

# Data Management and Software Centre

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Head of DMSC

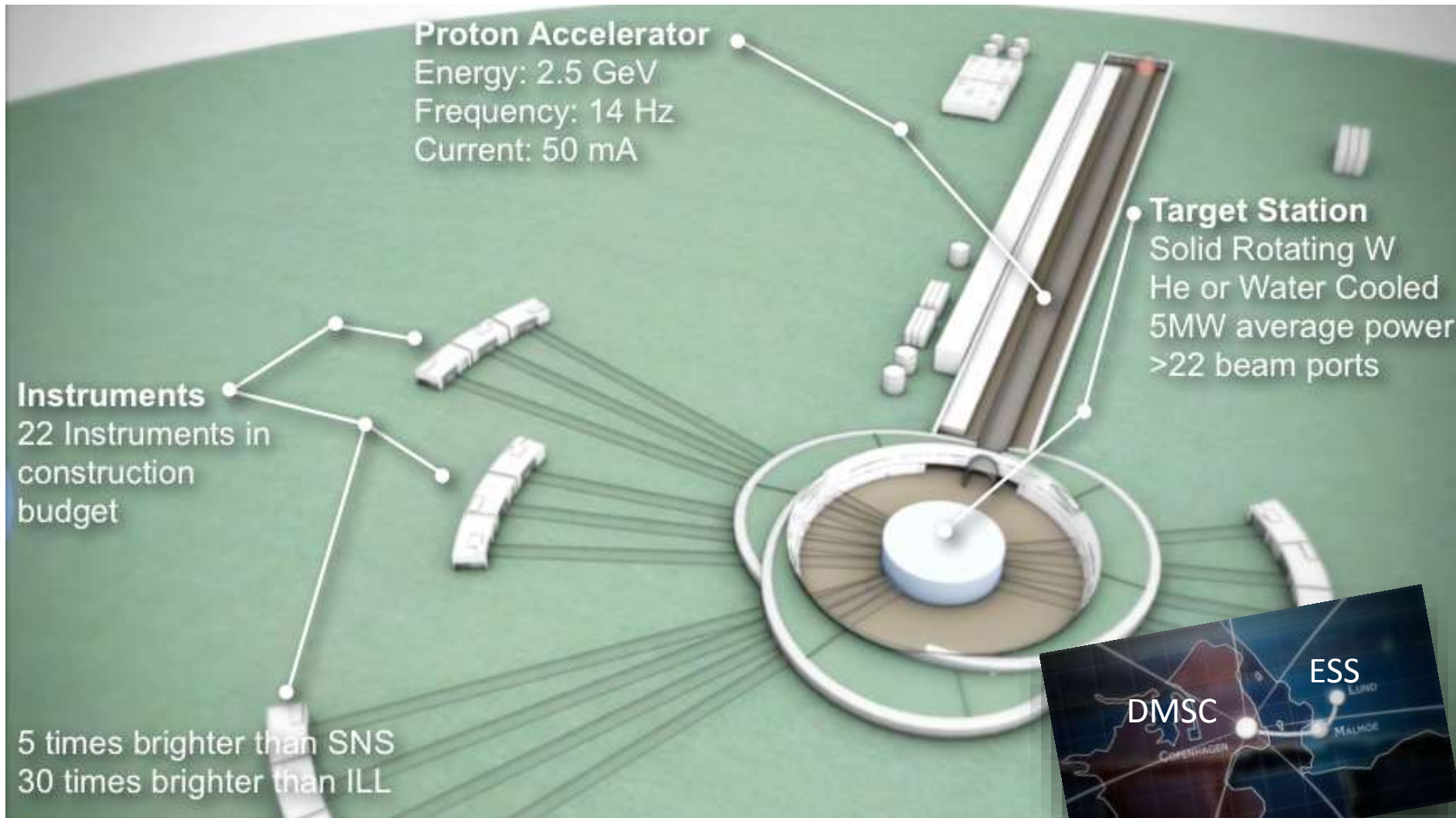
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NOBUGS-10, KEK, Tsukuba, September 2014

- European Spallation Source (ESS)
  - High level overview of ESS technical
  - Overview of ESS project
  
- Data Management and Software Centre (DMSC)
  - What is DMSC and it's scope?
  - Inst. Control, Data Acq. & Data Reduction Framework
  - Data Analysis, Modeling and Simulation
  - Organization

