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Other techniques: a comparison with neutron scattering

Non-scattering Neutron techniques

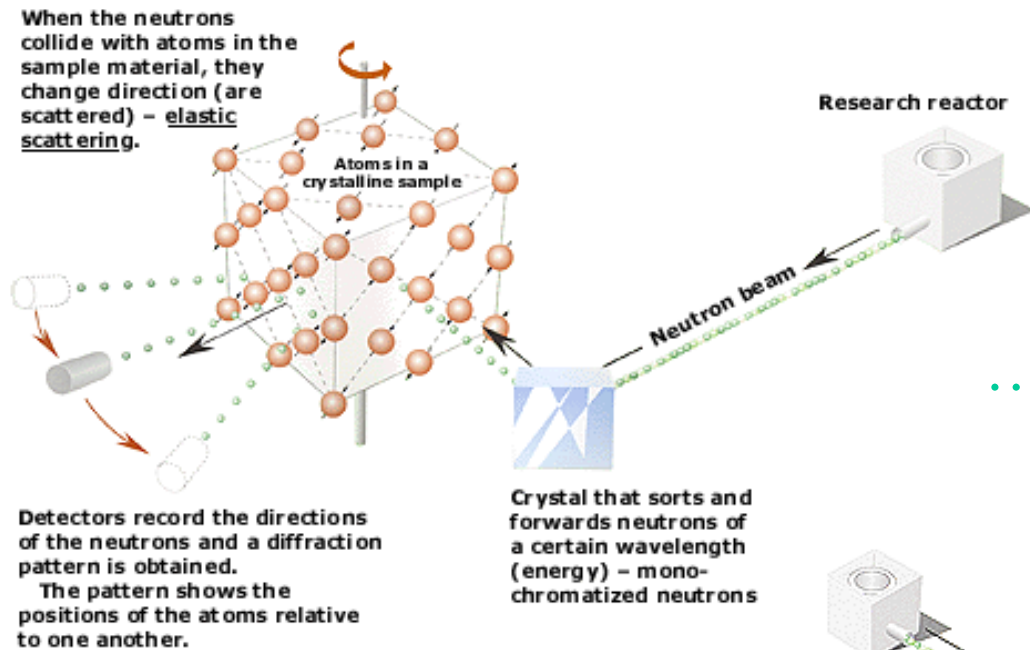
Constructability

Robert McGreevy

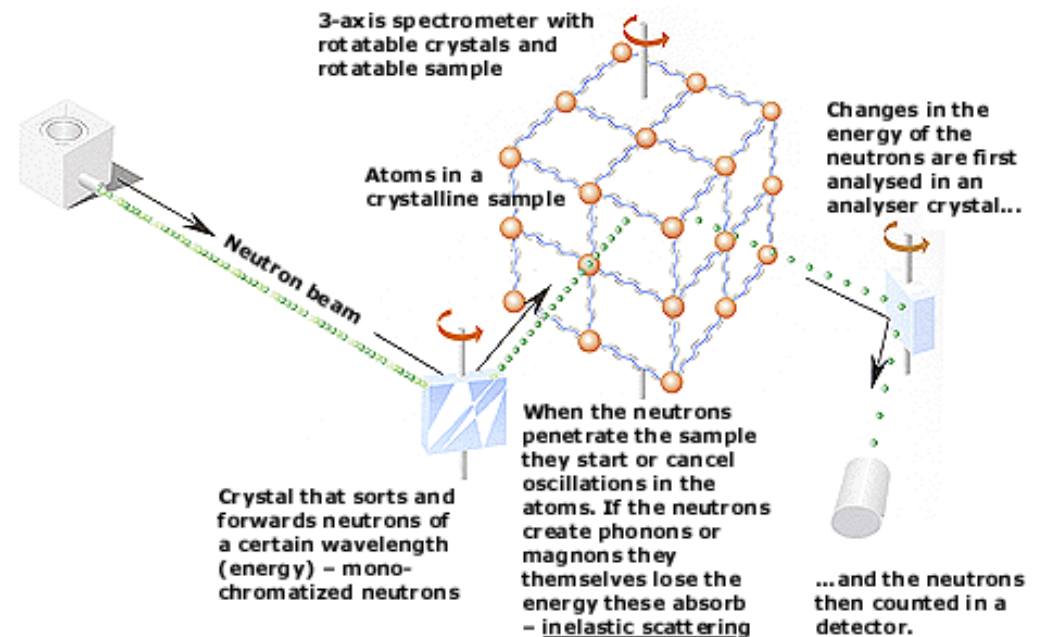
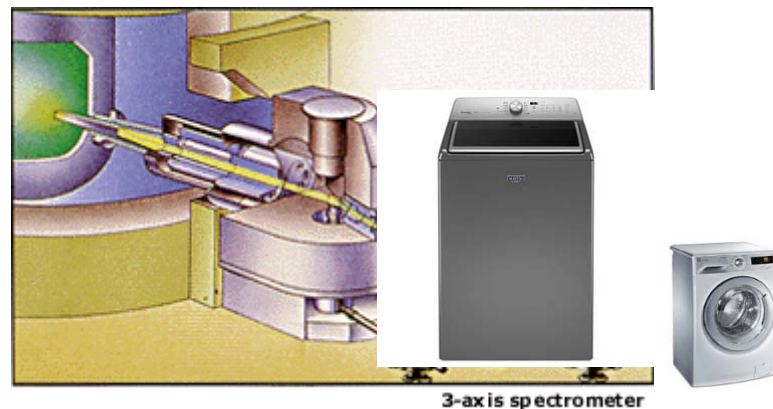
ISIS, STFC Rutherford Appleton Laboratory, UK

The 1994 Nobel Prize in Physics – Shull & Brockhouse

Neutrons show where the atoms are....



...and what the atoms do.





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Why do we build neutron instruments?

To do science

Not to be better than other neutron instruments

...which is usually the first thing people do ...



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Why are we learning about other techniques?

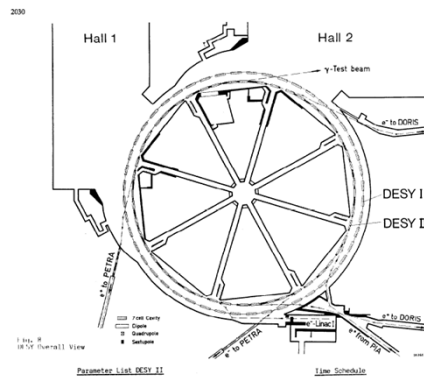


Eddie the Eagle

Because being a heroic failure is not a business strategy!
(at least in science)



Why are we learning about other techniques?



