Neutron Scattering Systems

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Latvian Partner Day, June 2nd, 2016

Academic Center for Natural Sciences, University of Latvia, Riga

Mark Hagen

European Spallation Source, Head of DMSC since Oct. 21 2013

Spallation Neutron Source, USA (2004 – 2013)
Data Analysis Group Leader (2010 – 2013)
Inelastic Scattering Group Leader (2007 – 2011)
HYSPEC Inst. Scientist/Project Manager (2004 – 2011)

ANSTO, Australia (2002 – 2004)
Wombat High Intensity Powder Diff. Inst. Scientist/Project Manager
(Echidna High Res. Pow. Diff., Taipan TAS)

ISIS Spallation Neutron Source & Keele Univ., U.K. (1987 – 2001)
Physics Dept. Staff at Keele University, UK
PRISMA instrument scientist at ISIS, RAL, UK

Ph.D & Post-doc
Post-docs – Institut Laue Langevin, France (1984); HFIR, ORNL, USA (1985-86)
Ph.D – University of Edinburgh , Scotland, UK(1980 – 83)

Thermal Neutron Scattering

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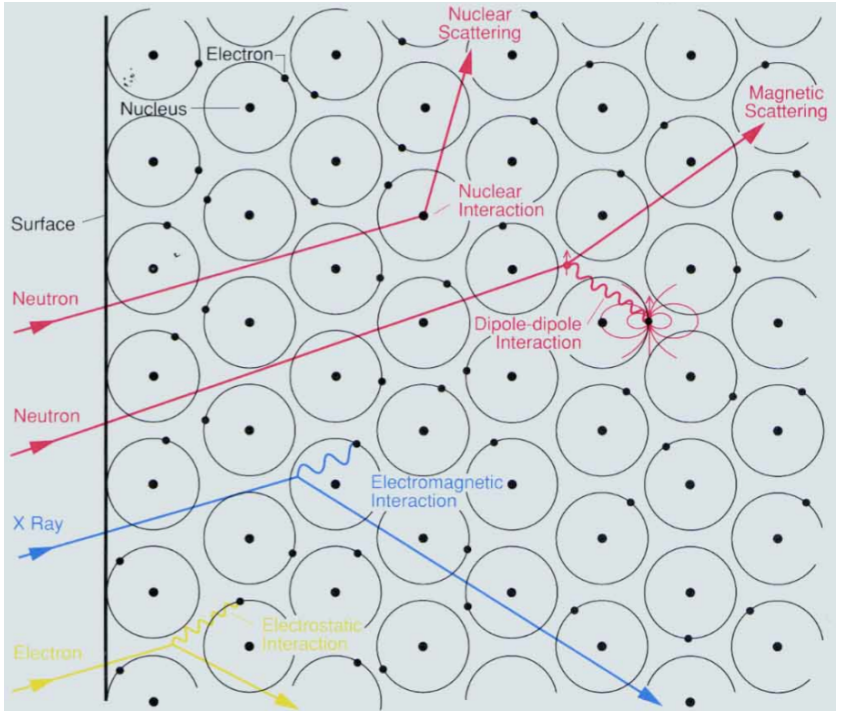
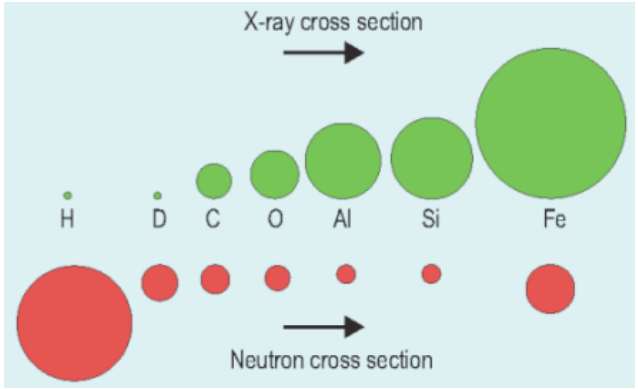
Charge neutral
Deeply penetrating