# What is the ESS?



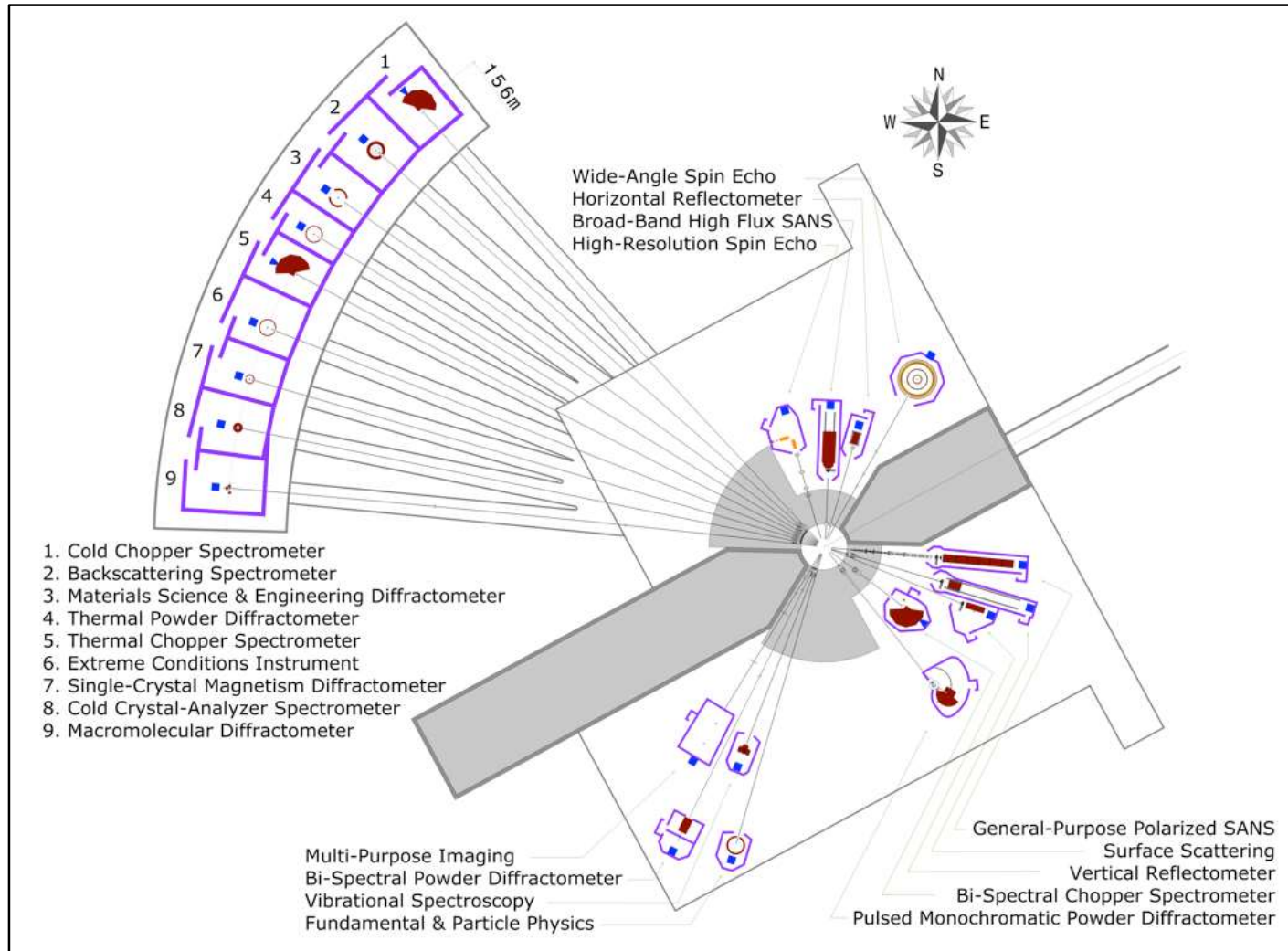
# ESS looking towards MAX IV



# ESS Target Building



# Neutron Instruments



# ESS, ISIS, SNS and MLF/J-PARC

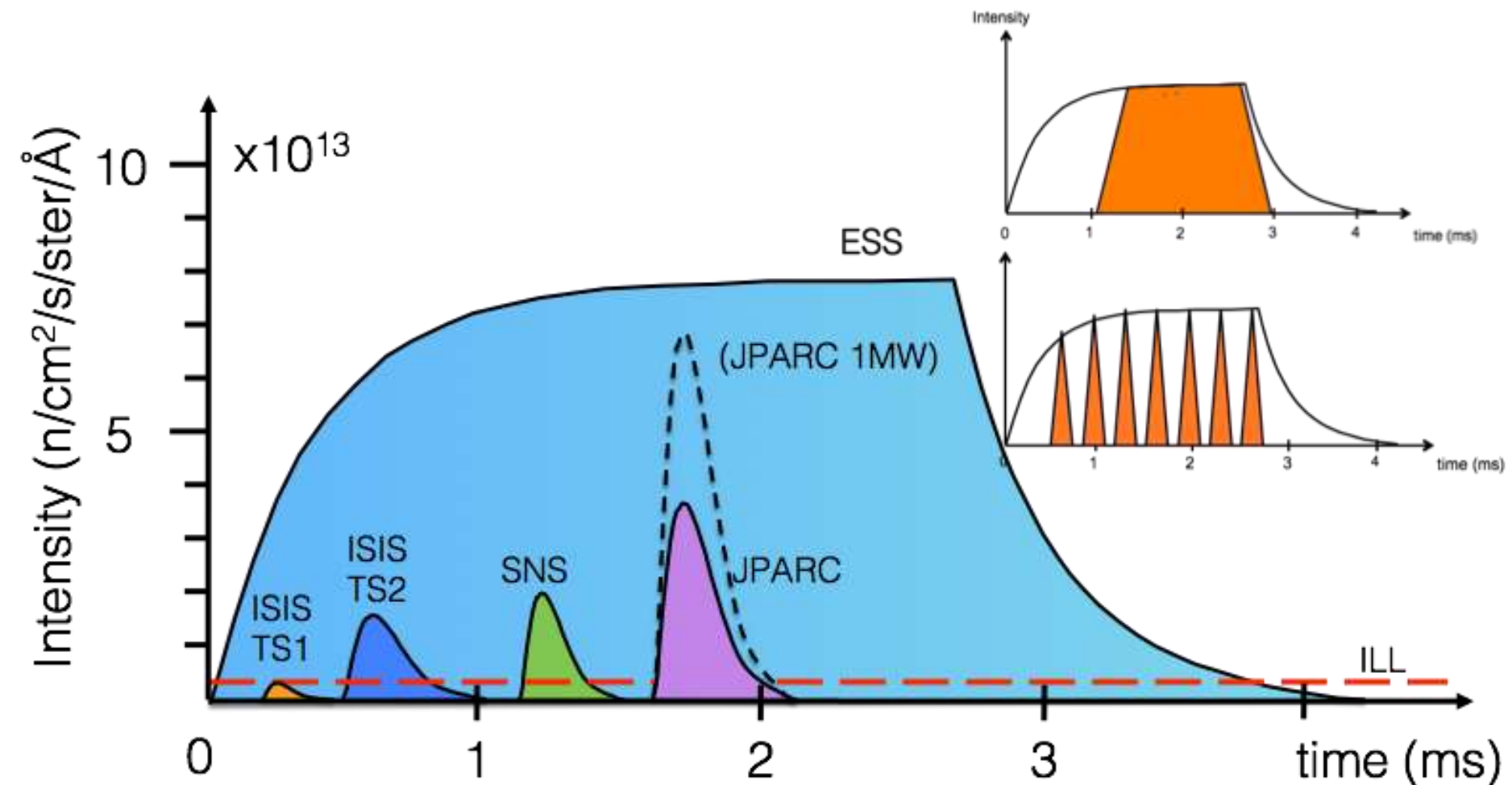


- **Things that are the same:**
  - Use protons to create neutrons via Spallation
- **Things that are different:**
  - ISIS & SNS have H- and rings
  - ESS will produce p from a plasma & only a Linac
  - ISIS has a single solid W target
  - SNS & MLF/J-PARC use Liq-Hg target
  - ESS will use rotating W wheel
  