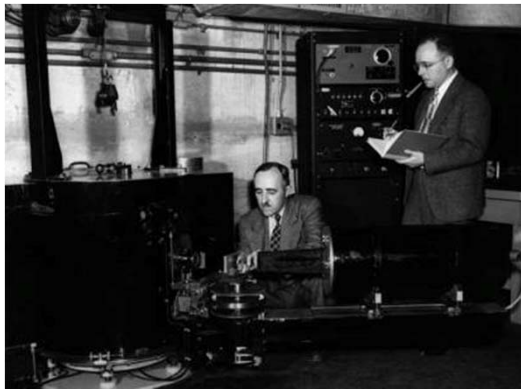
Synchrotron x-rays have evolved from parasitic to custom built
Brightness increase is orders of magnitude more than cost increase



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Why are we learning about other techniques?



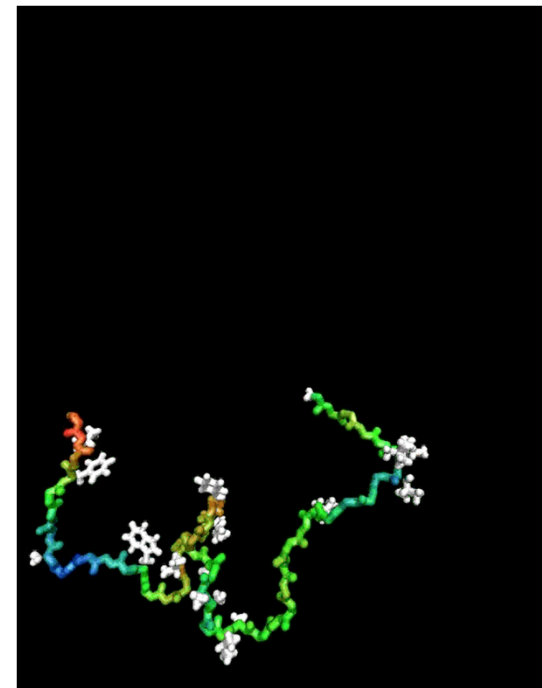
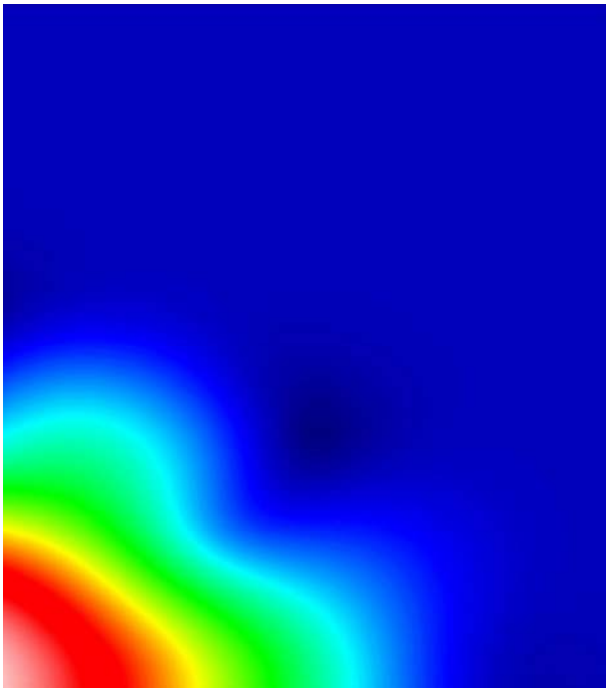
Neutron scattering sources have also evolved from parasitic to custom built
Brightness increase matches cost increase



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Why neutrons? – five good reasons



Length and time scales

$10^{-11} - 10^{-1}$ m

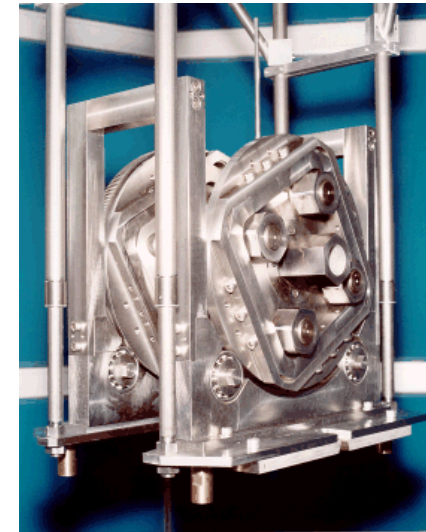
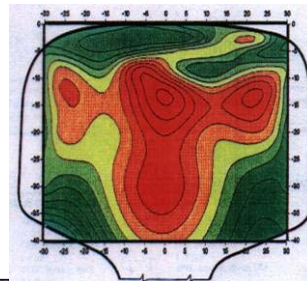
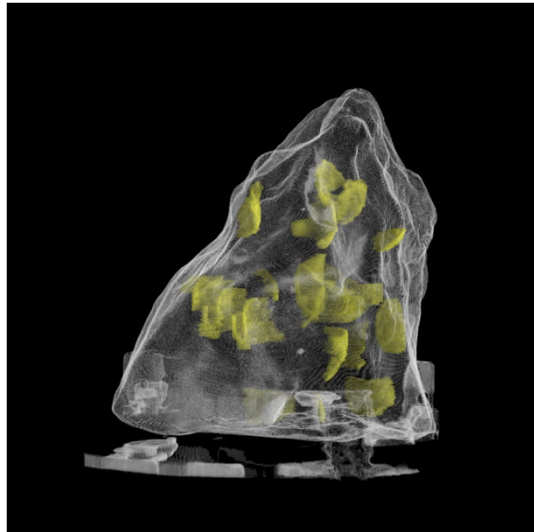
$10^{-14} - 10^4$ s



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Why neutrons? – five good reasons

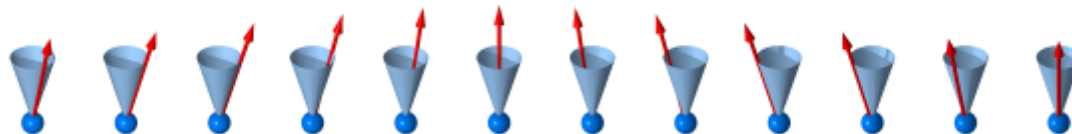
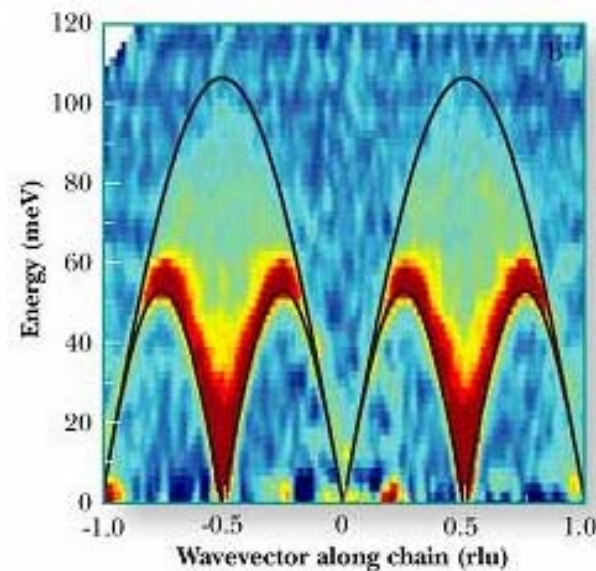
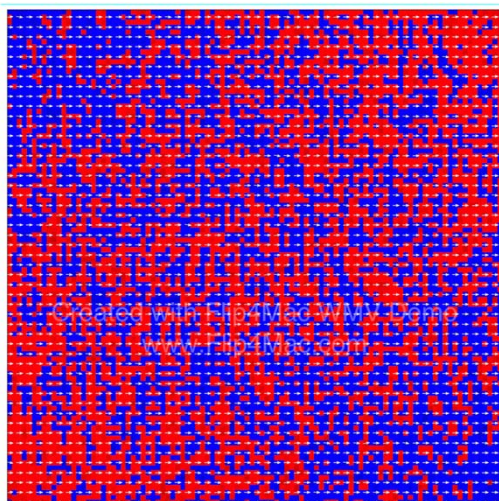


