Science & Technology Facilities Council

The ISIS Facility: Present State and Future Prospects

IX School of Neutron Scattering

Francesco Paolo Ricci

27 September 2008

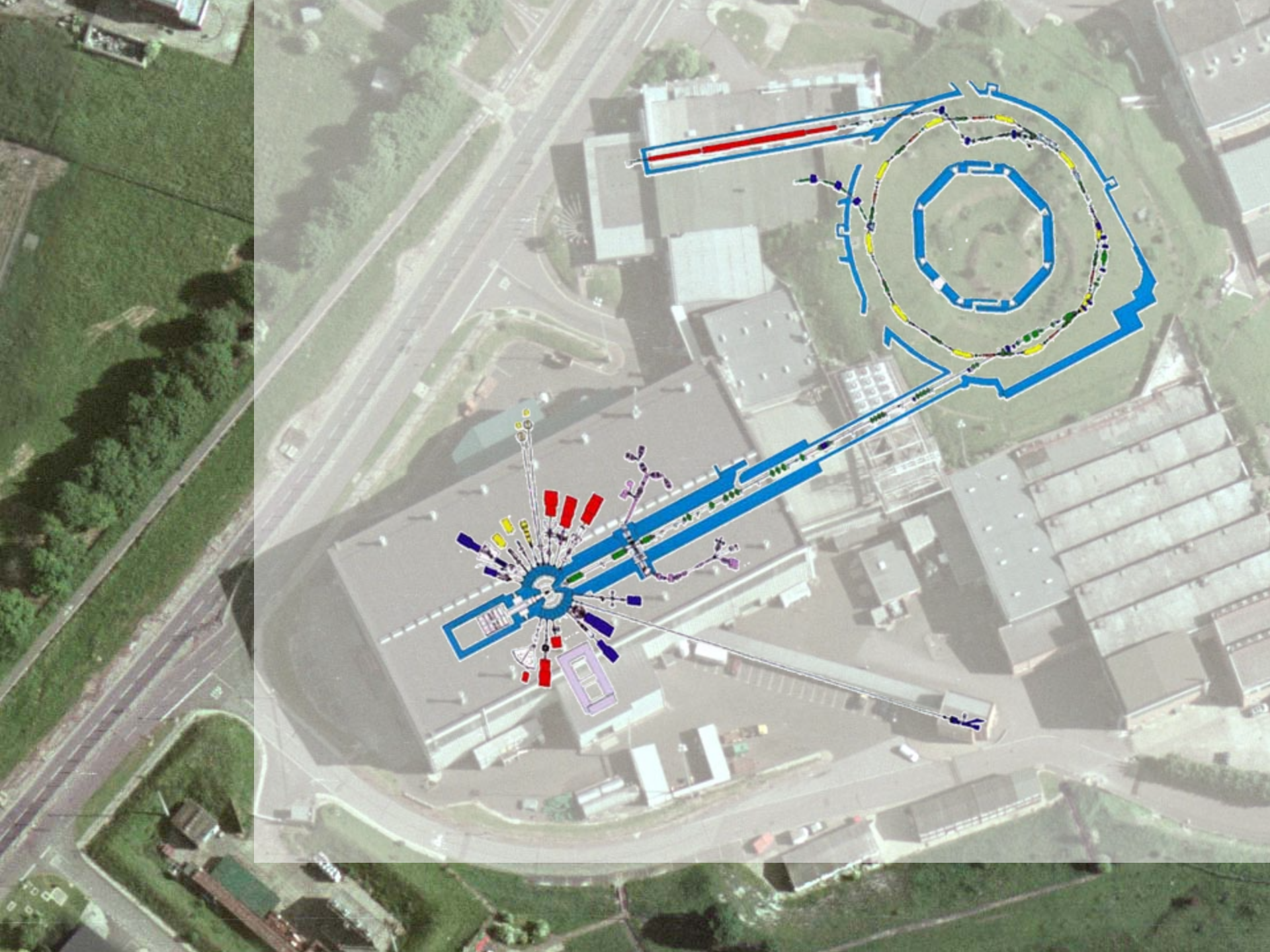
Andrew Taylor

Science & Technology Facilities Council

ISIS

is the world's leading pulsed neutron and muon research centre

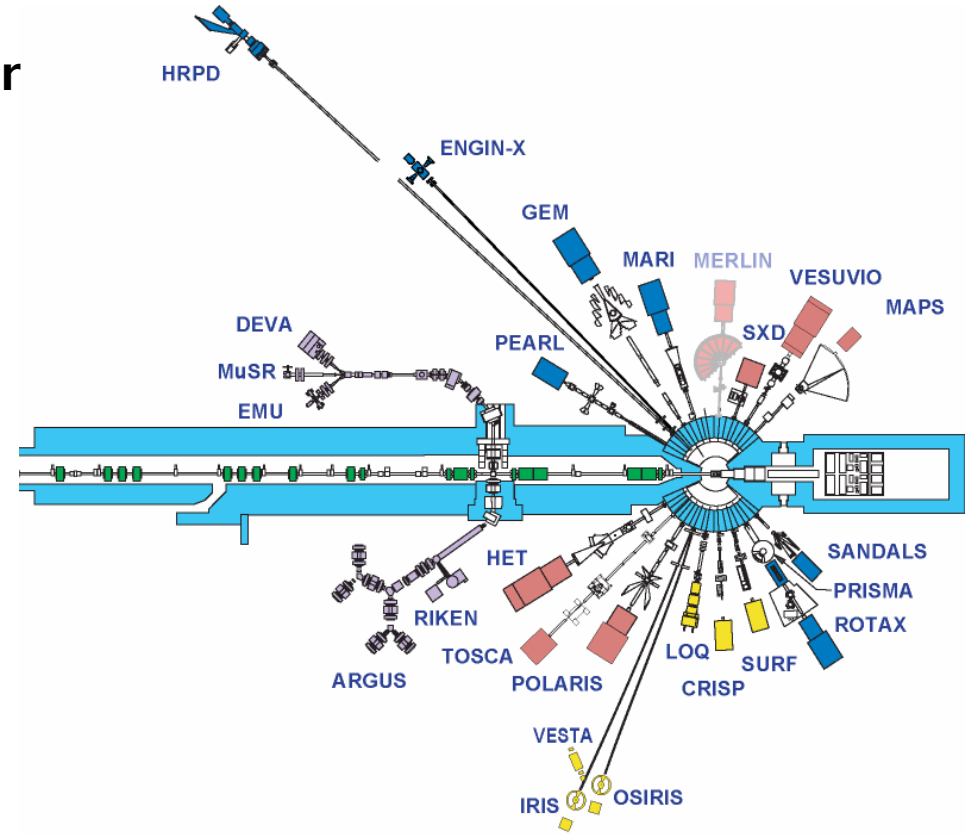
Science & Technology Facilities Council
ISIS




WT 17 TON
M108
RADIATION HAZARD

A World Centre for Research in the Physical and Life Sciences with Neutrons and Muons

- **Internationally Competitive**
- **Broad Academic Base ~1500/yr**
- **700 Experiments/ yr**
- **500 Publications/ yr**



Science & Technology Facilities Council
ISIS

ISIS 20

ISIS

is the world's leading pulsed neutron and muon research centre

Science & Technology Facilities Council
ISIS

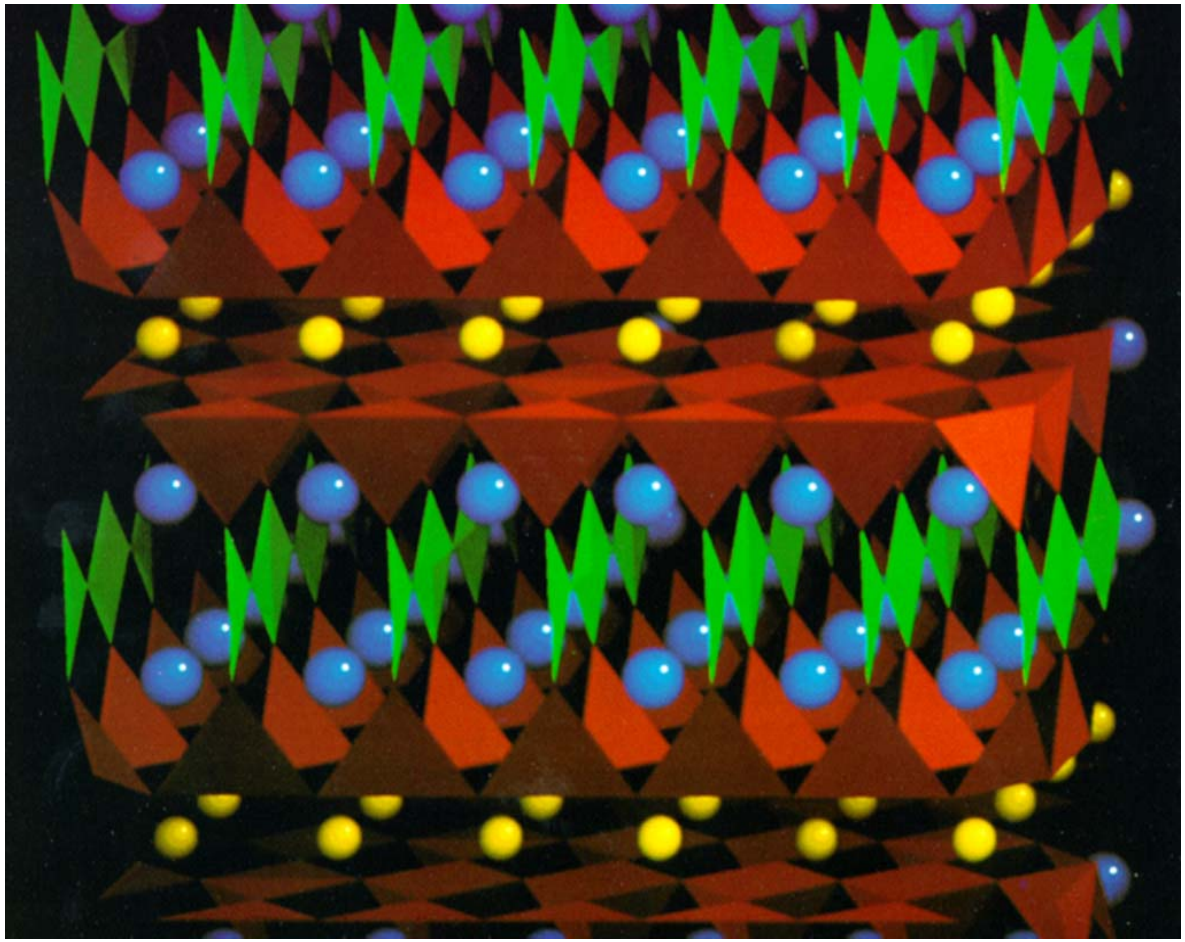
Science & Technology Facilities Council
ISIS

ISIS - riding the wave of materials research

- High Tc Superconductors
- Buckyballs
- GMR / CMR
- Residual Stress
- Surfactants
- Macromolecules
- *In Vivo* Studies

Science & Technology Facilities Council
ISIS

ISIS - riding the wave of materials research



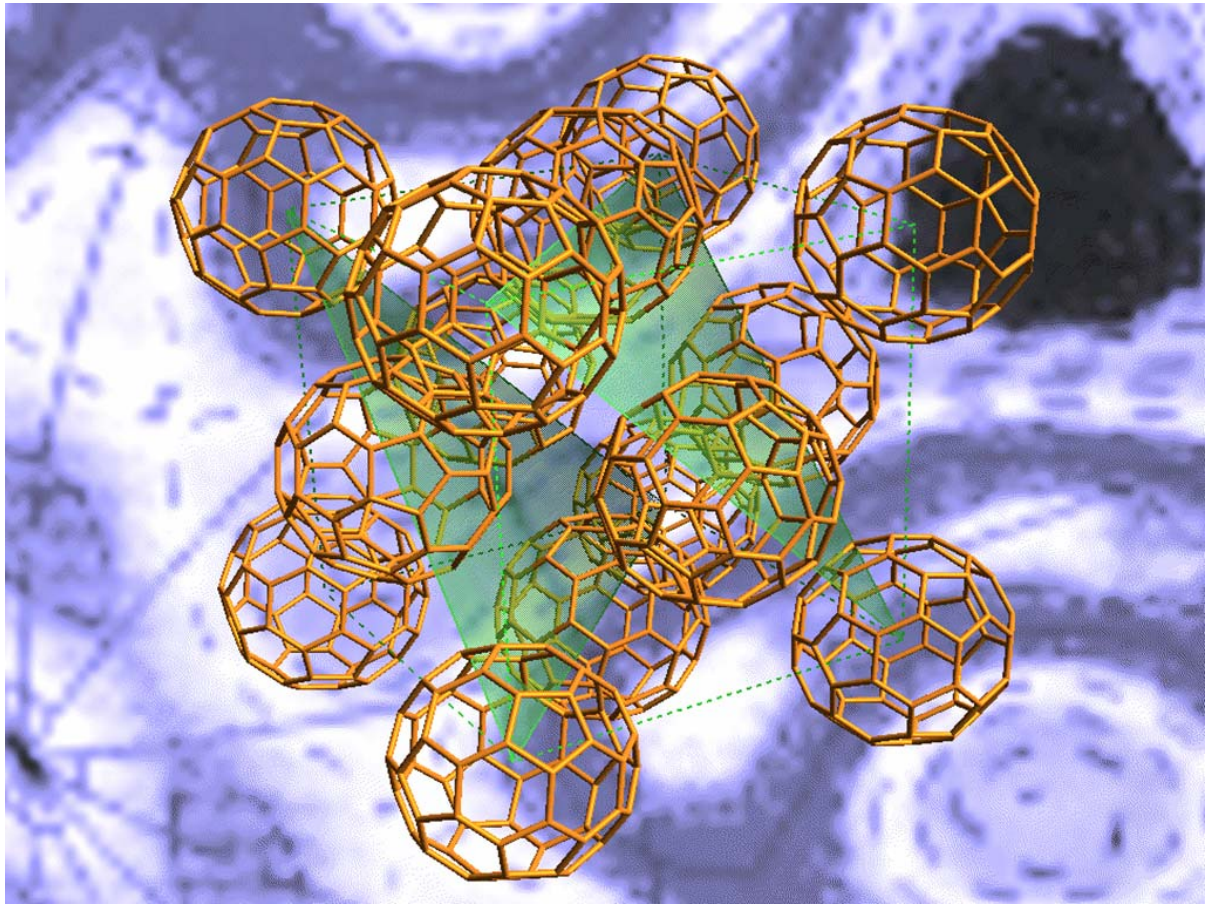
1987
High temperature superconductivity

The crystal structure of $YBa_2Cu_3O_7$ determined by neutron powder diffraction. This material has a variable oxygen content that is dependent on sample preparation. Superconductivity is crucially related to oxygen content. Neutron diffraction gave very precise information on the role of oxygen.

Nature (1987) **327** 310-312

Science & Technology Facilities Council
ISIS

ISIS - riding the wave of materials research



1991
C_{60}, fullerenes and fullerides

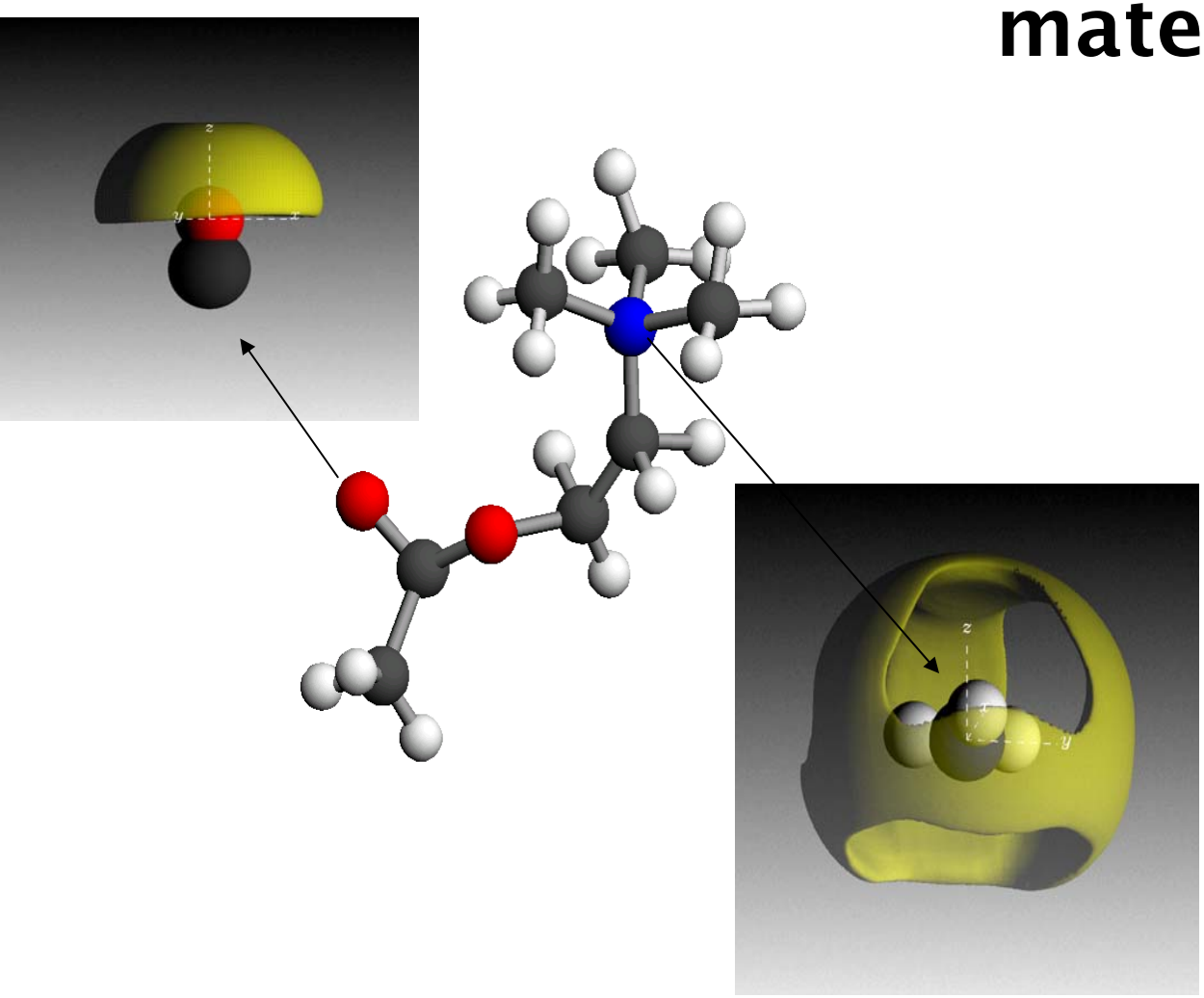
The crystal structure of C_{60} as determined by high resolution neutron powder diffraction.

Nature (1991) **353** 147-149

Office of Basic Energy Sciences
Serving the Present, Shaping the Future

Science & Technology Facilities Council
ISIS

ISIS - riding the wave of materials research



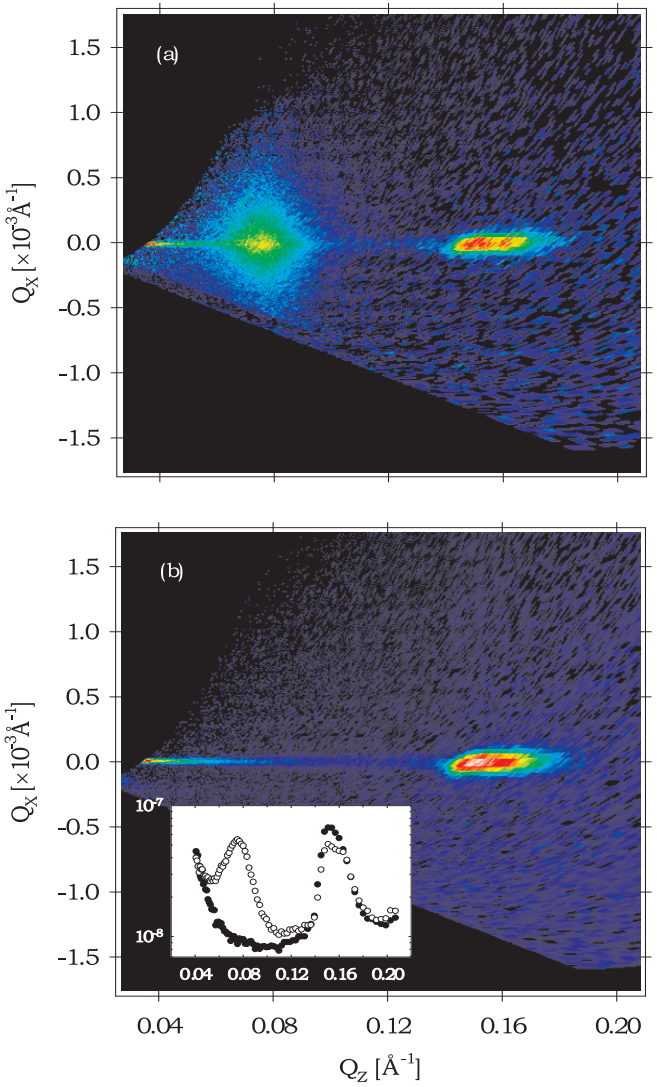
1996 Hydration Shells around molecules in solution

The neurotransmitter Acetylcholine. Absence of strong hydrogen bonding *to* water *from* methyl hydrogens.

Biophysical Journal (1996)

Science & Technology Facilities Council
ISIS

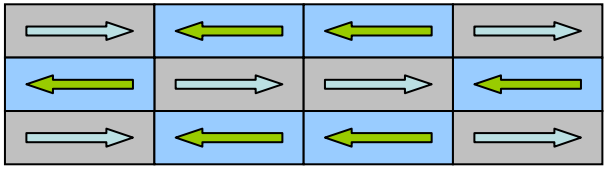
ISIS - riding the wave of materials research



2000
Complexity in Magnetic multilayers

The work on a[Co(20)/Cu(20)]x50 multilayer gives a full insight into the nature of GMR in this system which in turn helps develop our basic scientific understanding in important technologies such as hard disk storage.

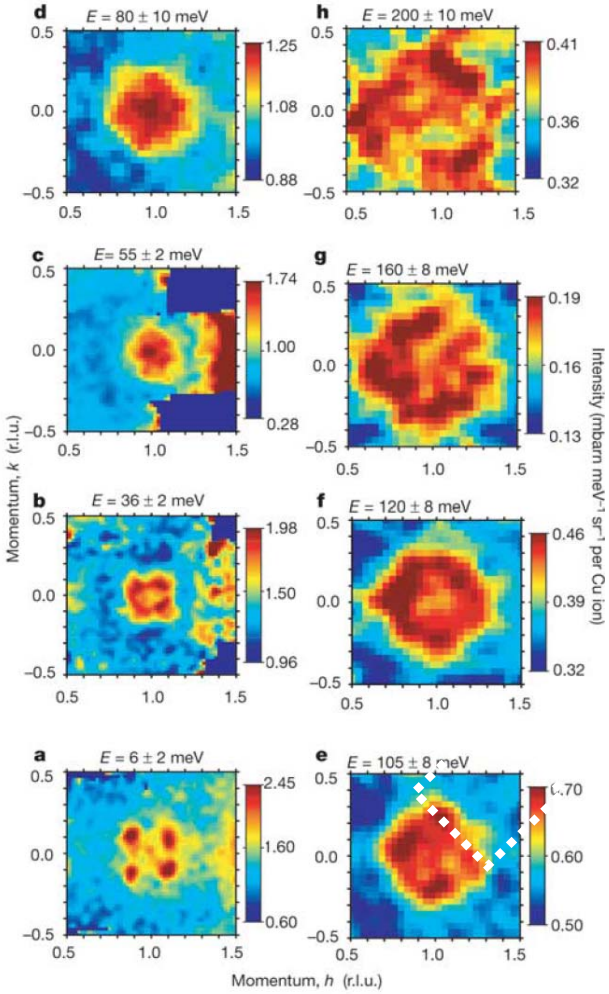
PRL 85 (2000) 4964



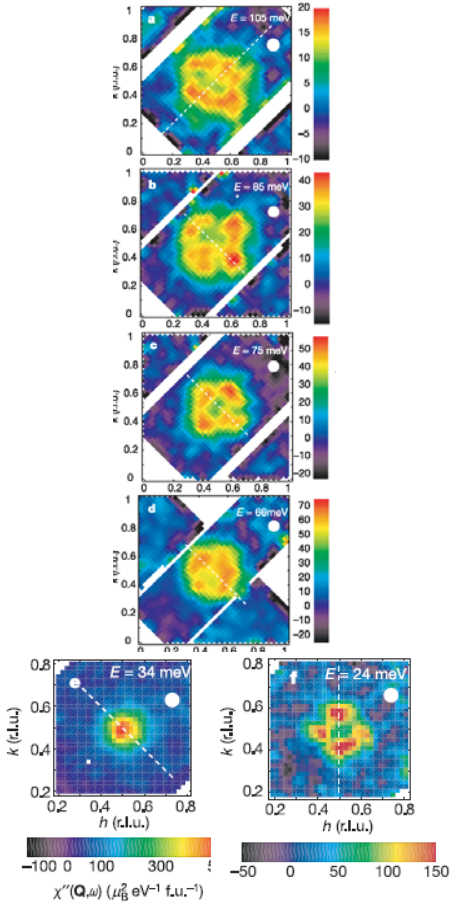
Science & Technology Facilities Council
ISIS

ISIS - riding the wave of materials research

$La_{2-x}Ba_xCuO_4$

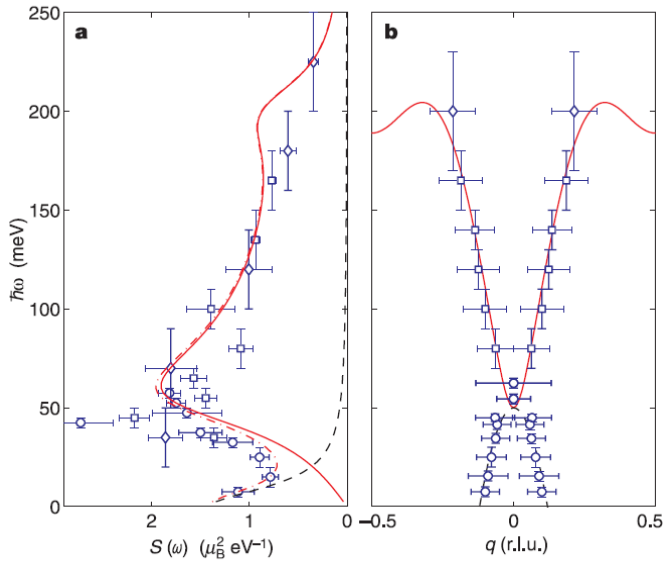


$YBa_2Cu_3O_{6+x}$



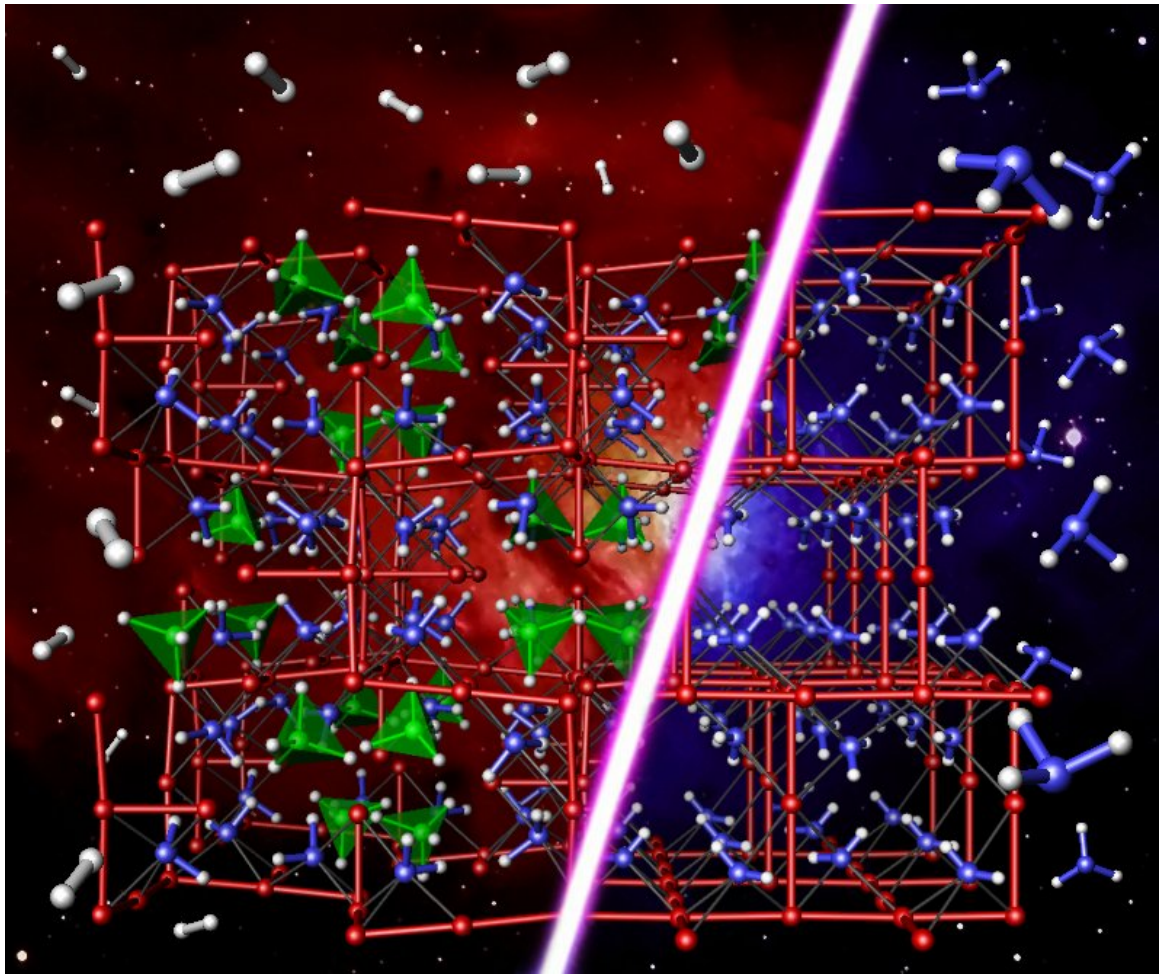
2004
High temperature superconductivity

S.M. Hayden et al., Nature (2004)
J.M. Tranquada et al., Nature (2004)



Science & Technology Facilities Council
ISIS

ISIS - riding the wave of materials research



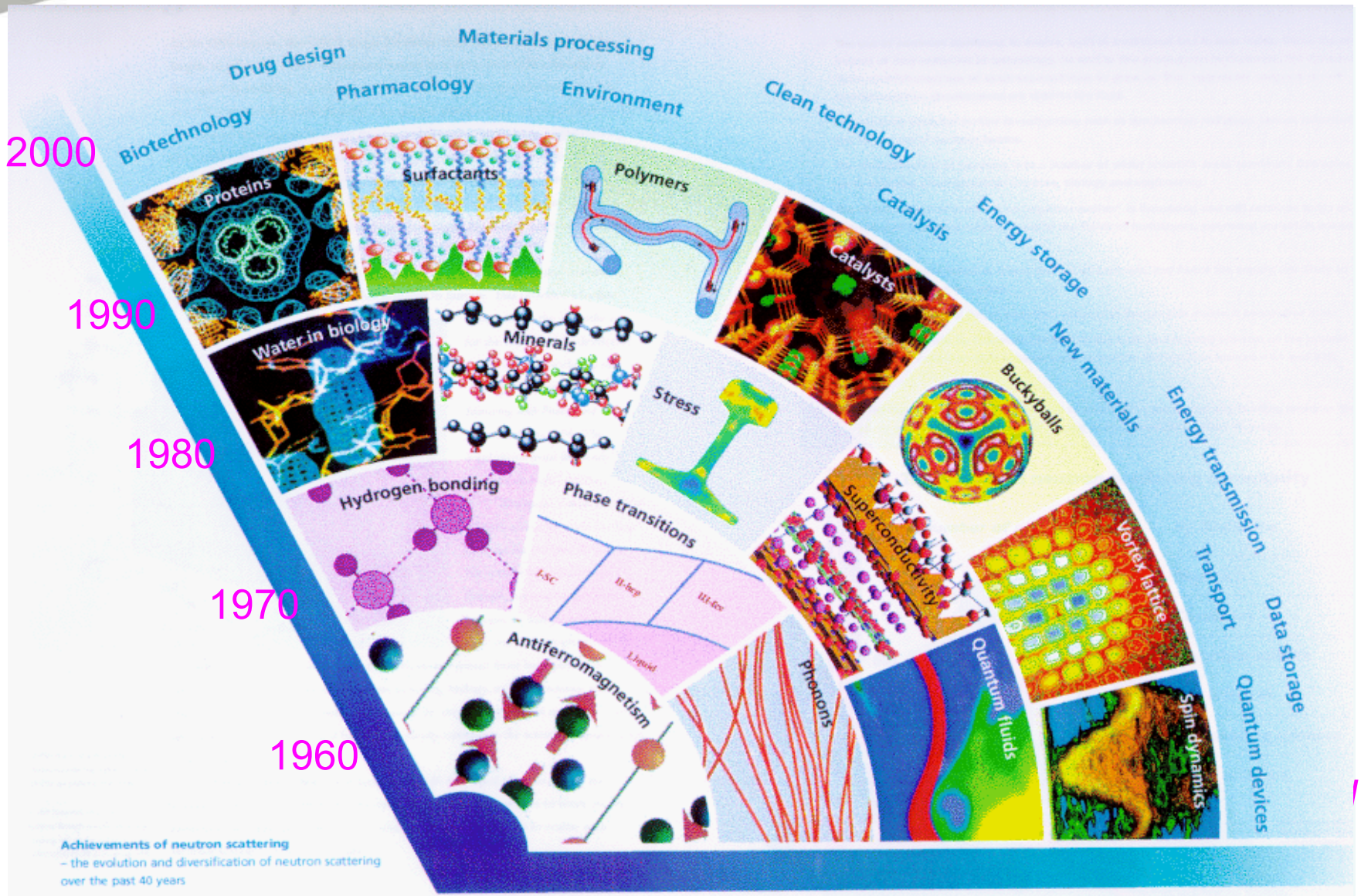
2006
H_2 storage materials

The crystal structures of $Li_4BN_3H_{10}$ and $LiNH_2$ as determined by high resolution neutron and X-ray powder diffraction.