  - ISIS & 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



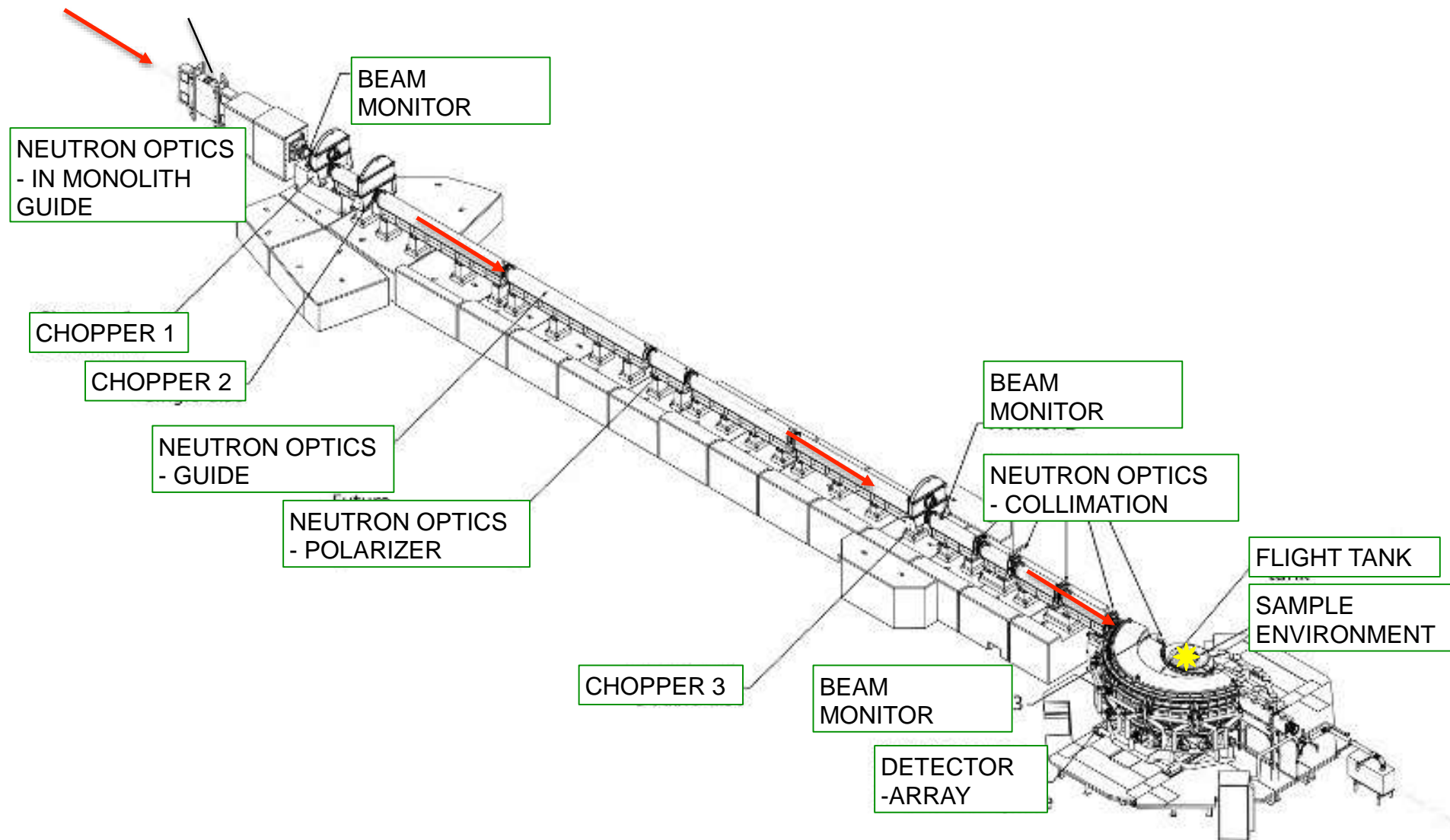
→ Don't reinvent the wheel

## The Long Pulse of ESS



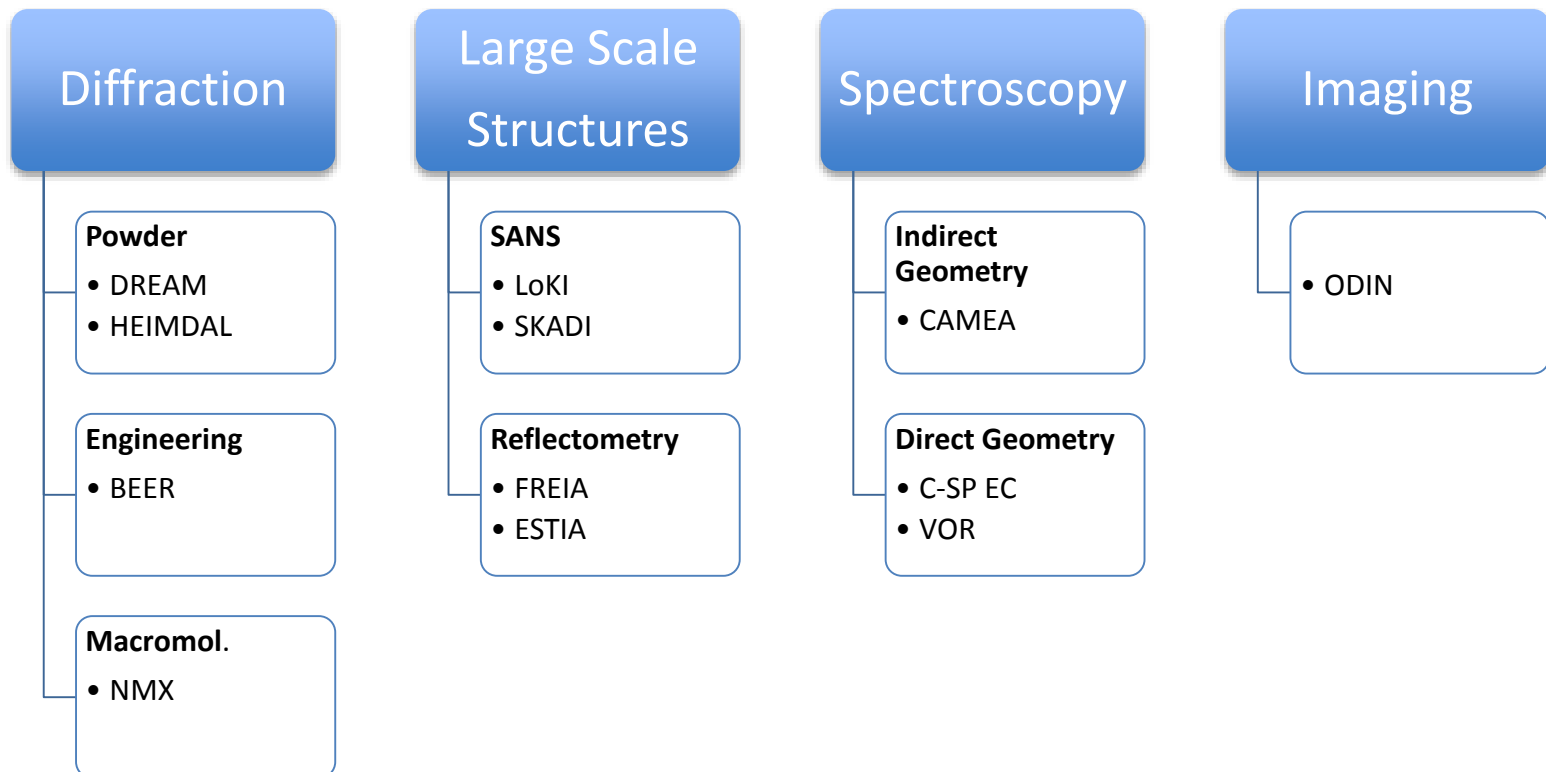


# Time of Flight Neutron Instruments



# ESS Neutron Instrument Suite

- Process: Proposals → Scientific & Tech. Advisory Panels → Science Advisory Council (SAC)
- ESS Steering Committee (STC) has approved 3 instruments (LoKI, NMX, ODIN) for suite
- SAC has recommended a further 9 instruments to STC for inclusion in suite
- Would leave 4 instruments to choose out of funding for 16 instruments



