 19 European facilities (+ SNS in US)

Data Acquisition, Reduction & Control

Data Streaming
ADARA
Aggregator
PVStreamer (link to EPICS)
Interface to detector readout
Streaming (HDF5) file writer
Data stream monitoring

Data Reduction, Cataloguing & Post-processing
MANTID
Reduction tailored to ESS instruments
Visualization
Live Listener (to data stream)
Live data visualization
Automated (post-acquisition) reduction
Cataloguing – ICAT

Instrument Control Interface
(Py) EPICS
Instrument server - user client
Generic interface toolset
+ instrument customization
Interface to ADARA
MANTID partner apps
Planning tool partner apps
Data analysis hooks for feedback



Data Systems & Technologies

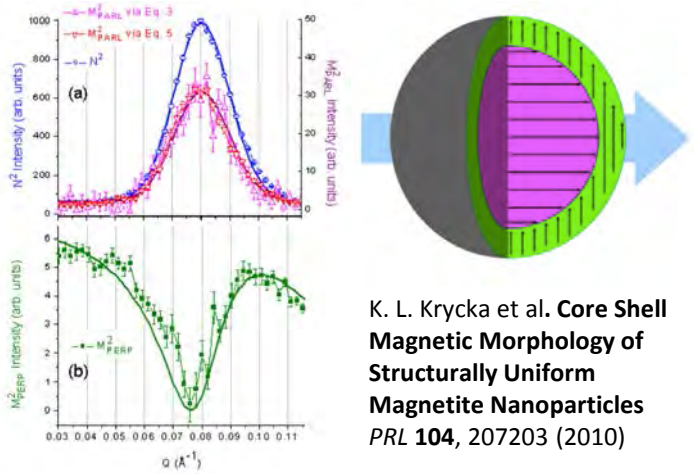
- DMSC will not be a “supercomputer” centre
- Data (disk) storage:
  - Back of the envelope ➔ ~4 PBytes/yr
  - Spectrum of file sizes: ~100MByte - ~10’s GByte – ~1TByte
  - Fast disk (200MByte/s) & Parallel File System (10GByte/s)
- Cluster(s) for data reduction & (modest) data analysis - ~2048 cores
  Architecture – CPU, GPU… visualization cluster/server

- Data download servers – sftp & gridftp
- Remote login capability for ESS users:
  - Re-reduce data using cluster
  - Data analysis software available for users
  - PaNDaaS (Photon and Neutron Data as a Service)
- Software development servers – repositories, bug trackers, build servers

Data Analysis

- 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

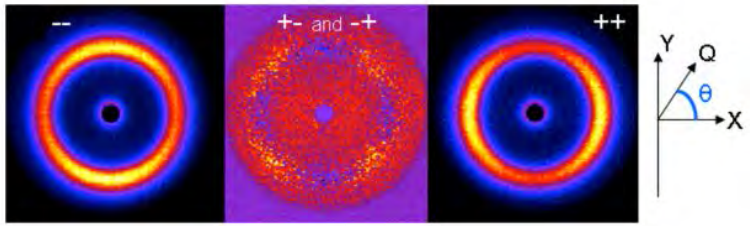
Structure of Nanomaterials



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.



Projects in addition to ESS funding

SINE2020

- EU Horizon 2020 proposal (INFRADEV-4)
- Five main partners:

Main topics:

- Innovation based on neutrons experiments
- Ready for ESS in 2020

Facility	Task
ILL+FZJ+PSI	Mantid for continuum sources
ESS	SANS (SASView)
FZJ	Reflectometry (BornAgain)
ILL	Modelling (nMoldyn)
ISIS	QENS (Mantid)
PSI	Imaging (MuhRec/KipTool)

Projects in addition to ESS funding

PaNDaaS (Photon and Neutron Data as a Service)

- EU Horizon 2020 proposal (INFRADEV-4)

- Twenty one partners:
  ESRF, Diamond, Soleil, Alba, Elettra, MAX-IV, DESY, E-XFEL,
  SLS/SwissFEL, KIT/ANKA, CYI, HZB (x-rays)
  ESS, ILL, ISIS, SINQ (neutrons), ELI-ALPS (light)
  SESAME, SLAC (SSRL/LCLS), SNS + 2 companies

- Provide pan-facility access to data, reduced data and analysis tools

How can e-Infrastructures help ESS??

- When the Users (researchers) at at the facility (e.g. ESS) the facility provides help
- Facilities provide reduced data (+ are working on pan facility access – PaNDaaS)

- Data analysis – "quick" analysis is done during experiment but…
  … major analysis is done "at home" when users return to Univ. etc.
  … typical timescale 2 years +/- 1 year

- What does the "analysis" involve??

- Modeling – "fitting" the reduced data to models of the material
- Semi-analytic models: Rietveld for powder diffraction, SANS models (hard spheres etc.)
  …
- Using simulation: Molecular dynamics and DFT

- Data on disk is useless ➔ it is data analysis (modeling) that leads to discovery

How can e-Infrastructures help ESS??