Chem Commun. (2006) 2439-2441

Science & Technology Facilities Council

Expanding the Frontiers



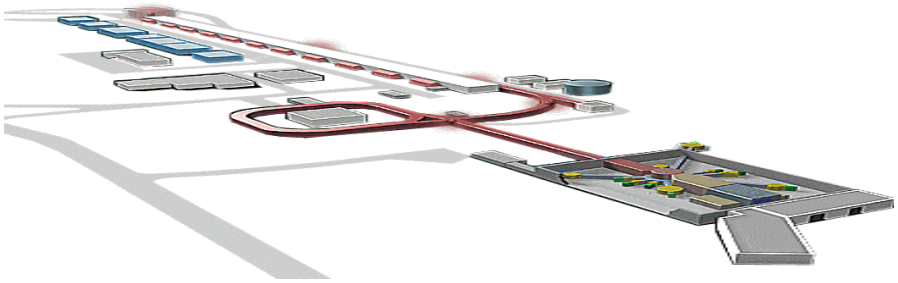
Achievements of neutron scattering
– the evolution and diversification of neutron scattering over the past 40 years

- **Europe has defined the field of neutron scattering over the past 25 years**
- **The European neutron scattering community enjoys world-leading capacity and capability**

International Challenges

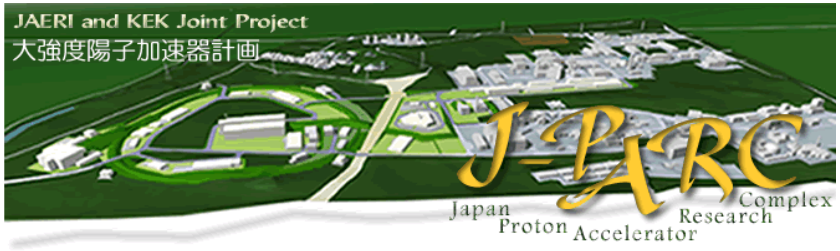
Revolution rather than Evolution

USA building 1.4 MW SNS $1.4B



Commissioning 2007
Science 2008
Source ~6x ISIS in 2012

Japan building 1 MW J-PARC $1.8B

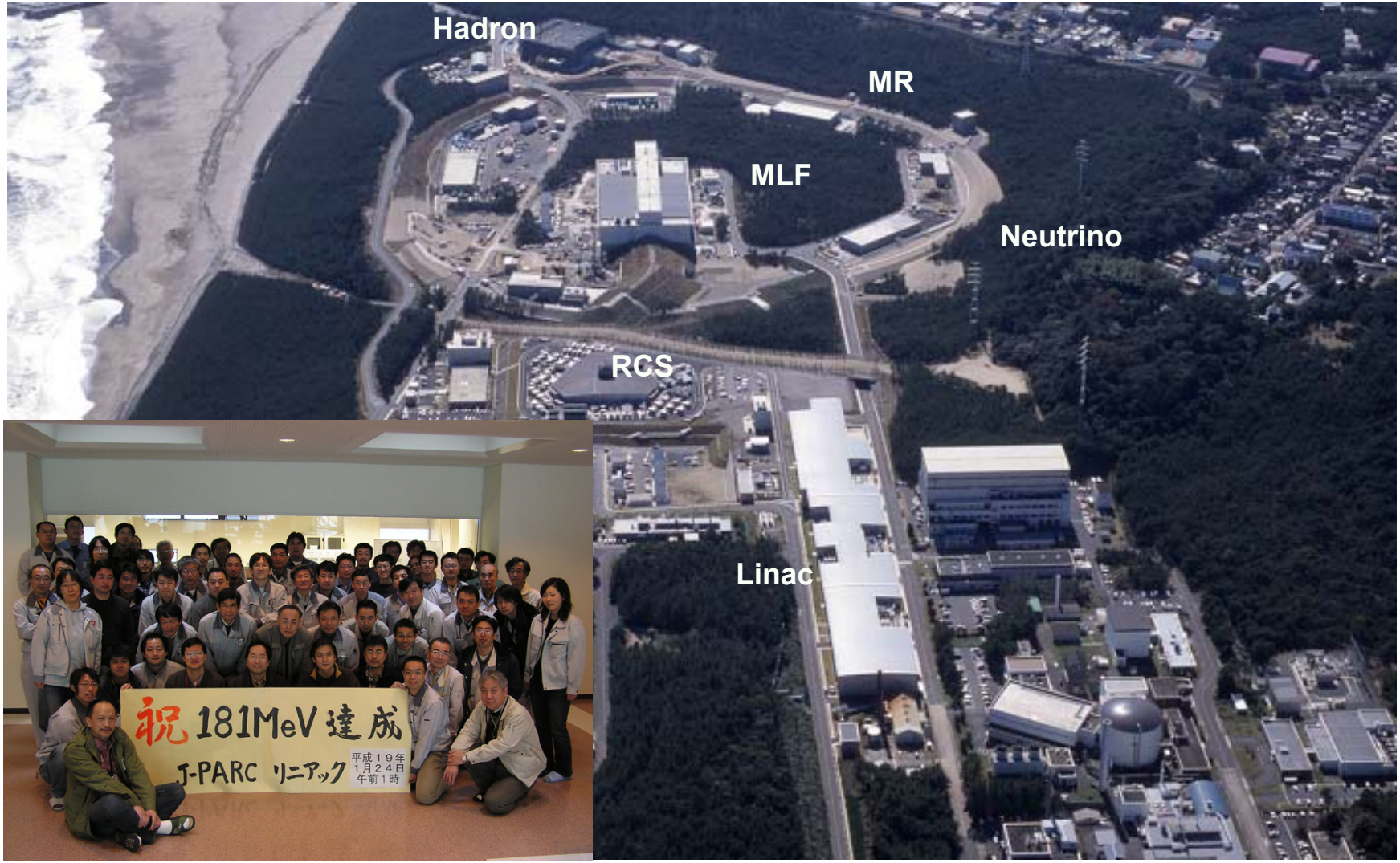


Part of Larger Accelerator Complex
Source ~ ISIS in 2008
Source ~ 4x ISIS in 2012

US Spallation Neutron Source

Science & Technology Facilities Council

JPARC – Tokai

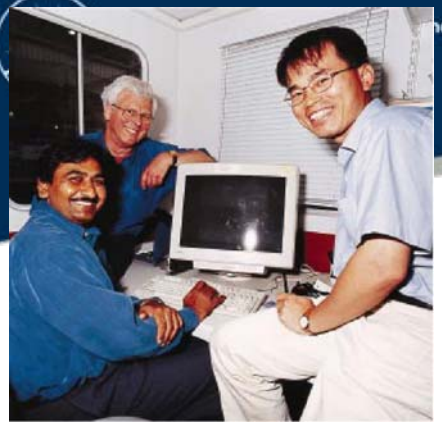


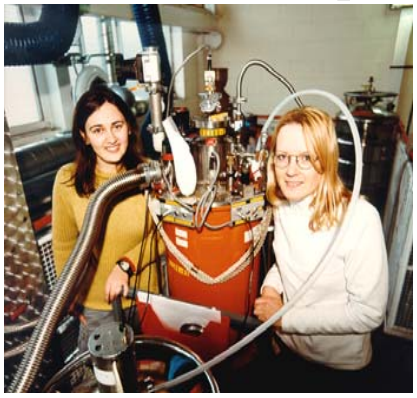
Science & Technology Facilities Council
ISIS

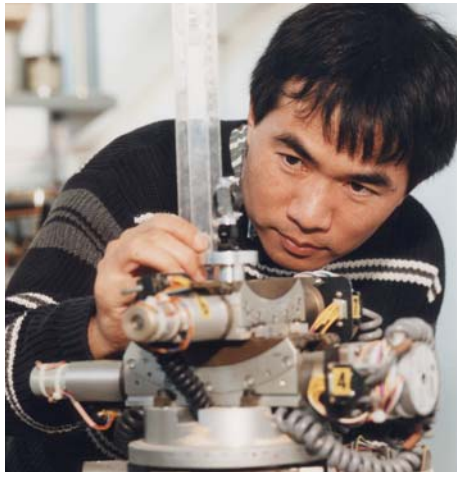
Facility Impact

Source
x
Leadership
x
Instrumentation
x
Innovation
x
Support
x
Investment
x
Cost Effectiveness
x
User Community

User Community



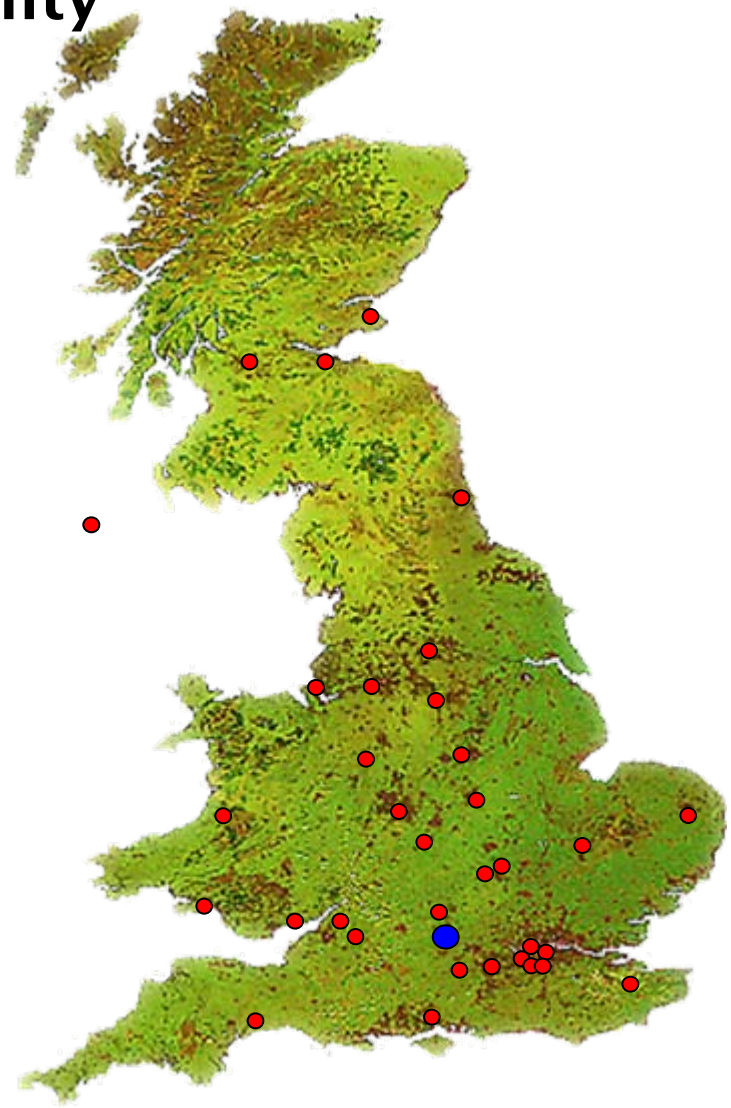




ISIS

ISIS UK Community

Aberystwyth
Bath
Belfast
Birmingham
Bristol
Cambridge
Cardiff
Cranfield
Durham
East Anglia
Edinburgh
Exeter
Glasgow
Keele
Kent



Leeds
Leicester
Liverpool
London
Manchester
Nottingham
OU
Oxford
Reading
Sheffield
Southampton
St. Andrews
Surrey
Swansea
Warwick

EPSRC

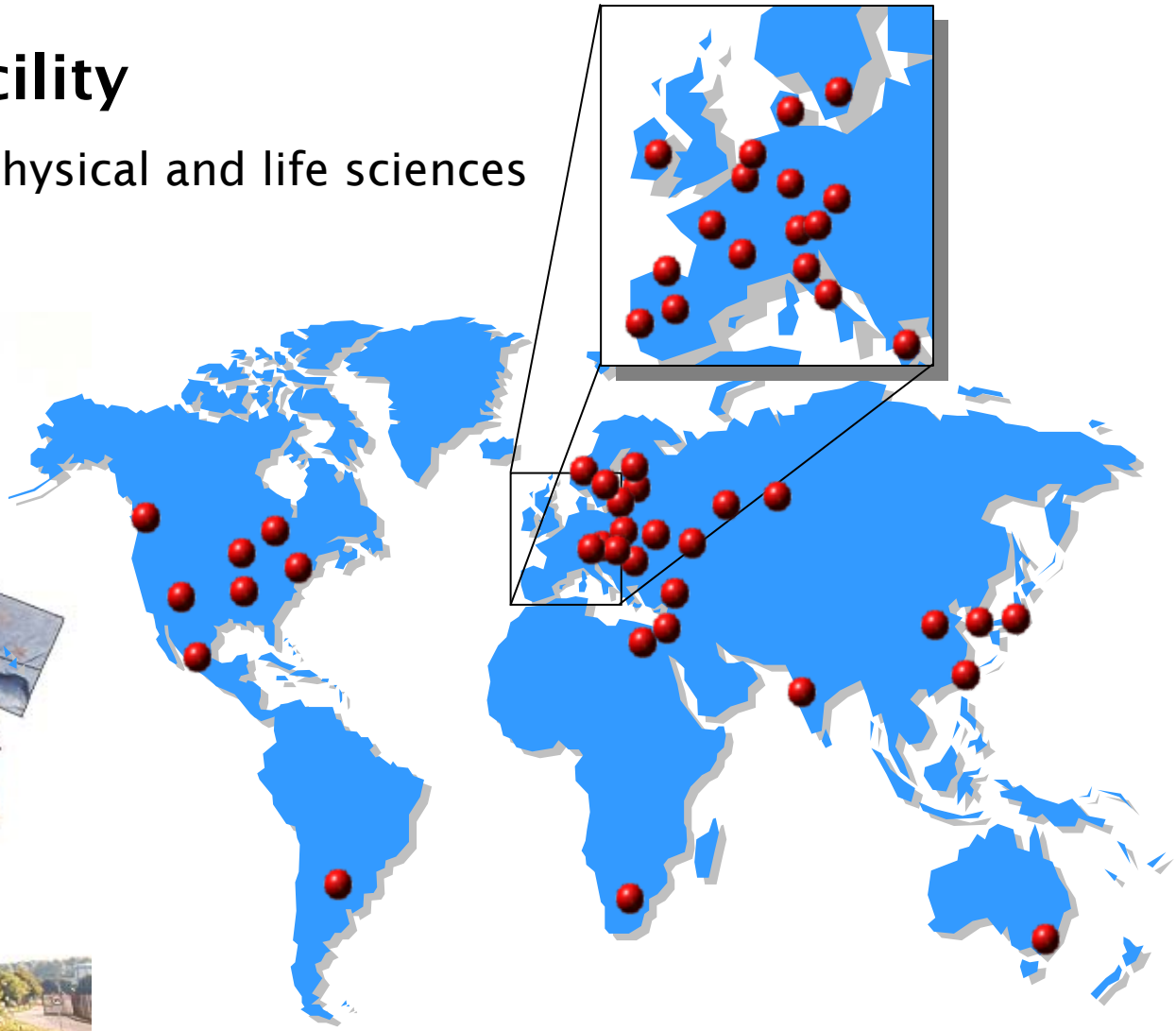
bbsrc
biotechnology and biological sciences research council

RESEARCH COUNCILS UK

Science & Technology Facilities Council
ISIS

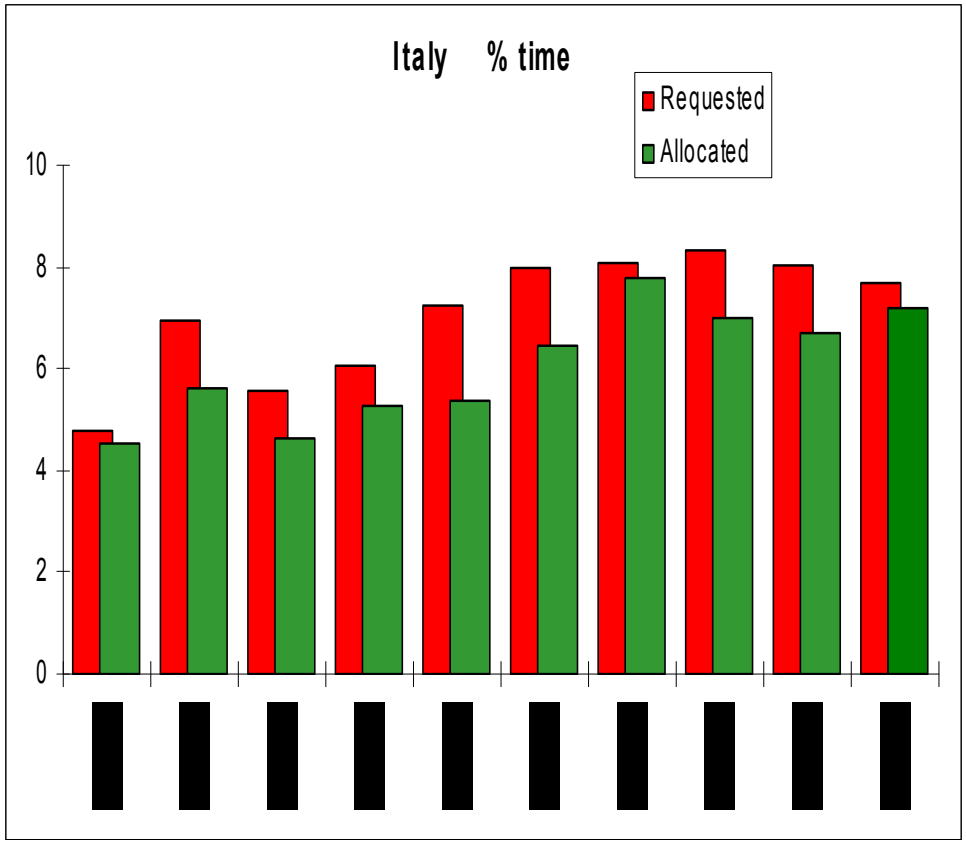
A world leading facility

for research in the physical and life sciences



Science & Technology Facilities Council
ISIS

Italy at ISIS



Partner since 1989

Major Science Programme

Strong Involvement in Instrumentation

Strong Involvement in technique development

> 300 Italian Users on ISIS Data base
> 200 ISIS publications in last 5 years

Science & Technology Facilities Council
ISIS

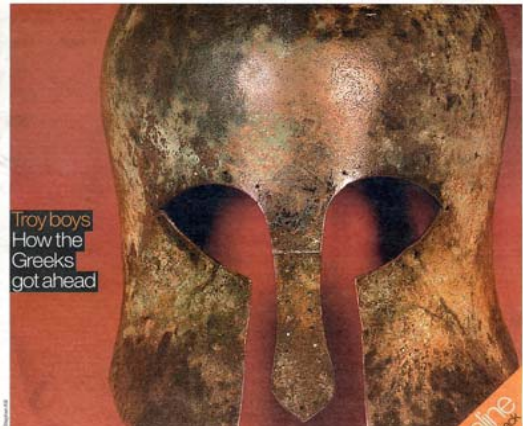
Science & Technology Facilities Council
ISIS

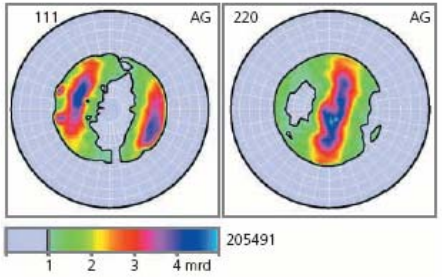
Science at ISIS

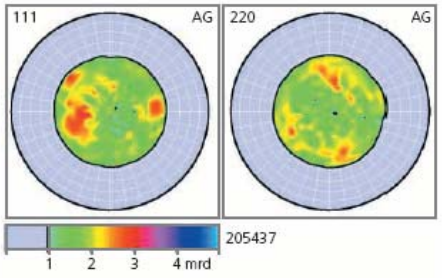
- Archeometry
- Bio-molecular
- Crystallography
- Engineering
- Hydrogen Storage
- Surfaces & Interfaces
- Superconductivity
- Quantum Complexity