# Funding is cash and in-kind deliverables

## Sweden and Denmark:

47,5% Construction

15-20% Operations

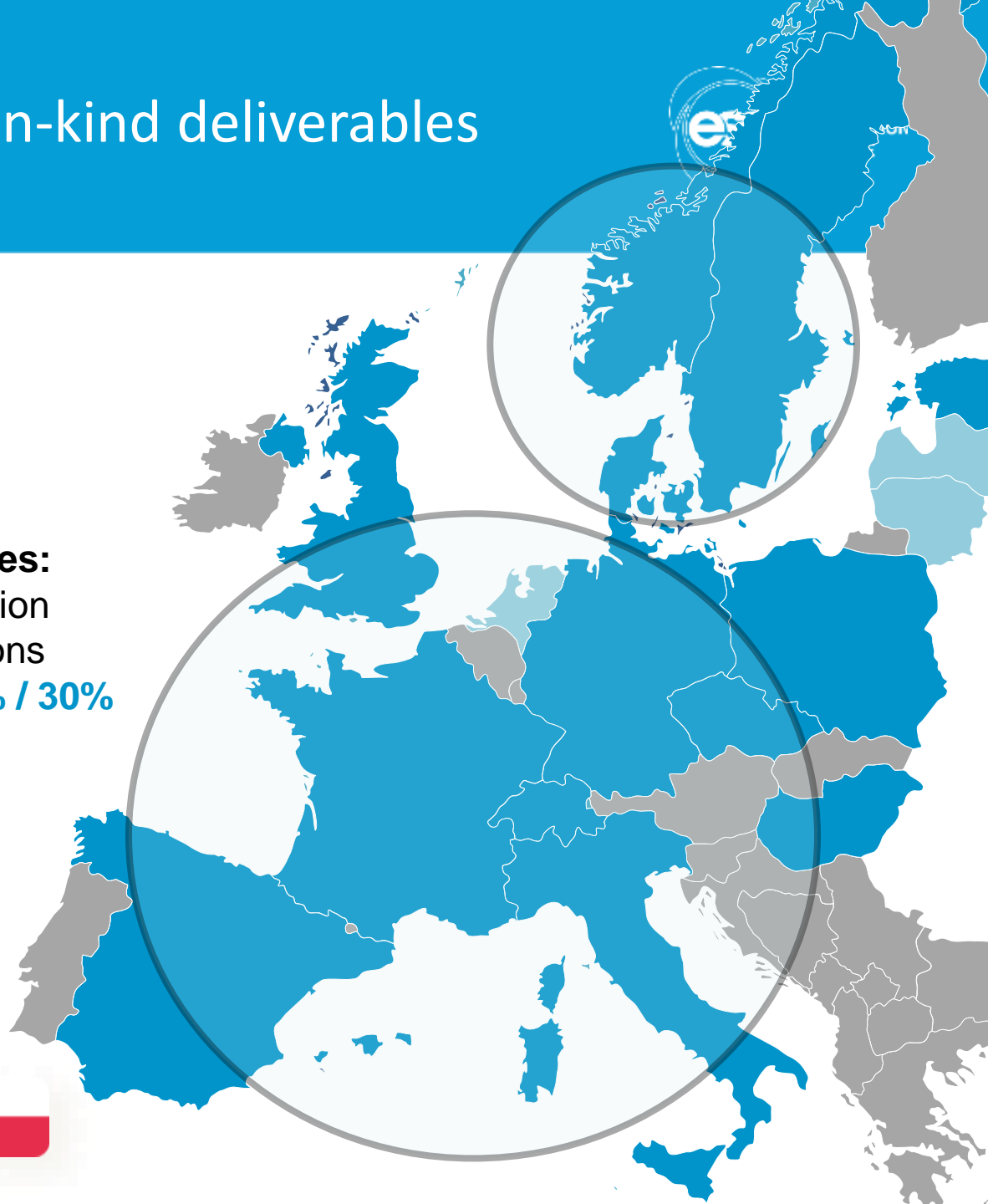
Cash ~100%

## Partner Countries:

52,5% Construction

80-85% Operations

IKC/Cash ~ 70% / 30%



## 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.

<b>ESS Construction Budget</b>	<b>M€<sup>1)</sup></b>
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 <sup>2)</sup>	123.7
Contingency	158.5
Conventional Facilities Funded by Host Countries <sup>3)</sup>	-93.0