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

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

ESS looking towards MAX IV

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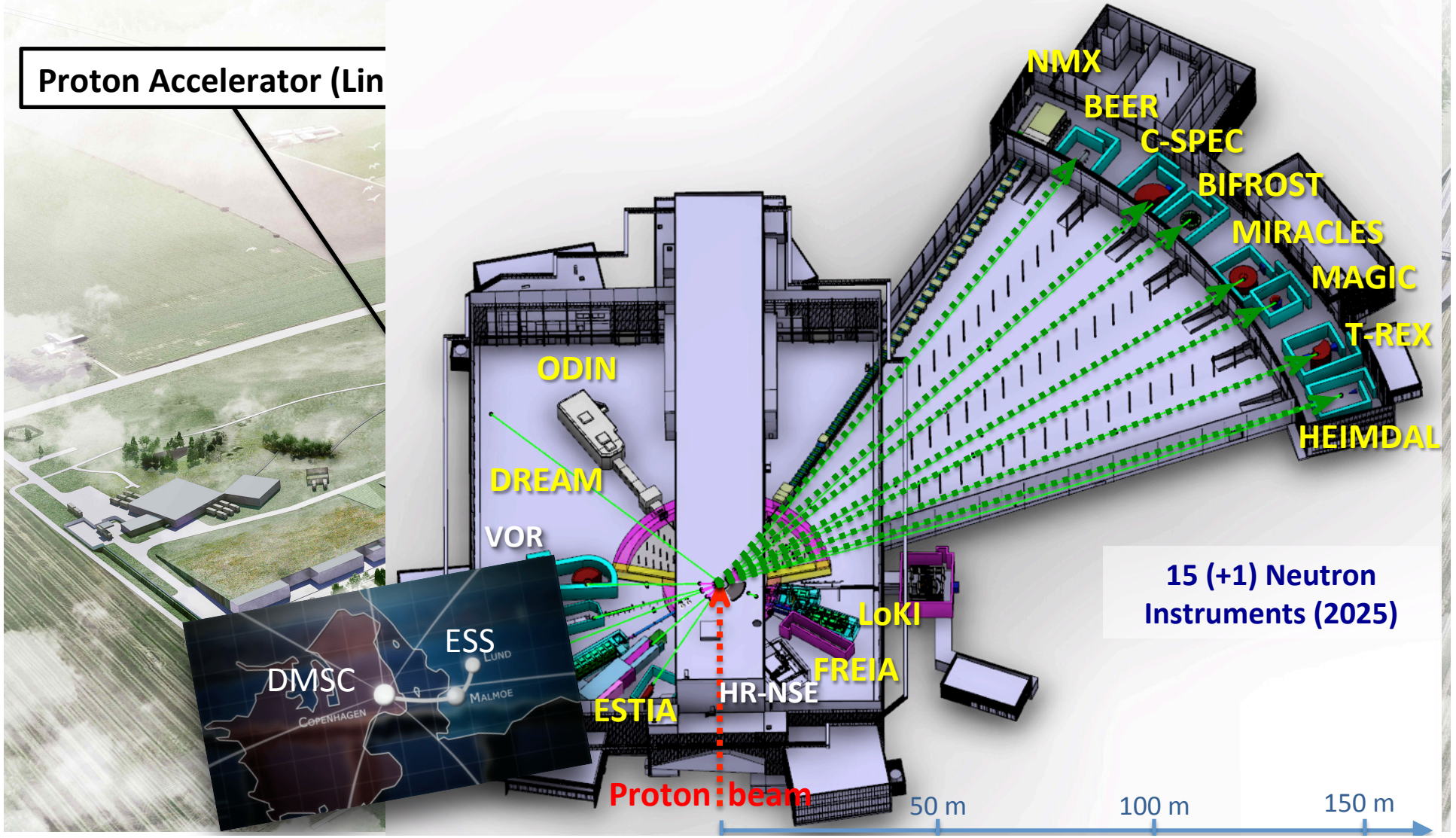
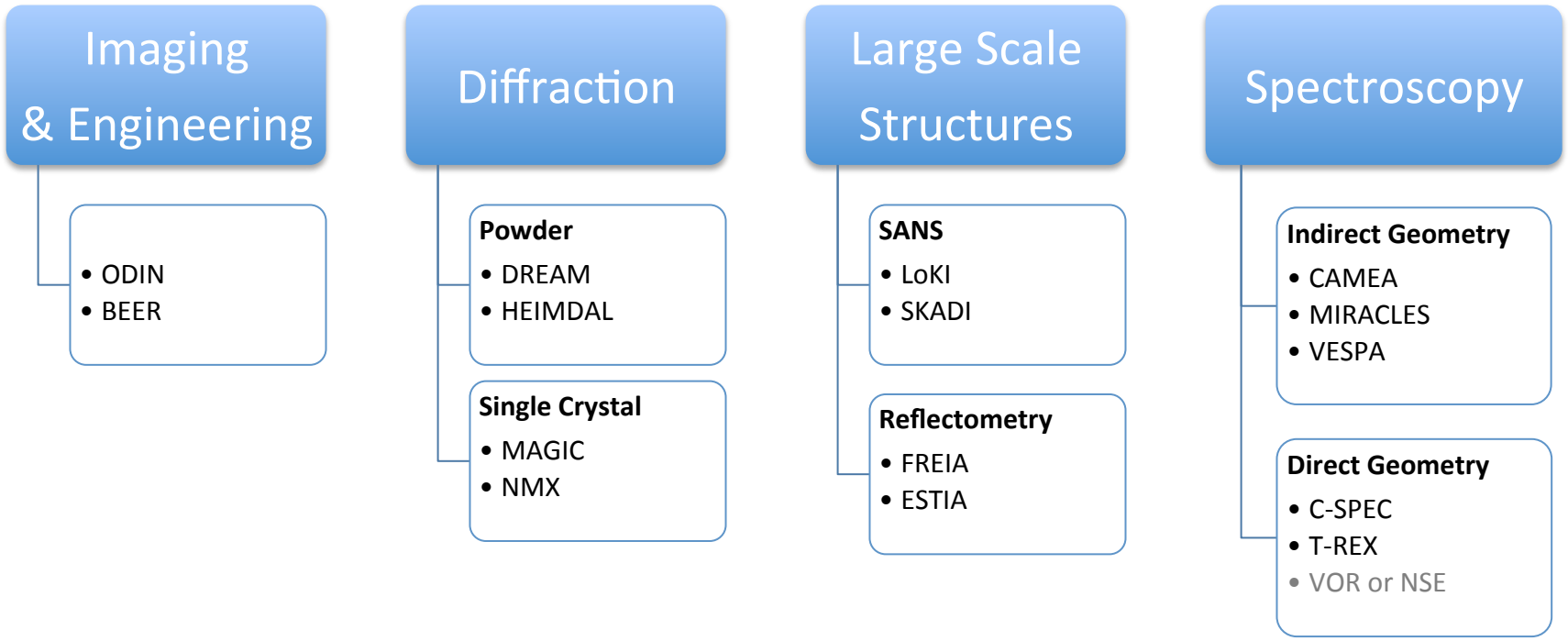


ESS Neutron Instrument Suite

Process:

Instrument Proposals → Scientific & Technical Advisory Panels →

Science Advisory Council (SAC) → ESS Council



Thermal Neutron Scattering

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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

LoKI

SANS for Soft Matter, Materials and Bio-Science

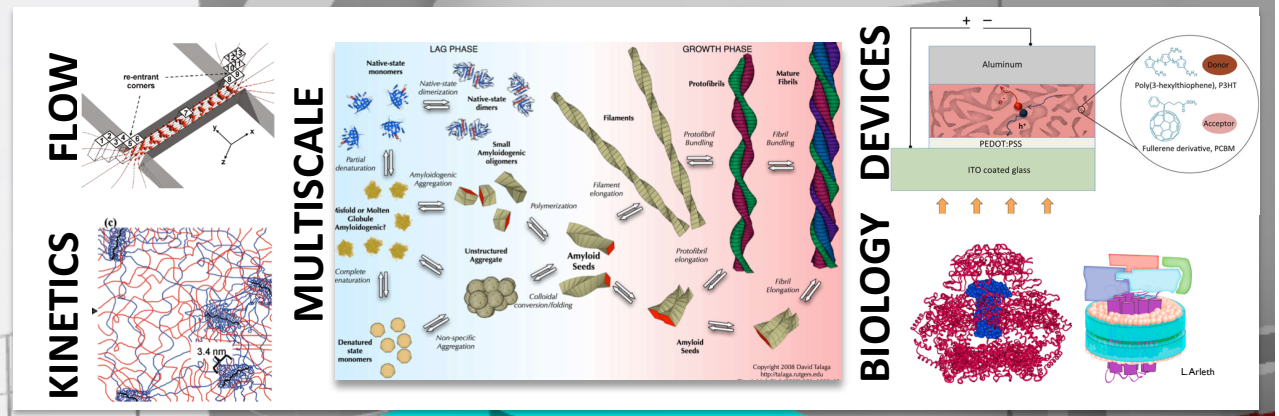
EUROPEAN SPALLATION SOURCE

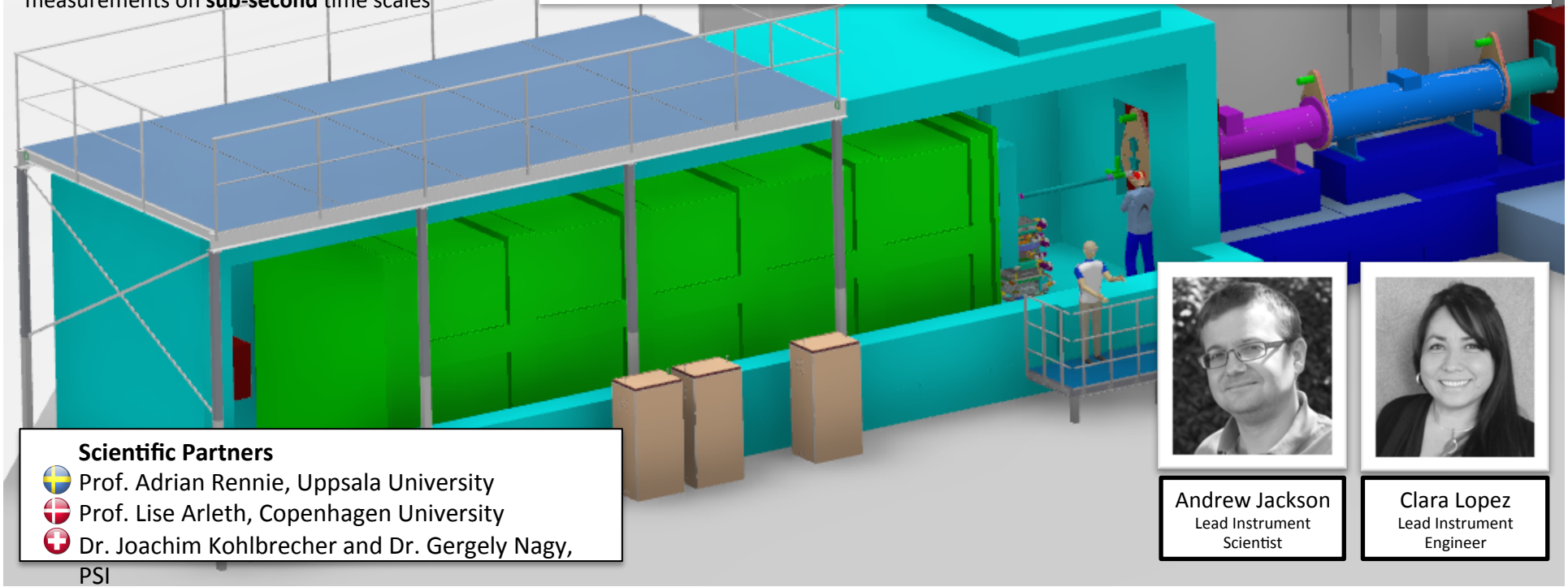
The combination of a **large solid angle** of detectors and a **broad wavelength band** will provide a **world leading** SANS instrument for the ESS.