Science & Technology Facilities Council

Archaeometry

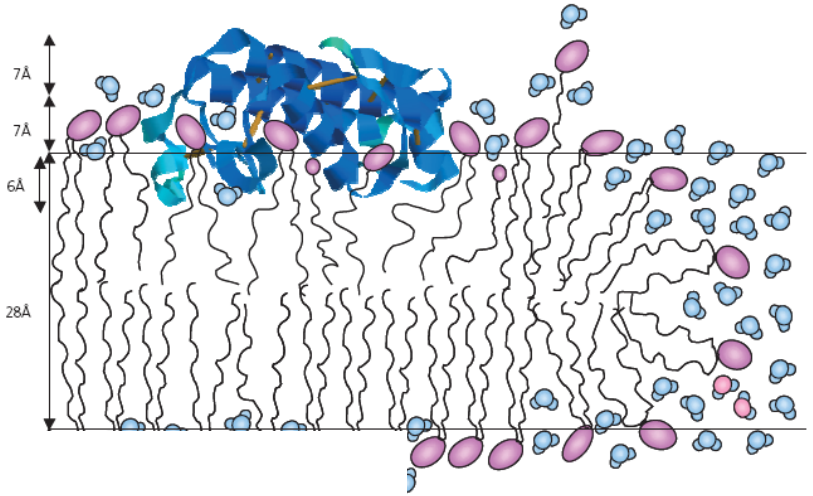




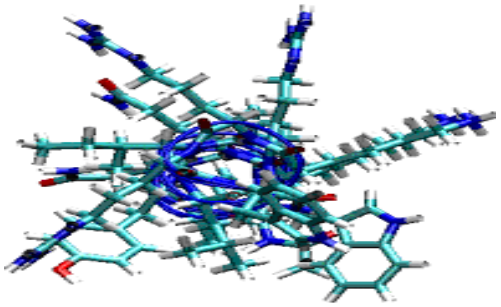


Science & Technology Facilities Council

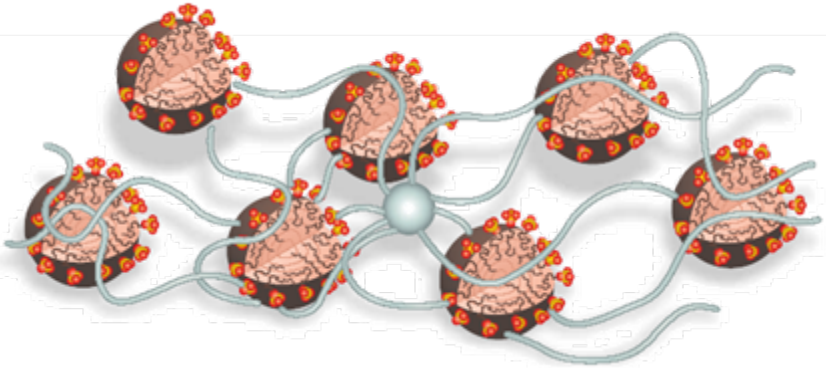
Bio-molecular Science

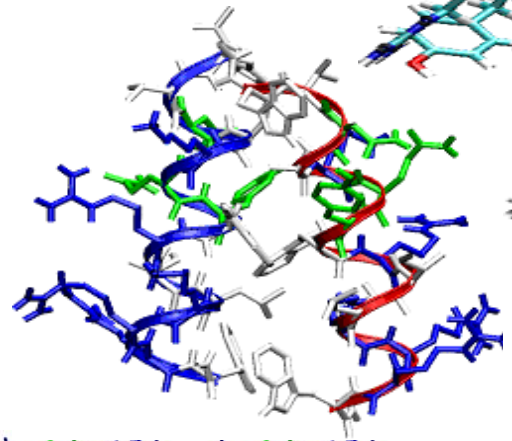


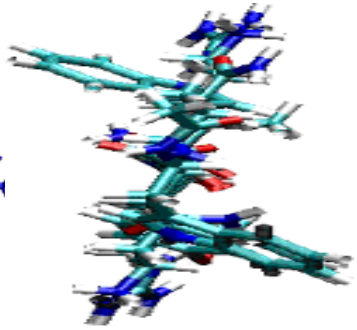
Cell membrane catalysts



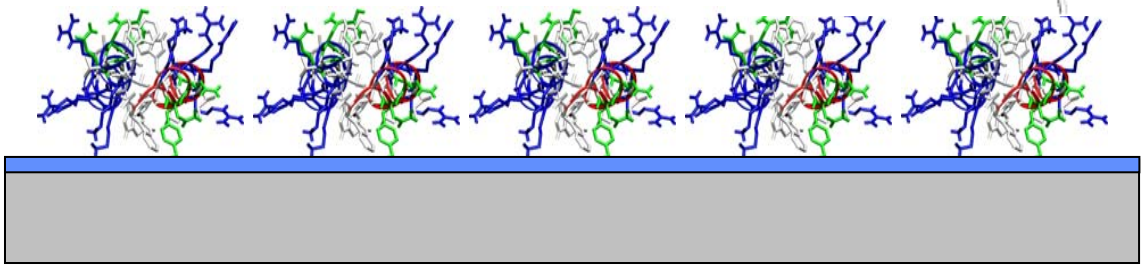
Snared polymer chains



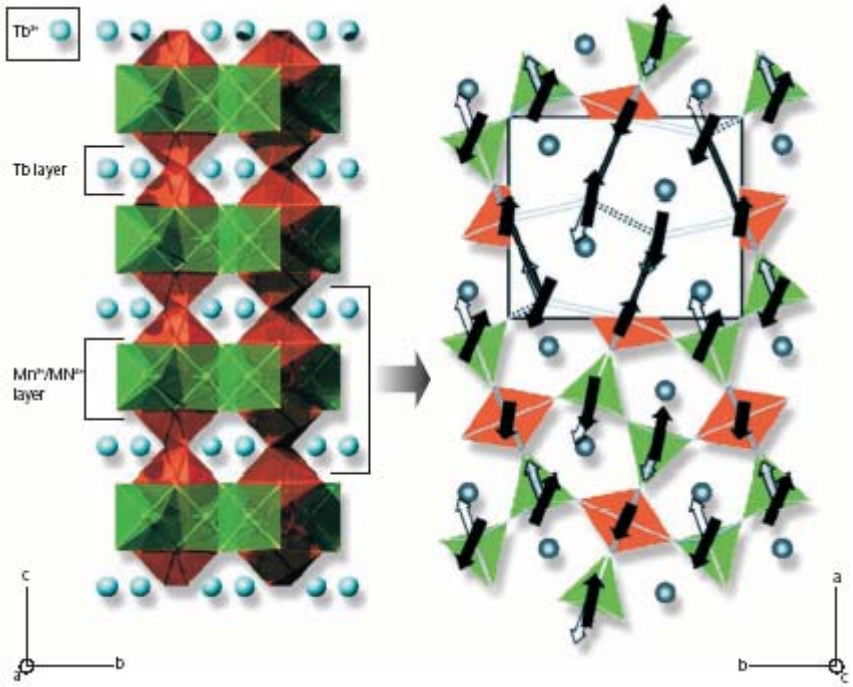




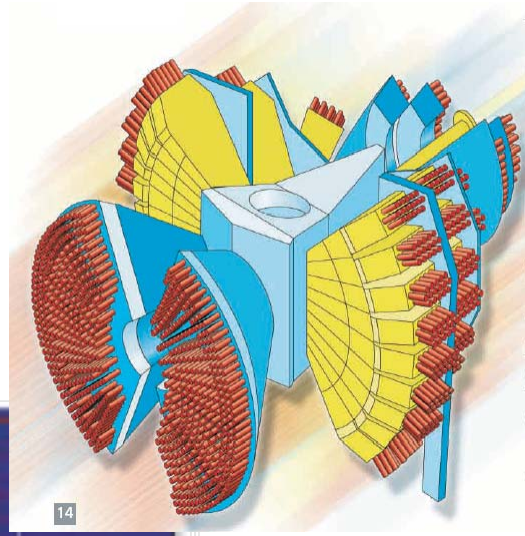
Bio-compatible membranes

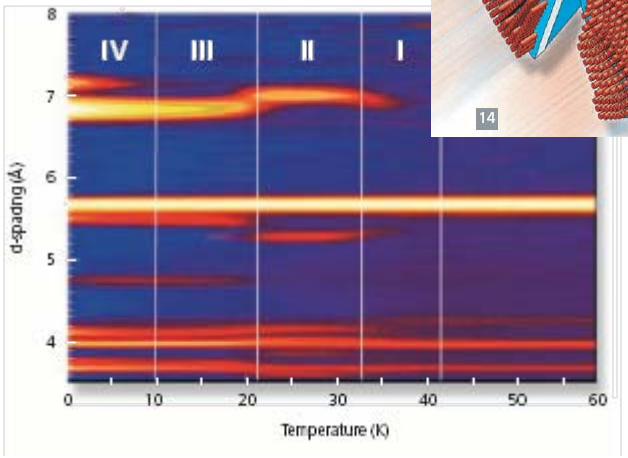


Crystallography

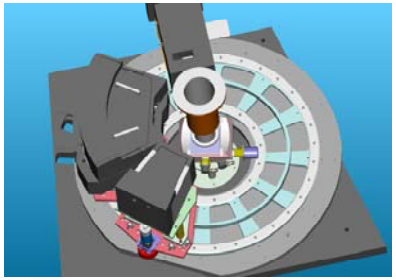


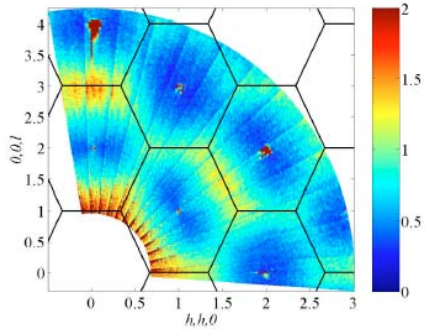
Ferroelectricity
$TbMn_2O_5$

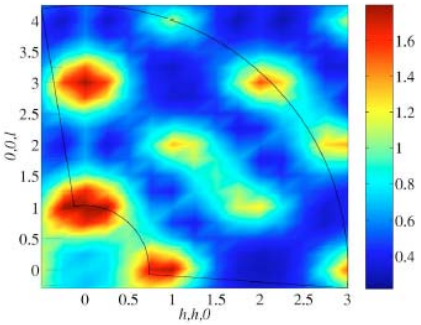




Frustrated magnetism



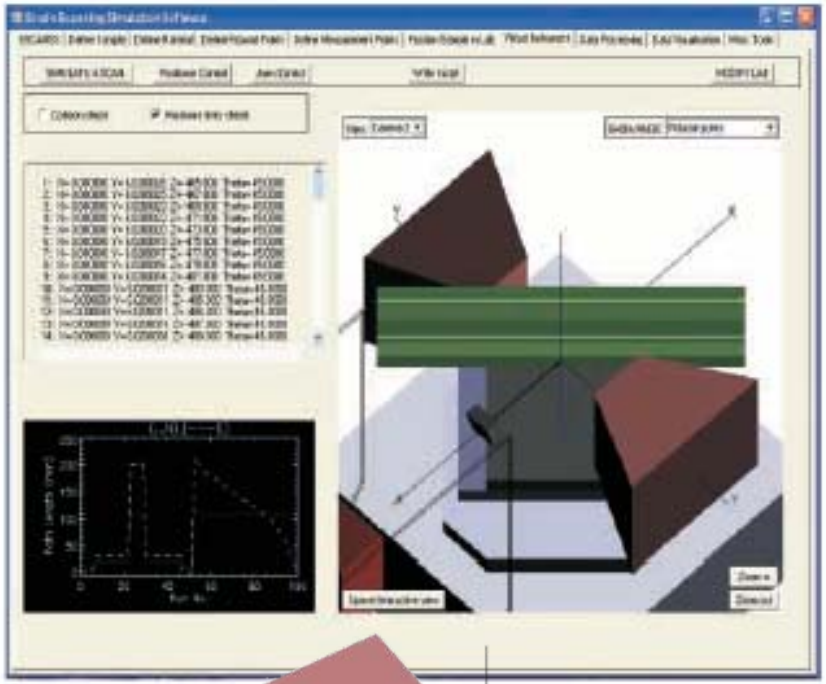


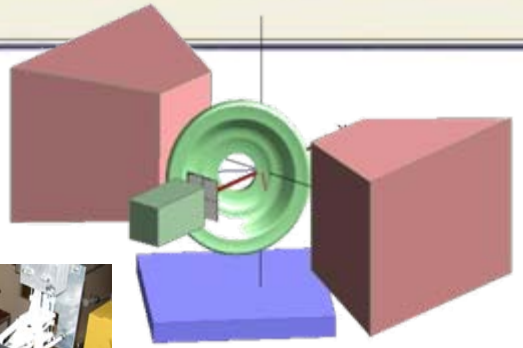


Science & Technology Facilities Council

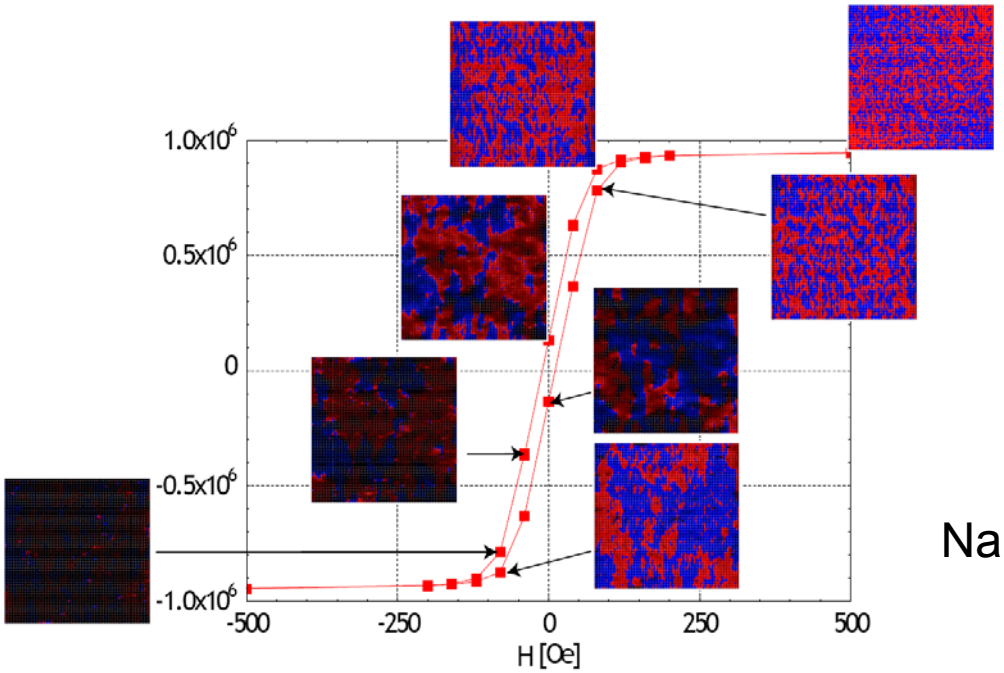
Engineering Science

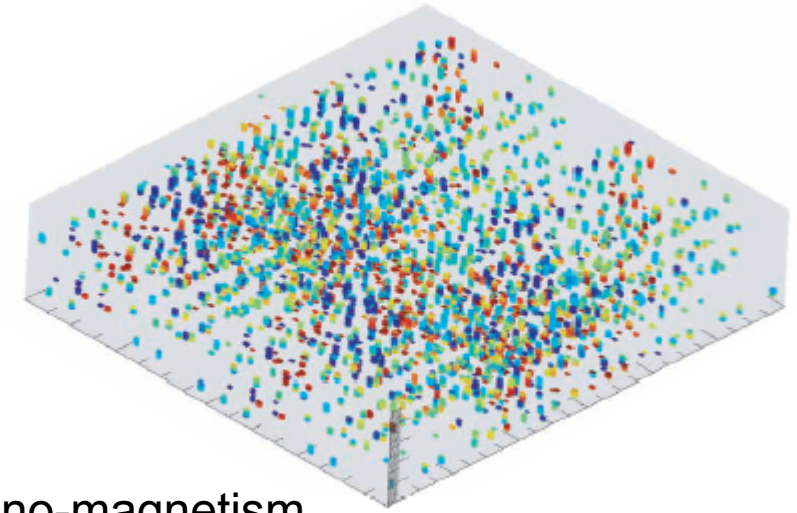
Airbus A380 Wing



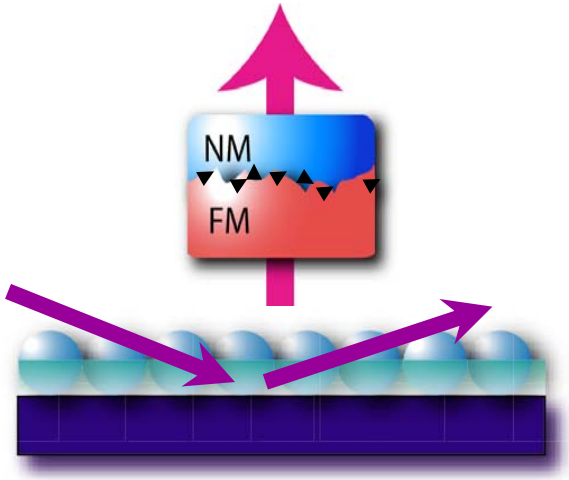


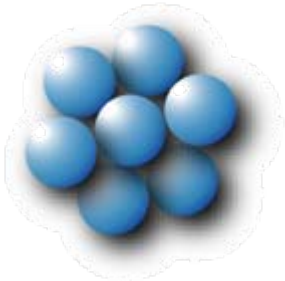
Spintronics



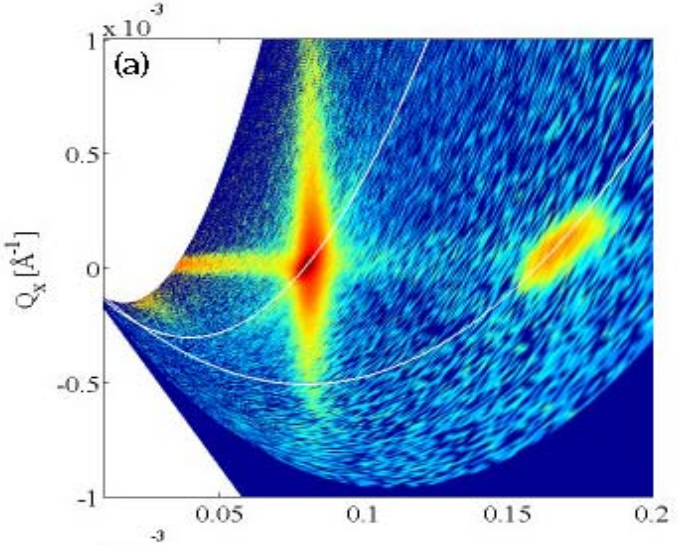


Nano-magnetism



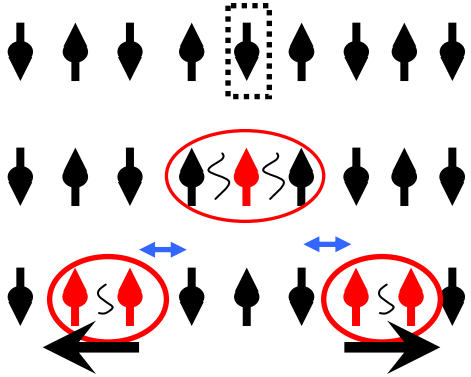


Surface patterning



Quantum Complexity

Theorists have predicted a new excitation

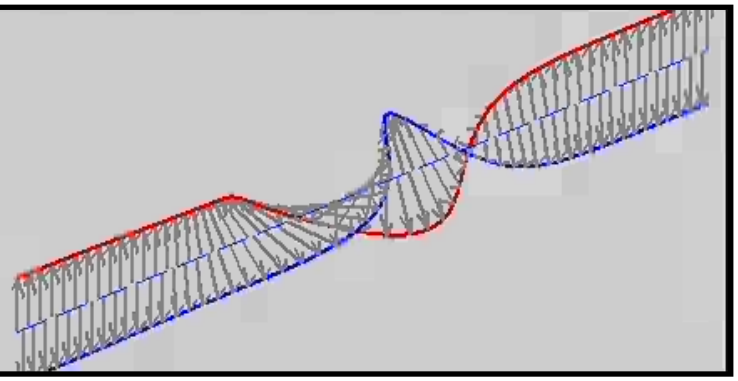


Normal anti-ferromagnet

Flip one spin

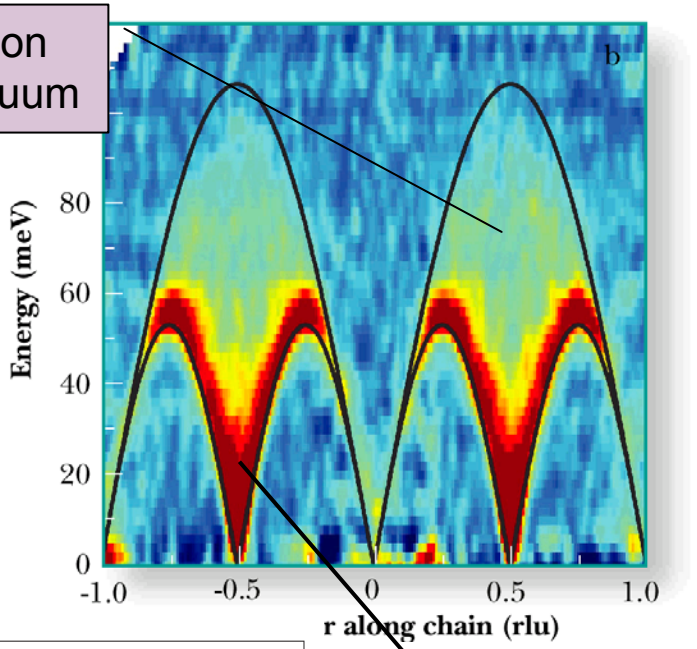
The bound pairs of spins propagate away

– these are *Spinons*

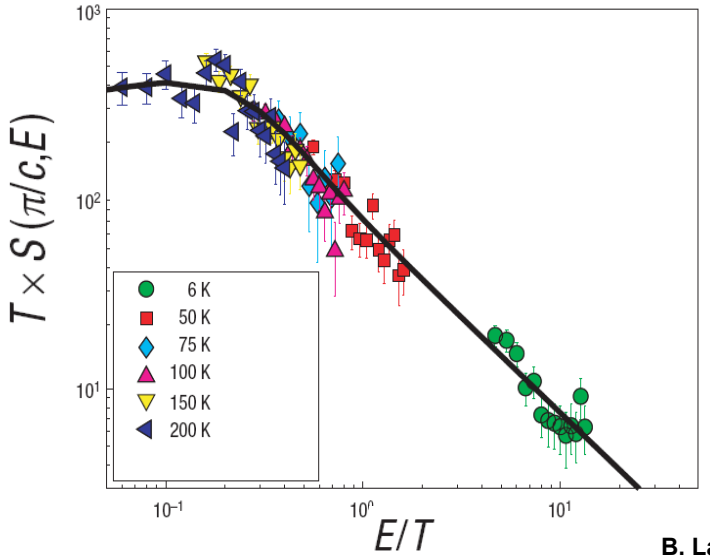


The signature of this excitation was seen using inelastic neutron scattering

Spinon continuum



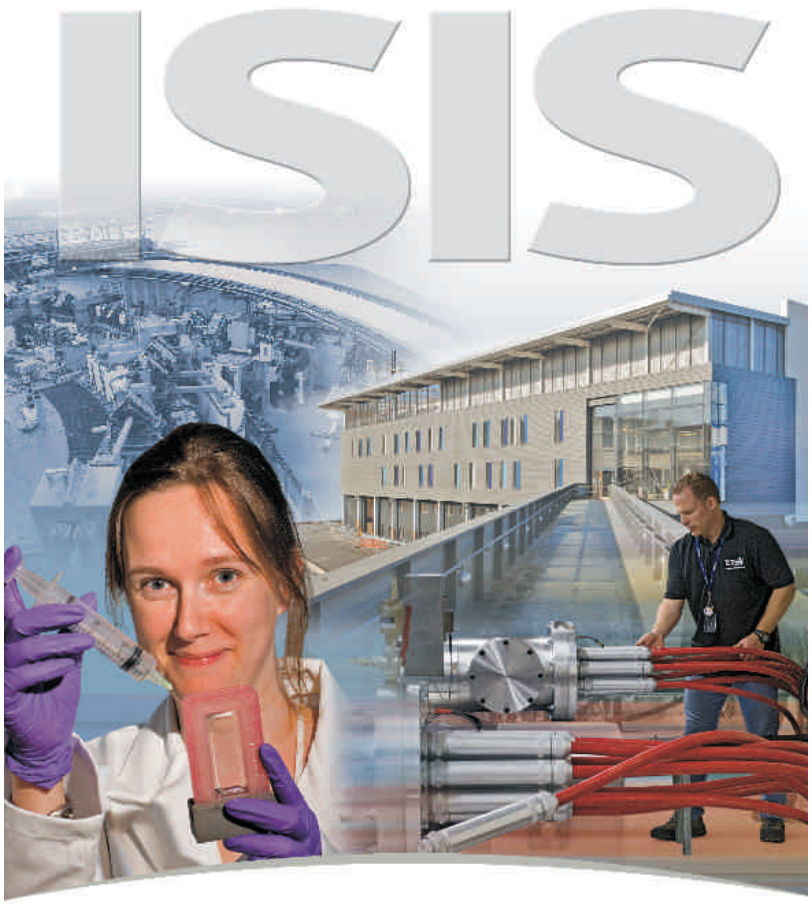
Normal spin wave



B. Lake et al., Nature Materials (2005)

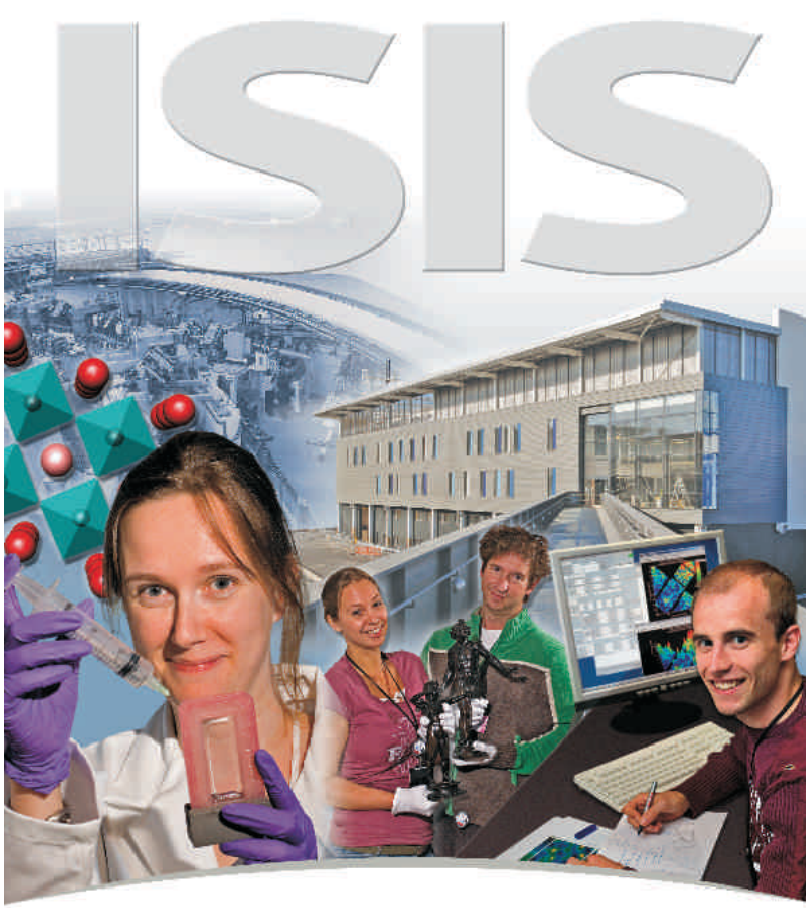
Science & Technology Facilities Council
ISIS

Science & Technology Facilities Council



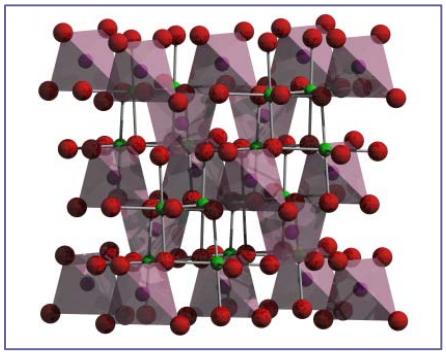
ANNUAL REPORT 2007

Science & Technology Facilities Council



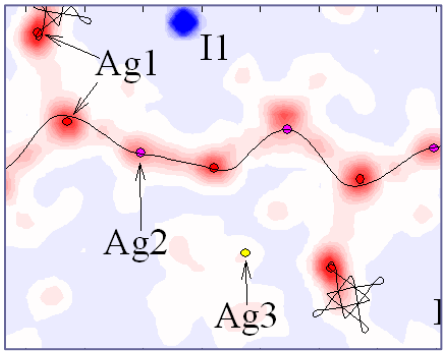
ISIS SCIENCE

Materials for Energy: current research at ISIS



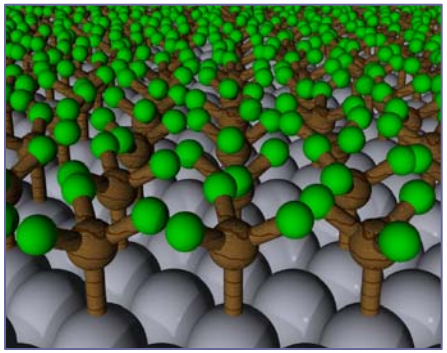
Battery materials:

High capacity Li+ battery cathode materials
(St. Andrews, ANL, Delft)



Fuel cells:

Pt/C catalysts for anodes in low temperature fuel cells
Protonic conductors for high temperature fuel cell
(Johnson Matthey, Degussa, Surrey, Nottingham)

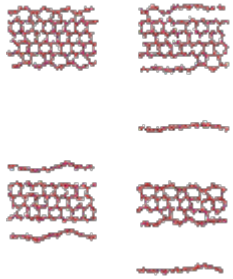


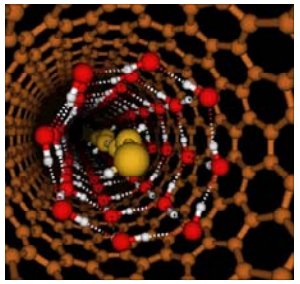
Catalysis:

Methyl chloride synthesis, deactivation processes in methane reforming and Fischer-Tropsch catalysts
(IneosChlor, Sasol, Berlin, Glasgow, Keele)

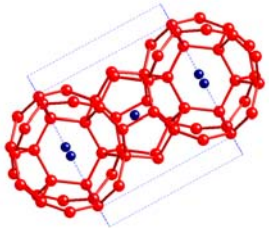
Science & Technology Facilities Council
ISIS

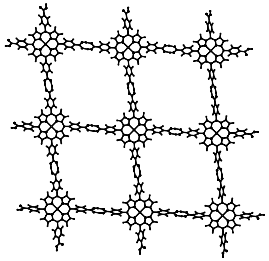
Structural Materials

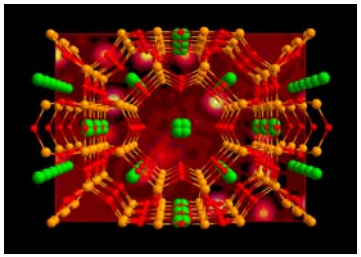


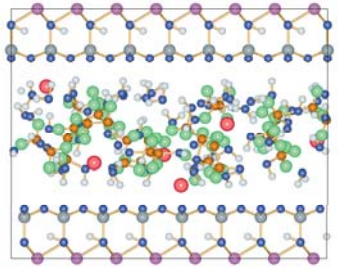


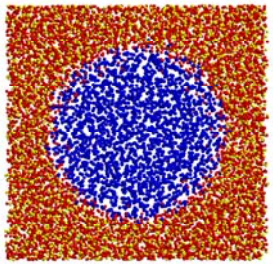
Carbon: fullerenes, nanotubes, nanohorns, graphenes



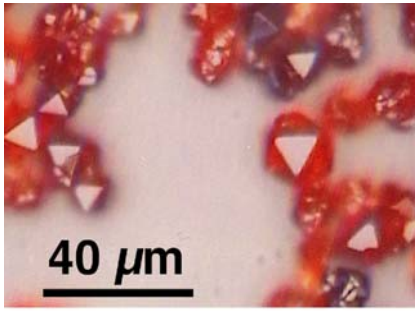


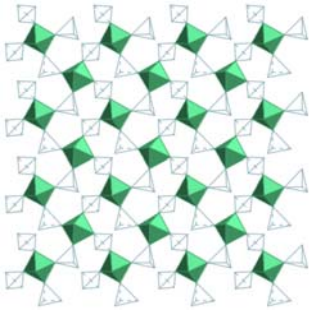


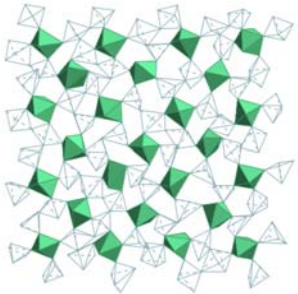


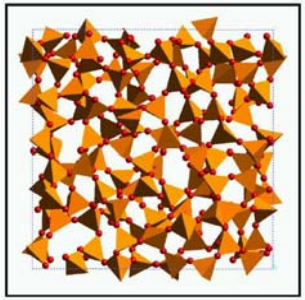


Framework and mesoporous materials e.g. clathrates, zeolites, silicates, clays









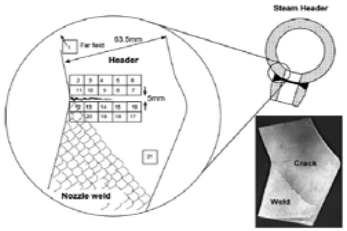
Ceramics e.g. ultrahard, negative thermal expansion

Glasses, aerogels, xerogels

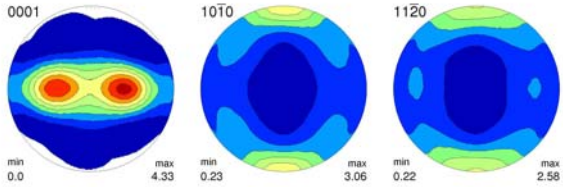
ISIS and Oxford, Cambridge, Liverpool, UCL, Durham, Edinburgh, Southampton, Heriot-Watt, Kent … plus international users

Science & Technology Facilities Council
ISIS

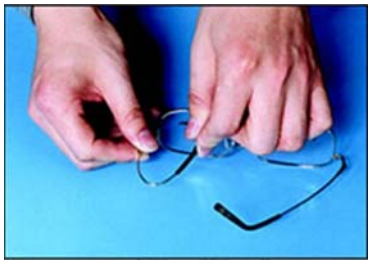
Structural Materials



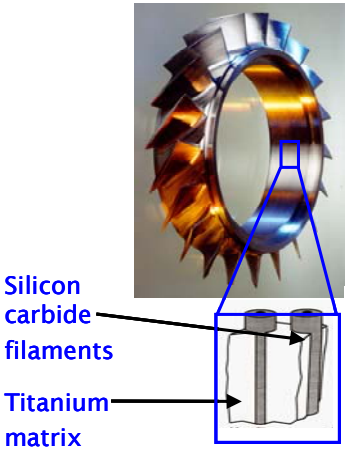
Creep cavitation



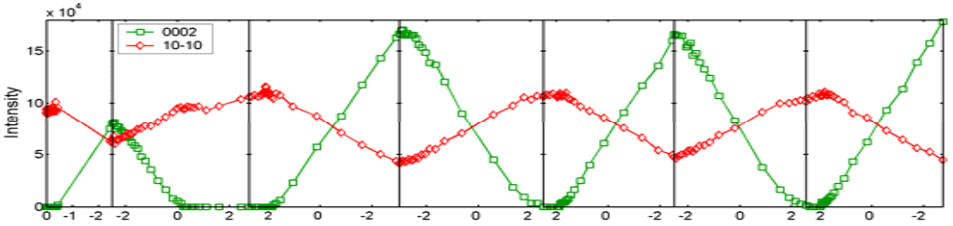
Texture



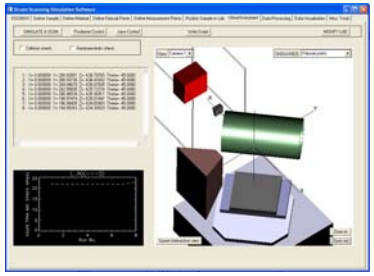
Alloys

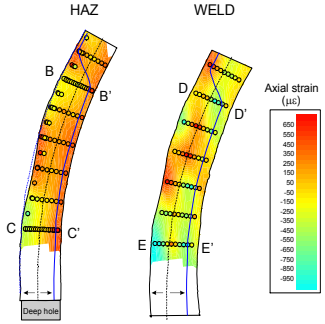


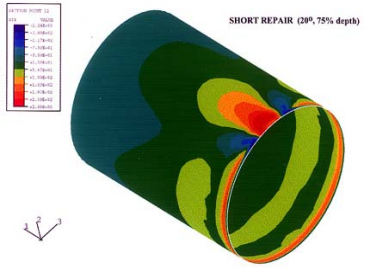
Composites

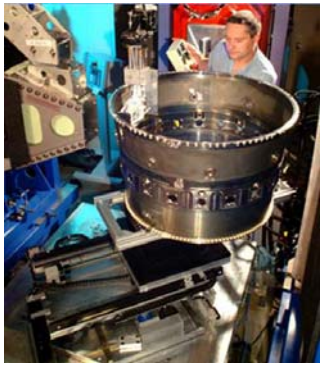


Fatigue







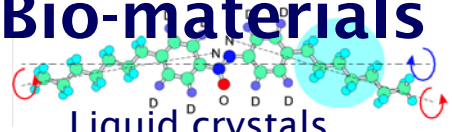


Welding, welds and residual stress

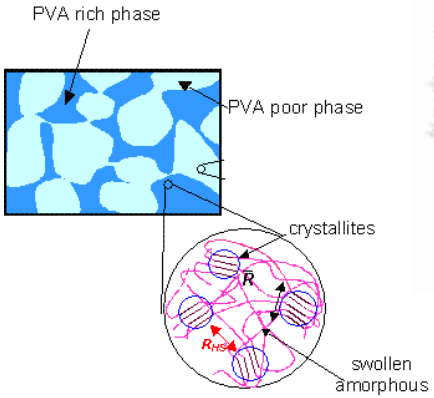
ISIS and Manchester, Open University, Sheffield Hallam, Cranfield, IC, Rolls Royce, British Energy … plus international users

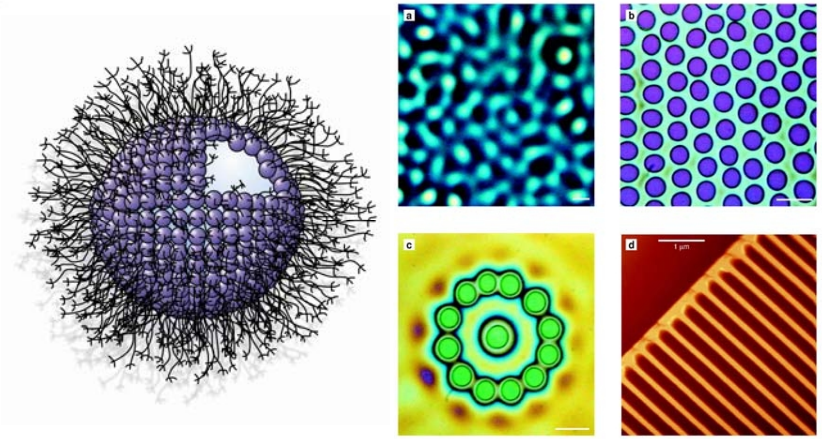
Science & Technology Facilities Council
ISIS

Polymers and Bio-materials

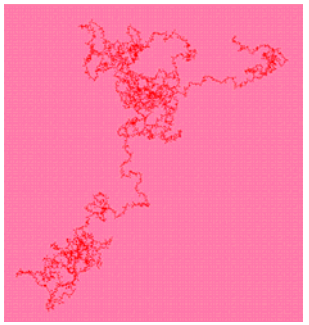


Liquid crystals

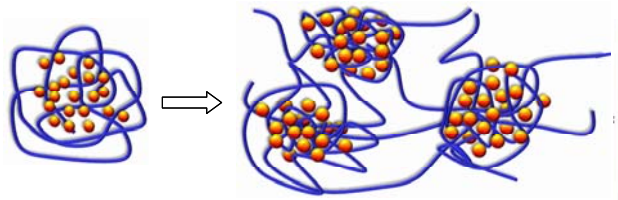


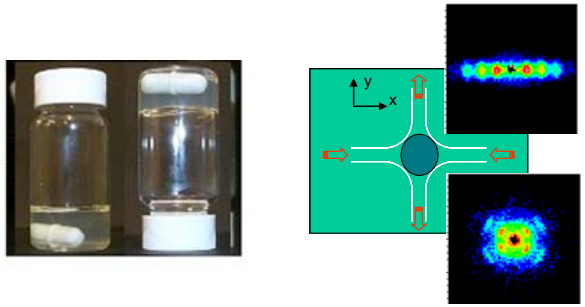


Colloids, microemulsions, self-assembly

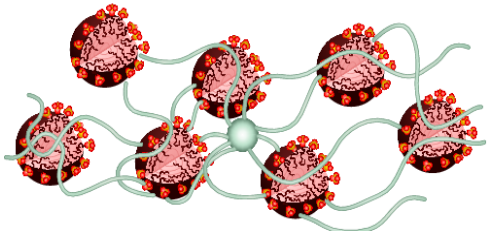


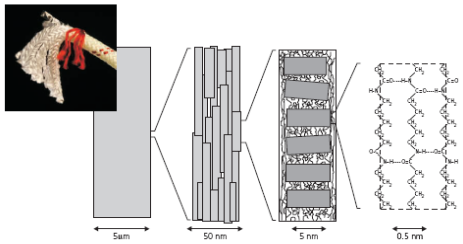
Block copolymers, ionomers, elastomers,



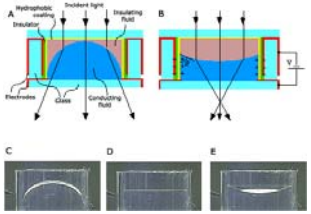


Phase separation, rheology





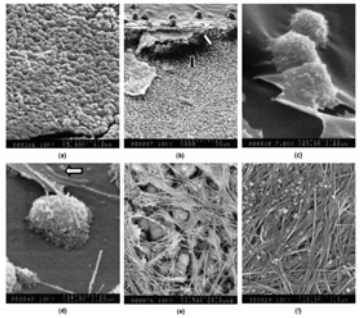
Fibres



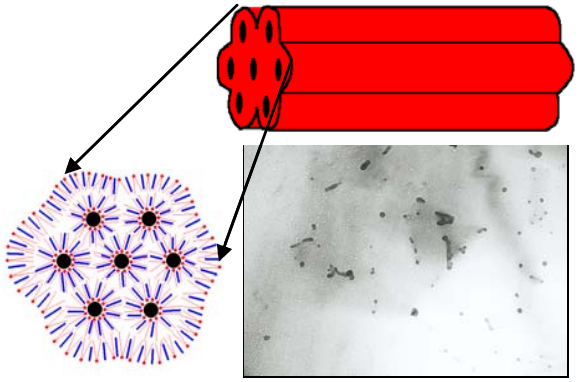
Interfaces

ISIS and Oxford, Leeds, Sheffield, Bath, Bristol, Manchester, Swansea, Cardiff, Reading, Unilever … plus international users