Penetration

Large samples, buried interfaces, extreme conditions, non-destructive



Why neutrons? – five good reasons

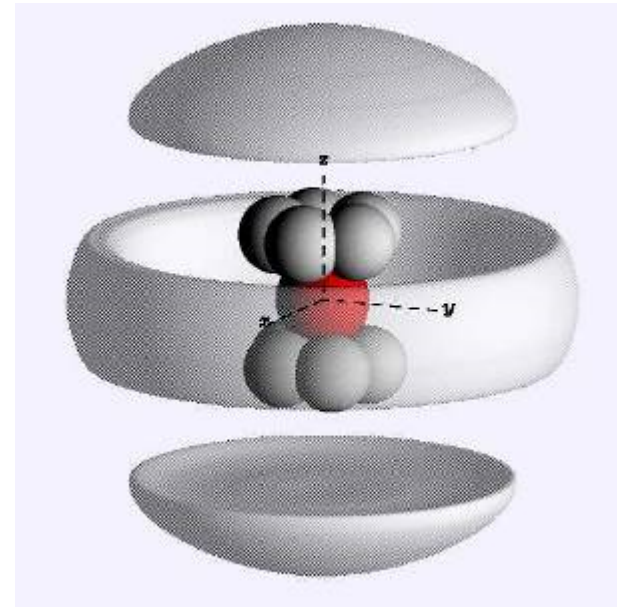
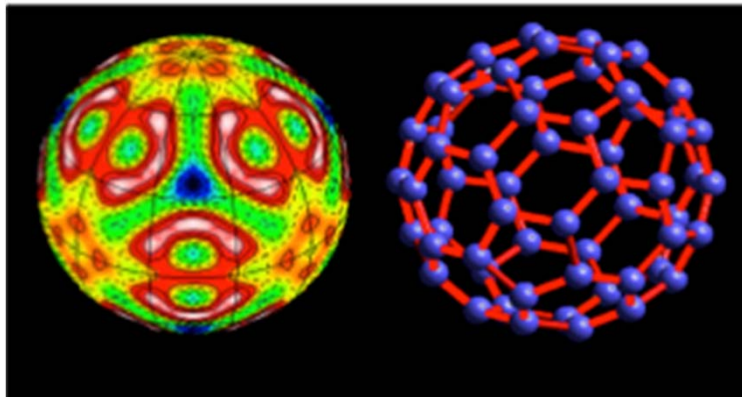