LoKI will have **high flux**, **wide simultaneous size range**, and a **flexible sample area**.

Small beams, making **scanning experiments** routine.

The ability to perform **"single-shot" kinetic** measurements on **sub-second** time scales





Scientific Partners

Prof. Adrian Rennie, Uppsala University
Prof. Lise Arleth, Copenhagen University
Dr. Joachim Kohlbrecher and Dr. Gergely Nagy, PSI

Andrew Jackson
Lead Instrument Scientist

Clara Lopez
Lead Instrument Engineer

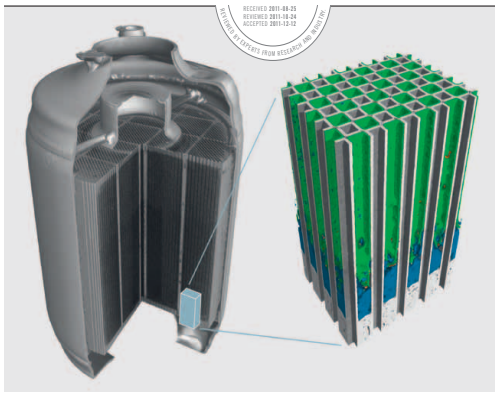
ODIN Optical and Diffraction Imaging with Neutrons
Multi purpose imaging instrument

M. Strobl

EUROPEAN SPALLATION SOURCE

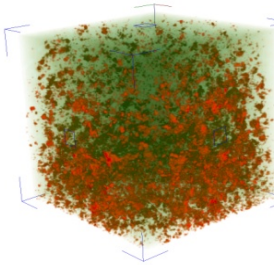
Conventional:

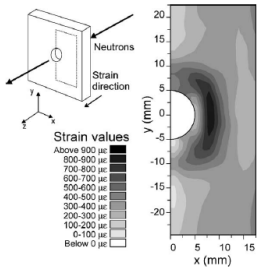
High resolution imaging:
Energy/Bio/Engineering/
Industry/Heritage/Soft M.

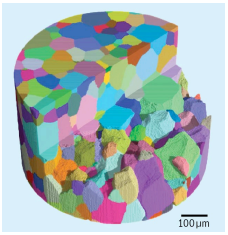


Advanced ToF methods:

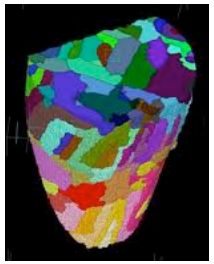
Bragg edge
Phases/
Grains/
Strains





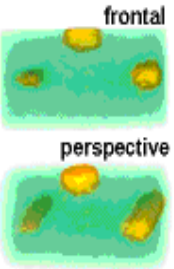


Dark-field
Domains/
Precipitates/
Porosity

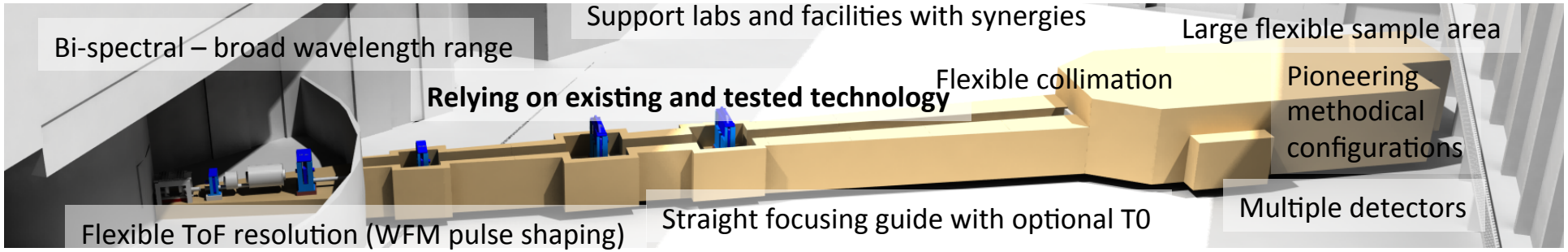


Nature Com. 2010

Polarized
Magnetism/
Supercond./
Phase trans.



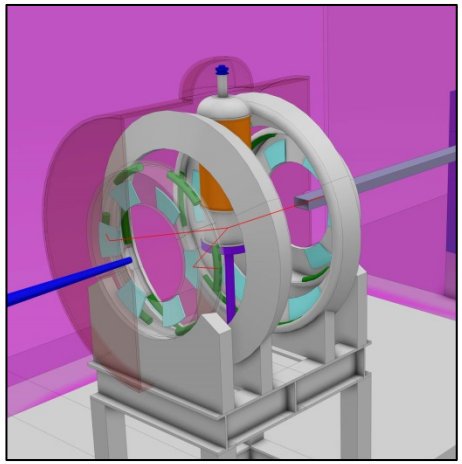
Nature Phys 2008



VESPA
Vibrational Excitation Spectroscopy with pyrolitic-graphite analyzers

EUROPEAN SPALLATION SOURCE

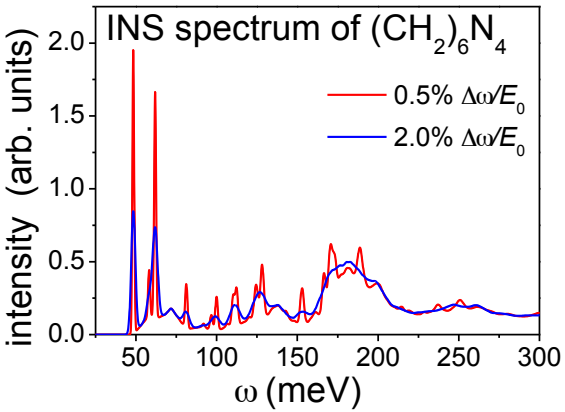
Proposers: **ISC-CNR** (Italy), **ESS** (Sweden), **University of Copenhagen** (Denmark).



VESPA: an indirect-geometry TOF spectrometer fully exploiting the long ESS pulse through wavelenght frame multiplication.

Specs: one-shot, high-resolution, high-intensity **neutron vibrational spectroscopy** in the 0-500 meV range.