Science & Technology Facilities Council
ISIS

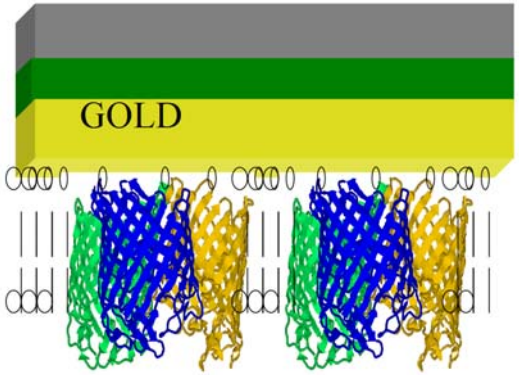


Biomineralisation, biocompatible ceramics

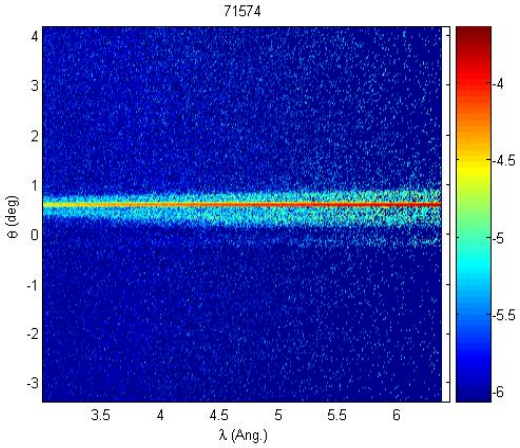


Biopolymers for drug delivery

Biopolymers, silks



Biosensors

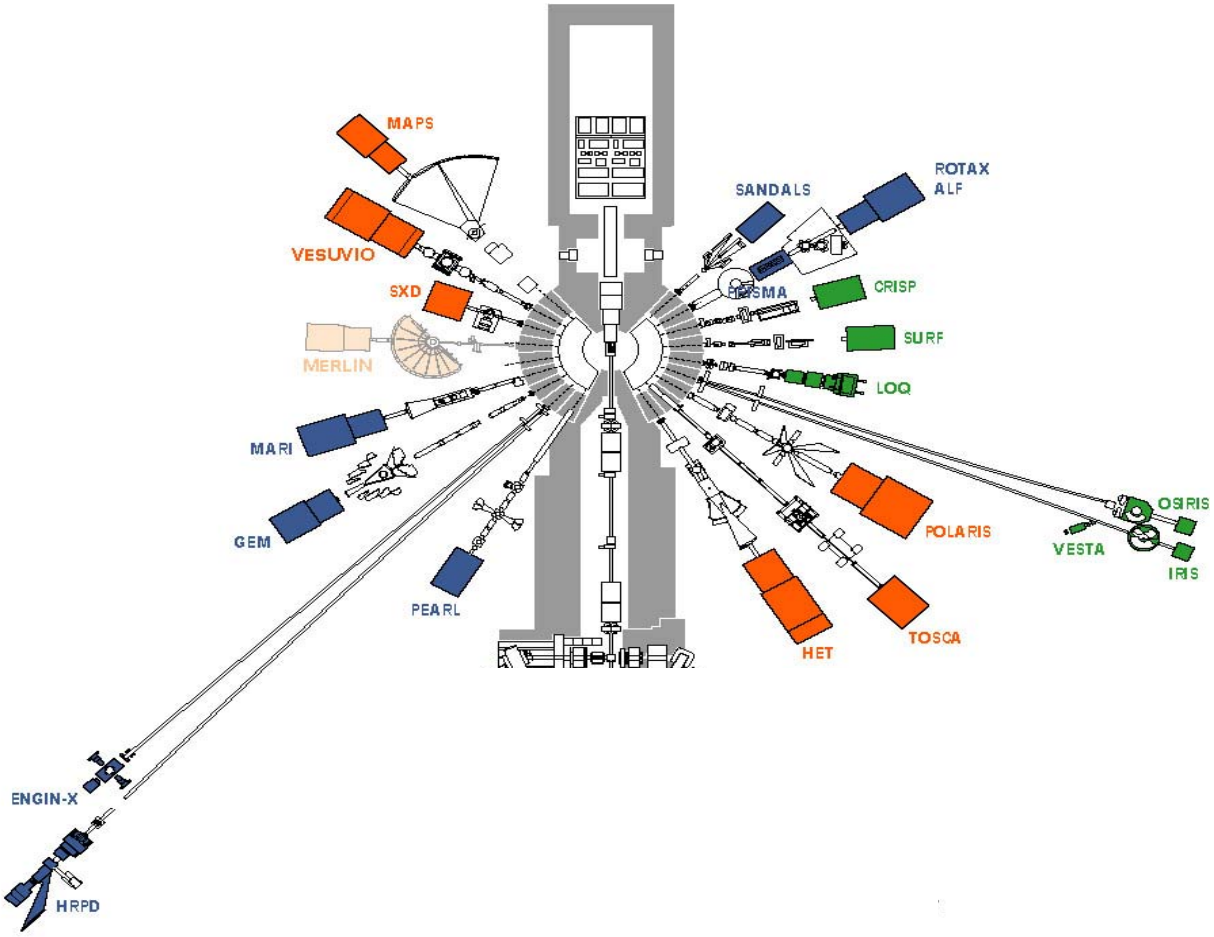


Model membranes

Polymers and Bio-materials

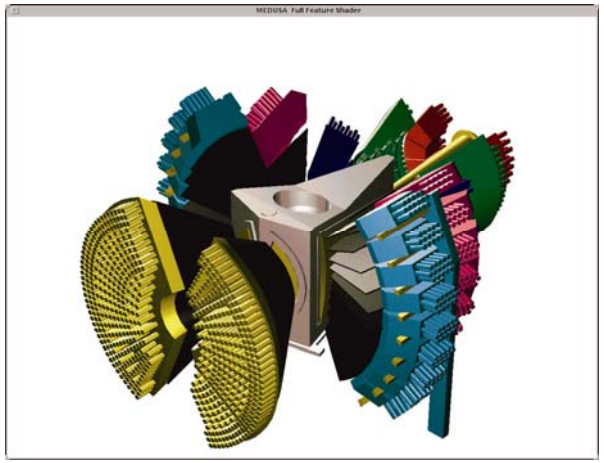
ISIS and Oxford, KCl, Kent, Edinburgh, Cardiff, Bristol,
QMC, Bath, Leeds … plus international users

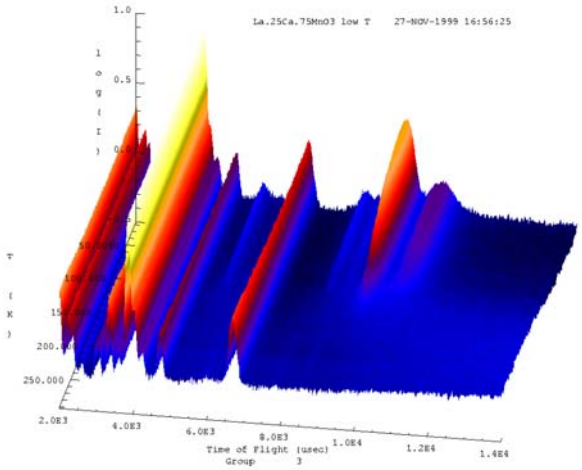
Science & Technology Facilities Council
ISIS



Instrument Developments

Instrument Developments





History of innovative instrument developments
Technology transfer from STFC Programmes

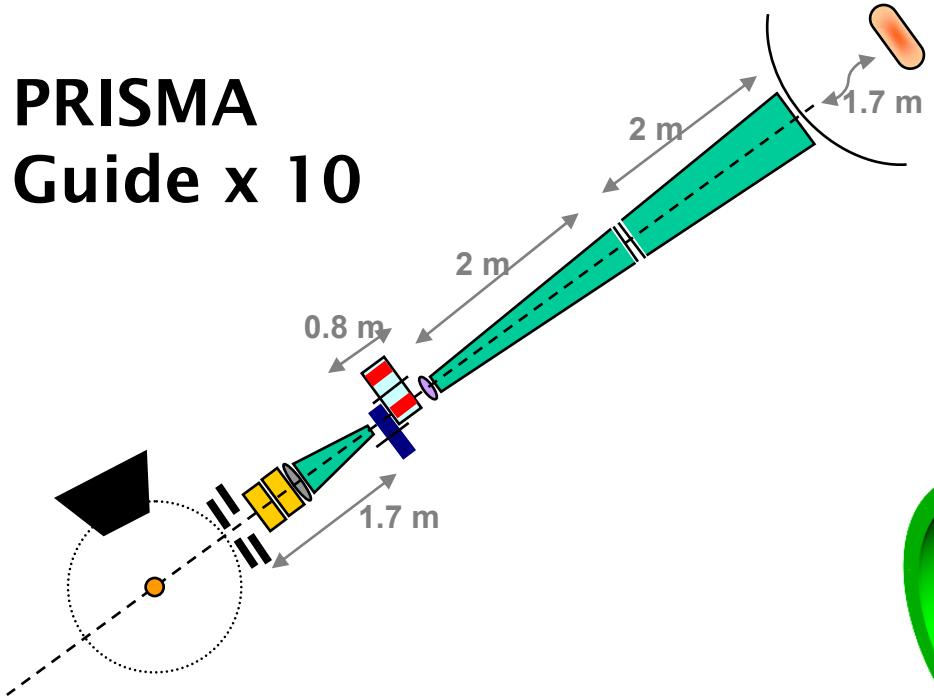
Working with University Consortia Facilitated by ISIS Staff
Substantial international support

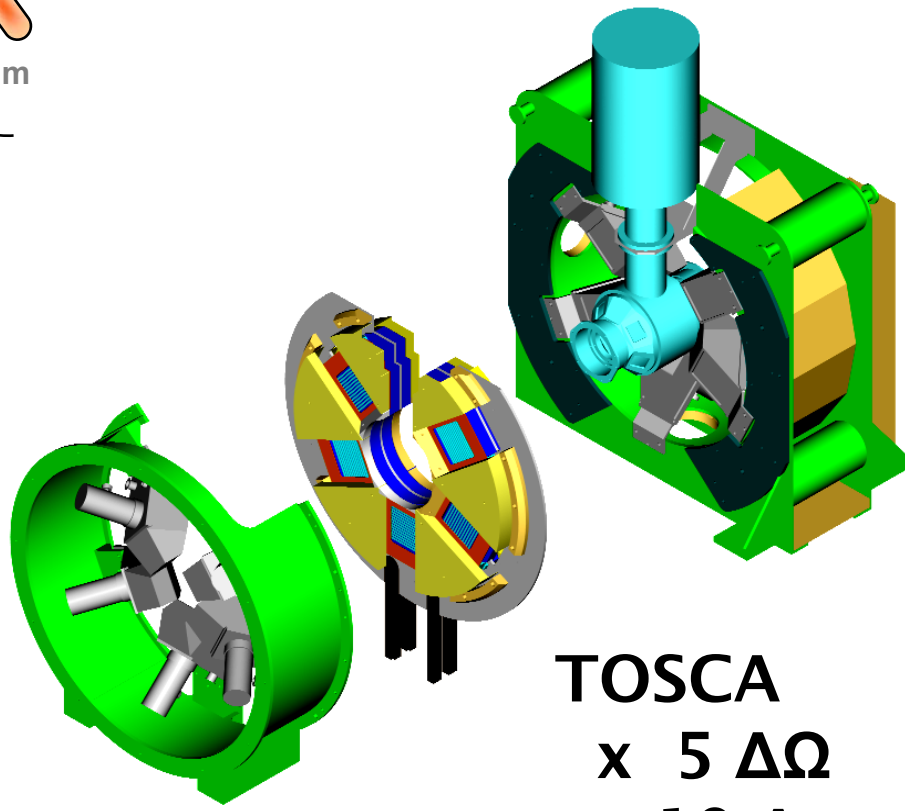
Responsive to ongoing demand for new scientific capabilities

Attracting new communities

Italian-led Developments

PRISMA
Guide x 10





TOSCA
x 5 ΔΩ
x 10 Δε

- **Vesuvio e-Verde INES**
- **Detector Development**
- **Ancient Charm Initiative**
- **Chip Irradiation**

Science & Technology Facilities Council
ISIS

Science & Technology Facilities Council

Rutherford Appleton Laboratory

World-class science made possible by

World-class Technology

Providing leading-edge science with the technological resources and skills to meet the exacting standards required for success

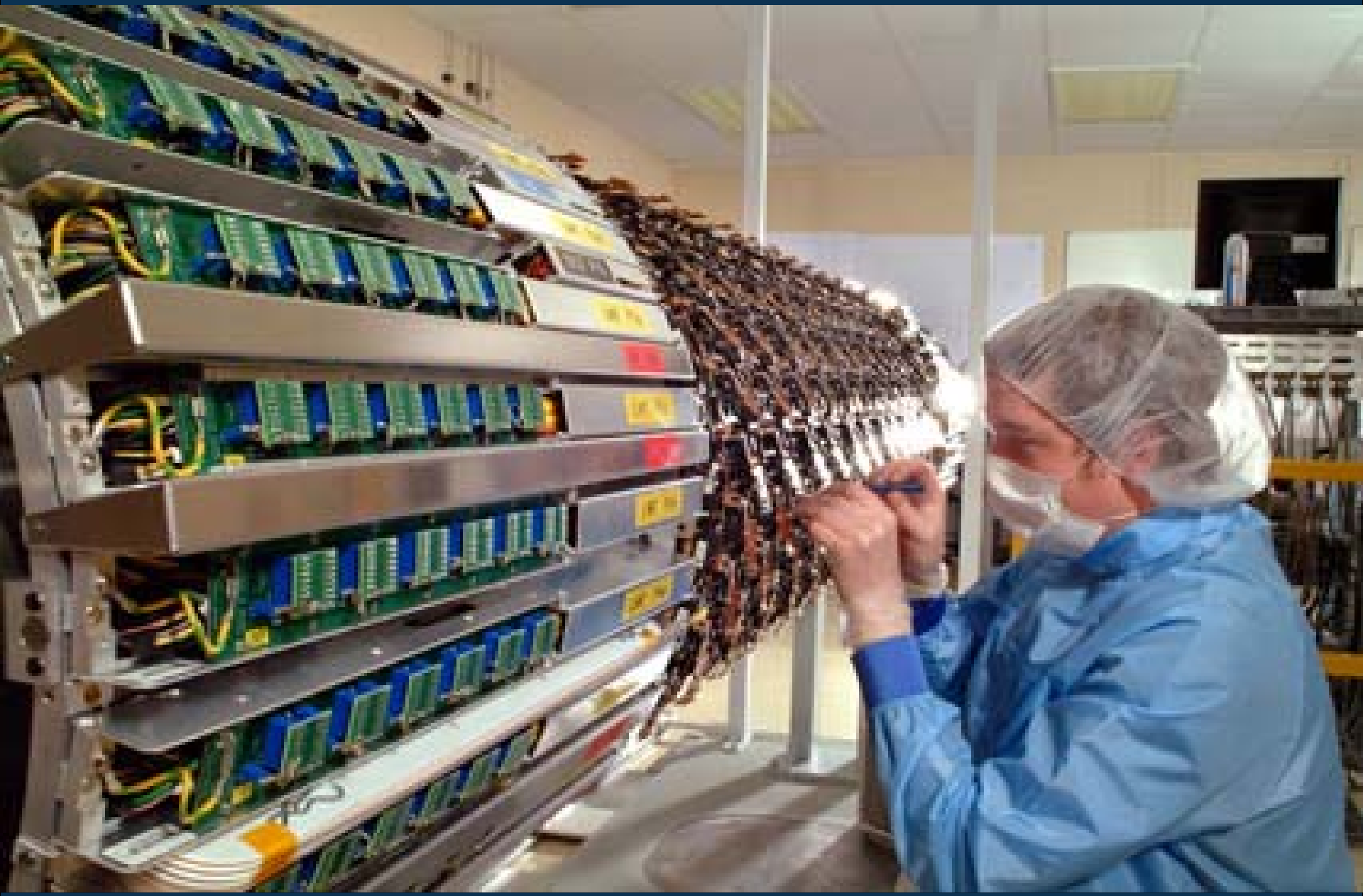
Science & Technology Facilities Council

Microelectronics Energy research Design *Metrology* Engineering
Advanced materials Research Instrumentation Sensors Detectors Computing
Bioscience Micro/Nano technology Cryogenics Mechanics

Technology

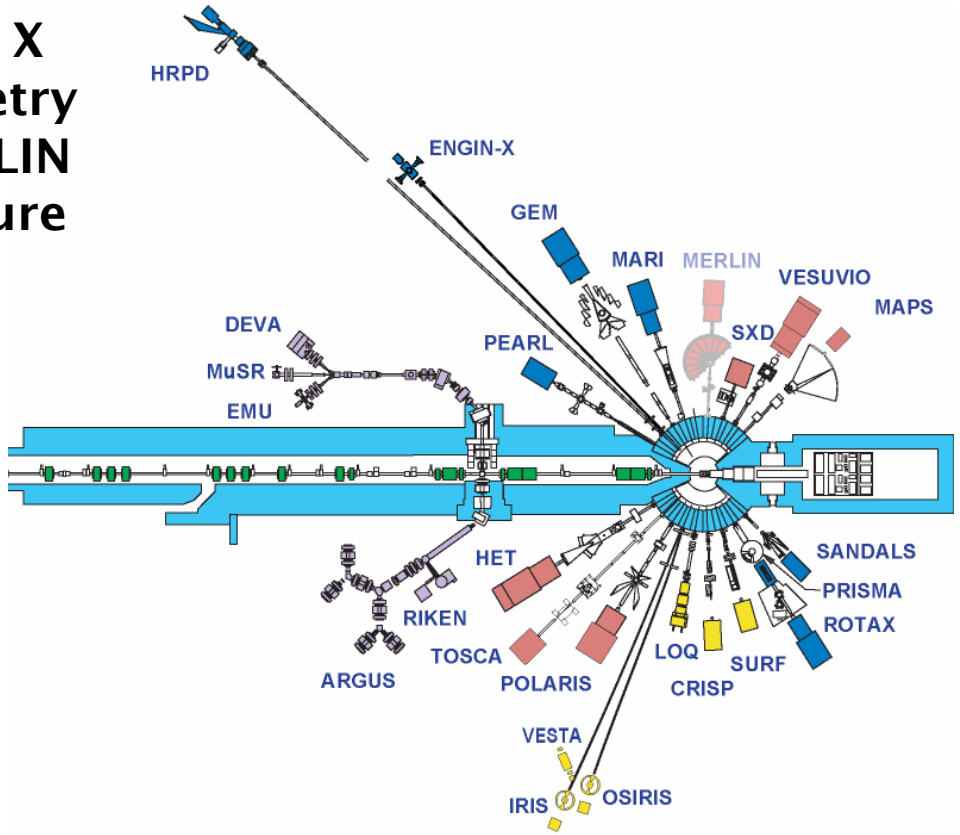
Science & Technology Facilities Council

Advanced Technology



Instrument Developments

- Detectors and Data Acquisition – GEM
- Guides and Backscattering - HRPD
- Engineering Science – ENGIN X
- Surface Science -- Reflectometry
- Data Analysis - MAPS / MERLIN
- Paris/Edinburgh Cell - Pressure
- Advanced SE

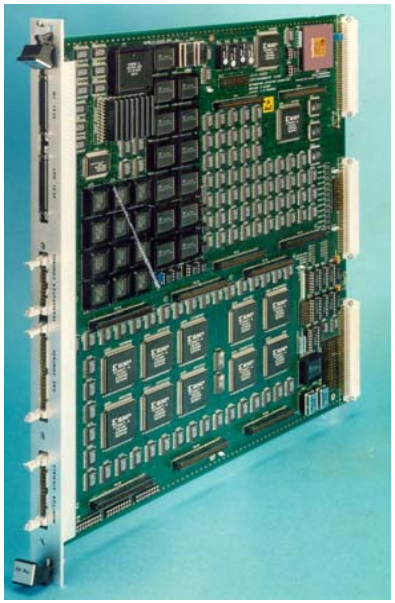


Science & Technology Facilities Council
ISIS

Science & Technology Facilities Council
ISIS

STFC Technology Transfer

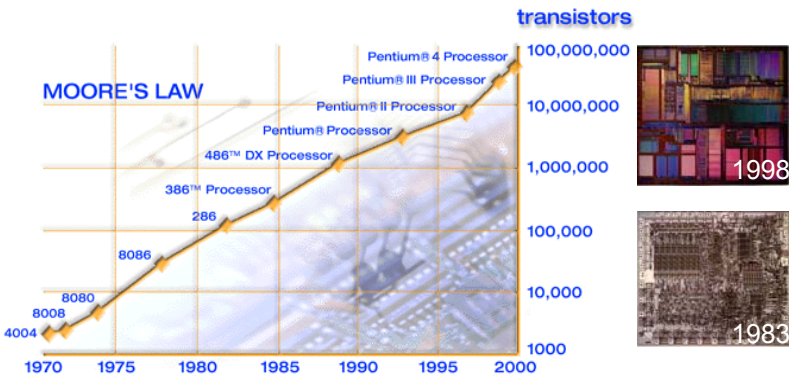
efficient large solid angle detectors...

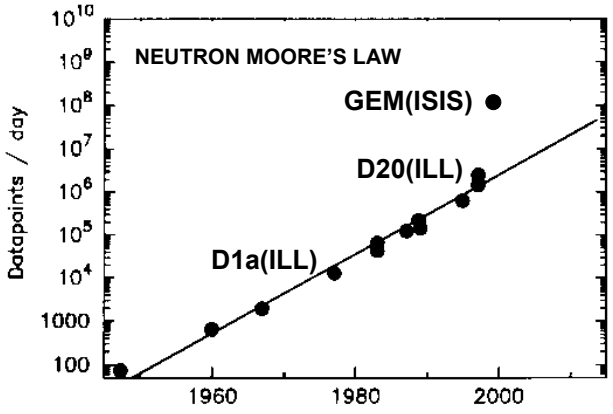


…fast electronics

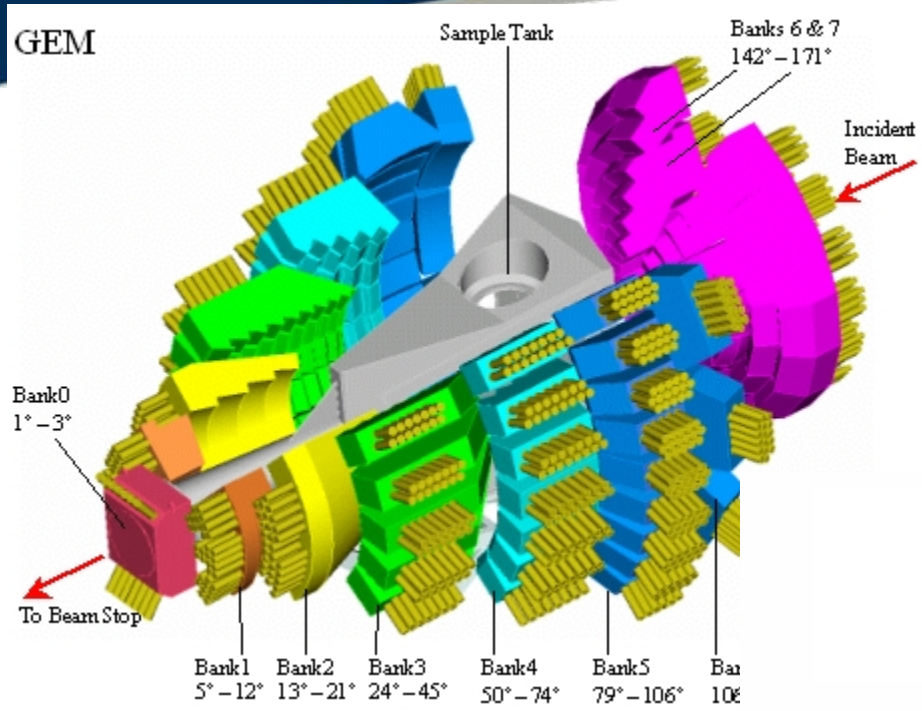
detectors and advanced data acquisition - unique synergy within STFC

4 orders of magnitude in 30 years





Neutron powder diffraction data rates (1950-2010) (4 orders of magnitude gain with ILL/ISIS alone)

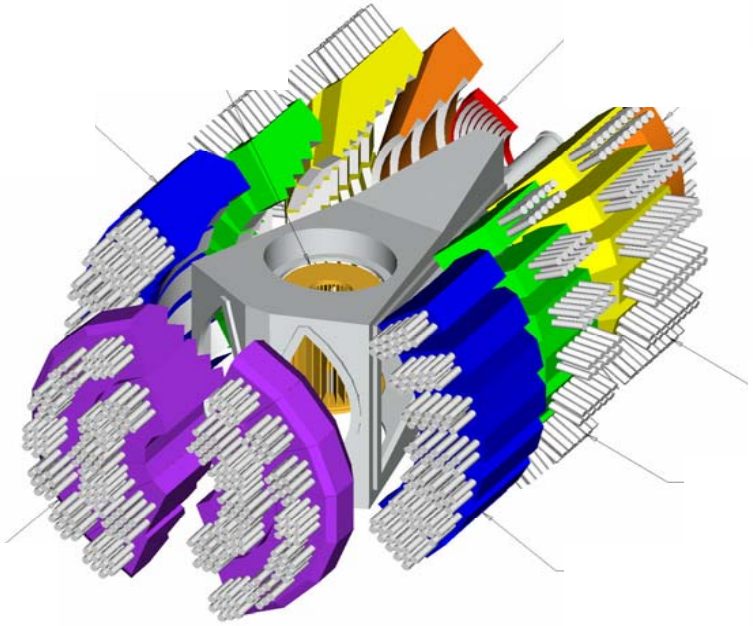


GEM: 2004

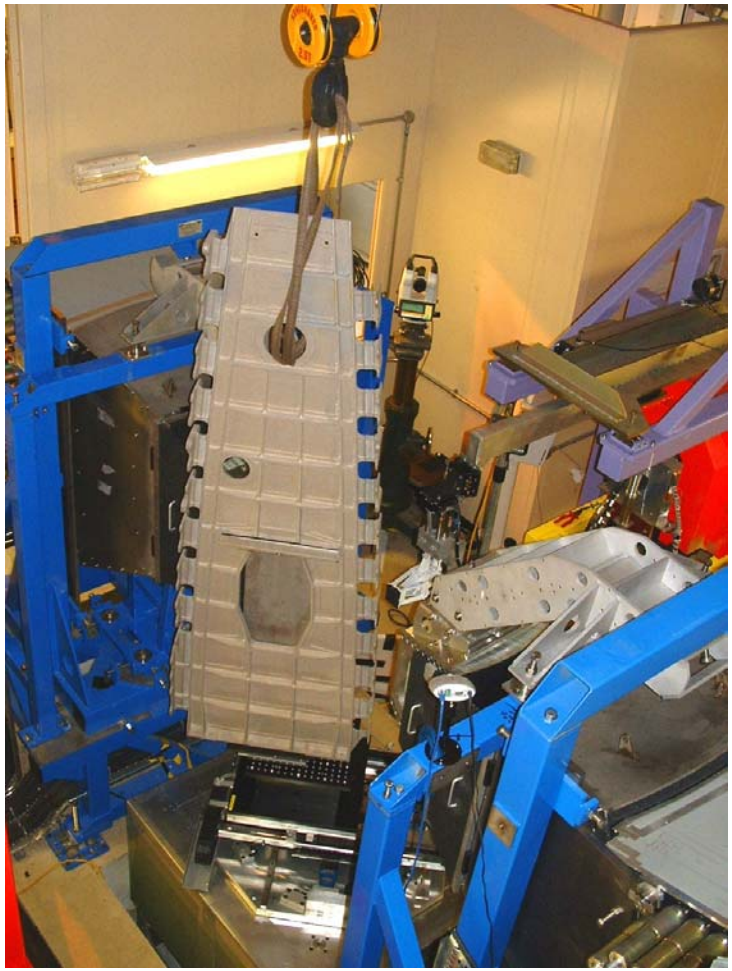
Medium resolution.
High intensity.
Powder diffraction.
Total scattering.
Glasses.
Archaeometry.

POLARIS+: 2008

Medium resolution.
High intensity
Powder diffraction.
Total scattering.