Magnetism

The neutron has a magnetic moment but no charge



Why neutrons? – five good reasons

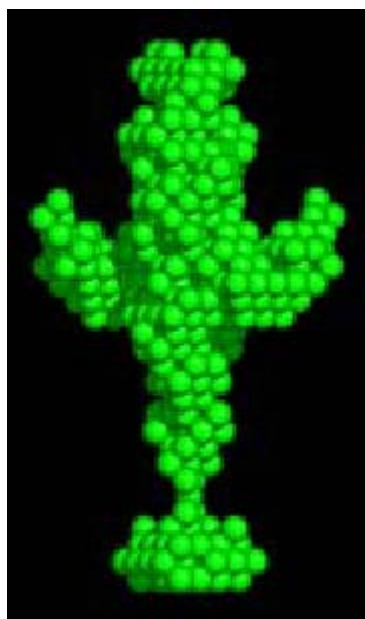


Precision

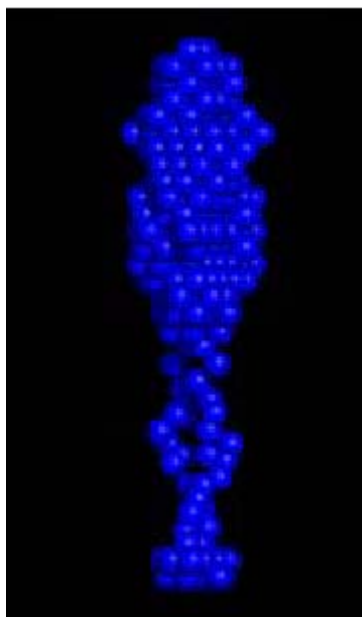
Weak interaction, simple interaction



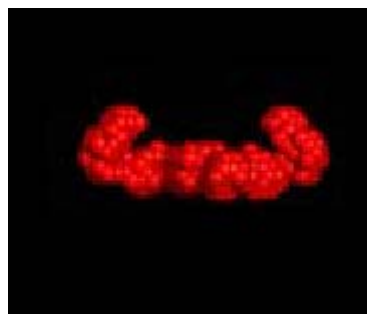
Why neutrons? – five good reasons



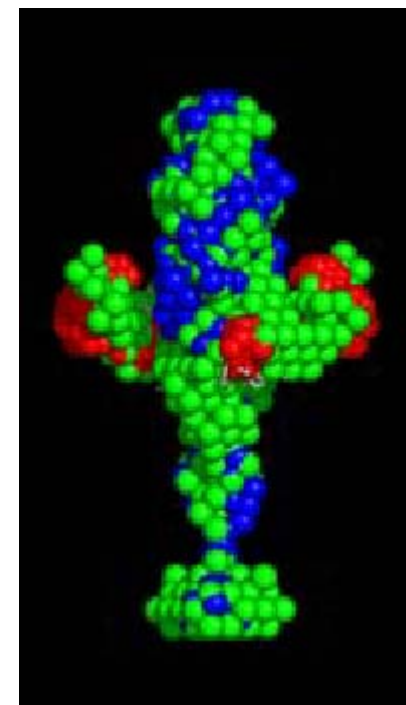
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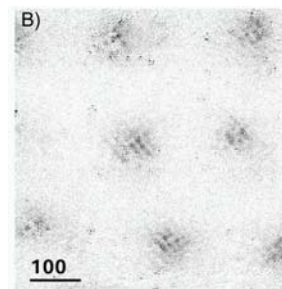
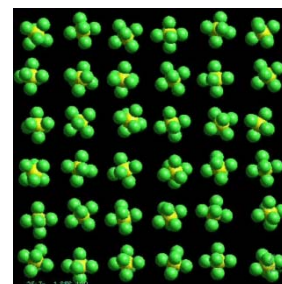
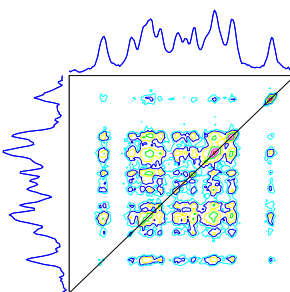
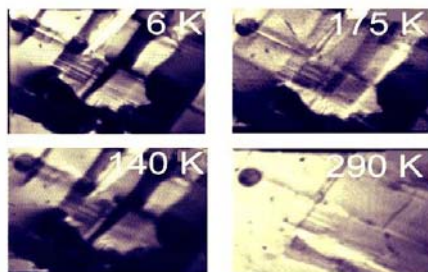
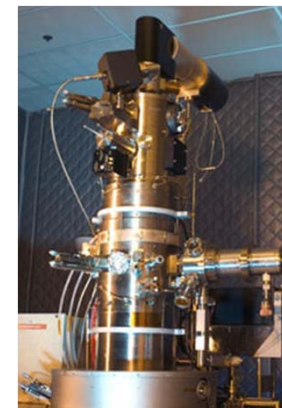
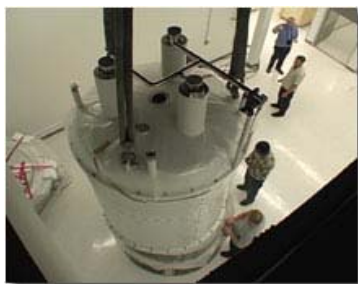


Sensitivity and selectivity

Isotopic substitution/contrast variation



But ...



Synchrotrons

NMR

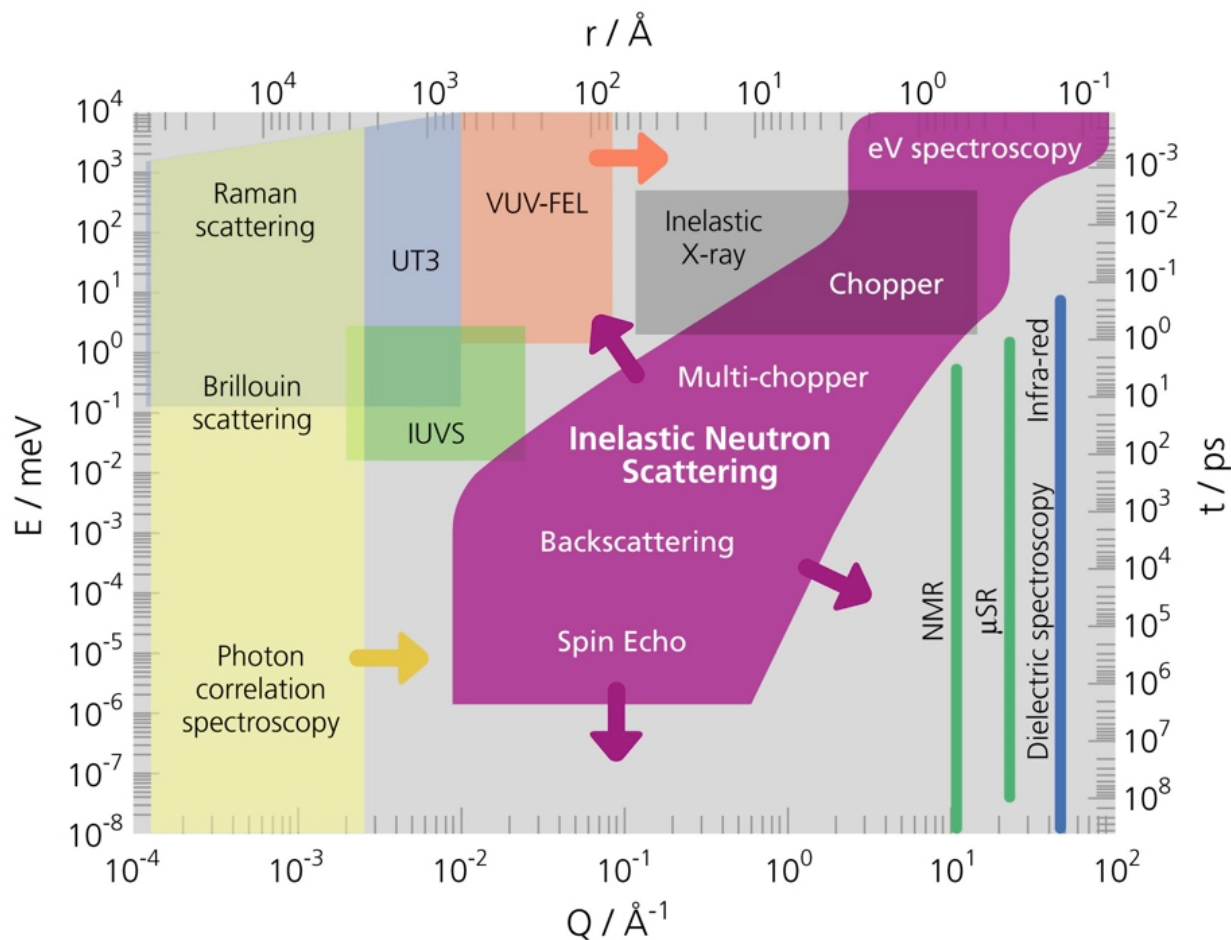
Computing

Microscopy

Most research that use neutron scattering also uses several complementary techniques