Science: devoted to *in-situ* spectroscopic studies - chemical reactions and catalysis, small samples, high pressure, renewable energies, geosciences, photo/electro-chemistry, pharmacy, advanced sample environments.



Gain factors:

- intensity on sample 10-100× larger than the current leading instrument.
- Relative resolution constant over wide range of energies.
- Trade of flux for resolution possible - resolution tunable from 0.4% to 1.1%.

Science Research Program (Operations)

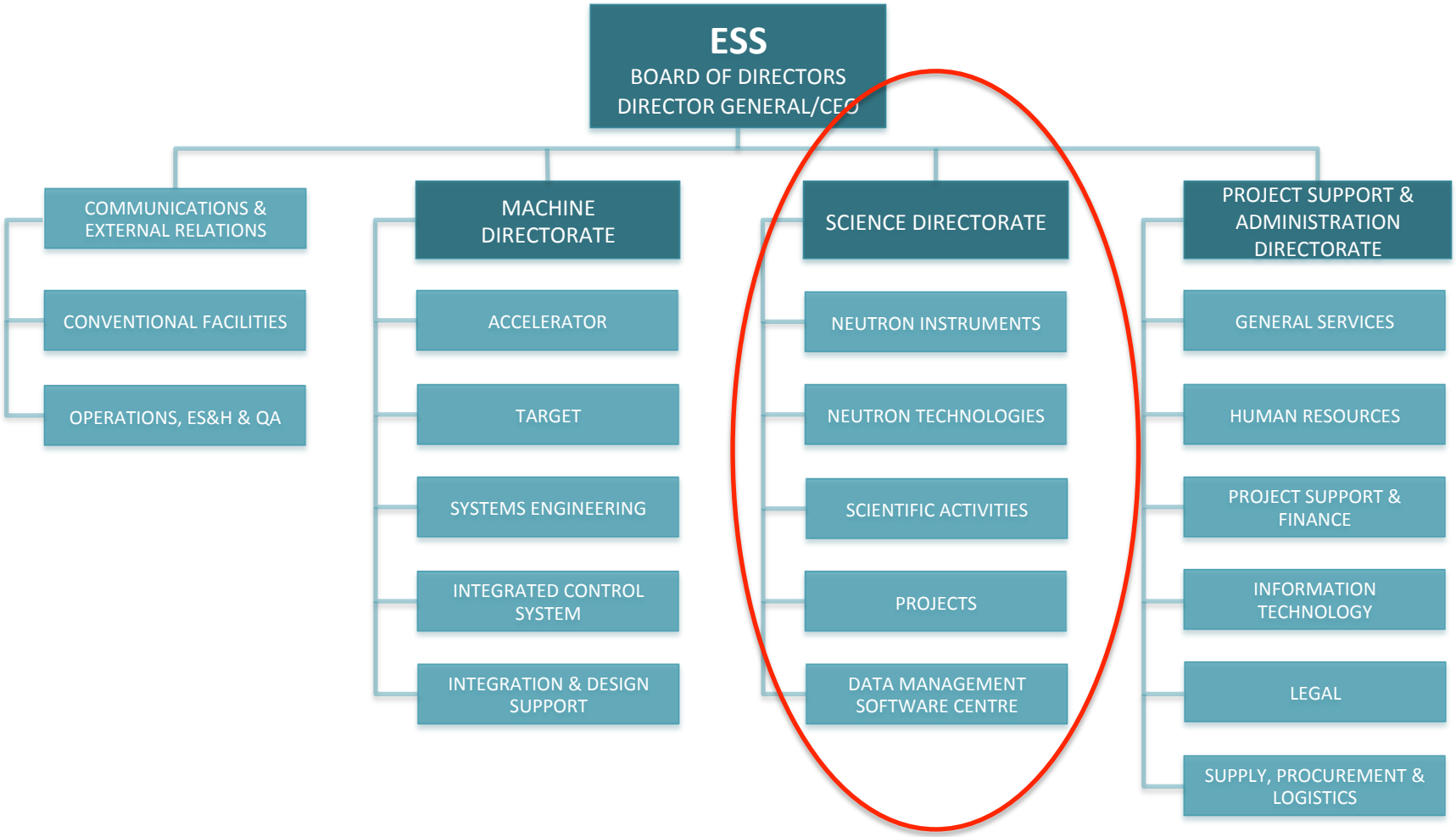
EUROPEAN SPALLATION SOURCE

User Facility (similar to I.L.L & ESRF)

- 1947: First neutron scattering experiments
- Nobel Laureate – Cliff Shull
- 1950/60's – neutron scattering done in small groups
- 1970's: (I.L.L.) 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 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

EUROPEAN SPALLATION SOURCE



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

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

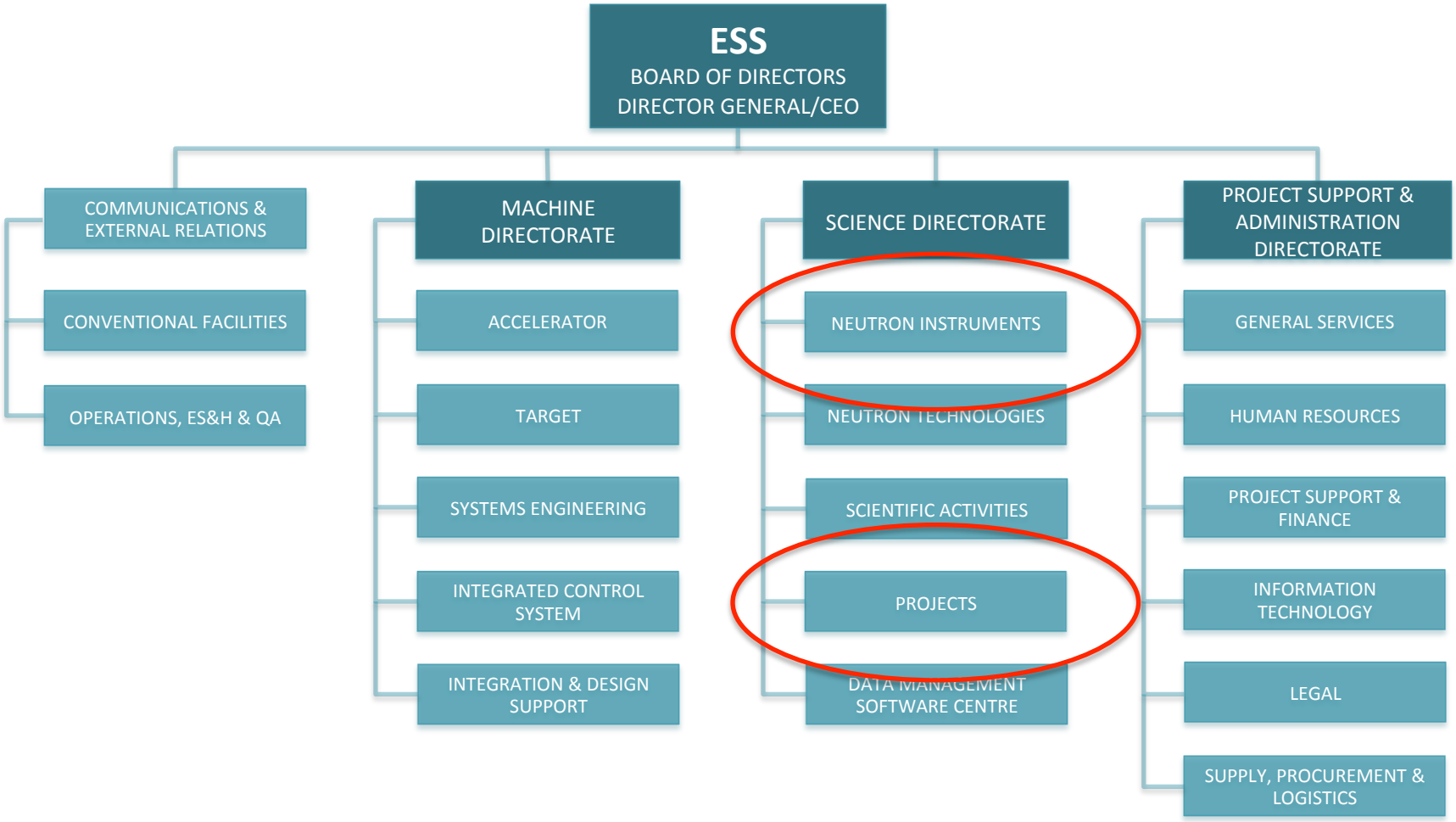
Neutron Technologies Division: Responsible for the specialized instrument components, choppers, guides, detectors.