New Developments–New Communities

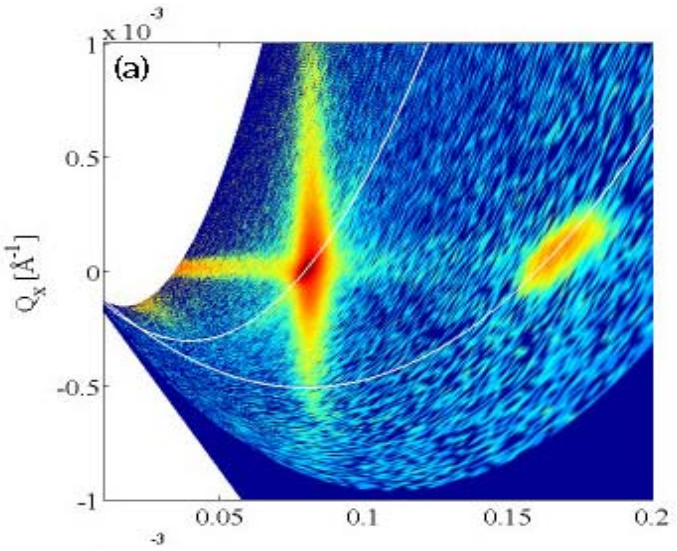


A380 wing section

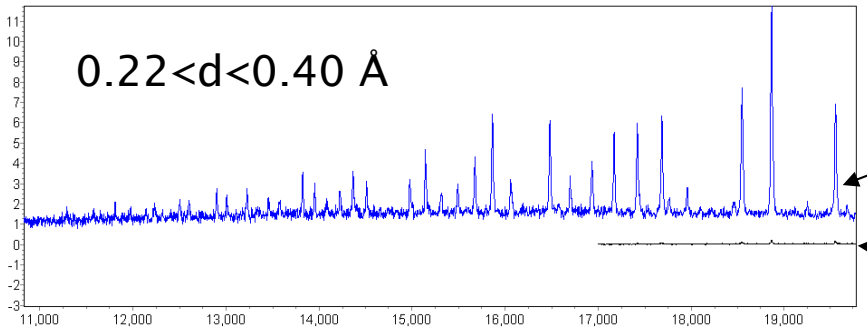
CRISP / SURF
- *Surface Studies*

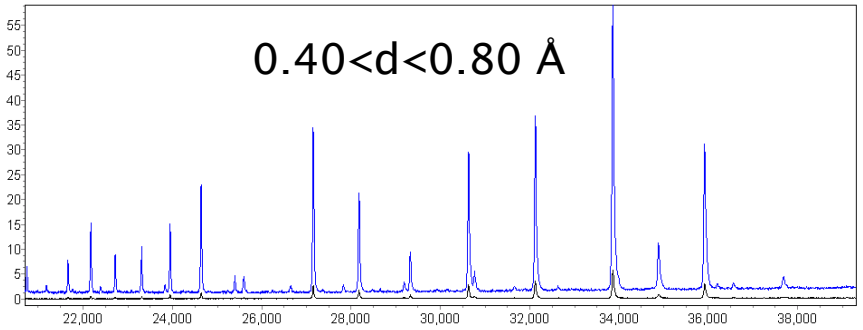
GEM
- *Parametric Studies*

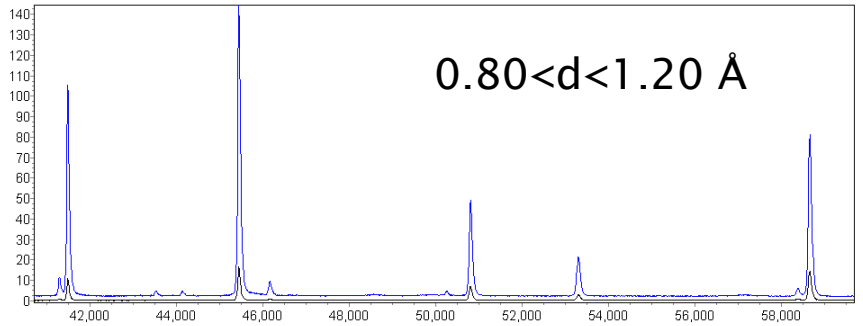
ENGIN-X
- *Neutron Strain Measurements*



HRPD Supermirror Guide – First results MgO





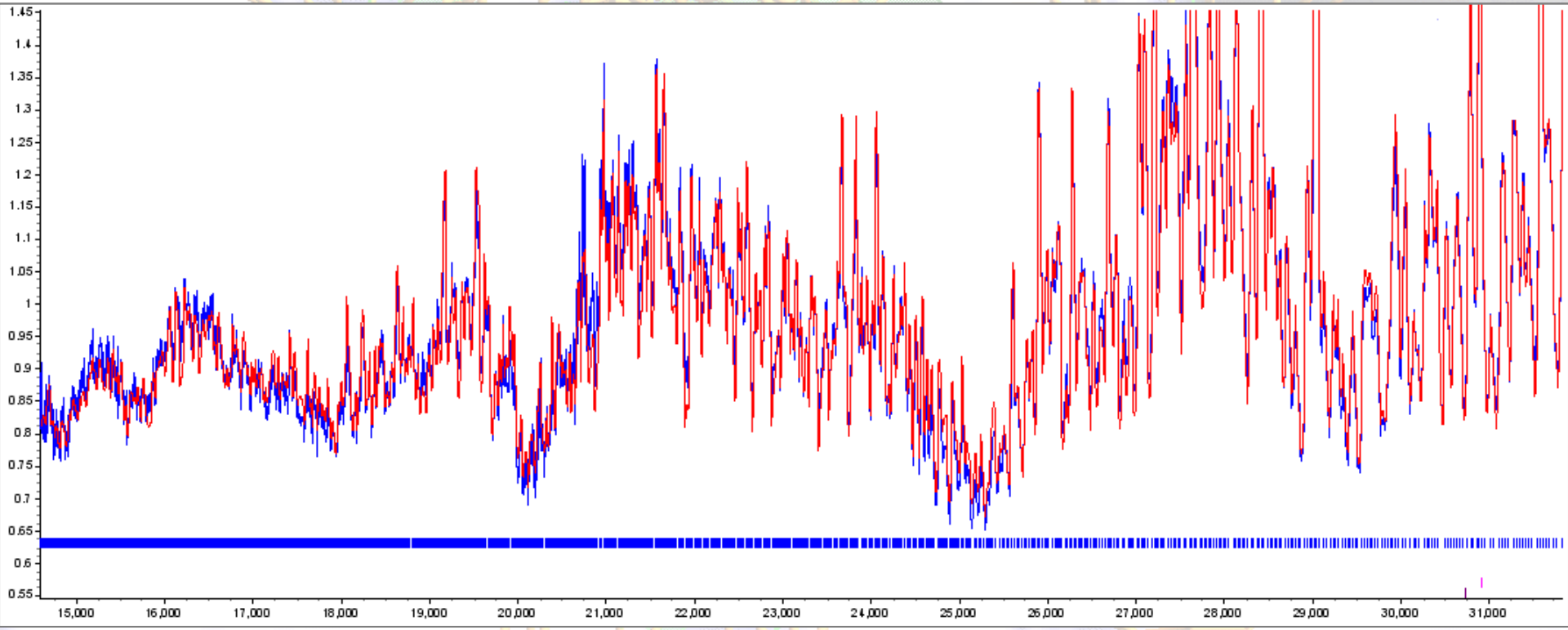


λ (Å)

Science & Technology Facilities Council

Science & Technology Facilities Council
ISIS

C_{60} revisited on HRPD – one of the best powder diffraction datasets ever collected



0.3Å

0.6Å

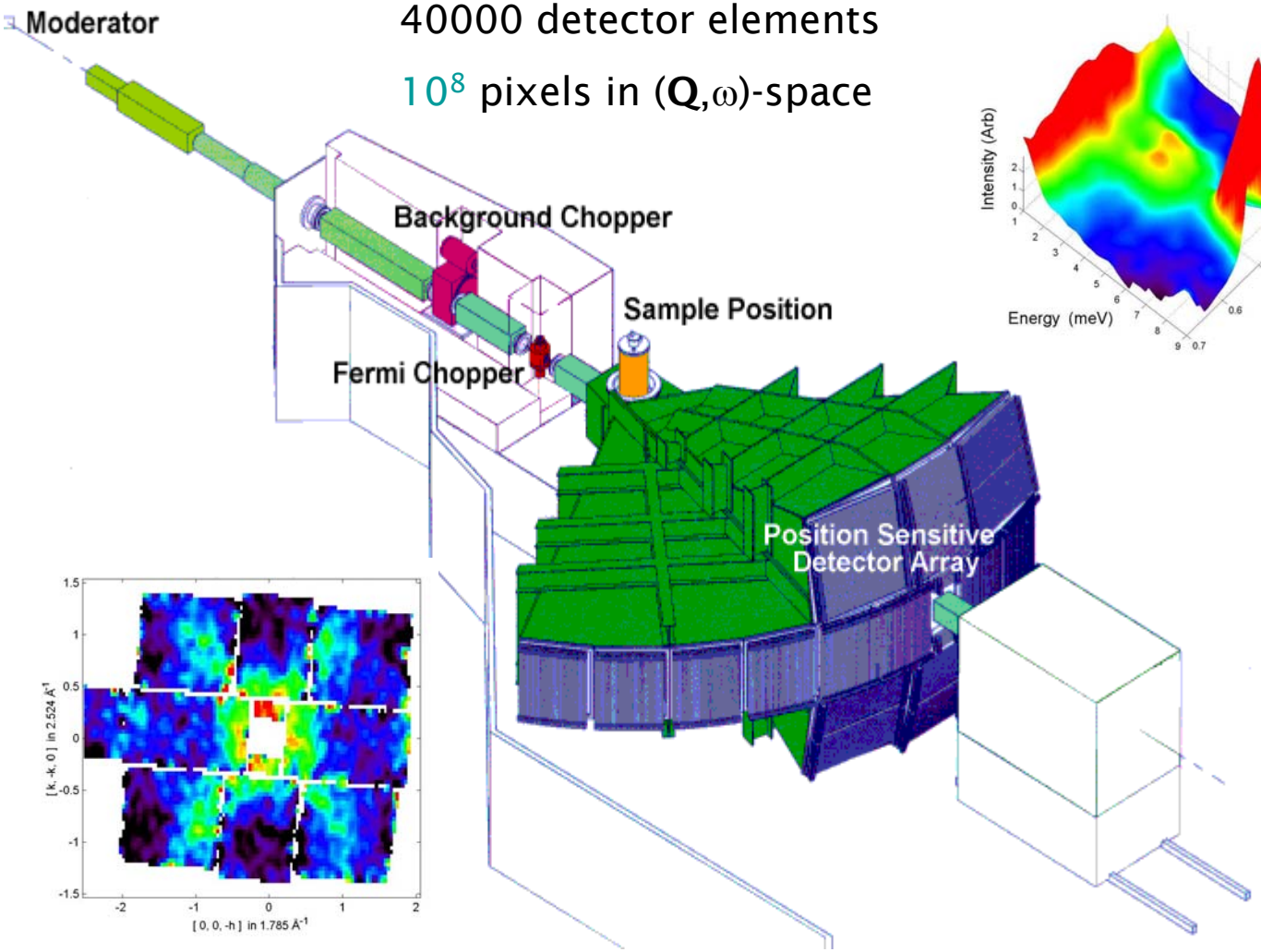
These data were not observed in 1992
*In 1992, there were **2,100** reflections to 0.6Å*
*In 2007, there are **17,820** reflections to 0.3 Å*

Science & Technology Facilities Council
ISIS

Making MAPS of Magnetism

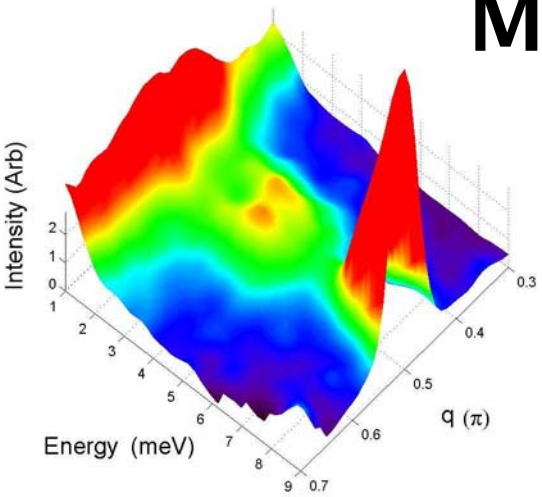
40000 detector elements

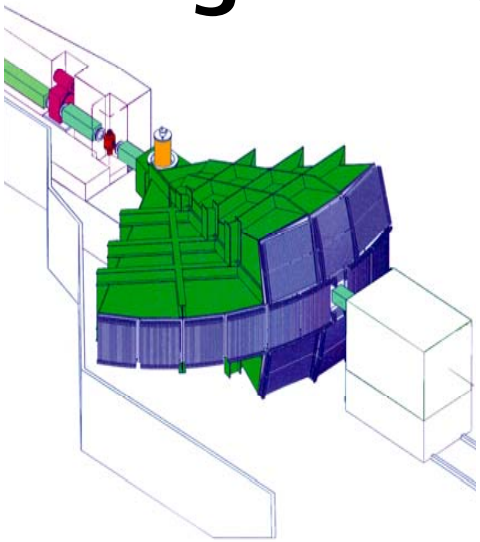
10^8 pixels in (**Q**,ω)-space

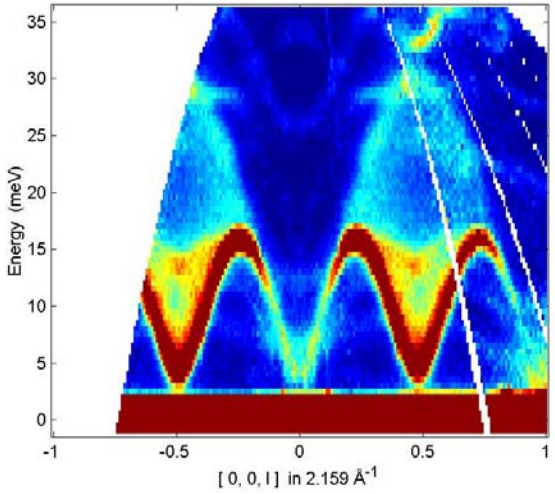


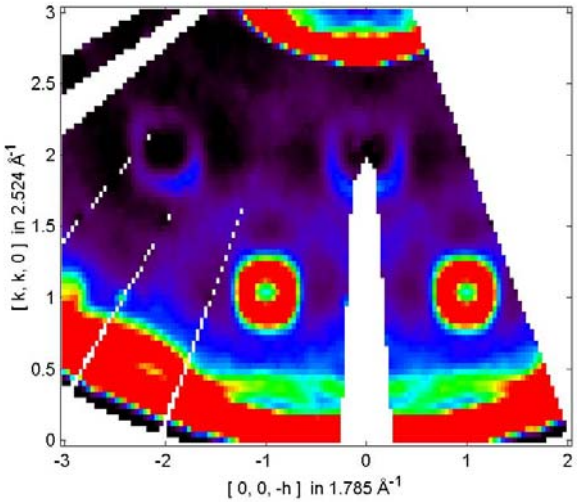
Science & Technology Facilities Council
ISIS

Making MAPS of Magnetism

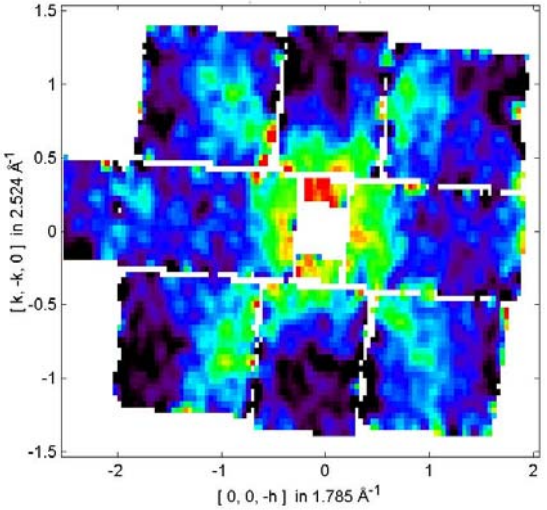








Pixel Power

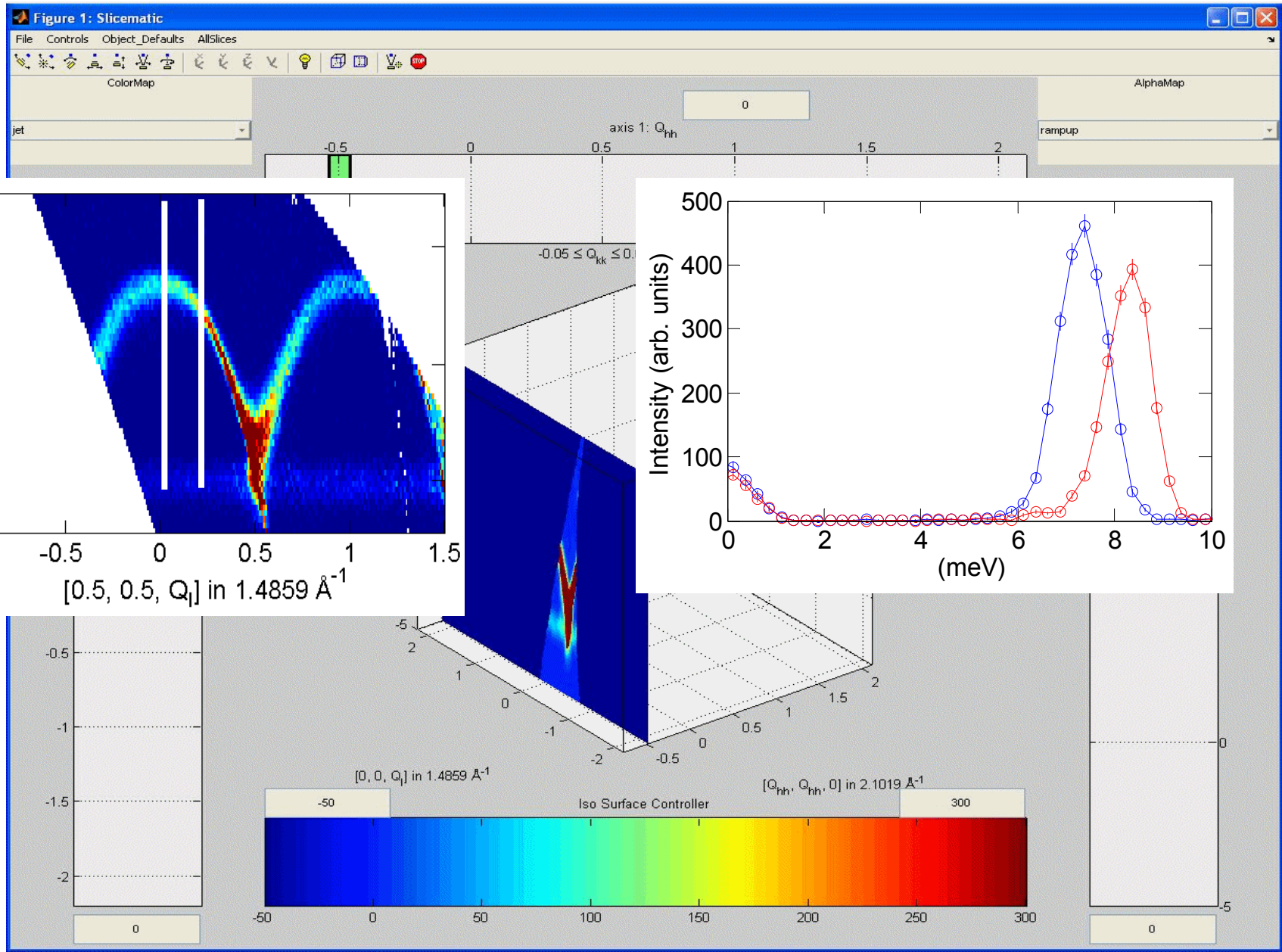


•Visualisation software

Combine ~200 datasets ⇒ full map of S(**Q**,ε)

40GB 10^9 pixels

Bespoke visualisation software ("HORACE")

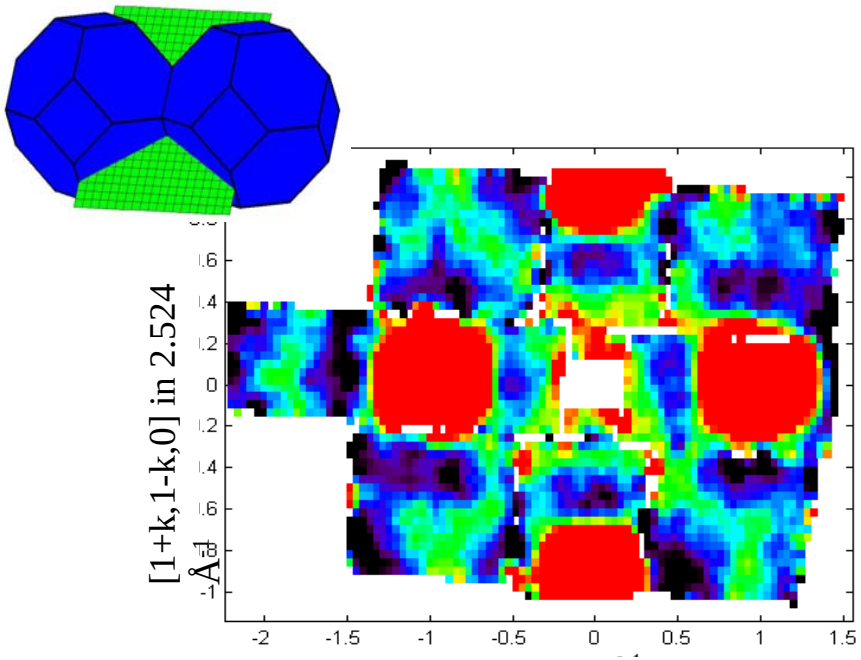


- Transition metal magnetism

- Fe, Co, Ni canonical examples of strongly correlated electron magnets
- Understanding dynamical susceptibility - $\chi''(\mathbf{q},\varepsilon)$ - requires account of electron exchange and correlation
- Interest in own right – BUT also of approximations that must be applied in calculations

Nickel

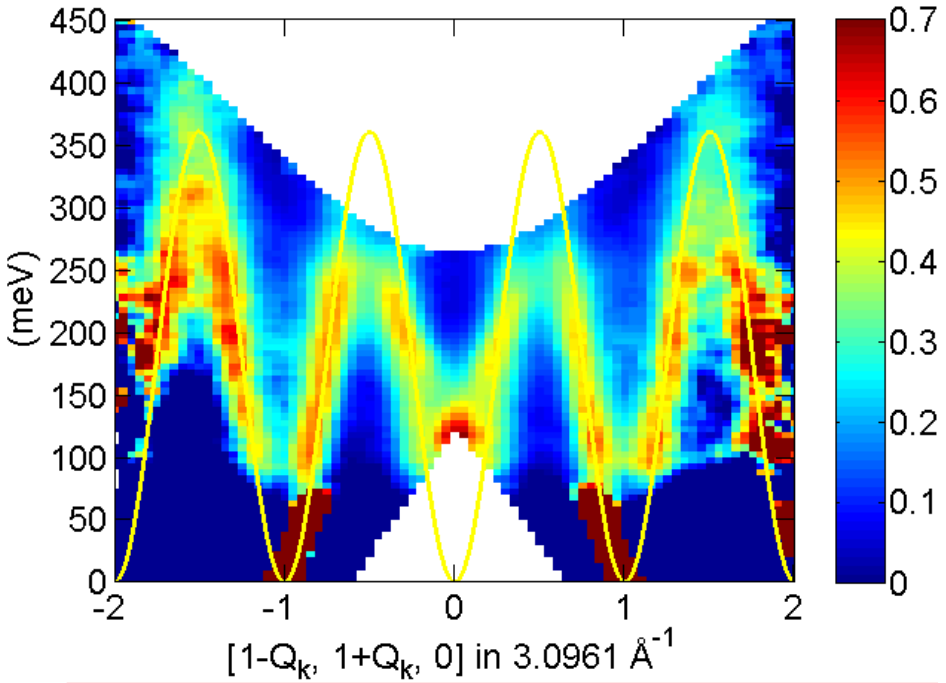
(Mook, Perring, Hayden, unpubl.)



[1,1, ℓ] in 1.785 Å^{-1}

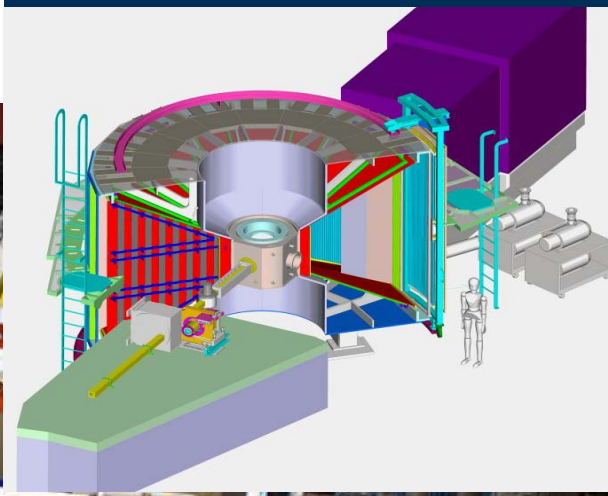
Iron

(Perring and Mook, unpubl.)

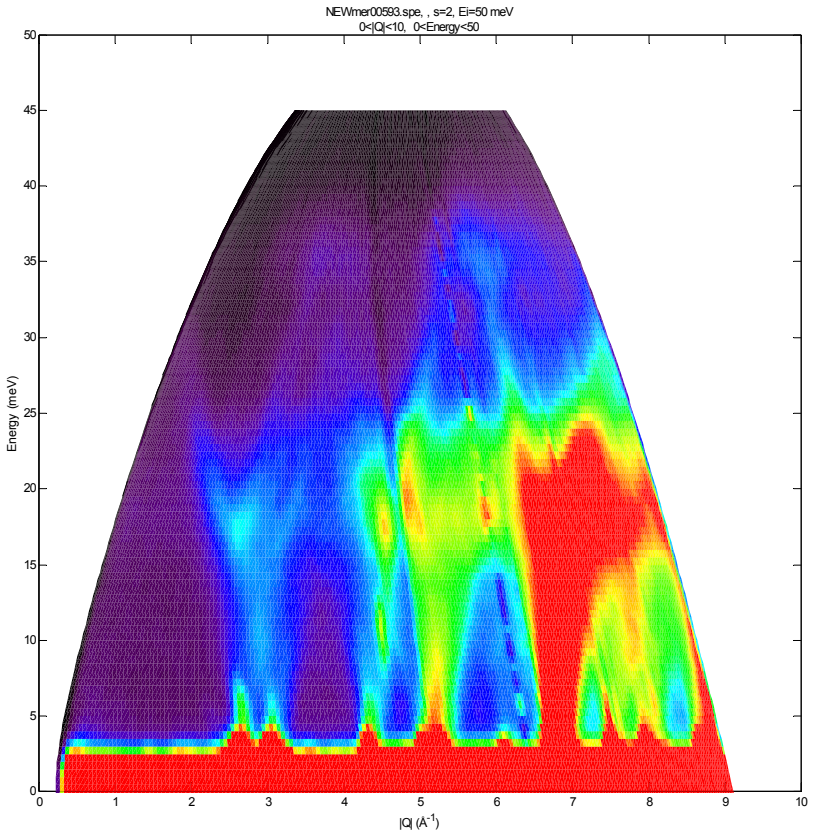


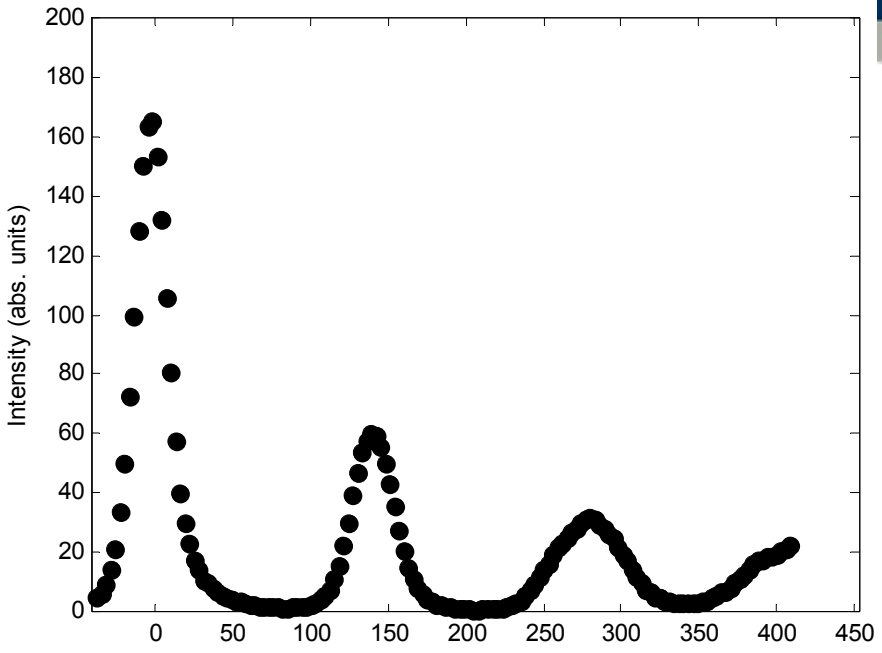
- **Complete measurement of ***ALL*** of S(Q,ε) to ~0.5eV**

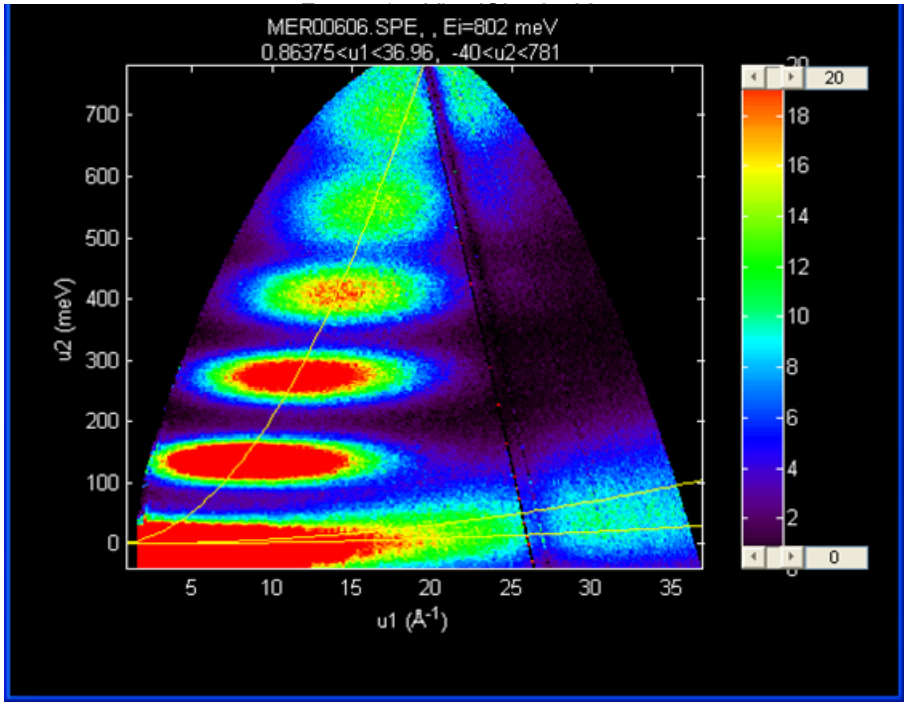
MERLIN – commissioning



Science & Technology Facilities Council
ISIS



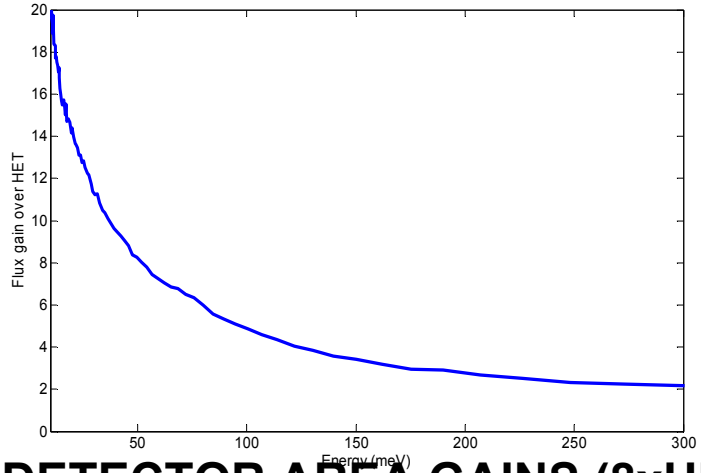




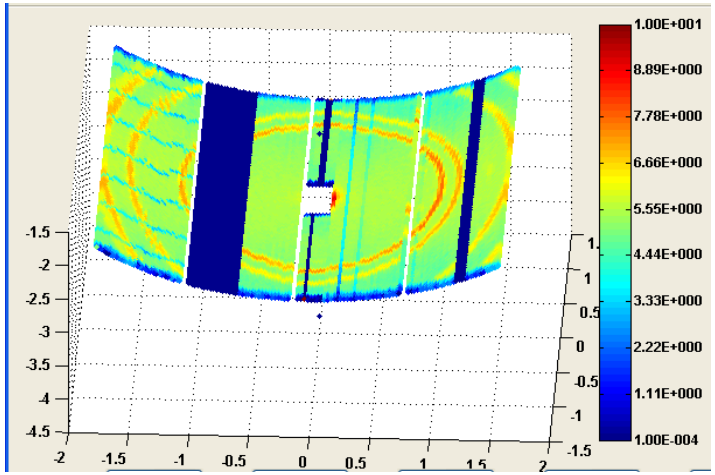
MERLIN commissioning

Science & Technology Facilities Council
ISIS

FLUX GAINS ON SAMPLE (20xHET)