<b>Total Construction Budget and ESS Cost Book Value</b>	<b>1843.0</b>

<sup>1)</sup> All costs are stated in January 2013 pricing

<sup>2)</sup> Project Support & Administration includes the DG Office and AD for Operations, ES&H and QA

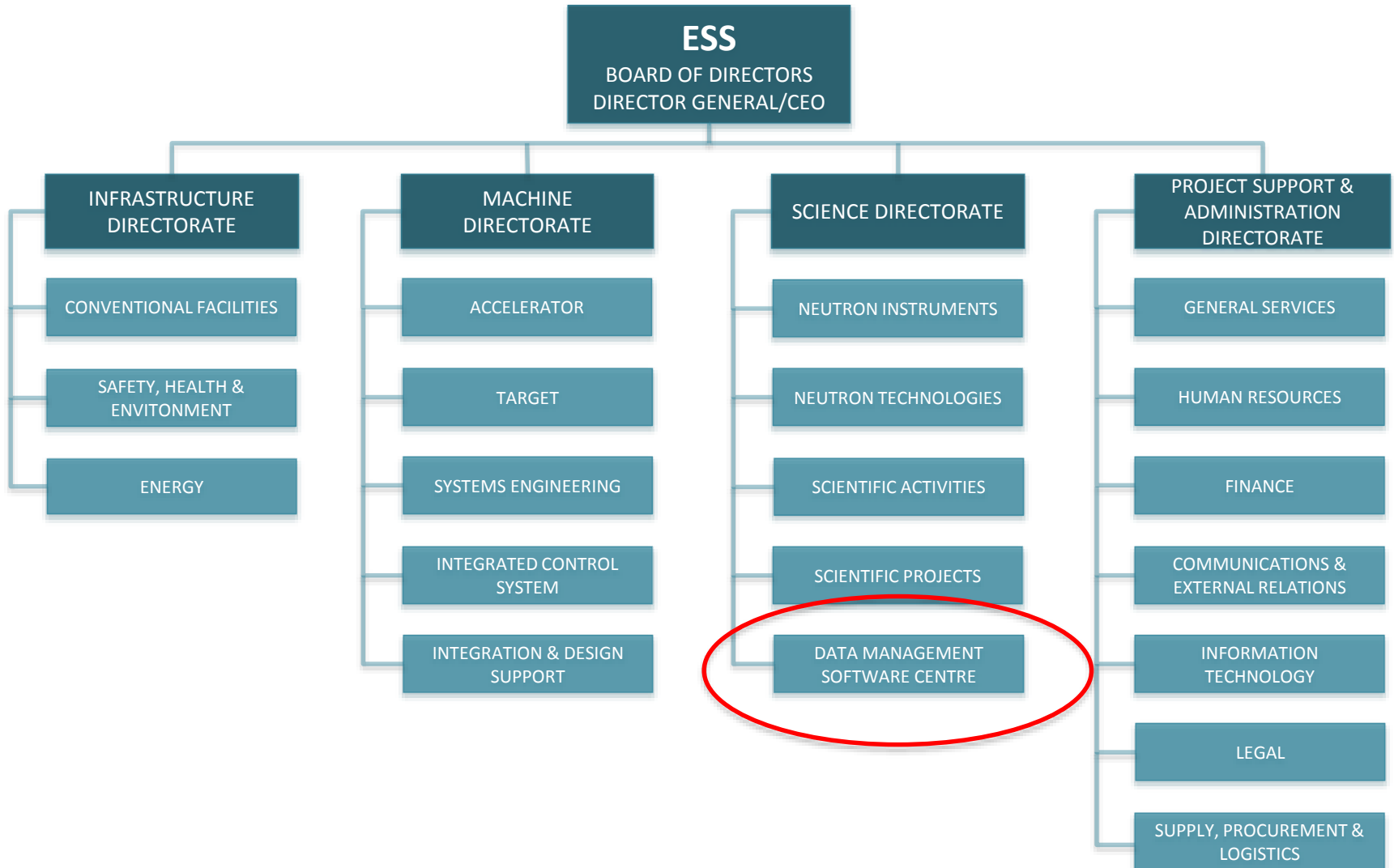
<sup>3)</sup> Conventional Facilities construction budget assumes Host Countries will cover costs and risk above the 423 M€ value described in the ESS Cost Report, dated December 2012.