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

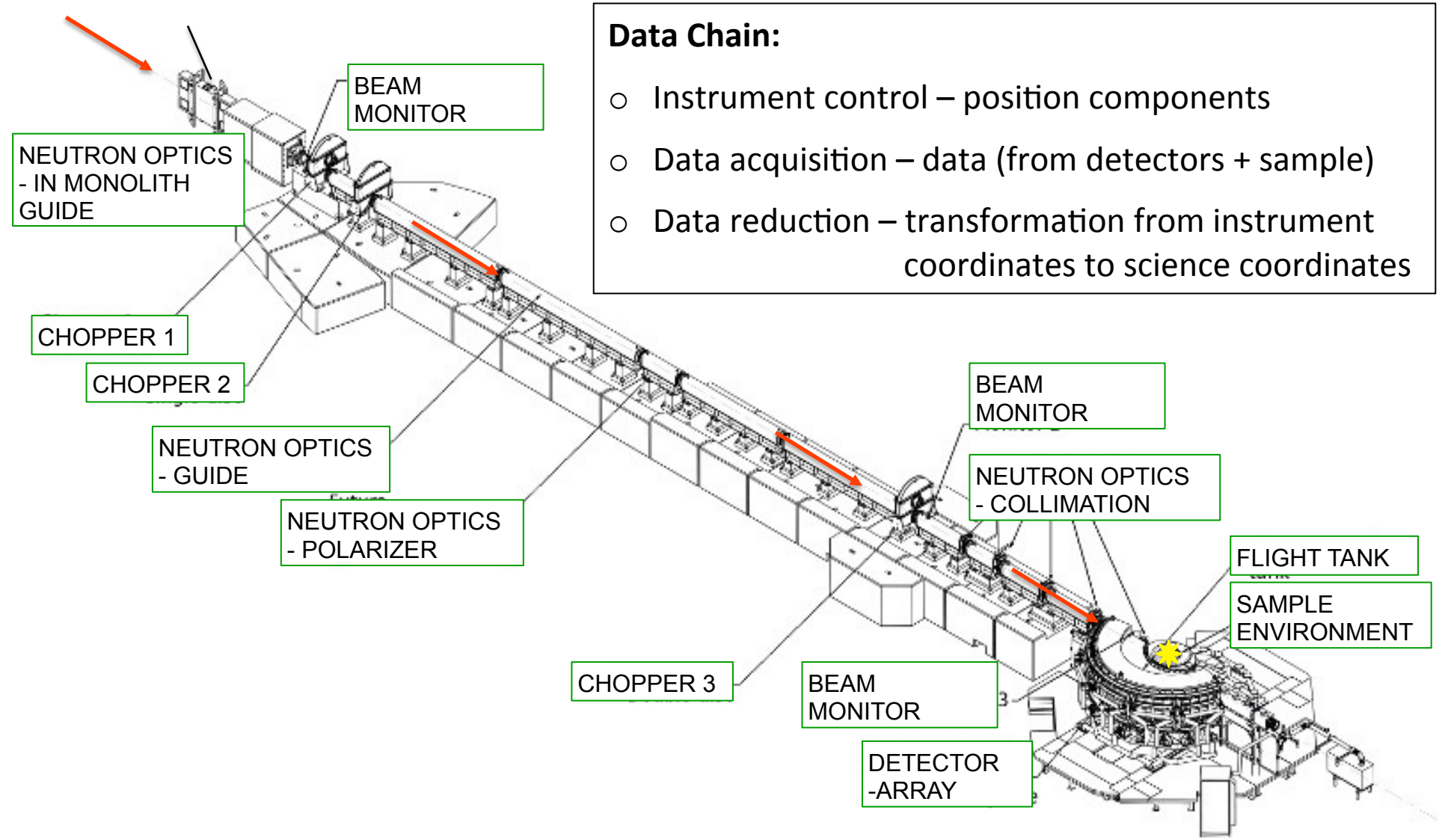
Data Management and Software Centre: Responsible for instrument control, data acquisition/reduction/analysis software and making data/software available to users.

ESS Organization

EUROPEAN SPALLATION SOURCE



Time of Flight Neutron Instruments



Data Chain:

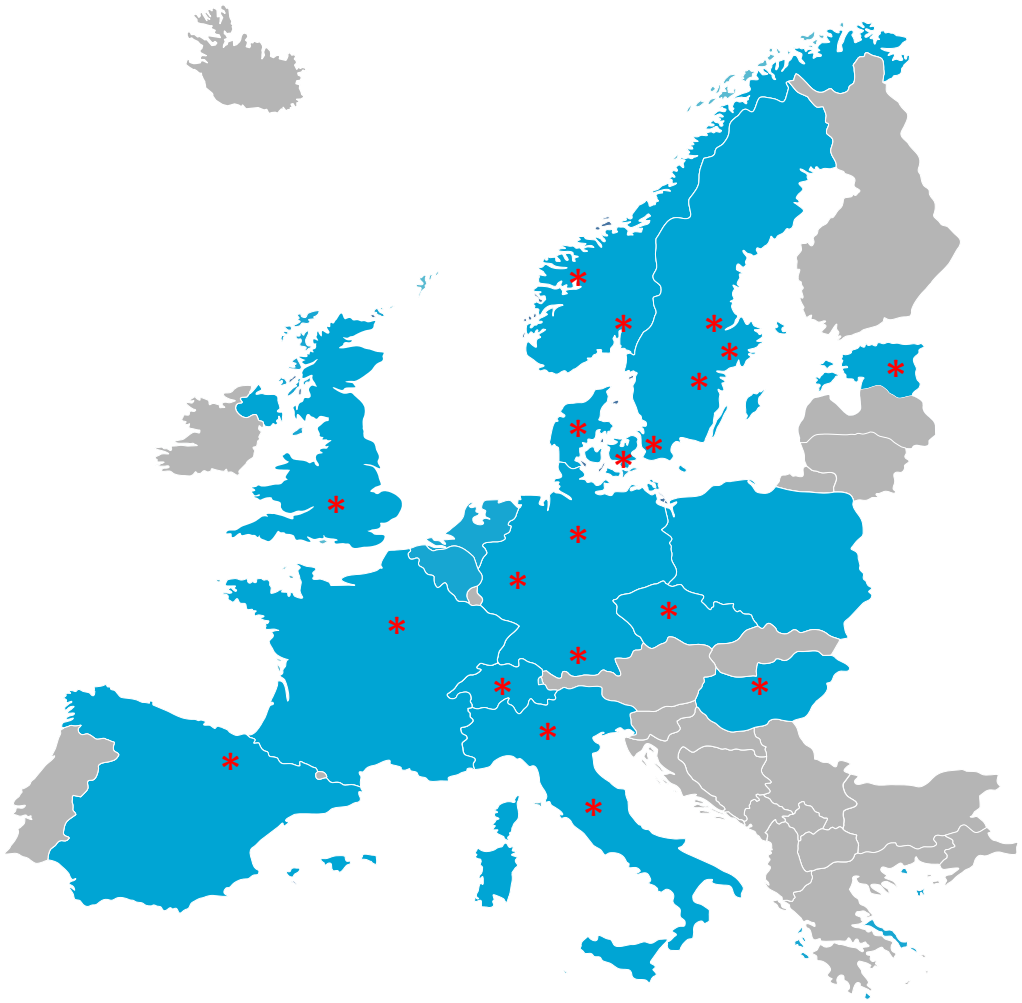
- Instrument control – position components
- Data acquisition – data (from detectors + sample)
- Data reduction – transformation from instrument coordinates to science coordinates