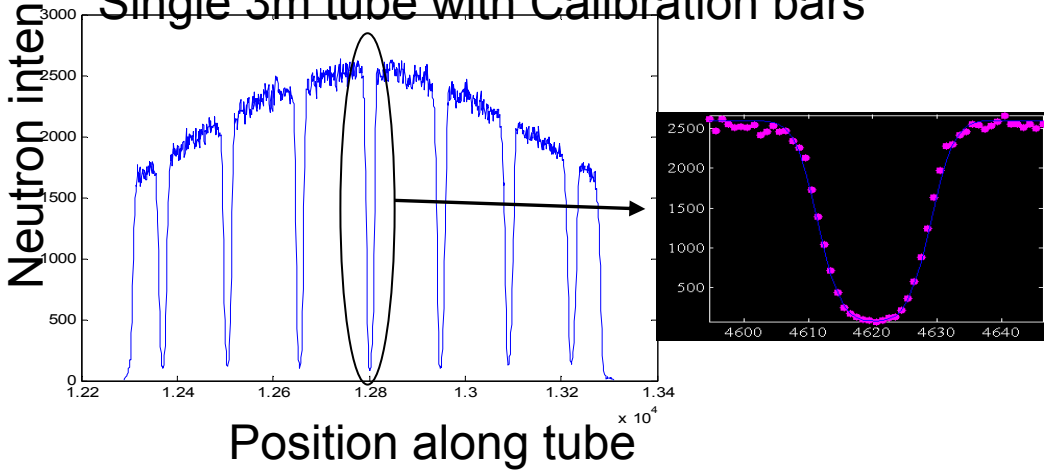


DETECTOR AREA GAINS (8xHET)



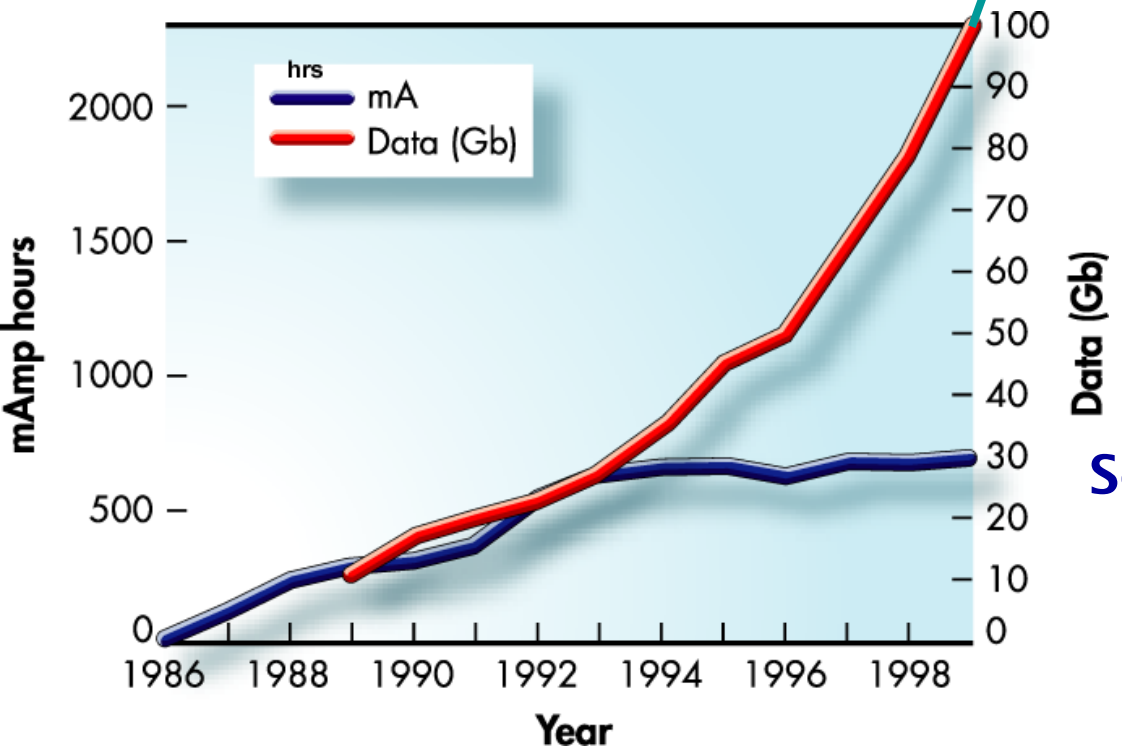
Ni powder rings on doors 1-4 of MERLIN

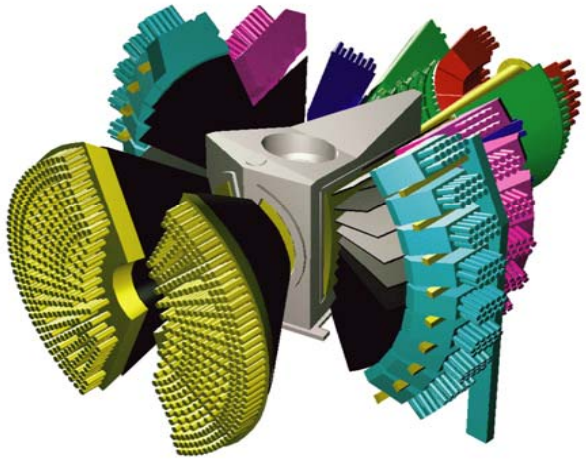
Single 3m tube with Calibration bars



Increasing Data Volume

800 Gbytes / year
2005

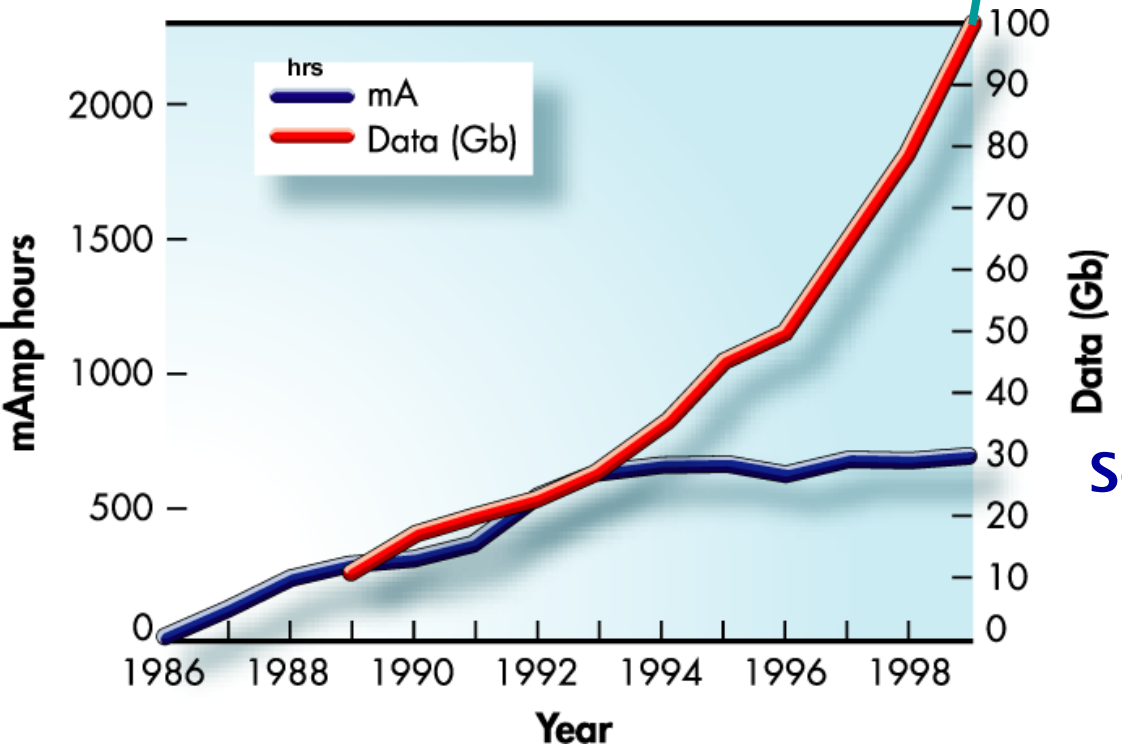


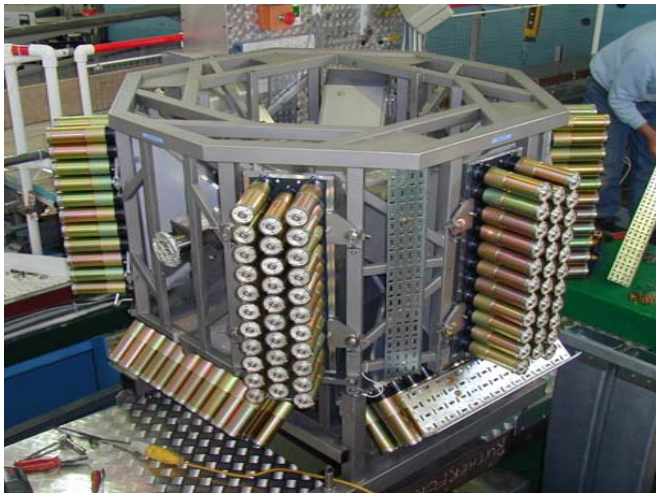


Source Strength

Increasing Data Volume

1200 Gbytes / year
2006



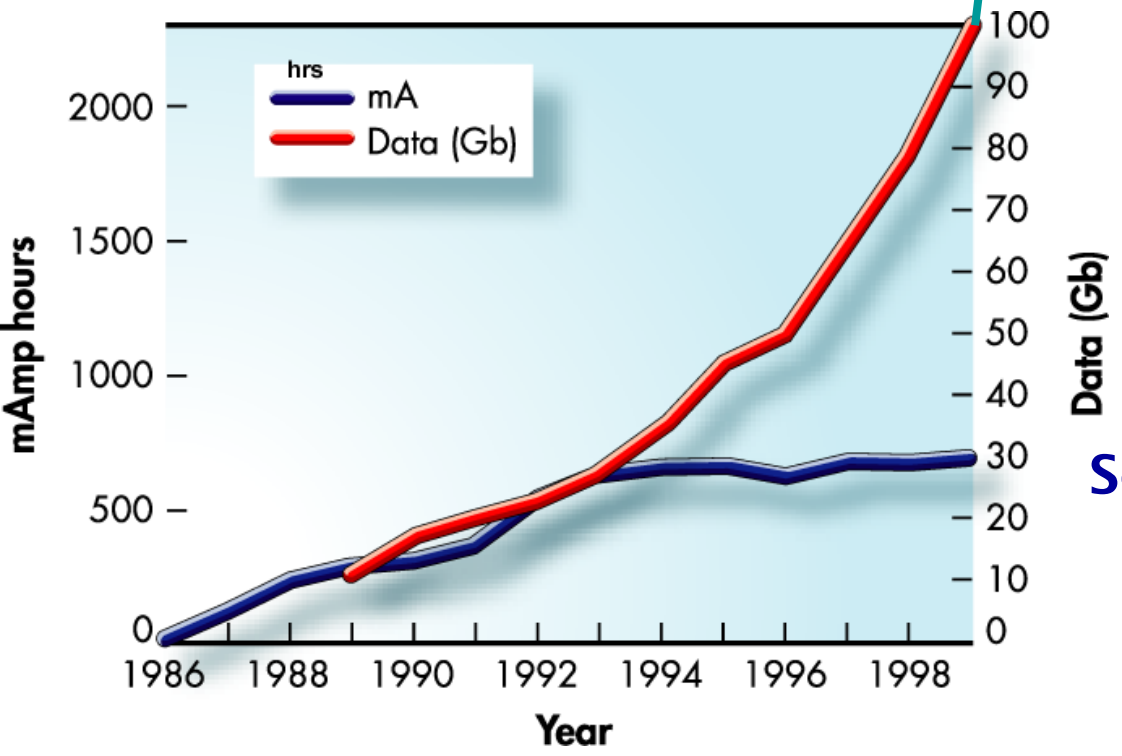


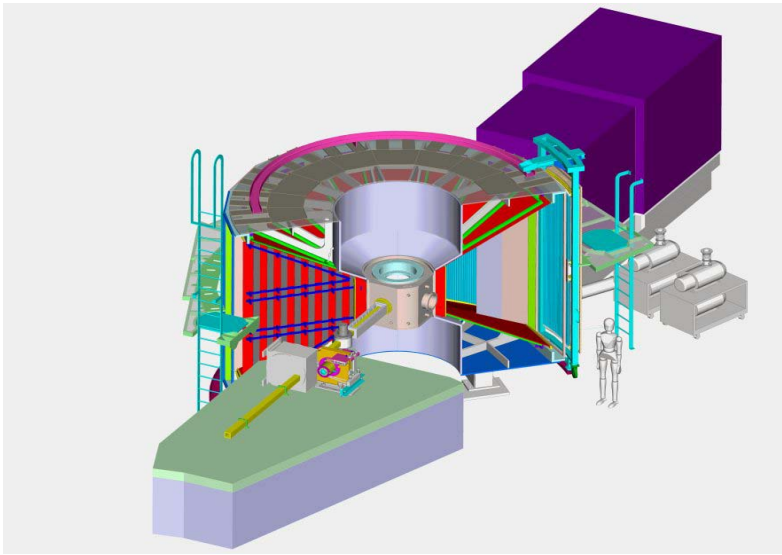
Source Strength

Increasing Data Volume

1800 Gbytes / year
2007

e-Science Grid technology

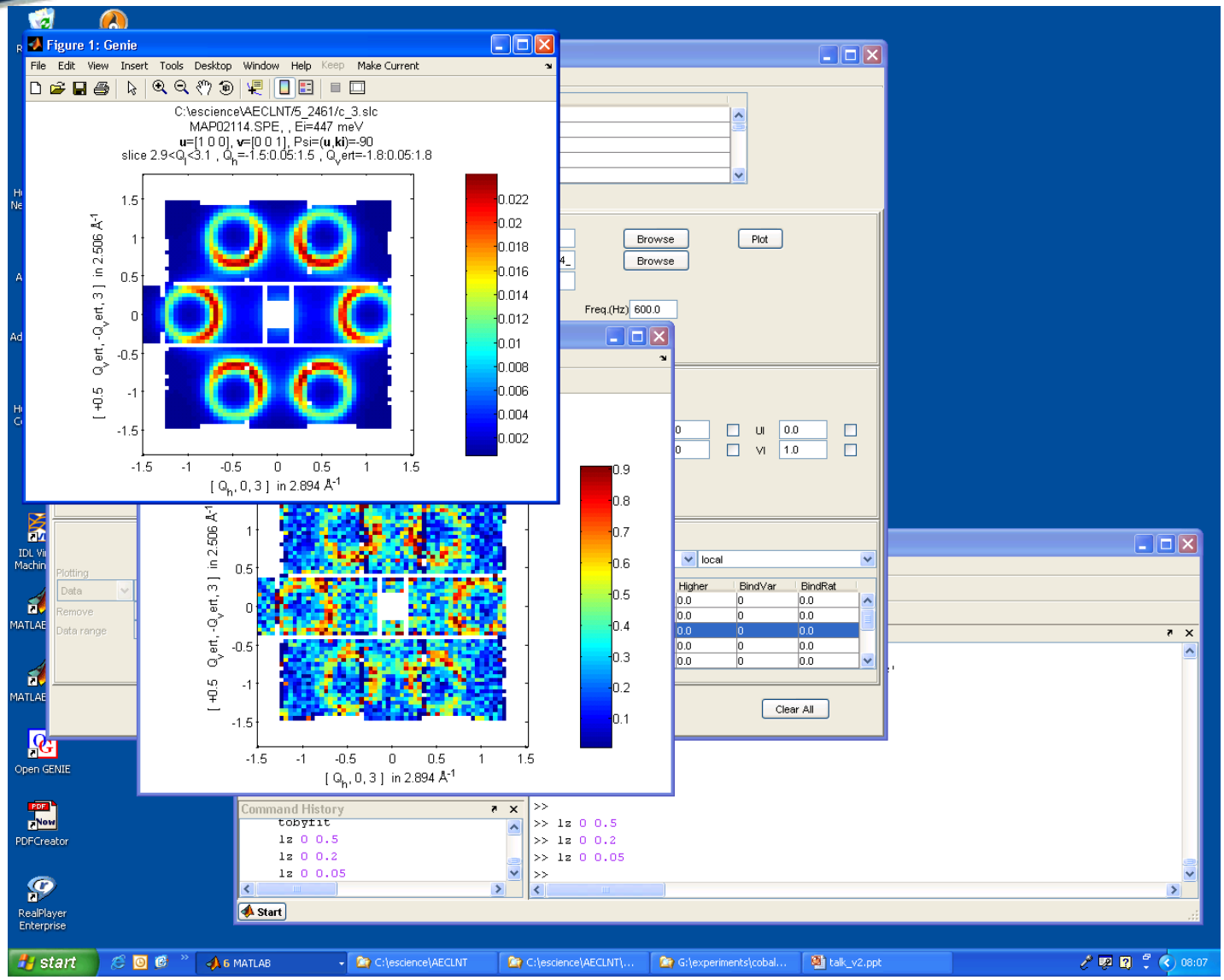




Source Strength

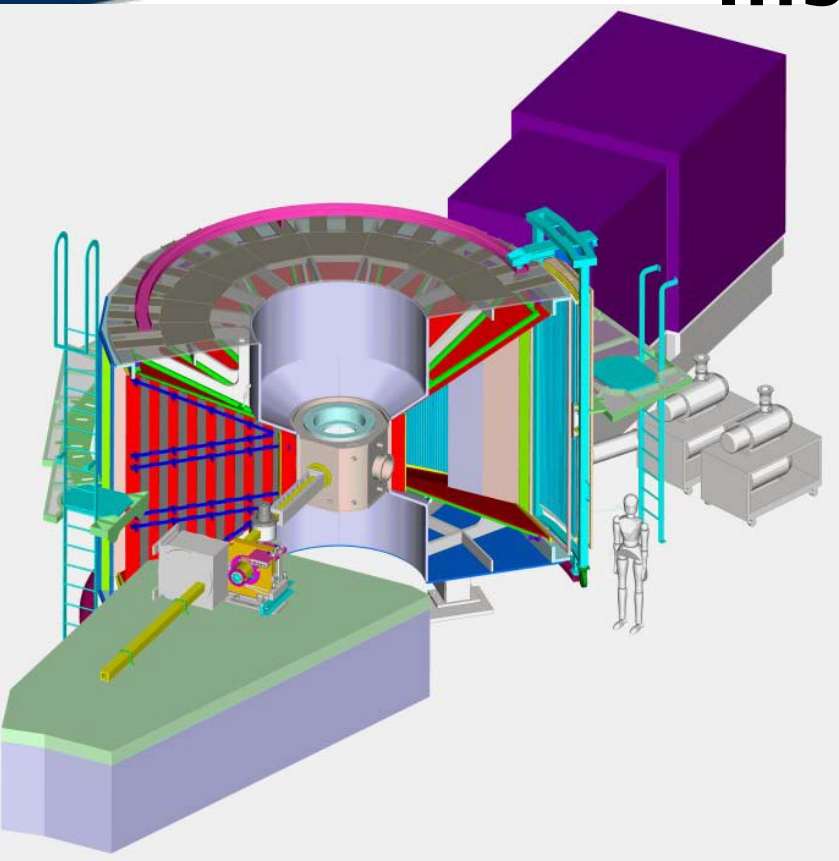
Science & Technology Facilities Council
ISIS

Grid Computing



Science & Technology Facilities Council
ISIS

Instrument Development



Detectors

LAD → GEM	x 30
ENGIN → ENGIN-X	x 20
HET → MAPS	x 25 → LET x3
SXD → SXD11	x 11 → SXD' x5

R&D

Detectors,

Smaller pixels, Higher Rates, Lower Costs

Optics, Filters, Choppers

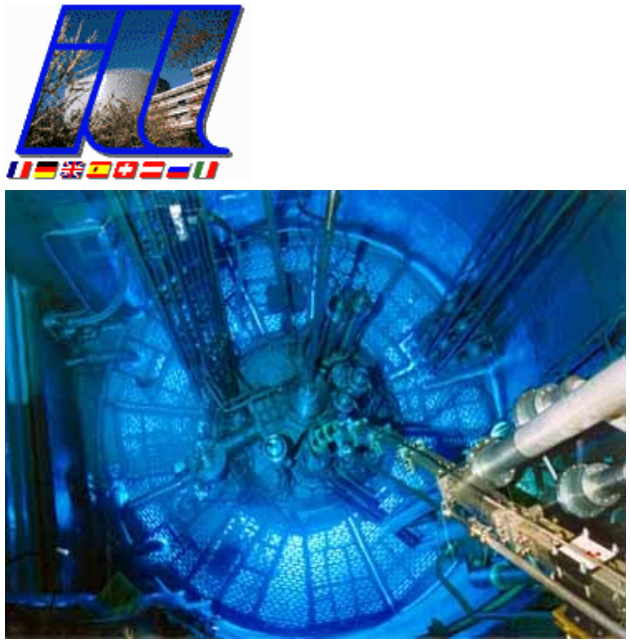
HRPD → HRPD' x 10

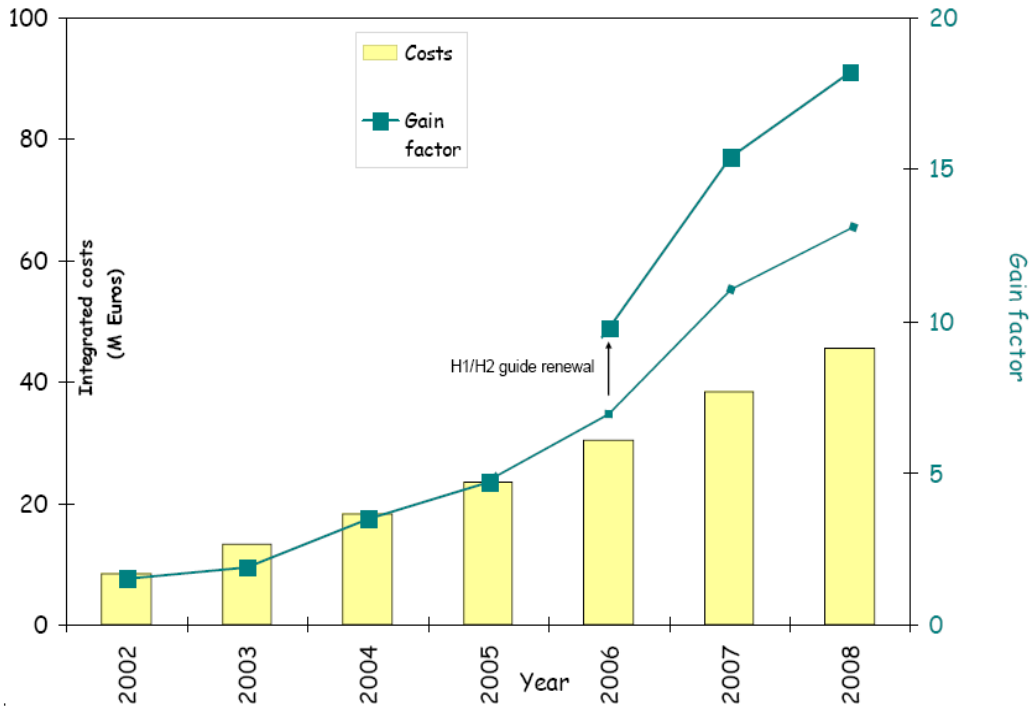
Software

Sample Environment

Investment in Instrumentation

Gain Factor from Millennium Programme x 14





Science & Technology Facilities Council

UK Neutron Strategy

- Neutron Scattering is an important tool for the UK
- Maximise return from ILL
- Maximise return from ISIS
- Plan to gain access to a next generation MW+ source within 15 years
- Address key technologies in an international context
- *Notes UK is a credible host*

Second Target Station Project

Science & Technology Facilities Council

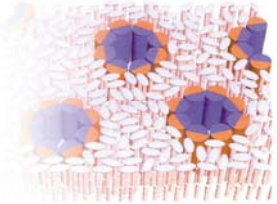
ISIS Second Target Station

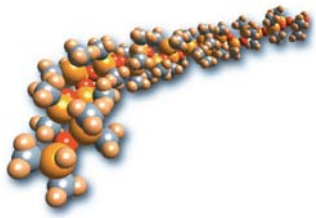
Budget ~ £200 M

Designed to meet future scientific needs in the key areas of:

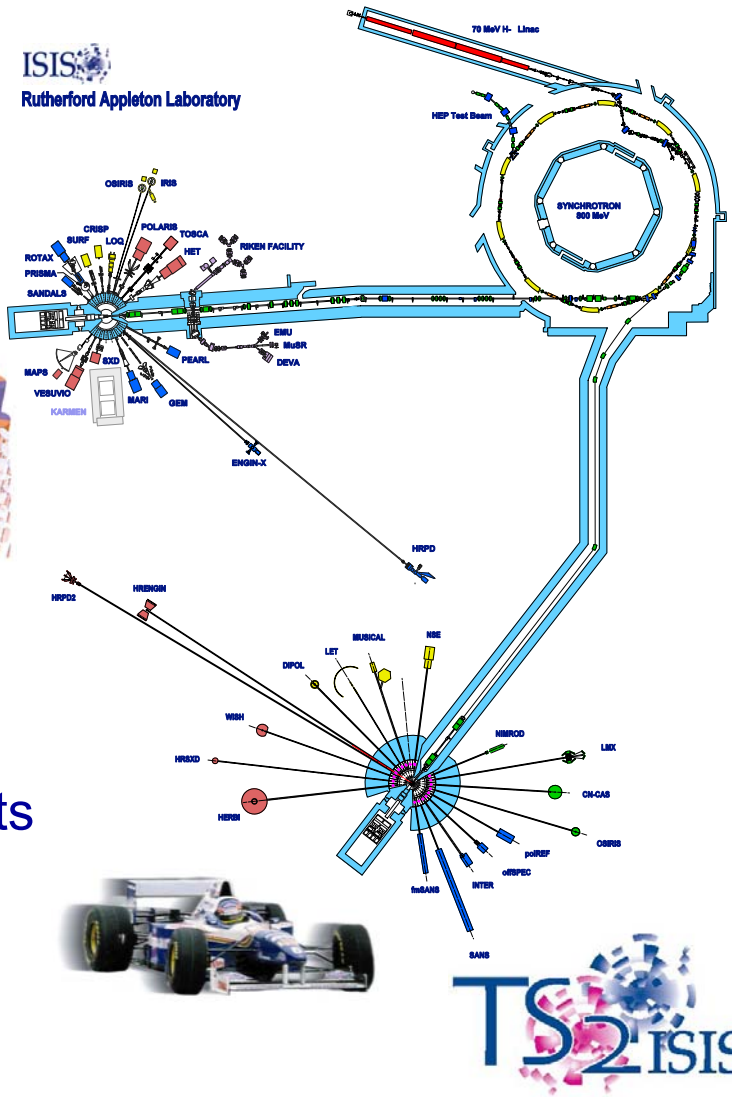
- Soft Matter
- Advanced Materials
- Bio-molecular Science

Nanoscience





- complex multi-phase or multi-component materials
- difficult or complex environments
- kinetic processes
- parametric studies
- smaller samples

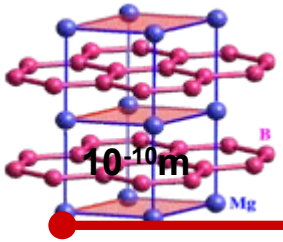


TS2 ISIS

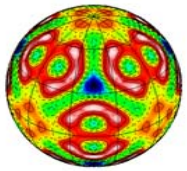
Science & Technology Facilities Council

Expanding the Frontiers

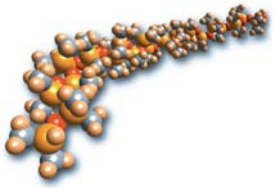
- Unique probe to study the structure and dynamics of Condensed Matter

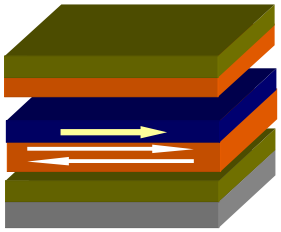


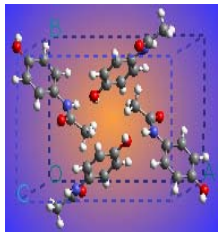
10^{-10}m

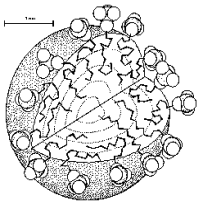


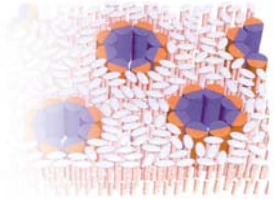
10^{-9}m



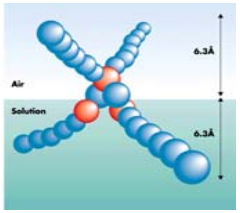


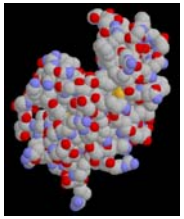




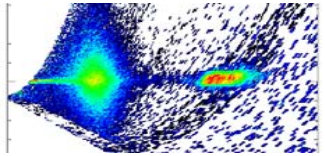


10^{-8}m





10^{-7}m



10^{-6}m

- The length scale from 10^{-10}-10^{-6} m covers a huge range of condensed matter science and technological applications