# 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 Organization



# 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  
(Universitetsparken, Københavns Universitet)
- DMSC building to be constructed in Copenhagen



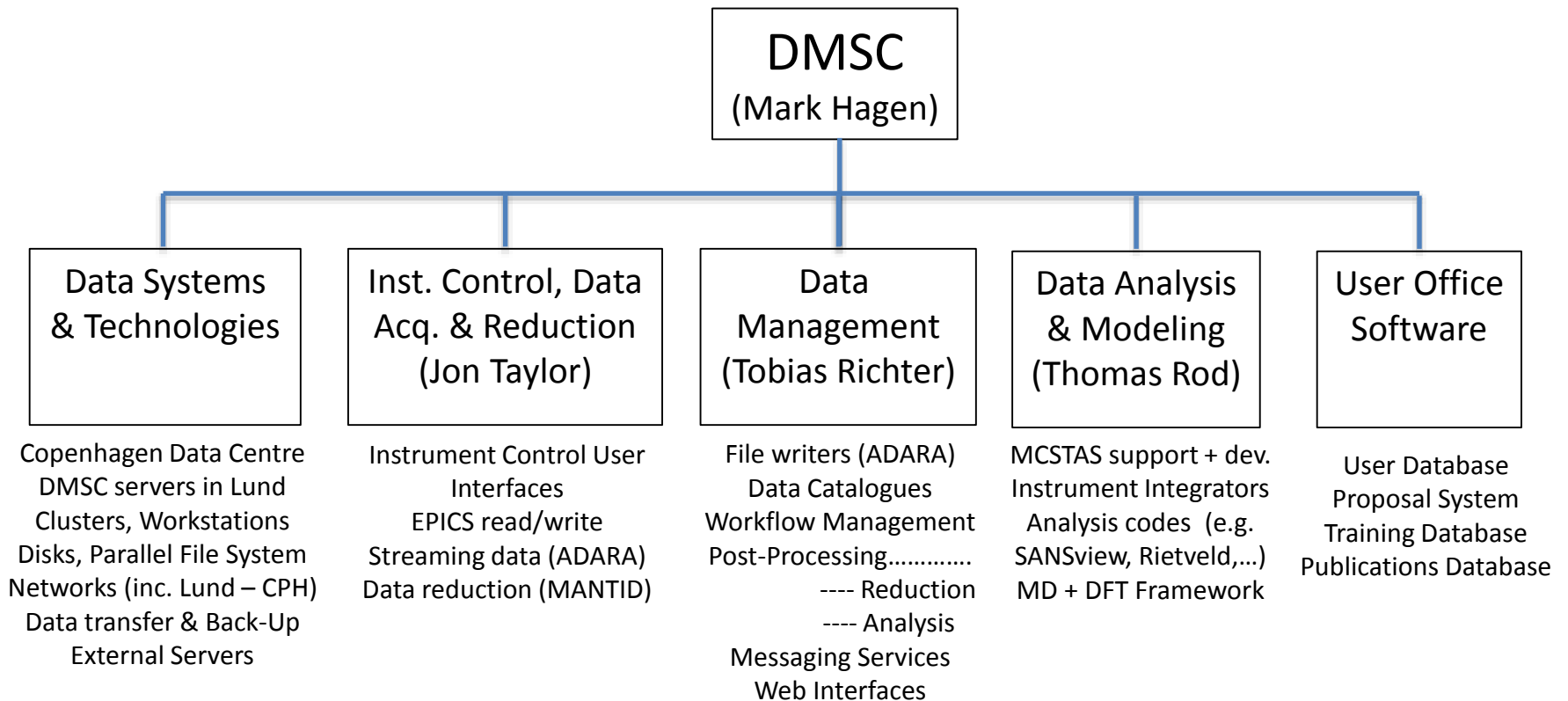


# What is DMSC's scope?

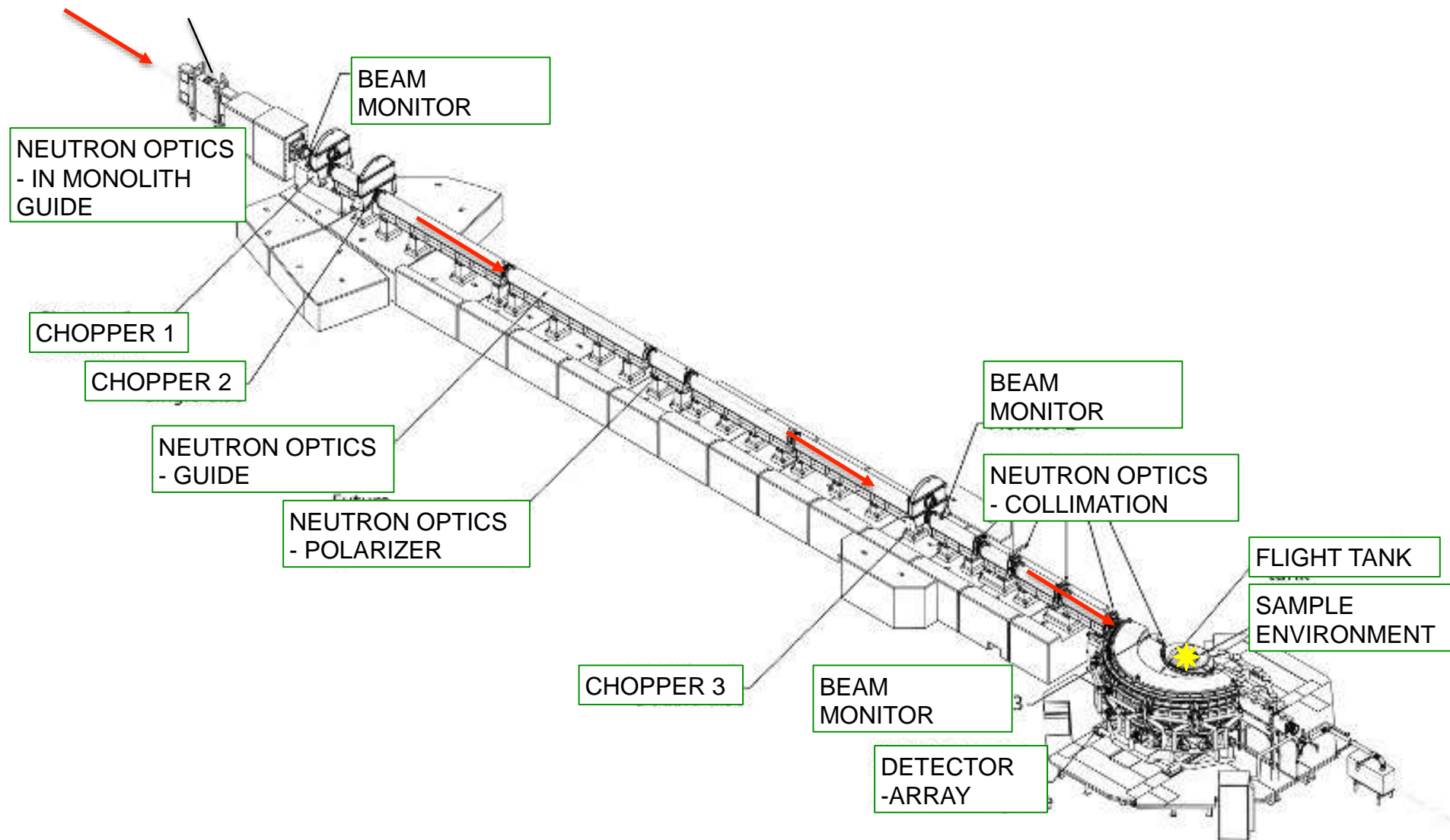


- Construction Phase of ESS (2014 – 2019) & Neutron Beam Instruments (2014 – 2025)