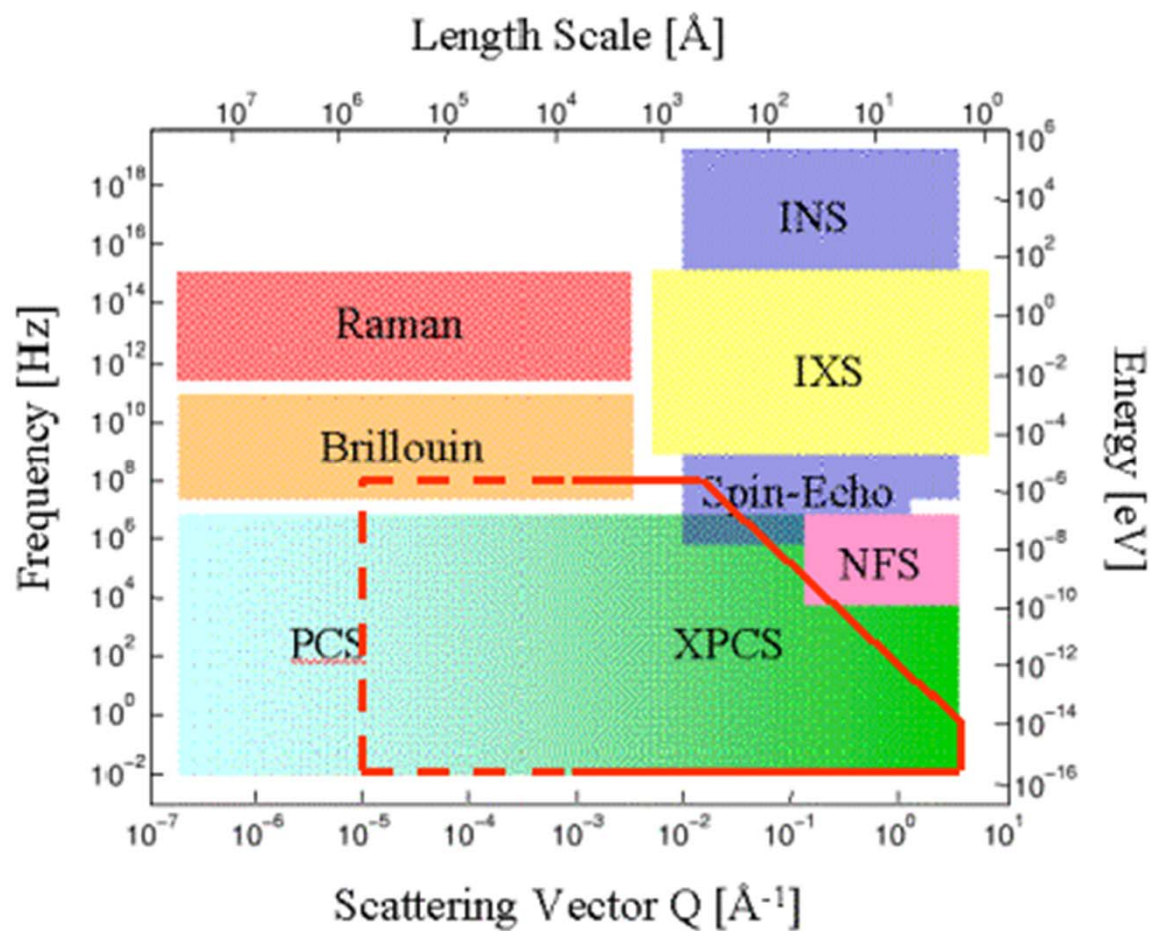
Why neutrons?



Neutron scattering 'simultaneously' covers a broad (Q, ω) range



Why not neutrons?



It may not look so broad when viewed from a different perspective!



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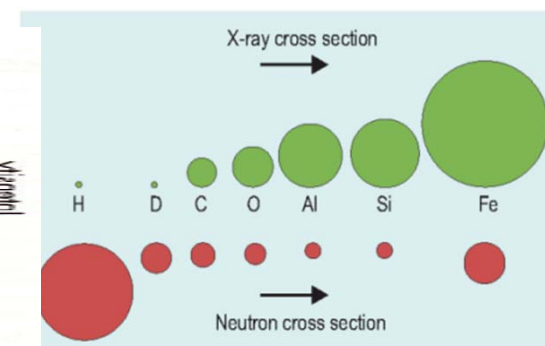
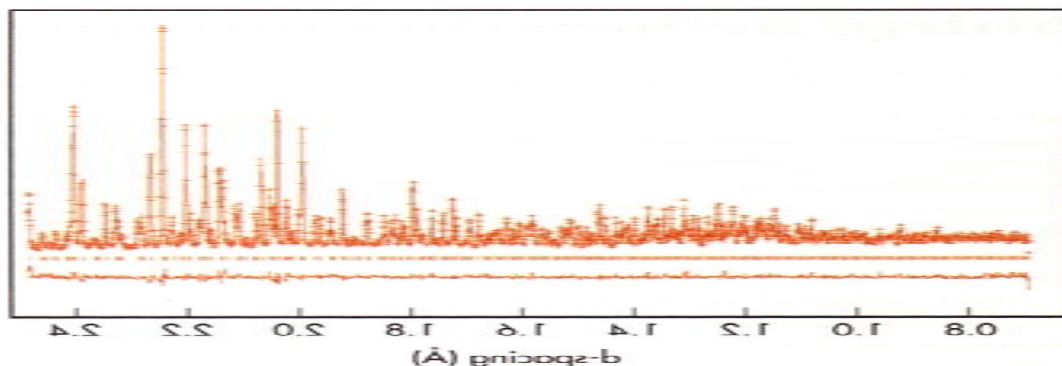
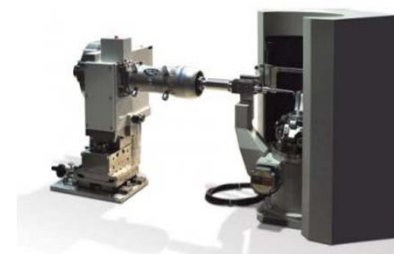
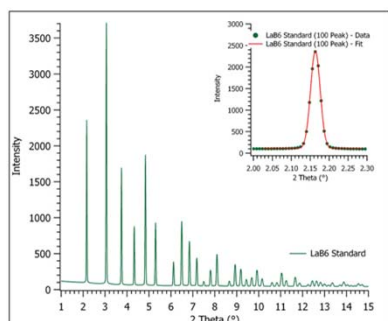
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Macroscopic property measurements

- Density
- Specific heat
- Conductivity
- Susceptibility
- ...



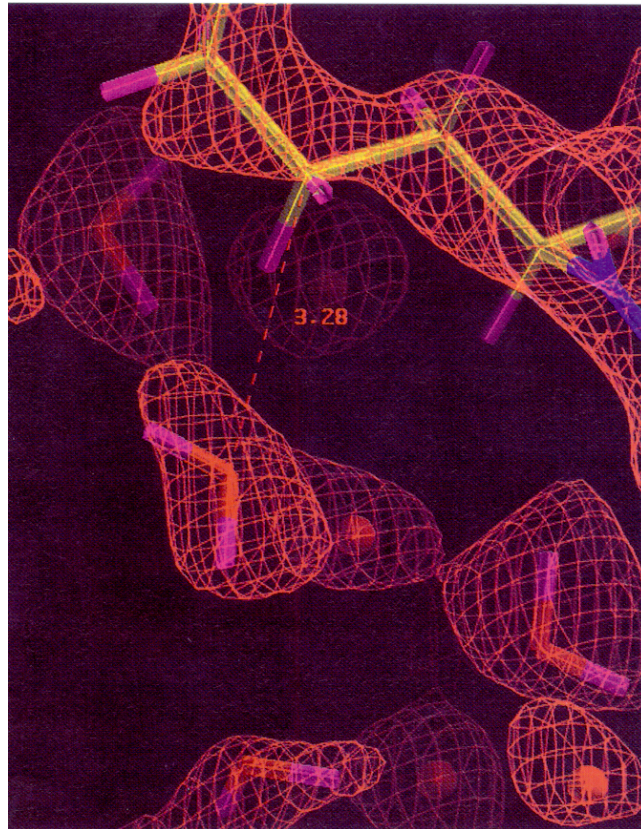
X-ray diffraction



X-ray diffraction is cheap, convenient and can do many, many things
Neutrons help for high Q, light atoms, similar Z atoms, magnetism