Science & Technology Facilities Council

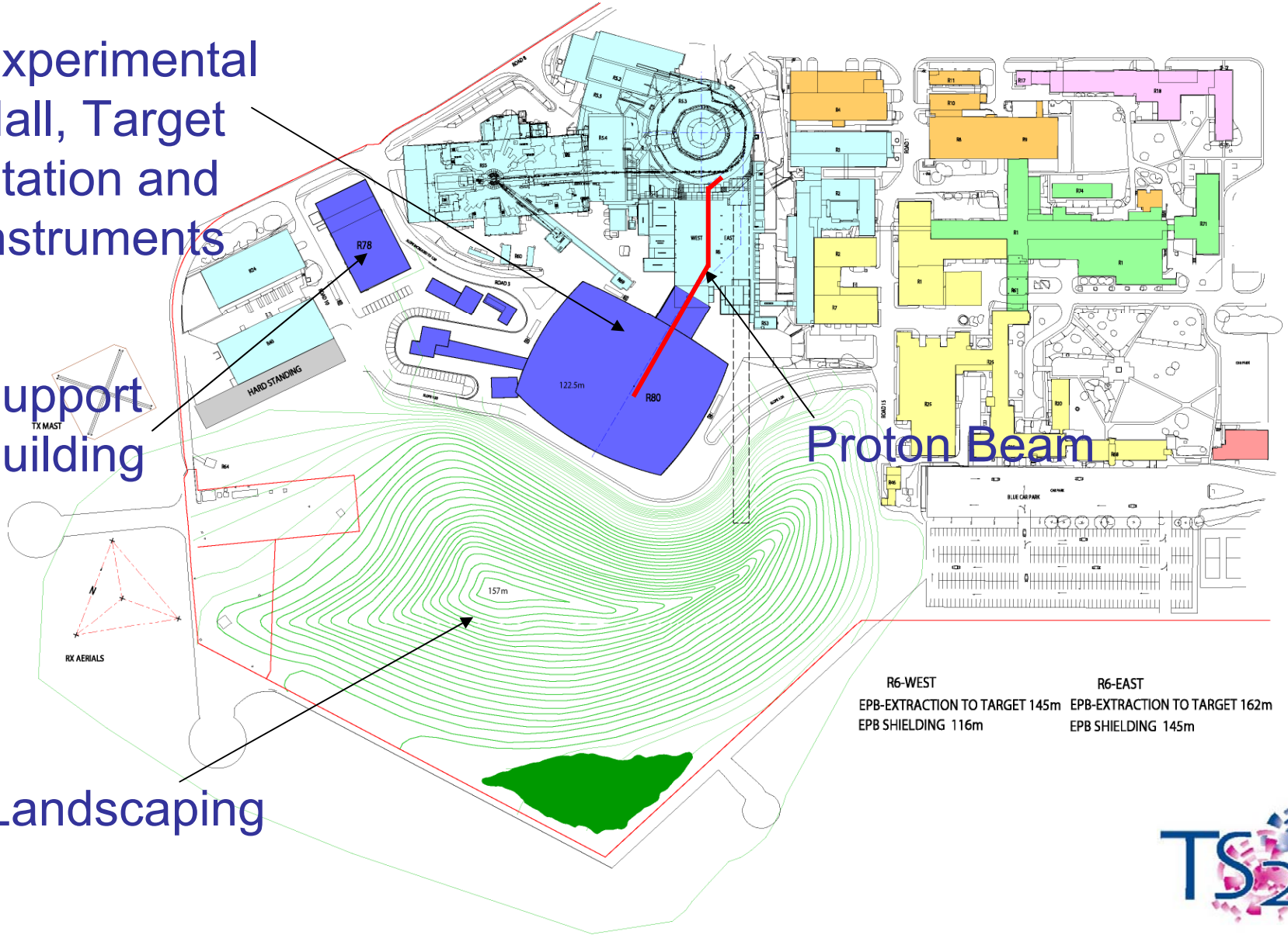
ISIS Second Target Station

Experimental Hall, Target Station and instruments

Support Building

Proton Beam

Landscaping



TS2 ISIS

Science & Technology Facilities Council

September 2003

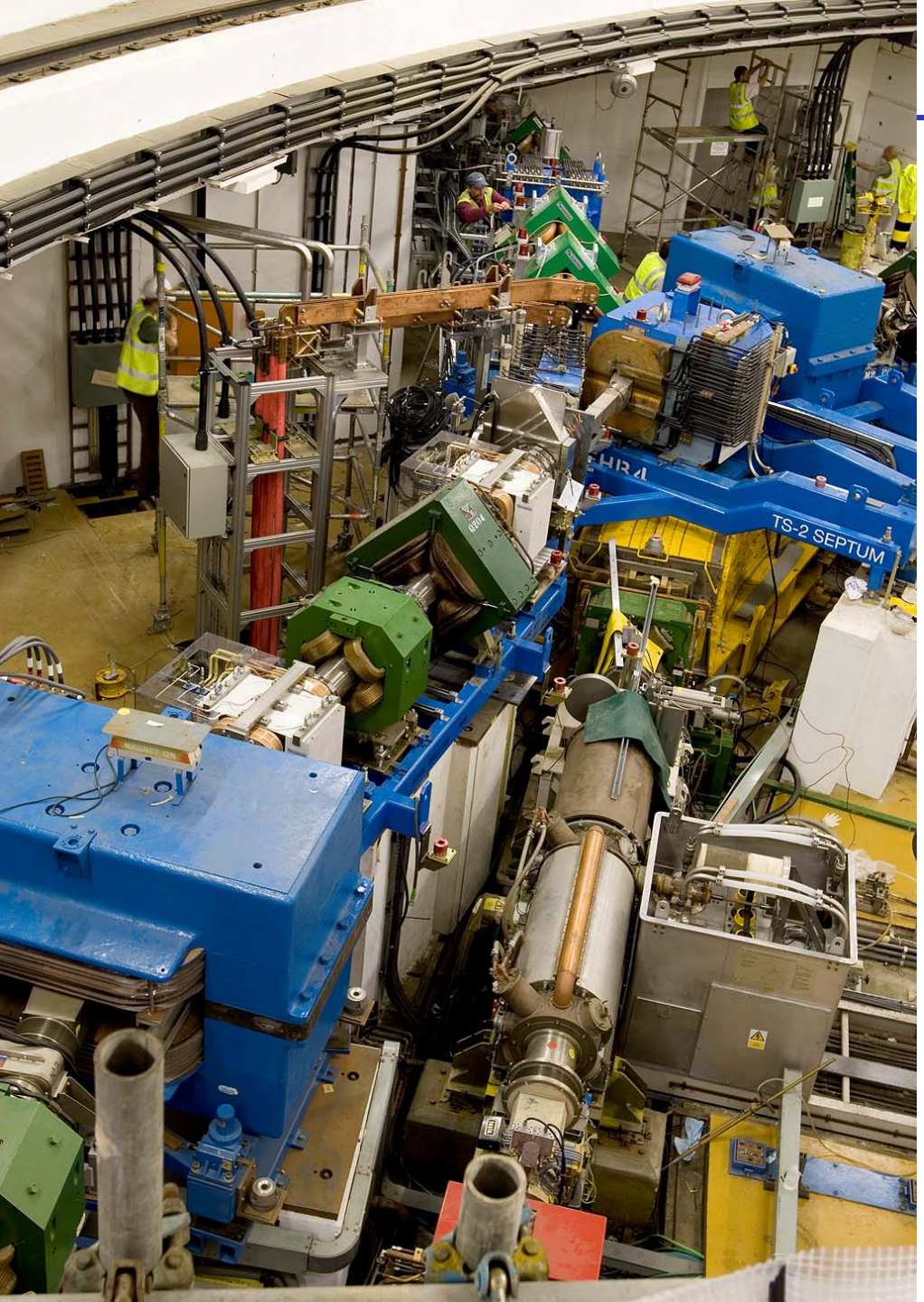
TS2 ISIS

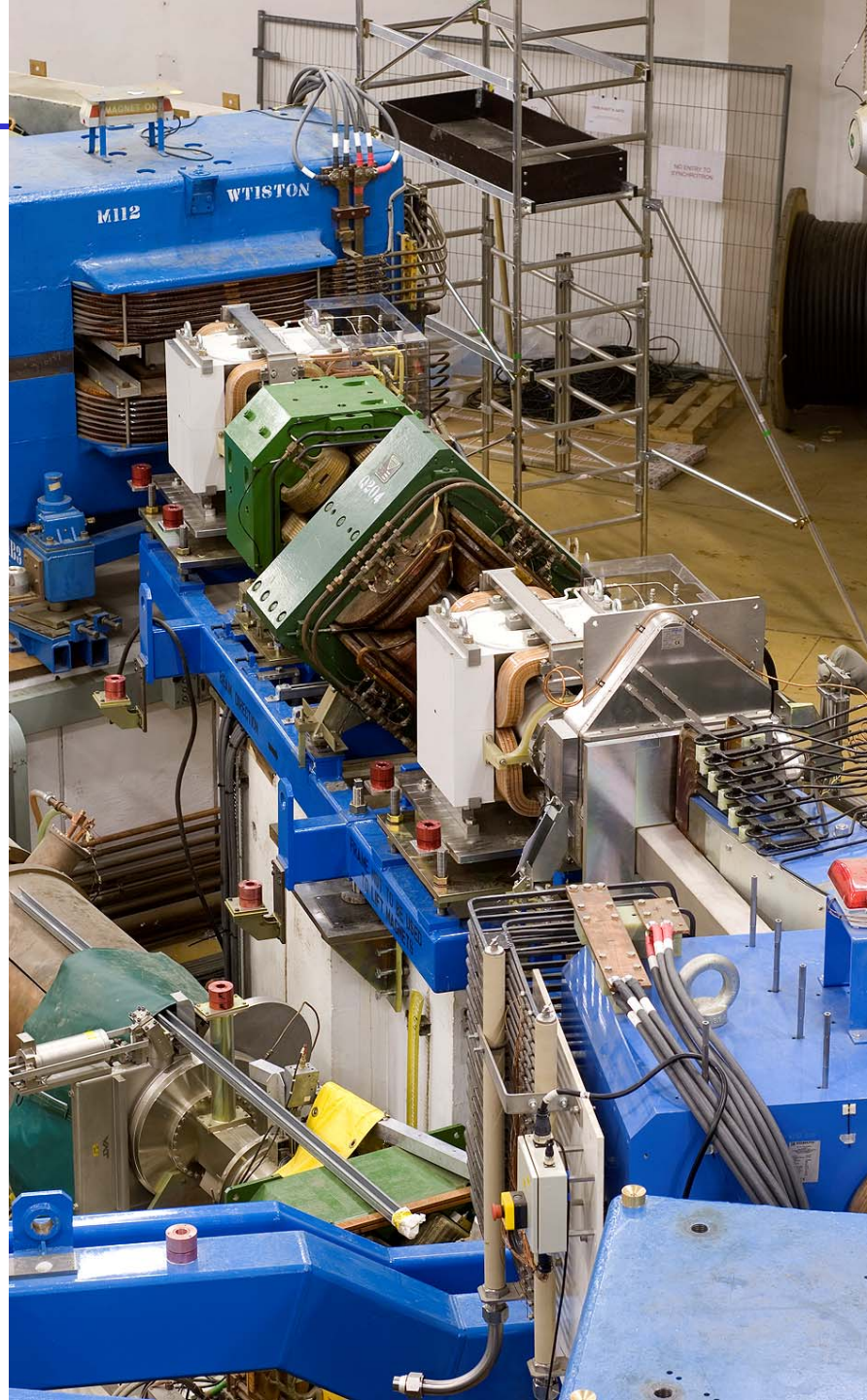
Science & Technology Facilities Council

March 2005

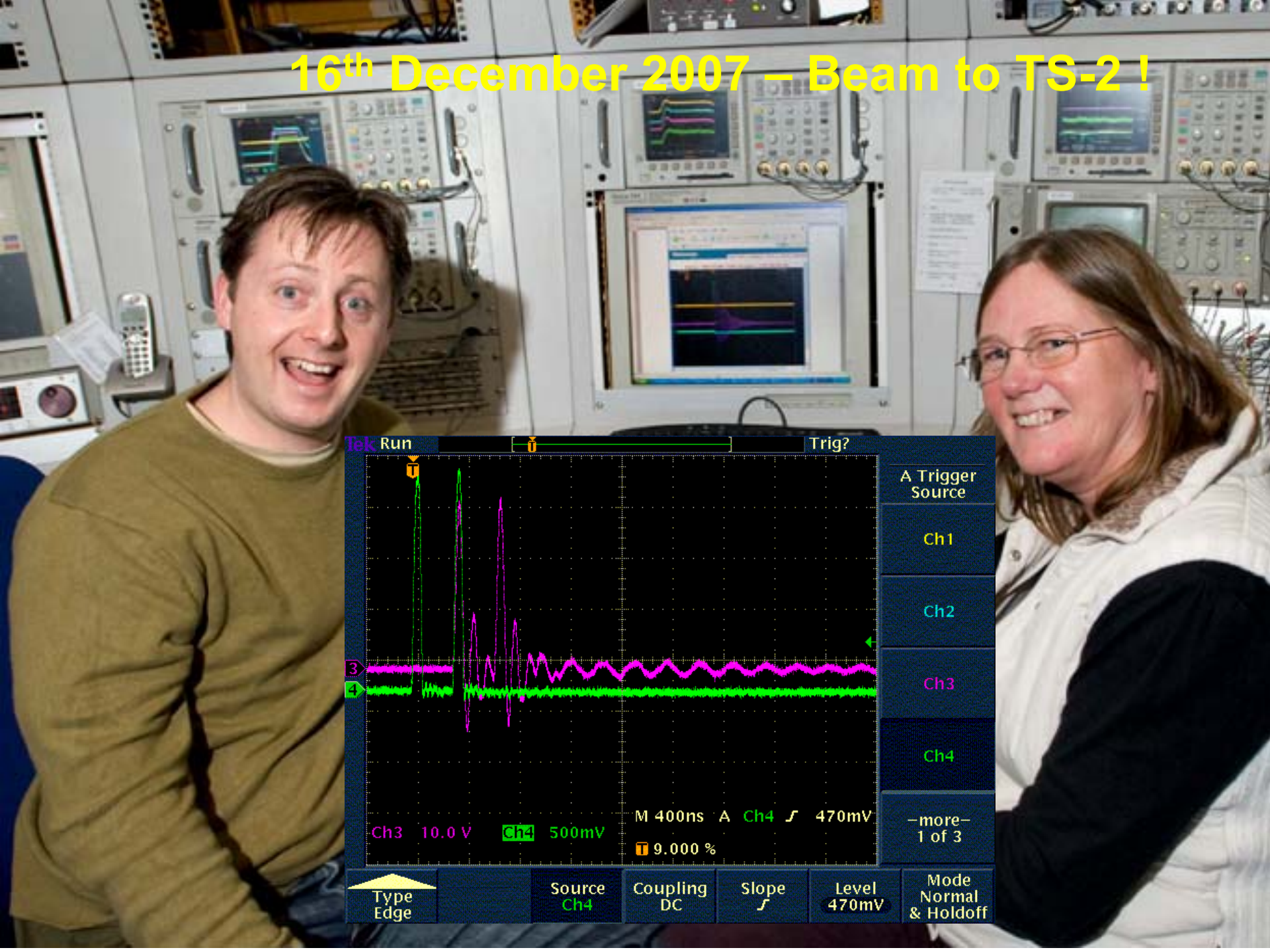
Science & Technology Facilities Council

June 2006


TS-2 SEPTUM

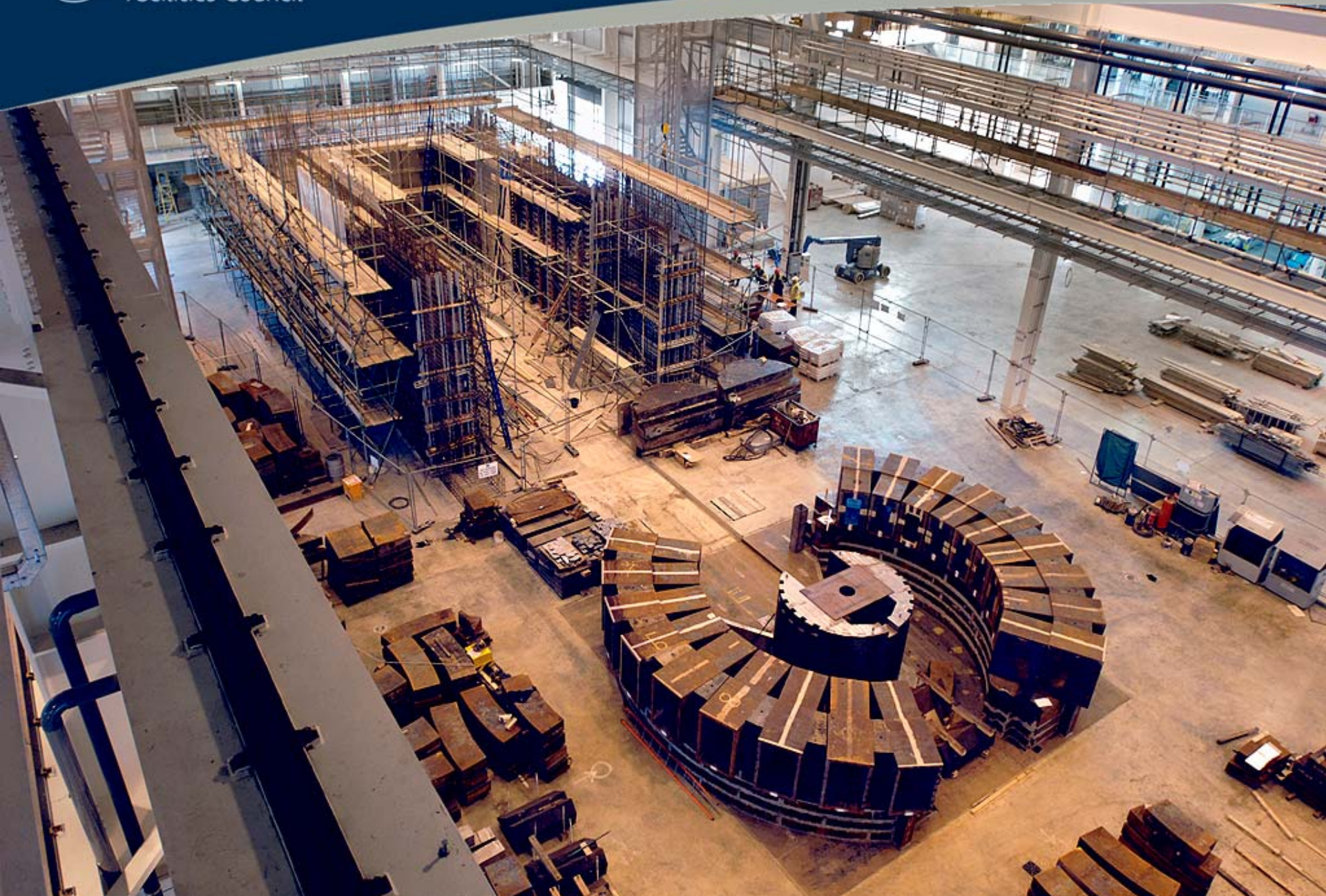

M112
WTISTON

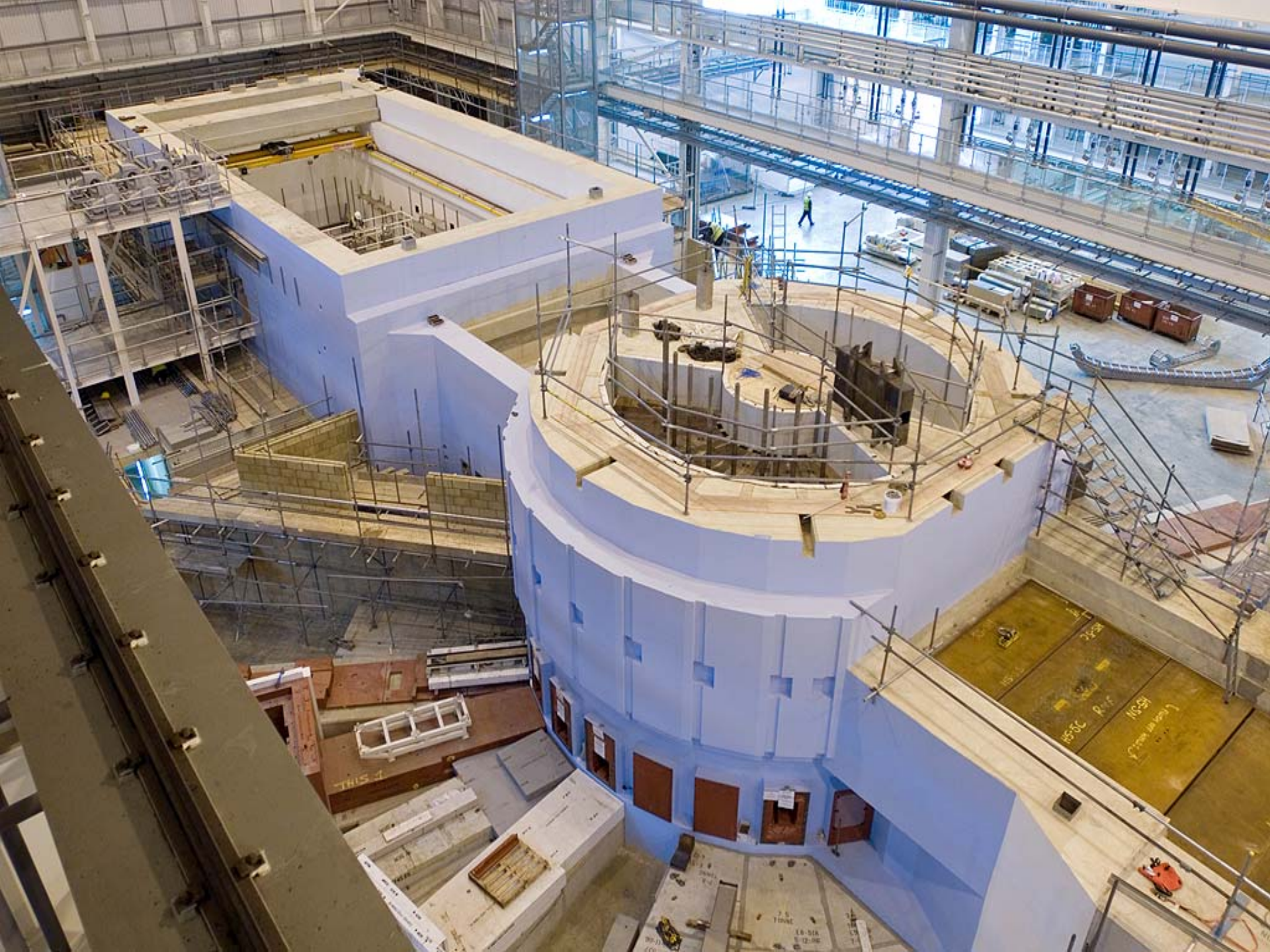
16th December 2007 – Beam to TS-2 !



Science & Technology Facilities Council

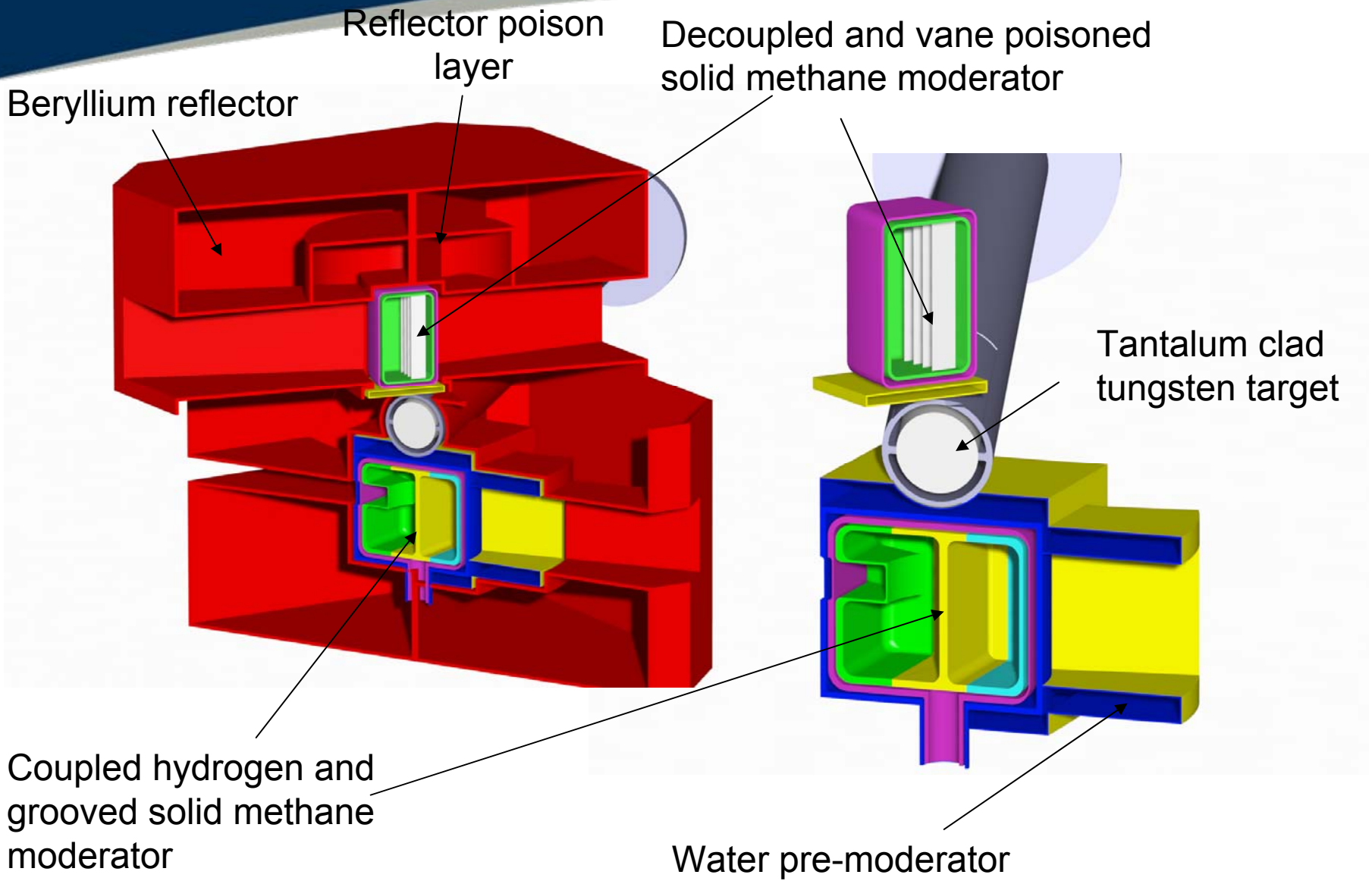
September 2006

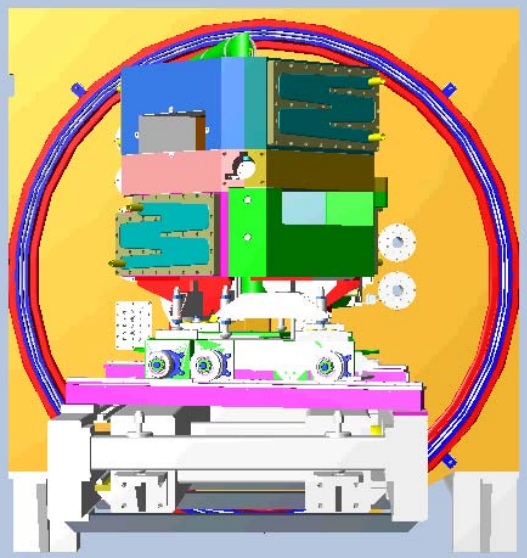




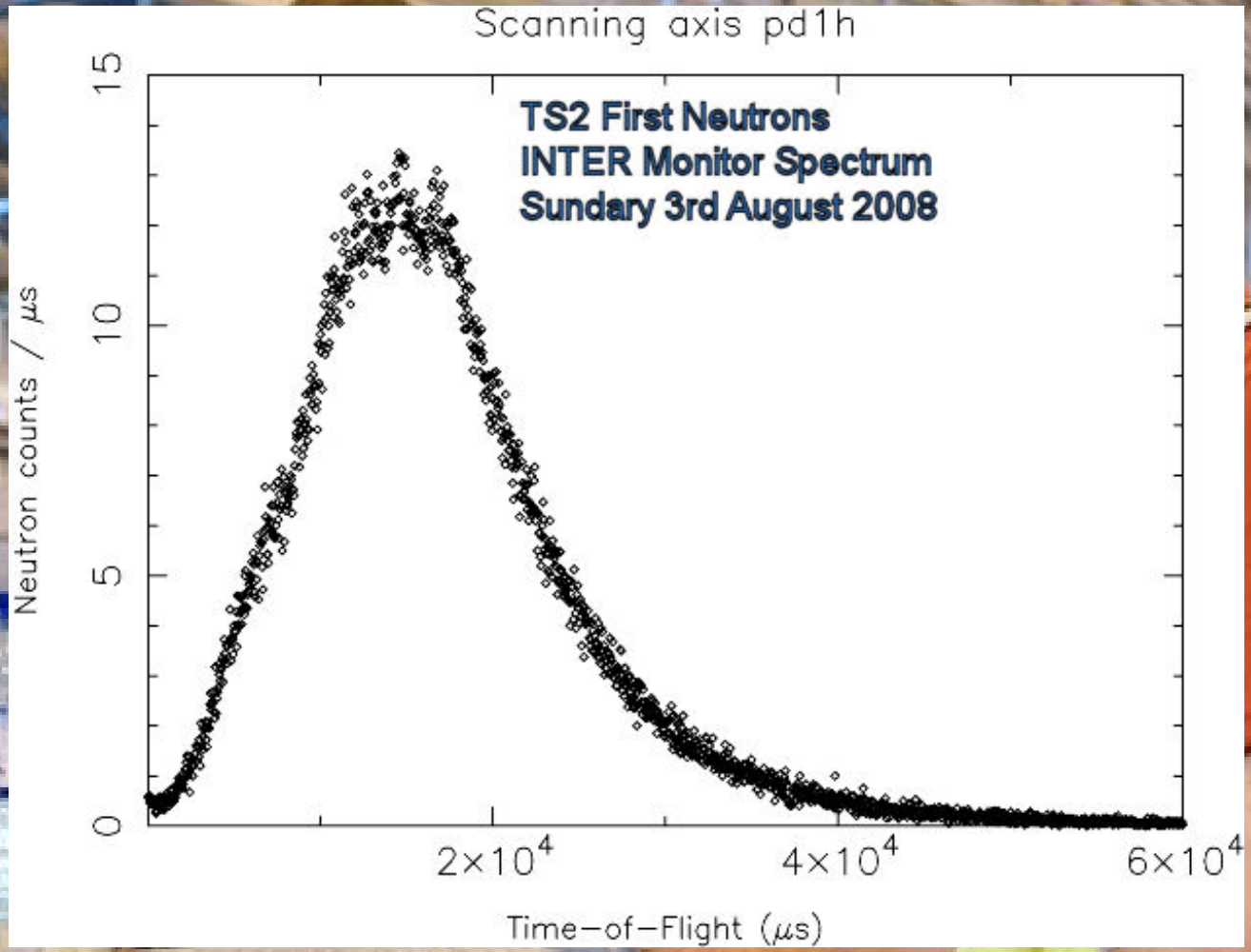
Science & Technology Facilities Council

Target-Moderator-Reflector





3th August 2008 – First Neutrons !