  - Software for the Inst. Control & Data Management (Acq., Reduction, etc.)
  - Software for Data Analysis
  - Software framework to do Live and Automated Data Reduction/Analysis
  - Software for managing the scientific 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

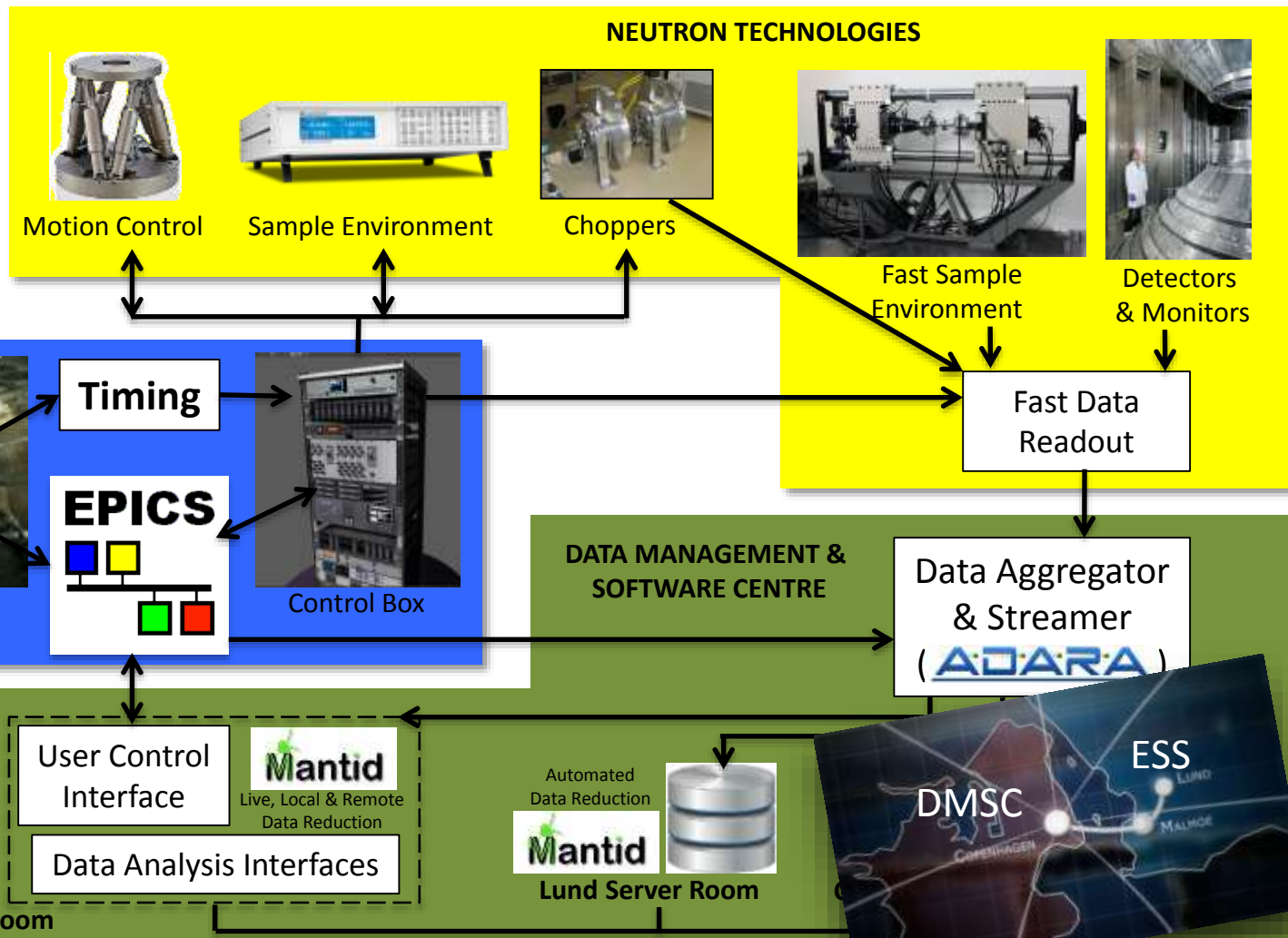
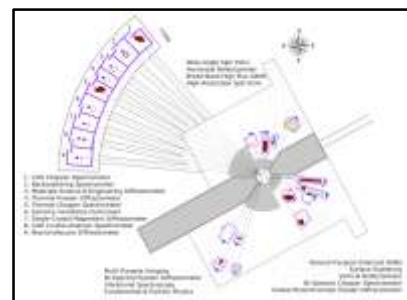
# DMSC Organization