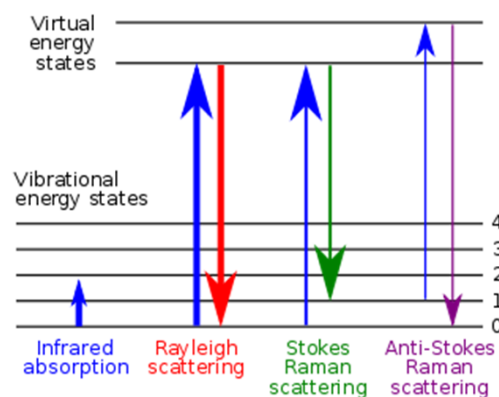
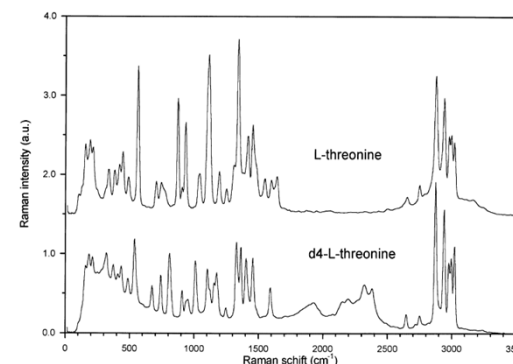
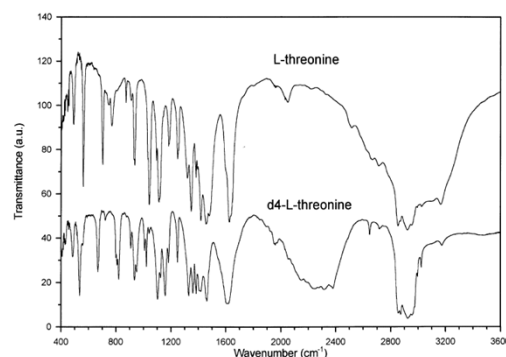
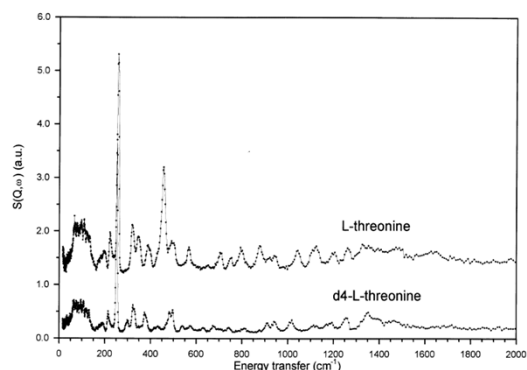
Lesson ...



Don't say 'X-rays can't see hydrogen'
Say 'neutrons can help see hydrogen better, when used together with X-rays'



Raman scattering/Infrared spectroscopy



Photons are cheap, convenient and can do many, many things
Neutrons give absolute intensities with no selection rules



Dynamic light scattering

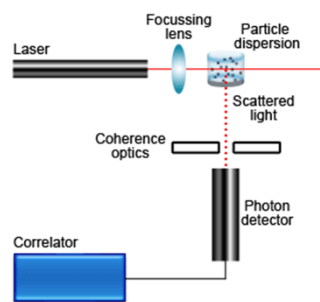
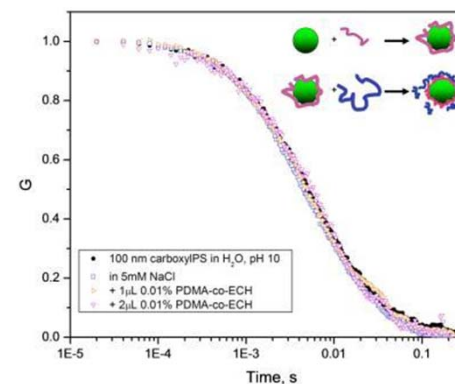
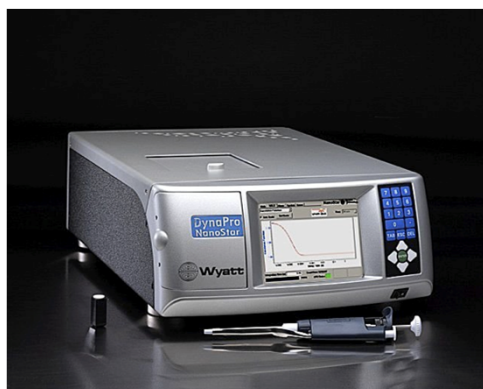
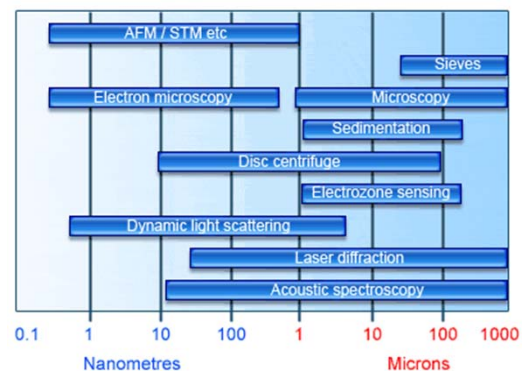