Neutron Beam Instruments & Lead Partners

EUROPEAN SPALLATION SOURCE

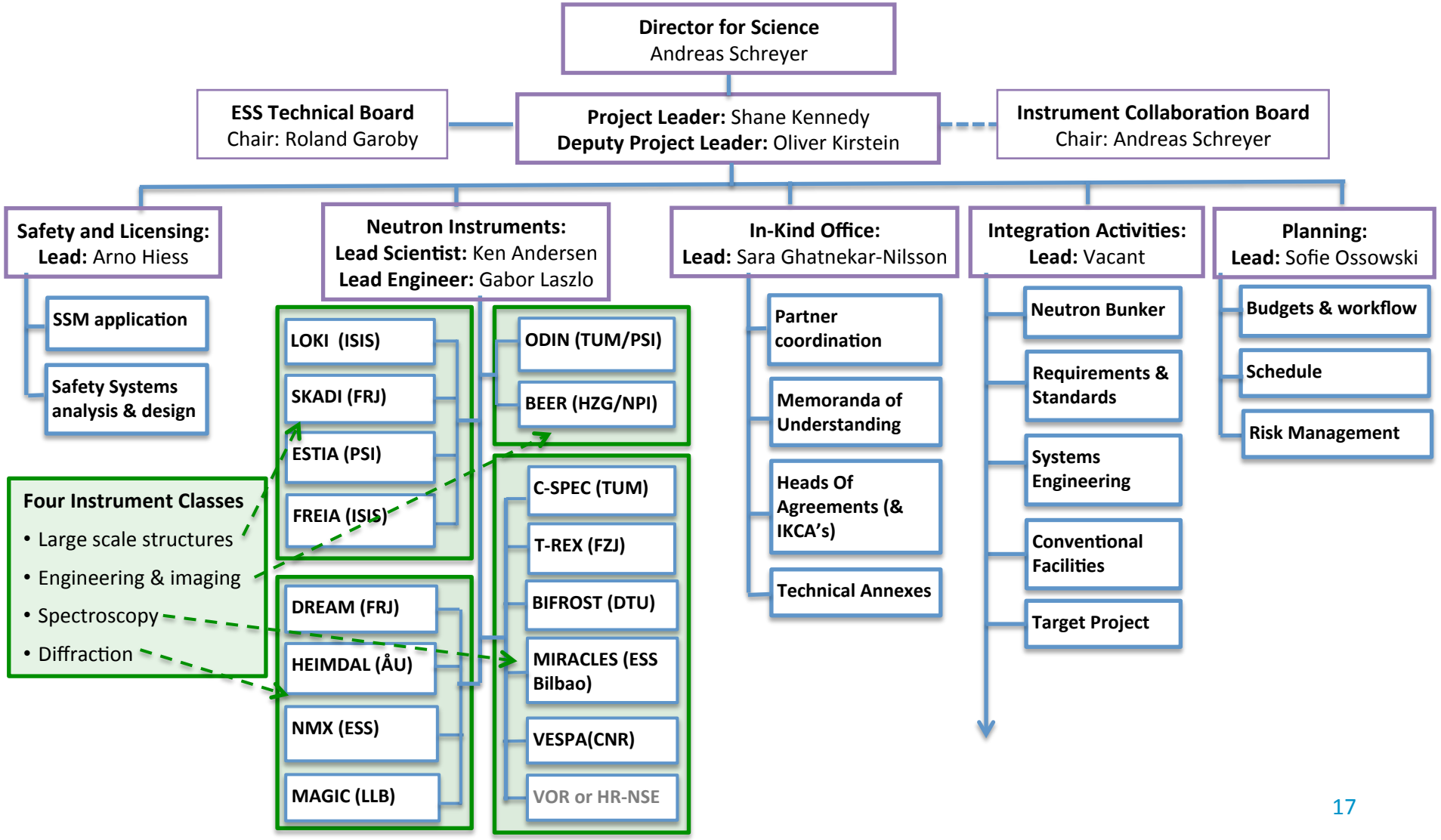
Instrument class	Neutron Instrument	Lead Partner(s)
Large scale structures	LOKI broadband SANS	ISIS (UK)
	SKADI general-purpose SANS	FZJ (DE)
	ESTIA focusing reflectometer	PSI (CH)
	FREIA liquids reflectometer	ISIS (UK)
Diffraction	NMX macromolecular crystallography	ESS
	DREAM powder diffractometer	FZJ (DE)
	HEIMDAL hybrid diffractometer	AU (DK)
	MAGIC magnetism single-crystal diffractometer	LLB (FR)
Engineering	BEER engineering diffractometer	HZG (DE) + NPI (CZ)
	ODIN multi-purpose imaging	TUM (DE) + PSI (CH)
Spectroscopy	C-SPEC cold chopper spectrometer	TUM (DE)
	BIFROST extreme-environments spectrometer	DTU (DK)
	T-REX bispectral chopper spectrometer	FZJ (DE)
	VESPA vibrational spectroscopy	CNR (IT)
	MIRACLES backscattering spectrometer	ESS-Bilbao (ES)
	16th Instrument **(VOR or NSE)**	TBD