- The ESS will produce “more” raw & reduced data than previous neutron facilities
  - More is not just data volumes it means more research (experiments) performed
  - More also means more new users who have not yet built experience

- The user community is diverse
  - Geographically diverse (pan-European & global)
  - Come from wide spread of disciplines
  - Wide range of computational skills + needs
  - Single investigator/small group but collaborative
  - Want to link to related data –
    X-ray (PaNDaaS) but also their own lab data (NMR, TGA, etc.)

- Supporting the user community to turn reduced data into discovery:
  - It’s the modeling tools + resources more than the data itself
  - Should it be driven by the facilities??
  - Should it be driven from the disciplines??
  - Should it be driven by the e-Infrastructures??

ESS Construction has Begun

- Construction on the ESS site has begun in 2014
- Accelerator + target & first neutrons in 2019
- Instrument rollout 2019 – 2025 (16 instruments)

ESS looking towards MAX IV

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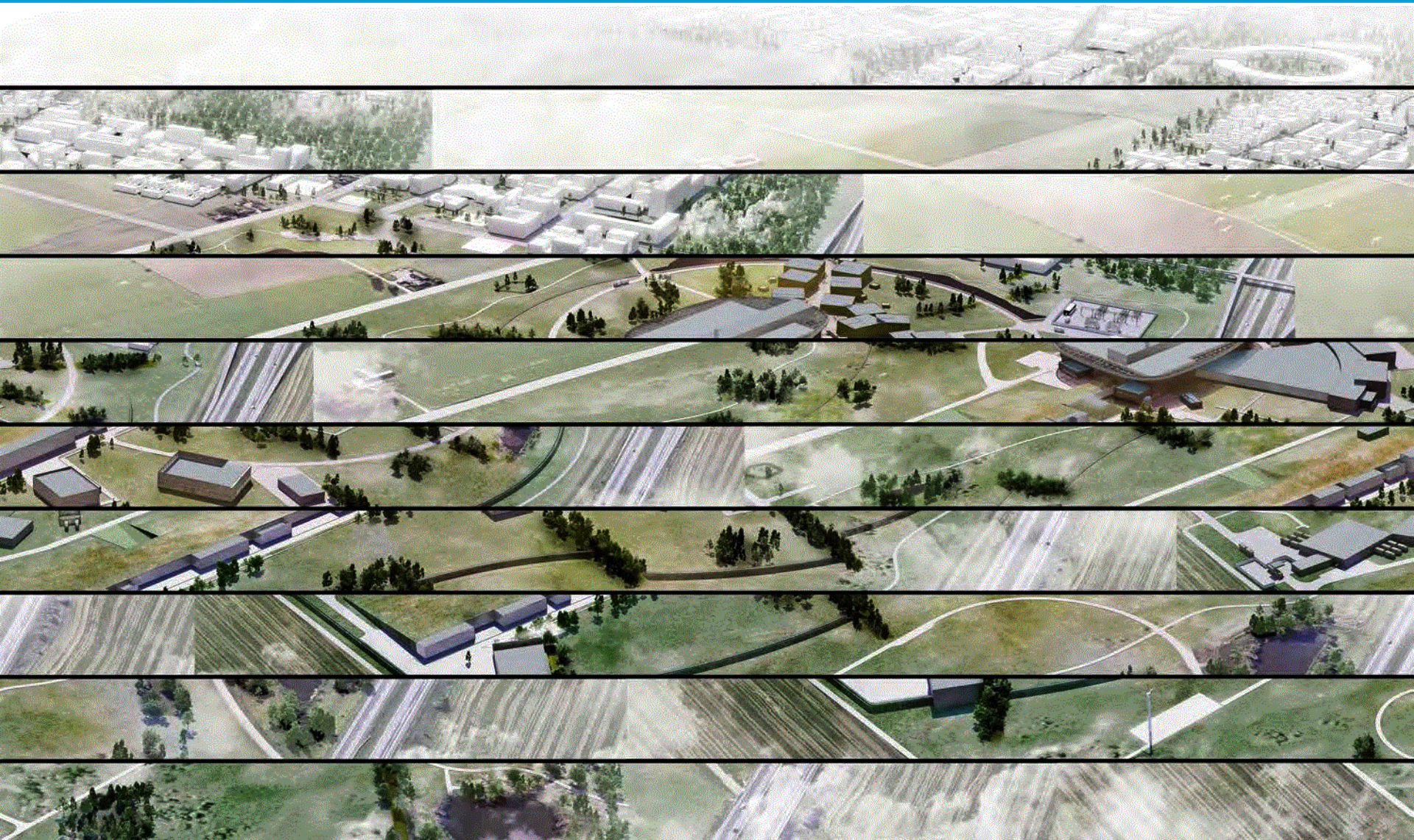

ESS Target Building

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QUESTIONS