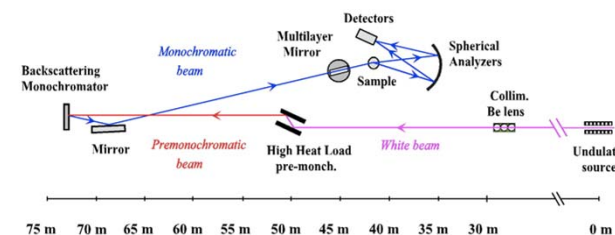
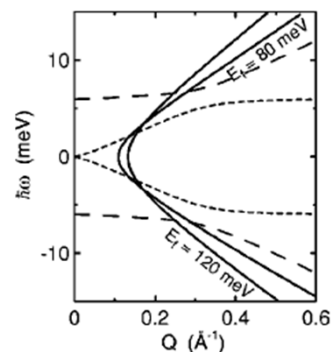
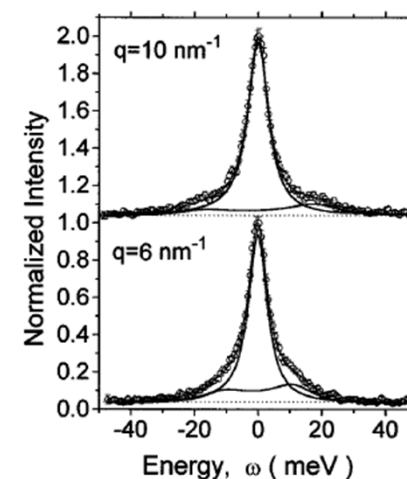
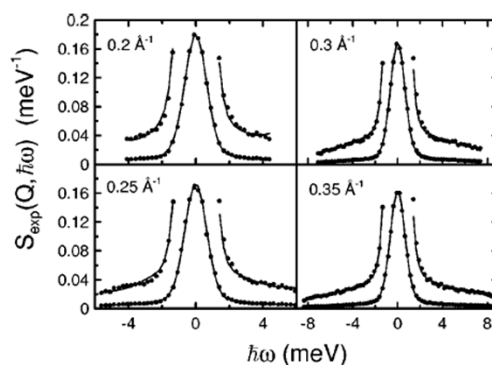
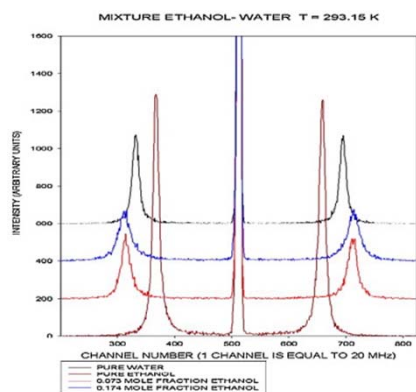
Figure 1: Schematic diagram of a conventional, 90° dynamic light scattering instrument.



DLS exploits coherence, covers many decades in time
1-D information only, needs transparent samples



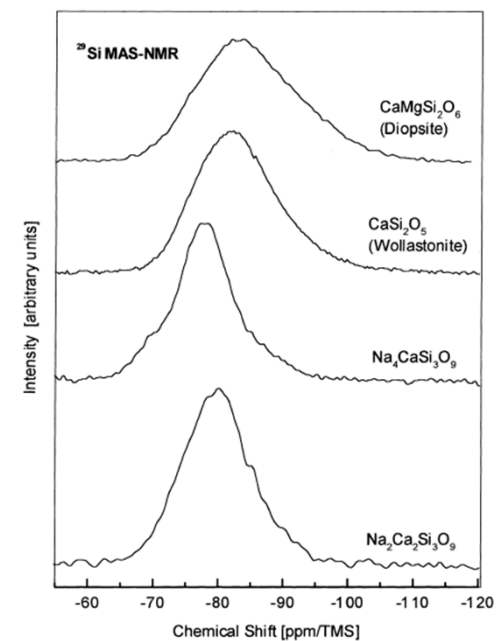
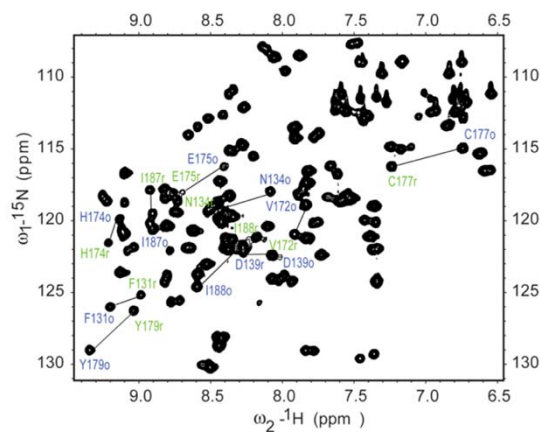
Brillouin scattering, Inelastic X-ray scattering



X-rays now 1-2 meV resolution; complementarity poorly exploited
Neutrons struggle at low Q because of kinematic restrictions



NMR (1D, 2D, FT, MAS ...)



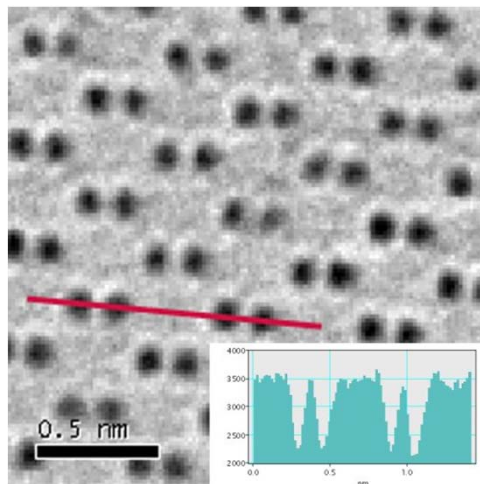
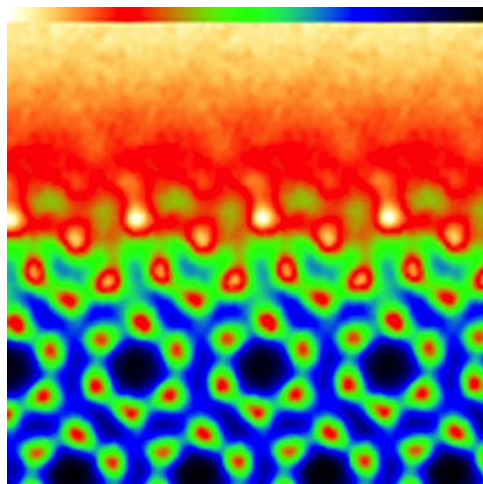
NMR naturally provides many-body correlations
In all normal circumstances neutrons provide only 2-body correlations