# Time of Flight Neutron Instruments



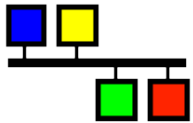
# Data Acquisition, Reduction & Control



# 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



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



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

## Data Management



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



# Data Acquisition, Reduction & Control

## Data Streaming

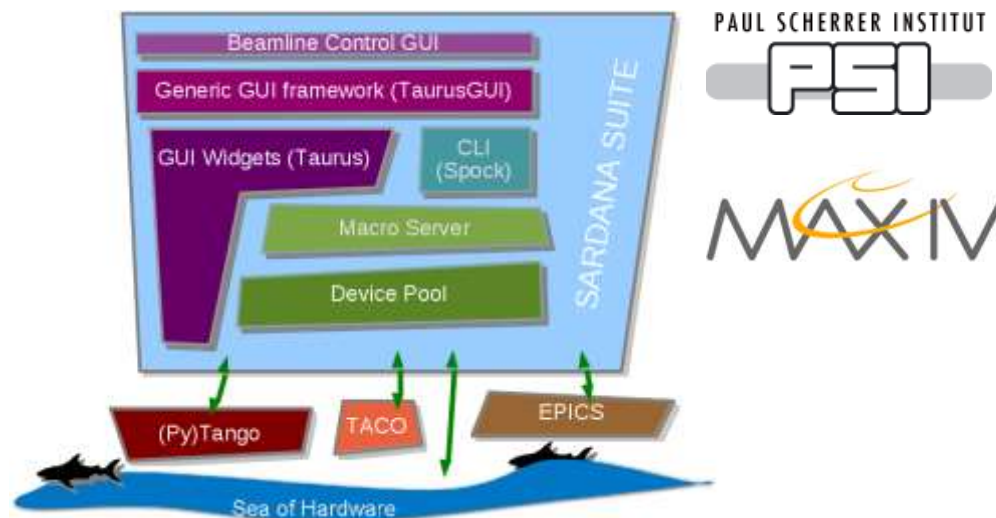
ADARA  
Aggregator  
PVStreamer (link to EPICS)  
Interface to detector readout  
Streaming (HDF5) file writer  
Data stream monitoring

## 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

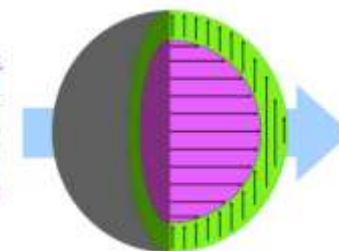
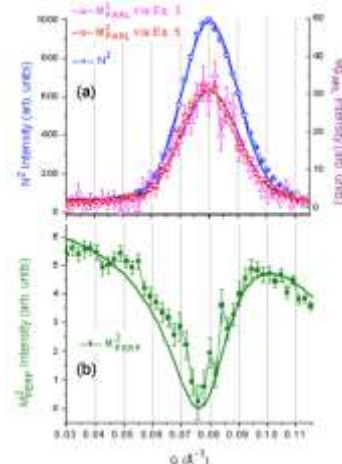
## Instrument Control Interface

(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 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

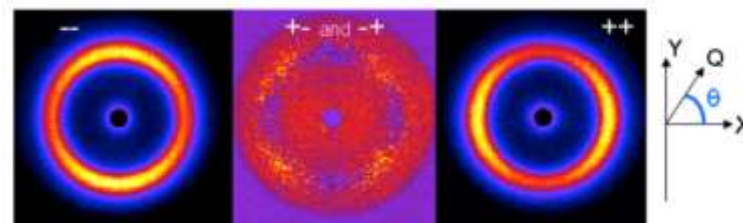
## Structure of Nanomaterials



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)



## **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

# 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



# QUESTIONS