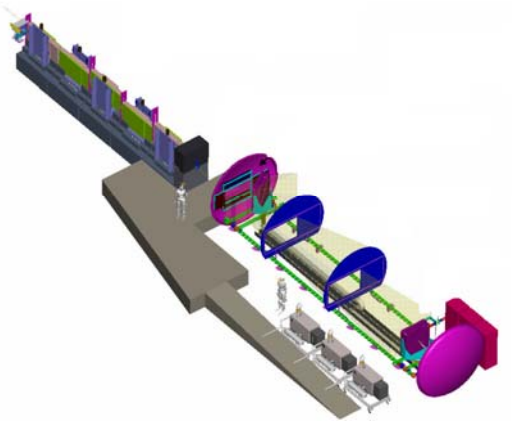


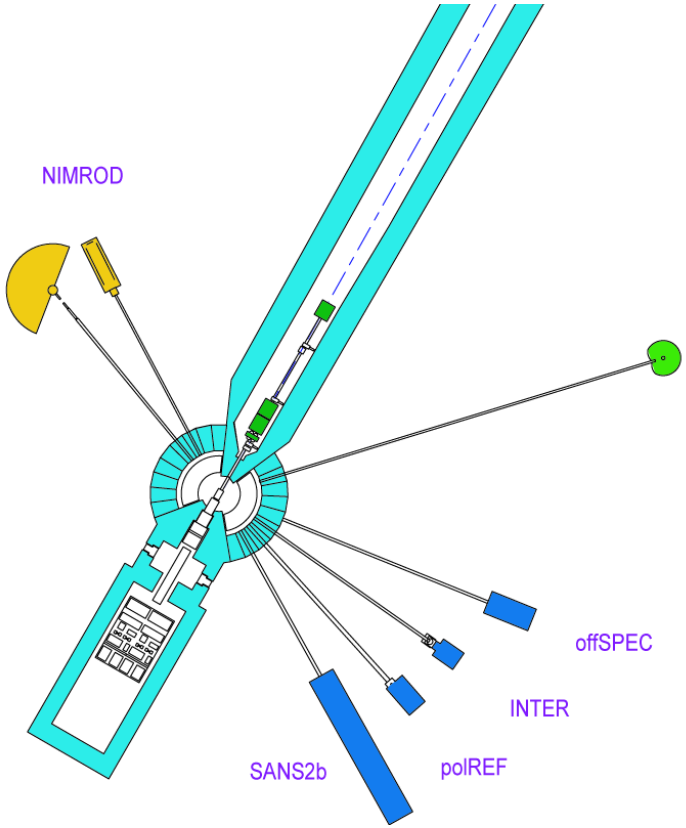
Science & Technology Facilities Council

TS-2 Phase One Instruments

Dynamics

LET High-resolution measurement of material energy scales



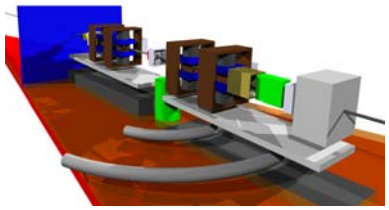


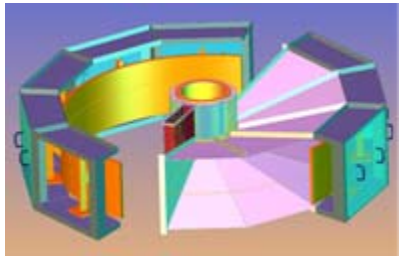
Structures

NIMROD Intermediate range order in liquids

WISH High-resolution magnetic structure

SANS2D Large molecule structure in multi-component systems





Reflectometry

INTER Air/ liquid/ solid interface interactions

OFFSPEC Structures of membrane, protein and liquid interfaces

POLREF Interface measurements in magnetic sensor devices

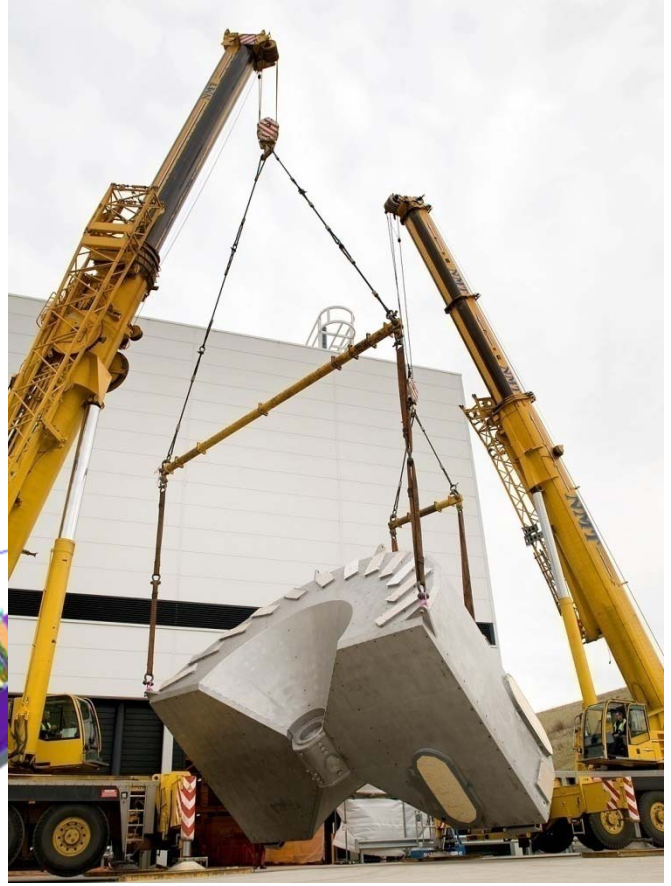
Reflectometers

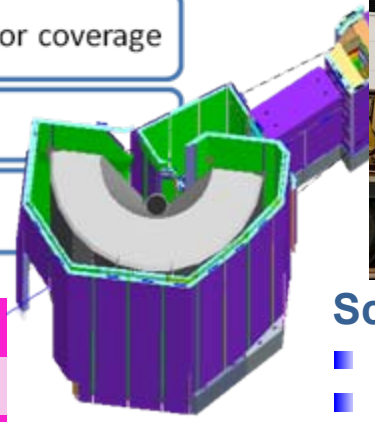
- Offspec
- Inter
- Polref

Spectrometers

LET

- High incident flux at low energies
- Large Solid Angle, -45º to 135º (± 30 º in the vertical)
- Pixelated detectors (50 000 pixels), No gaps in detector coverage
- High energy resolution
- Broad energy range (0.5 meV to 80 meV)





Energy range	1 – 80 meV
Moderator	CH_4 / H_2 – 26K coupled
Primary flight path	25m (m=2/3 supermirror guides)
Secondary flight path	3.5m -45° - 135° (PSD ^{3}He tubes)
Beam size	40 x 50 mm
Resolution	5μeV at E_i = 1meV 260μeV at E_i = 20meV

Scientific Opportunities

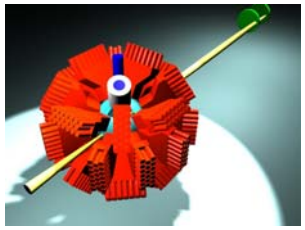
- Strongly correlated electron systems
- Magnetism
- Quantum fluids
- Functional materials
- Polymers and bio-molecular materials
- Phonons

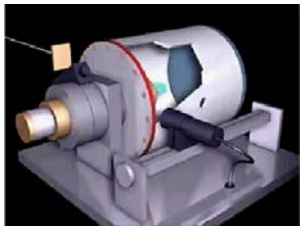
Science & Technology Facilities Council

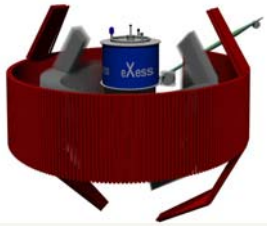
Science & Technology Facilities Council

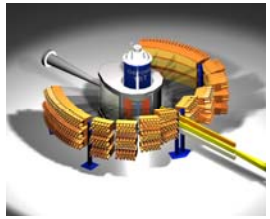
Phase 2 Instruments

LMX	Macromolecular Crystallography
Proteus	Biological structures
Bounce	Ultra-small angle neutron scattering
Spiral	Real space structure correlations
Zoom	Small-angle scattering from kinetic processes
eXess	Extreme sample environments spectrometer
eXeed	High-pressure crystallography
Nessie	Ultra-slow dynamics spin-echo spectrometer
Tomcat	Neutron tomography and cultural heritage
U-Hrpd	Ultra-high resolution powder diffraction
Hr-Engin	High-resolution beamline for engineering
Herbi	High-resolution back-scattering spectrometer









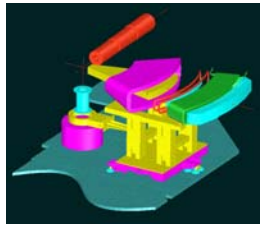
Strategic Development Programme:

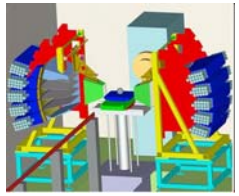
- Detectors

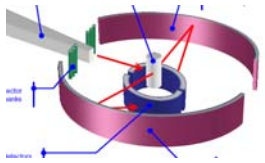
- Optics

- Spins

- Software

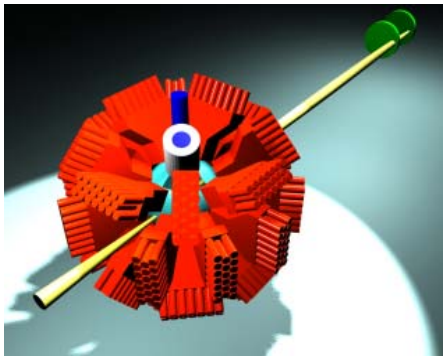


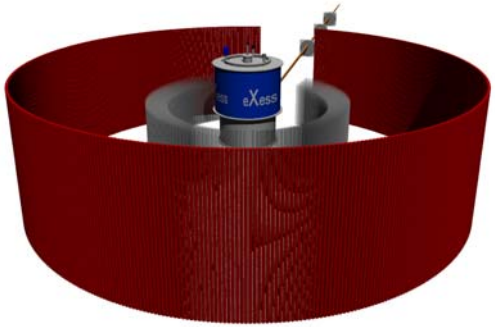


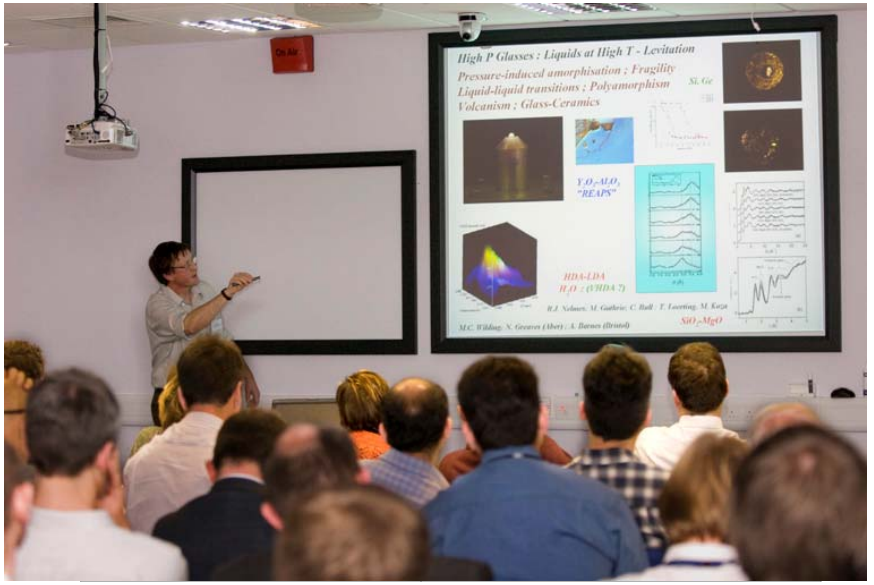


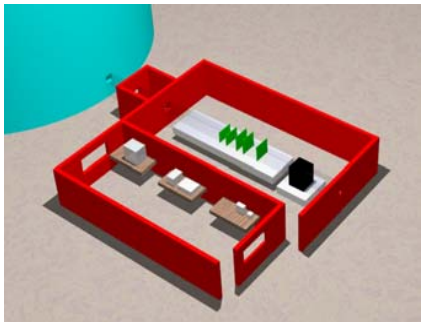
TS2 Phase 2 – Users Meeting

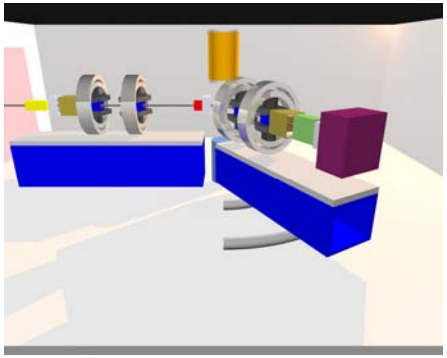
Science & Technology Facilities Council

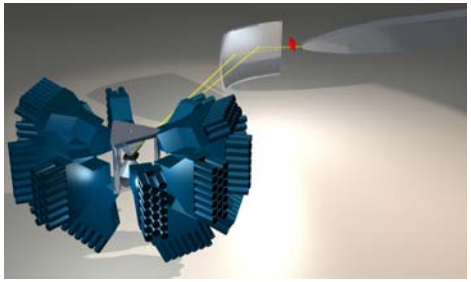


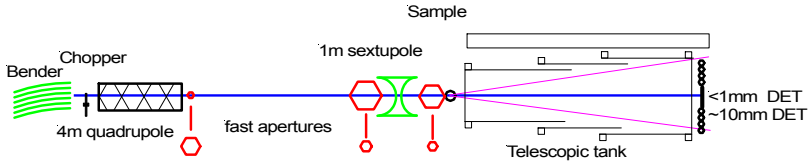


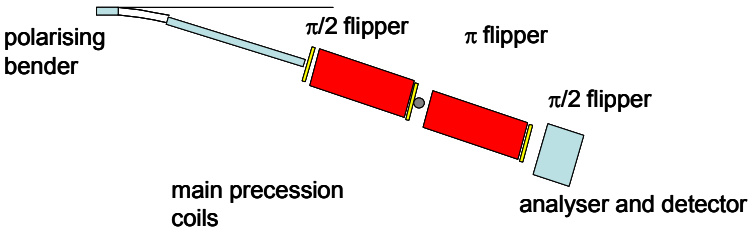


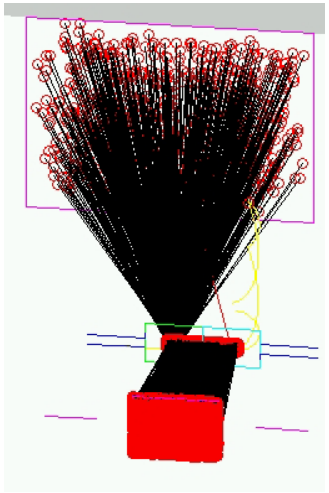




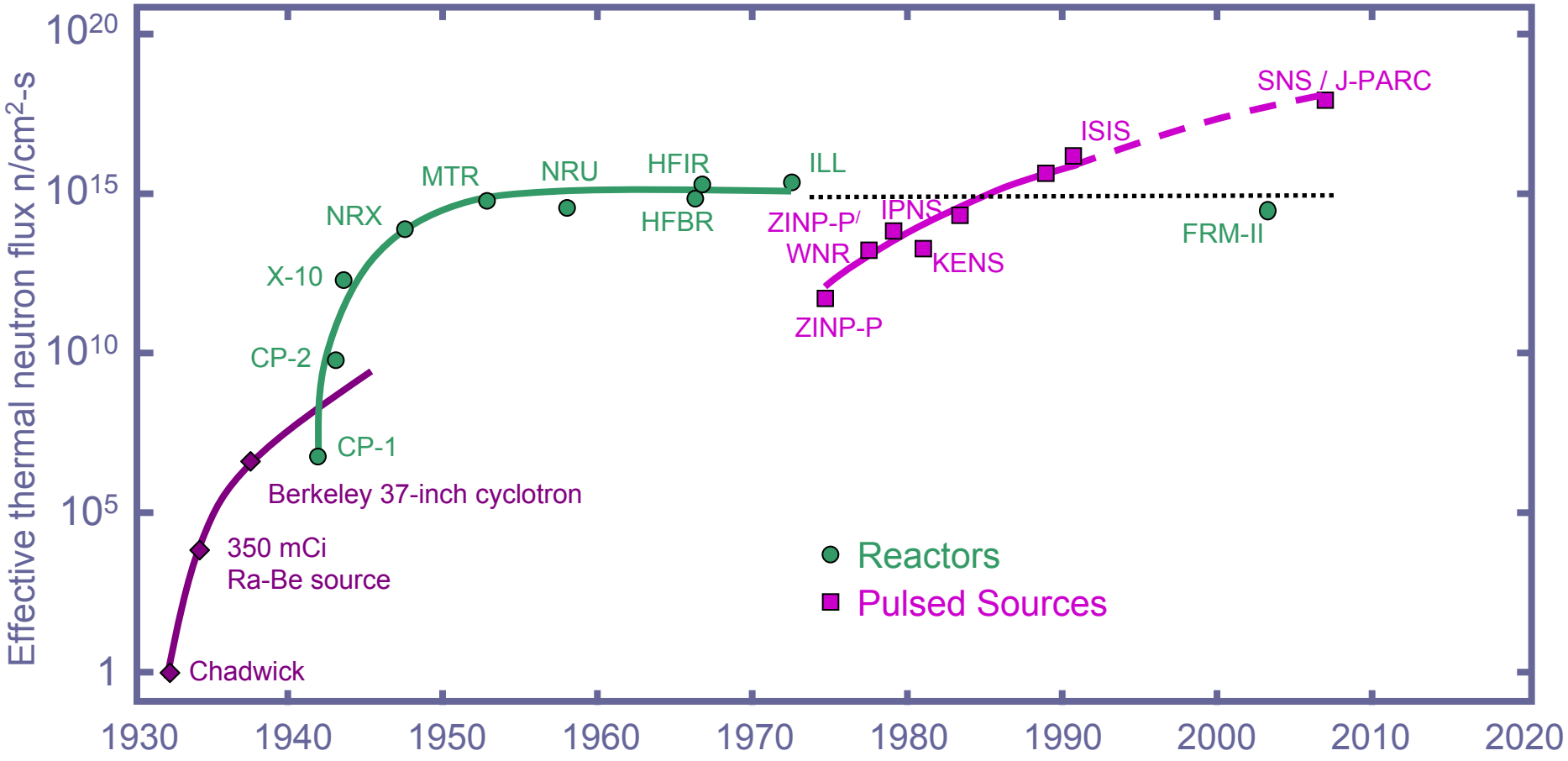




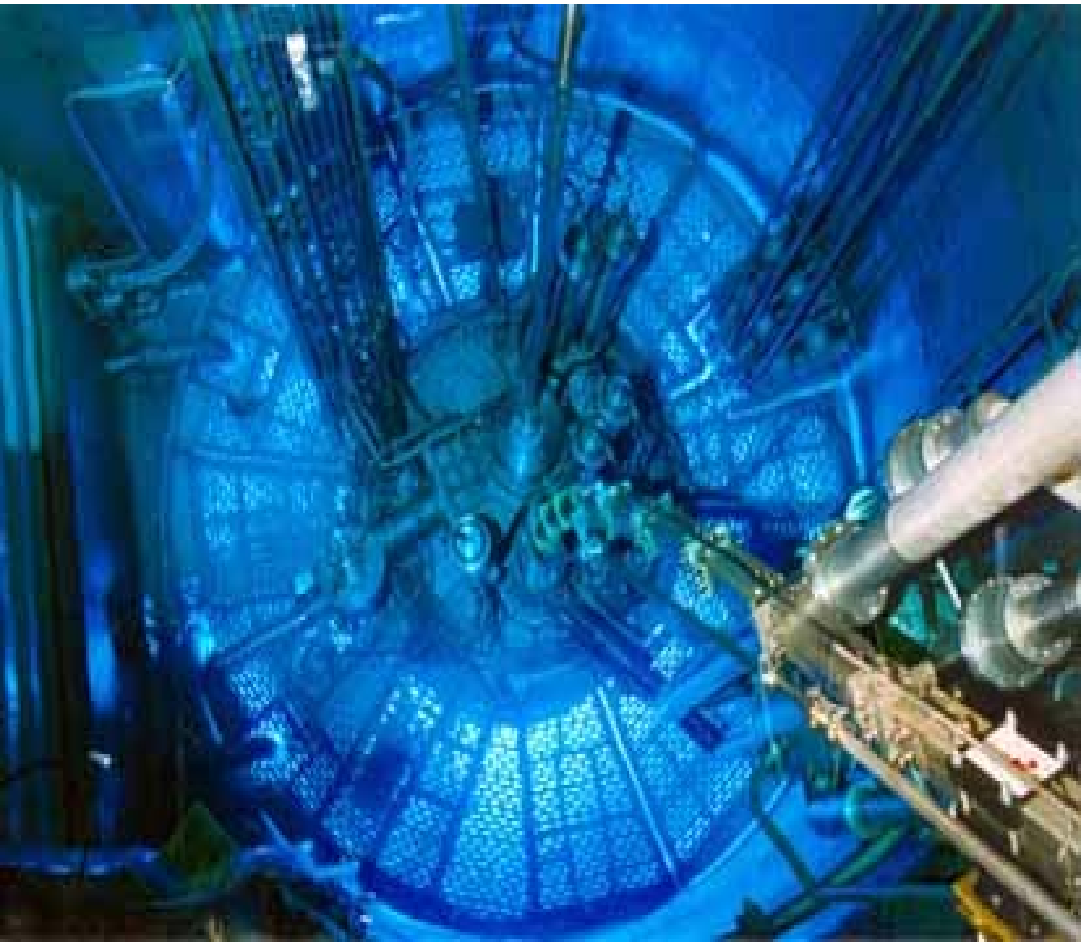




International Challenges



(Updated from *Neutron Scattering*, K. Skold and D. L. Price, eds., Academic Press, 1986)



Source

x

Leadership

x

Innovation

x

Instrumentation

x

Support

x

Investment

x

Cost Effectiveness

x

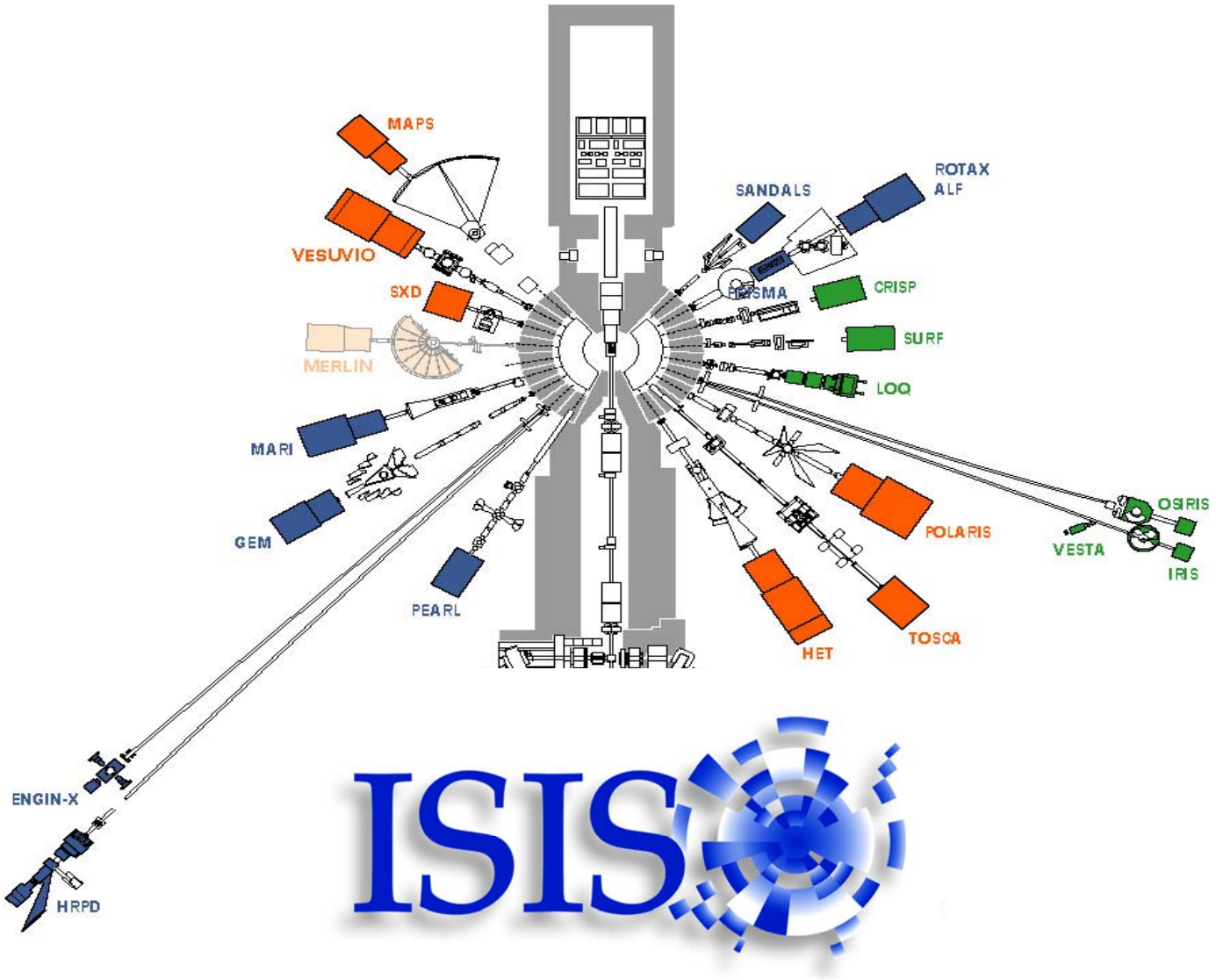
User Community

Neutrons in Europe

150 instruments supporting 5000 users

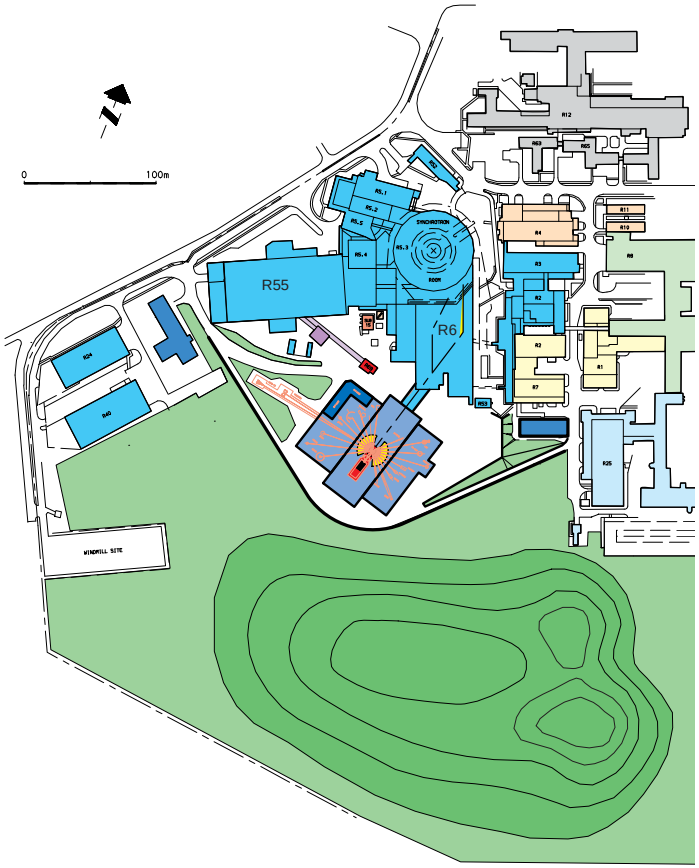
Science & Technology Facilities Council

30 Instrument at ISIS - 2008

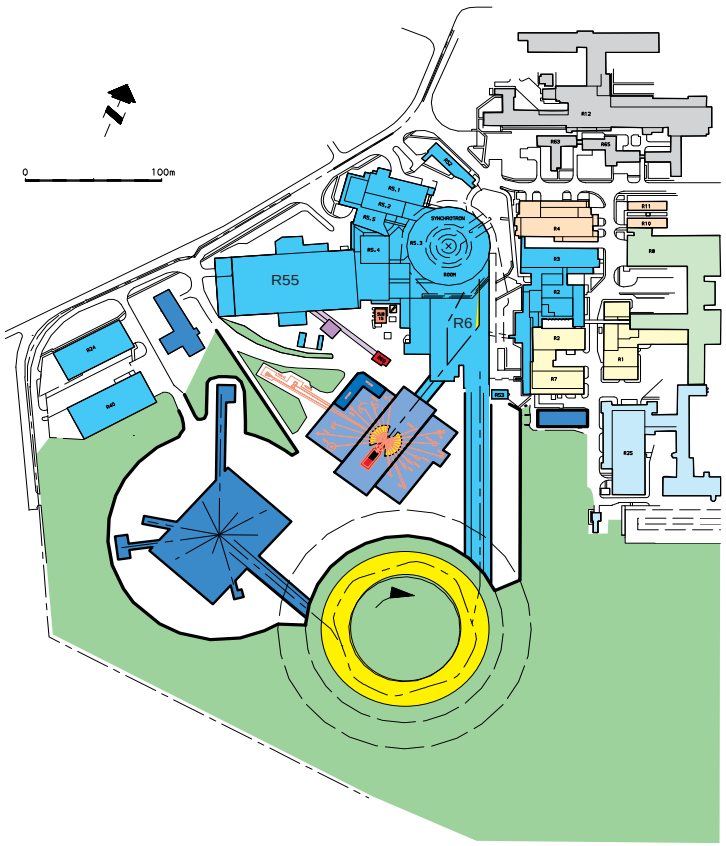


Future Options

Second Target Station

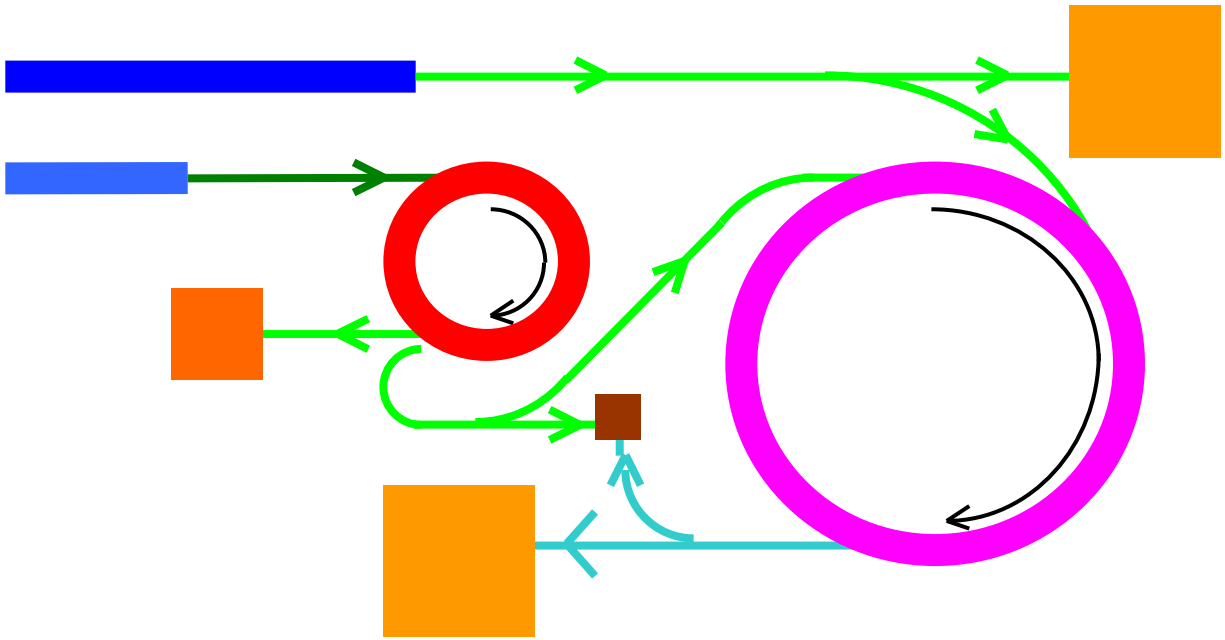


ISIS MW Upgrade



Increase Beam Power to MW+ with a 3.3 GeV Synchrotron

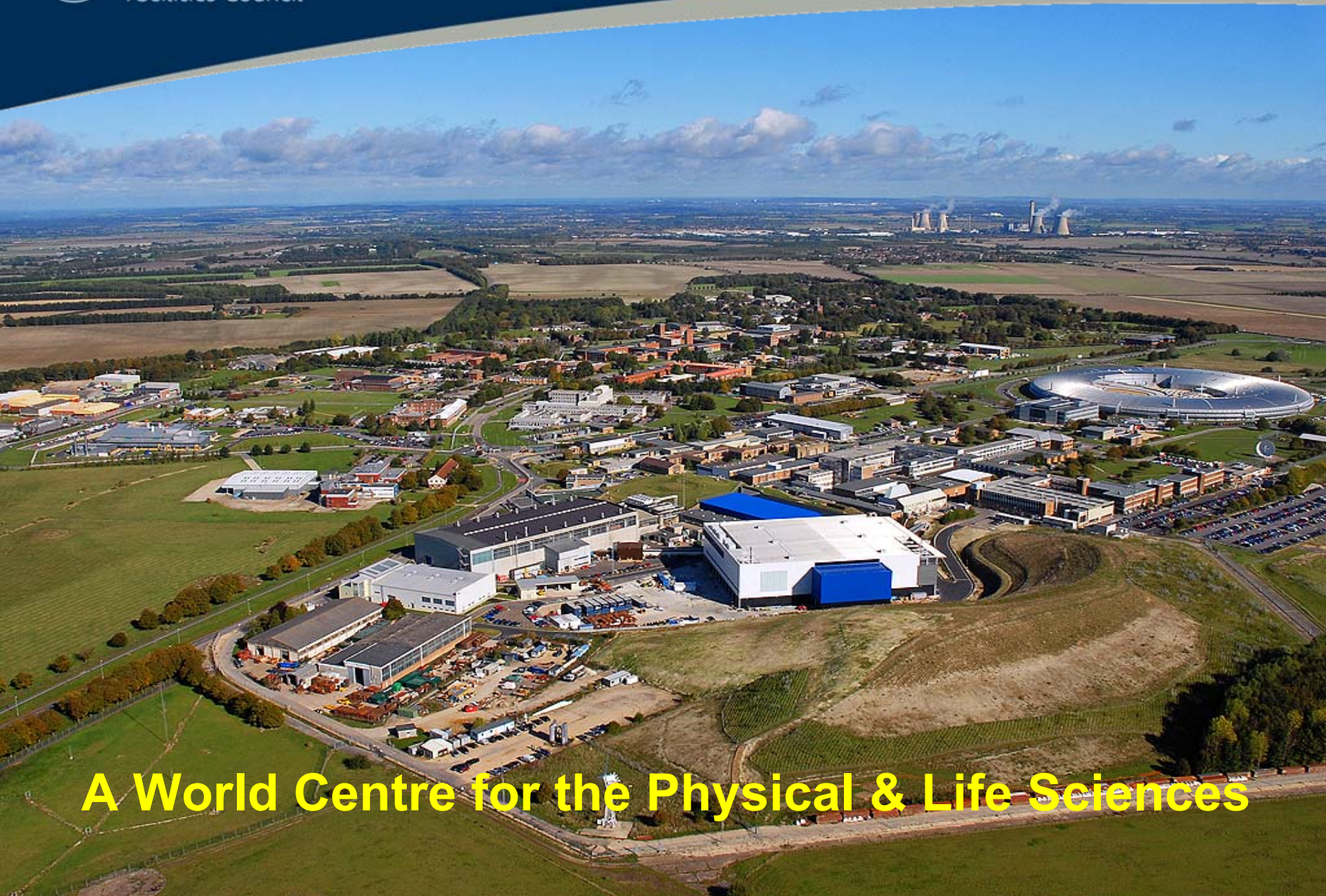
Possible Future options



2.5 MW LPSS + 2.5 MW SPSS

Science & Technology Facilities Council

Harwell Science & Innovation Campus



A World Centre for the Physical & Life Sciences