NSS Partners



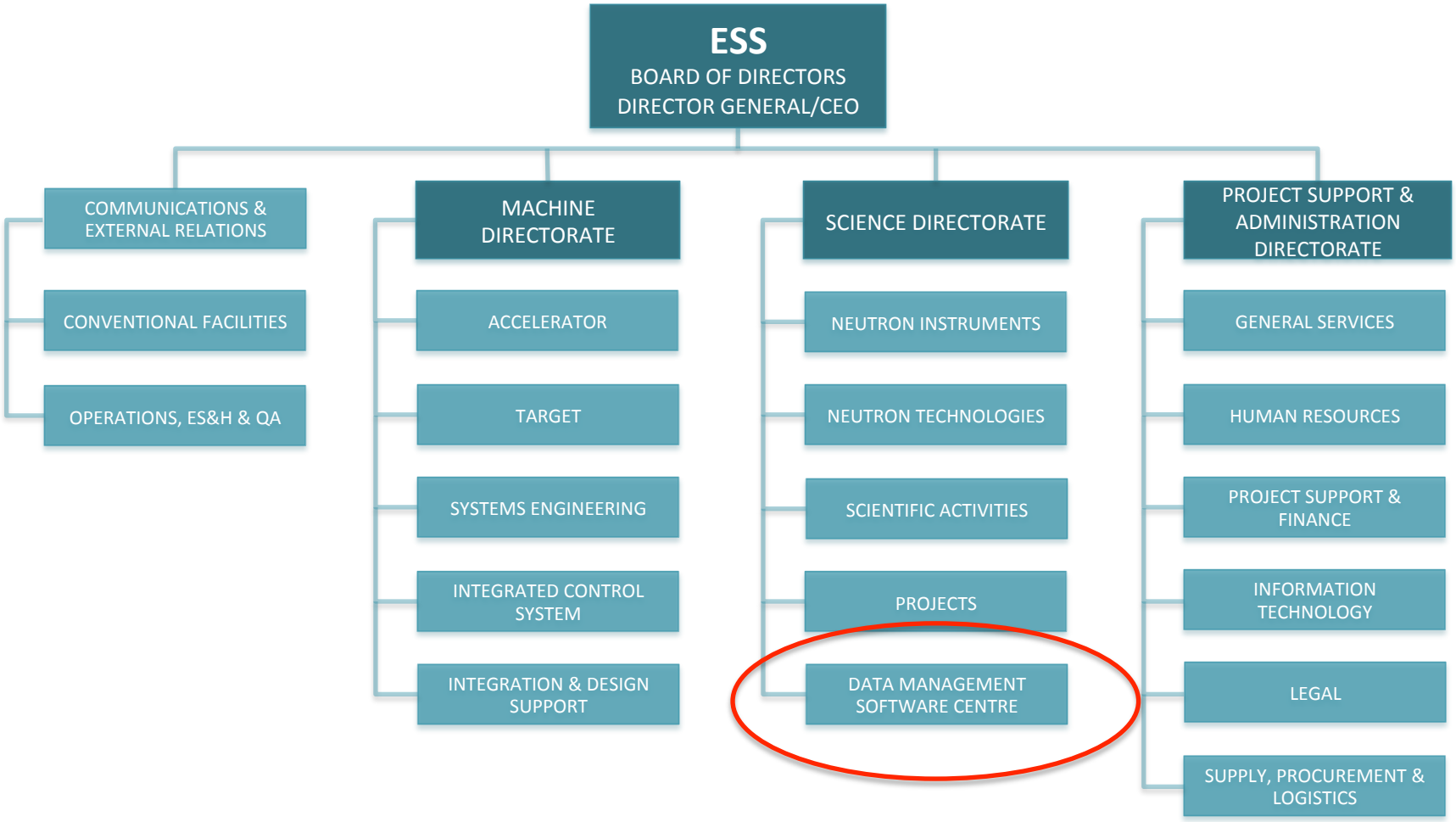
Partner Institutes:
Czech Republic: NPI
Denmark: Aarhus University, DTU, KU, Roskilde University
Estonia: Tartu University
France: LLB (CEA-CNRS)
Germany: FZJ, HZG, TUM
Hungary: Wigner Institute, Centre for Energy Research
Italy: CNR (Perugia and Milano University)
Norway: IFE, Bergen University
Spain: ESS Bilbao
Sweden: LU, LiU, UU, KTH
Switzerland: PSI
United Kingdom: STFC

NSS Instruments & Project Divisions



ESS Organization

EUROPEAN SPALLATION SOURCE



DMSC's Scope

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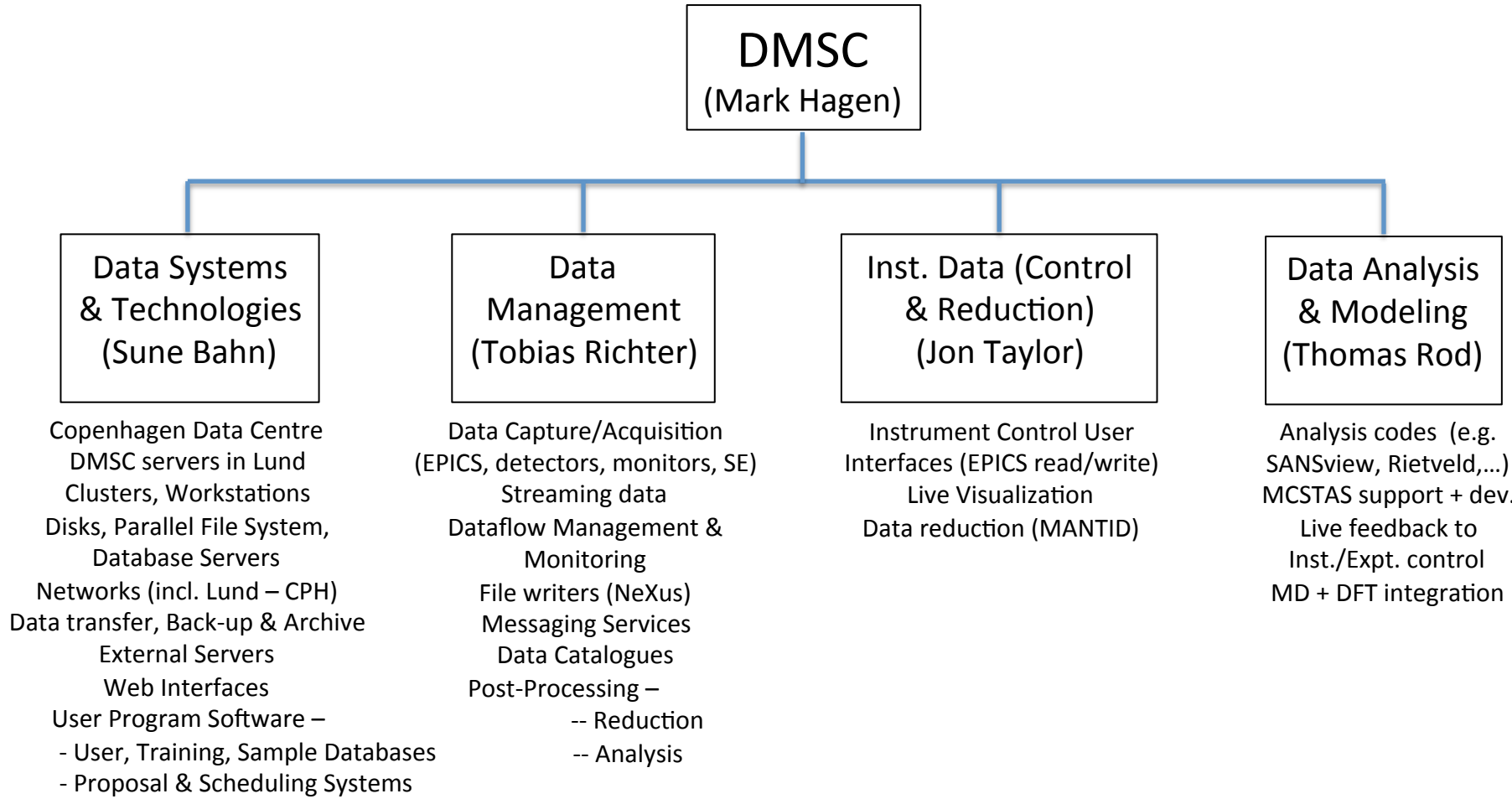
- Construction Phase of ESS (2014 – 2019) & Neutron Beam Instruments (2014 – 2025)
  - Software for the Inst. Control & Data Management (Acq., Reduction, etc.)
  - Software for Data Analysis
  - Software framework to do Live and Automated Data Reduction/Analysis
  - Software for managing the scientific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



DMSC's Scope: Experiment Data Chain

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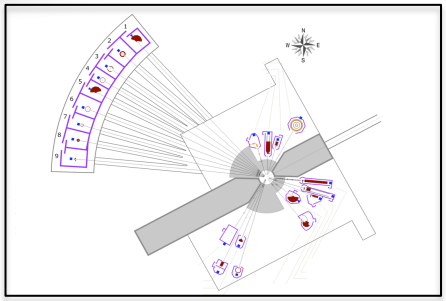
Data Management and Software Centre

- ~75% Software development
- ~25% Hardware (cpu/disk)
- Software to collect data
- Software to turn data into science



Data Analysis

Fitting
Modeling
Simulation

Instrument Data

Control
Reduction
Visualization

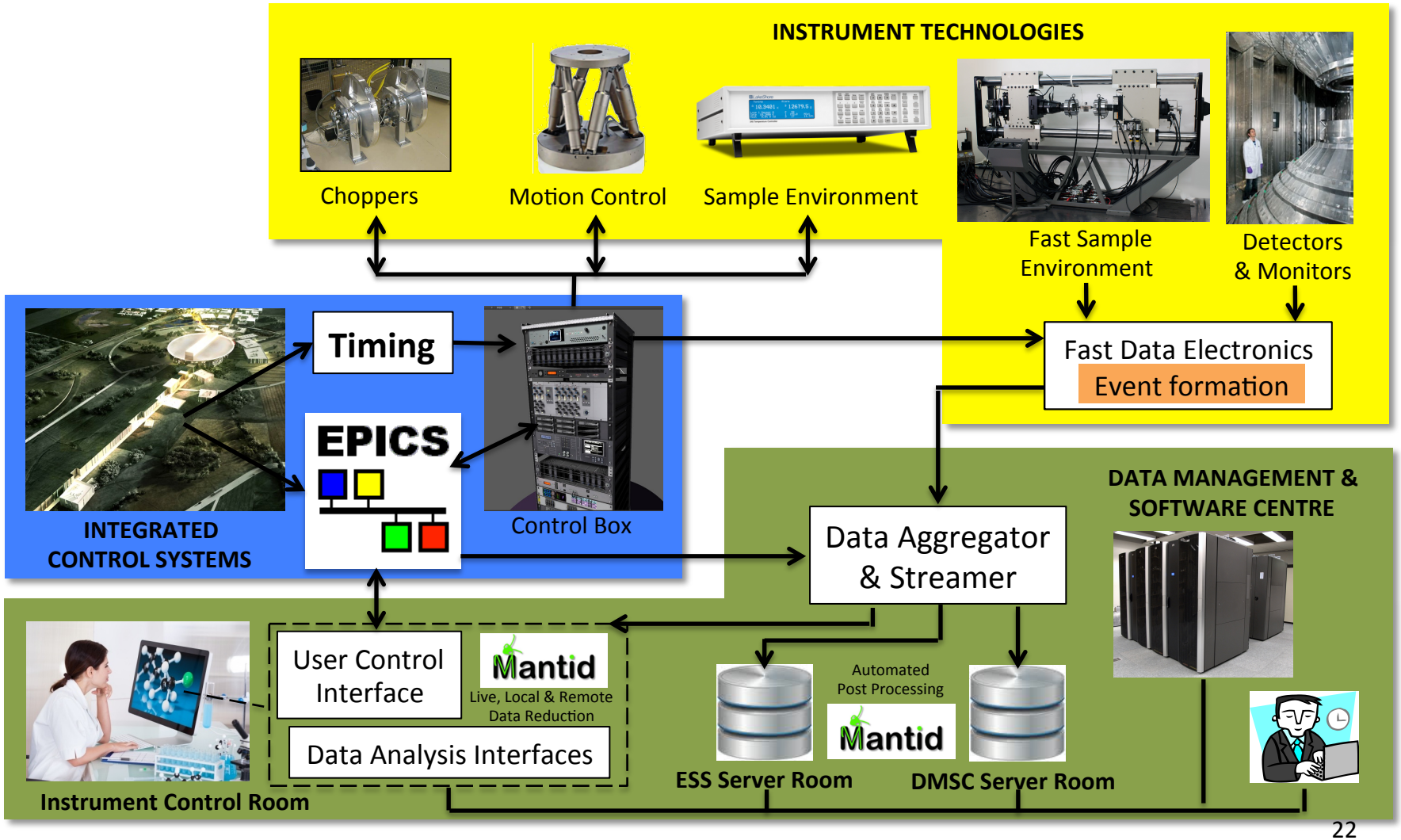
Data Sys. & Tech.

CPUs (Cluster)
Disk, Network
Logins

Data Management

Detector Event Formation
Data Acq./Agg./Stream
File creation/Cataloguing

DMSC's Domain and Interfaces



Core Software Frameworks (+ In-Kind)

EUROPEAN SPALLATION SOURCE

(Live) Data Analysis

ESS bilbao · JCNS · PAUL SCHERRER INSTITUT PSI

Instr.	LOKI, SKADI – ESTIA, FREIA	C-SPEC, TREX – BIFROST, MIRACLES, VESPA	DREAM, HEIMDAL – MAGIC, NMX – BEER	ODIN
Instr. Class	Large Scale Structures (SANS - Reflectometry)	Spectroscopy (Direct – Indirect)	Diffraction (Powder – Xtal – Eng)	Imag -ing

(Live) Data Reduction Framework

ISIS · Mantid

Instr. Class	Large Scale Structures (SANS - Reflectometry)	Spectroscopy (Direct – Indirect)	Diffraction (Powder – Xtal – Eng)	Imag -ing

(Live) Data Management

PAUL SCHERRER INSTITUT PSI · ISIS · NeXus · ICAT · ZeroMQ · EPICS

Experiment Control Framework

ISIS · PAUL SCHERRER INSTITUT PSI · EPICS

Instr. Class	Large Scale Structures (SANS - Reflectometry)	Spectroscopy (Direct – Indirect)	Diffraction (Powder – Xtal – Eng)	Imag -ing

Instrument Data Group · Data Management Group · Data Analysis Group

Data Systems & Technologies

EUROPEAN SPALLATION SOURCE

- Software development servers – repositories, bug trackers, build servers etc.
- Estimated data storage for ESS (at full power) is ~10 PBytes/yr:
  - Neutron scattering data rates are ~10-100 MBytes/s
- In 2019-22 accelerator is low power + instruments rolling out – need less compute/disk than in full ops

  2019: Compute – 59 nodes, 2 PB (Cph) + 2 PB storage (Lund)
  2022: Compute – add 76 nodes, add 28 PB storage (Cph)
  2025: Compute – add 116 nodes, add 45 PB storage (Cph)
- Instrument computers: event formation, user control + reduction, aggregation and streaming
- Remote login access nodes for users
  Data download nodes (sftp, gridftp)
- Servers and software for User Office

Questions

EUROPEAN SPALLATION SOURCE

Thank You