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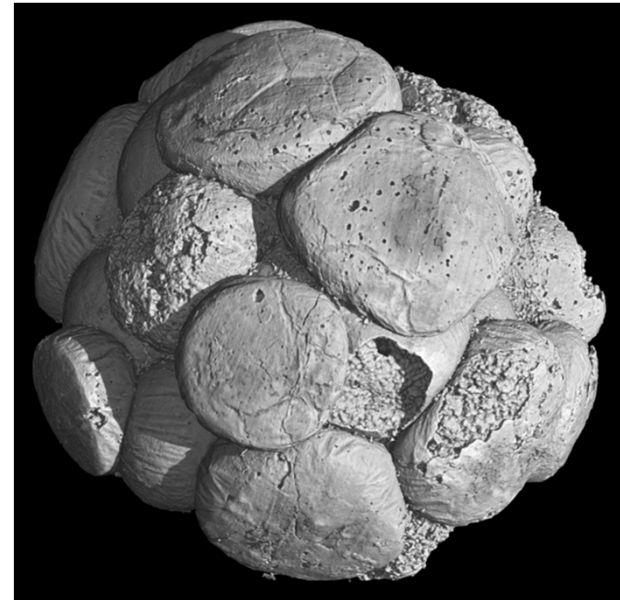
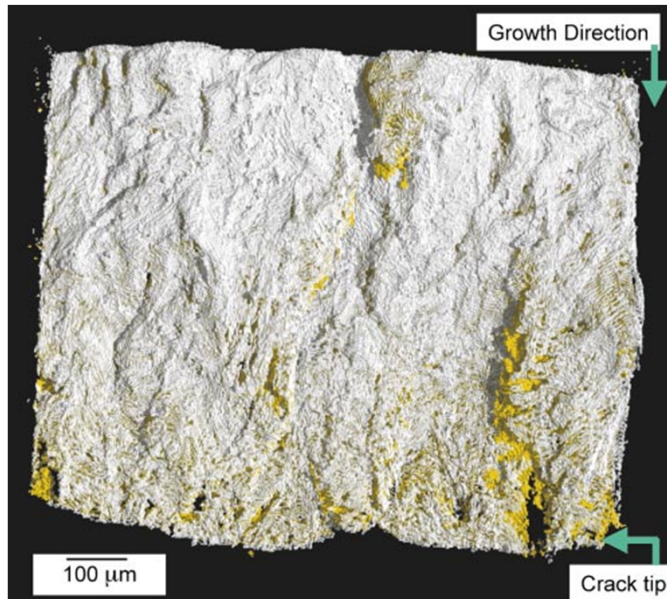
Electron diffraction/microscopy



Now close to 1 Å resolution; can do liquids and glasses
Small samples, 'local' structure



Imaging

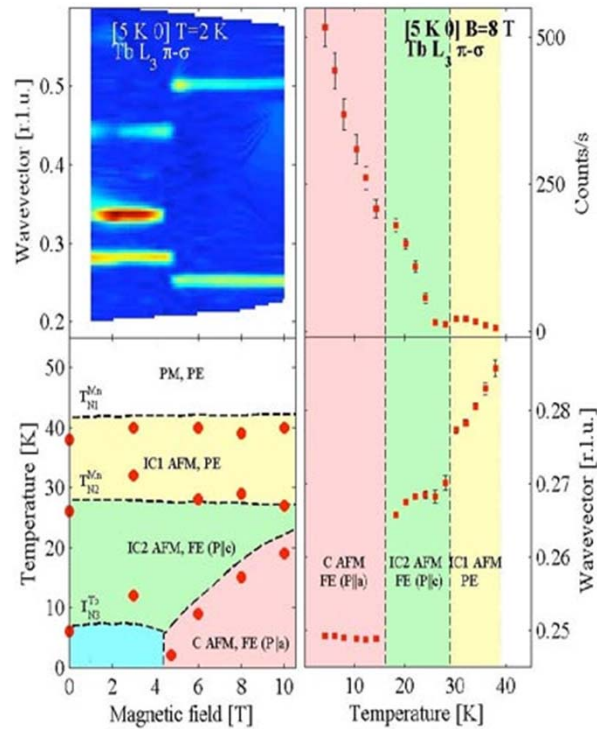


<http://paleo.esrf.eu/>

Sub- μm resolution; keV x-rays give high penetration
Neutrons only 50 μm , but better for light elements



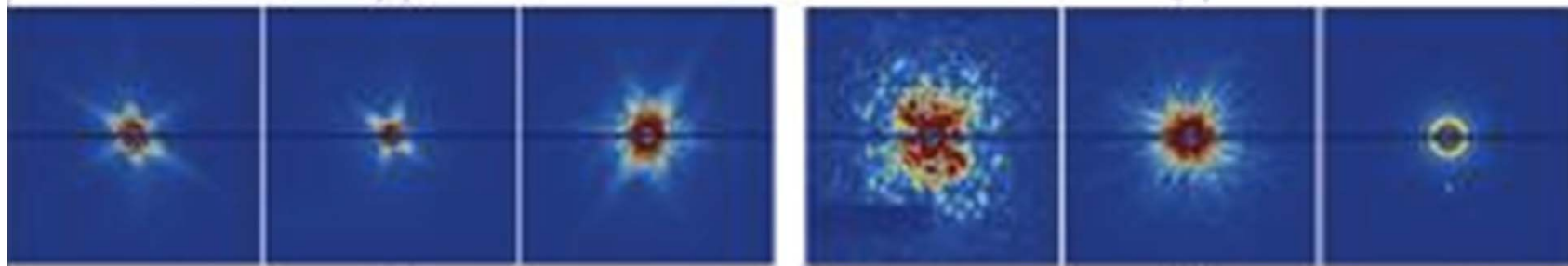
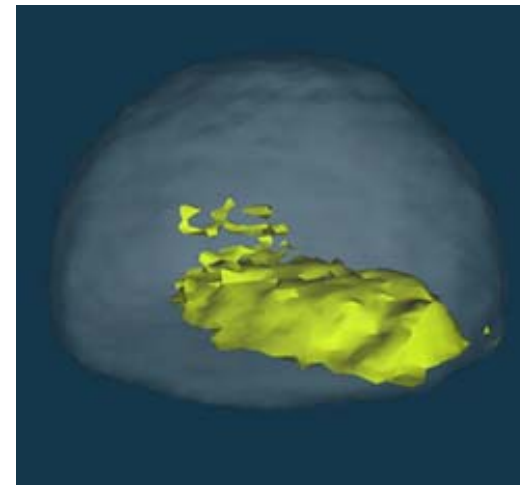
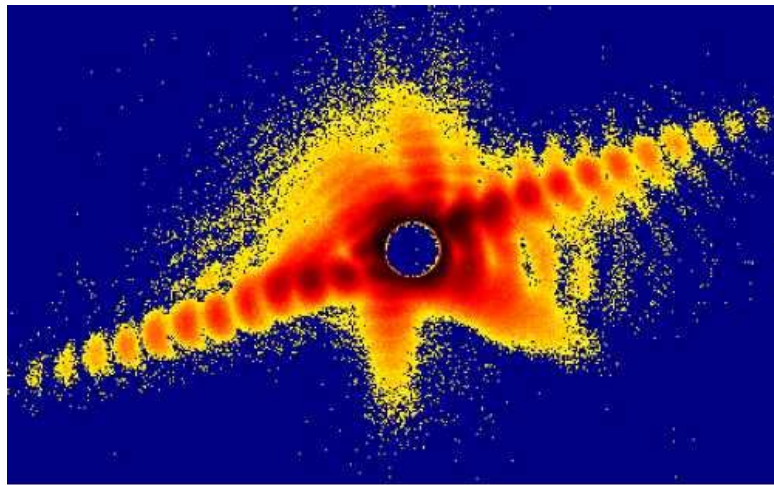
Resonant X-ray scattering



Element and electron shell selective (e.g. orbital ordering)
But probably can't interpret without neutron data as well ...



Coherent X-ray diffraction, FEL



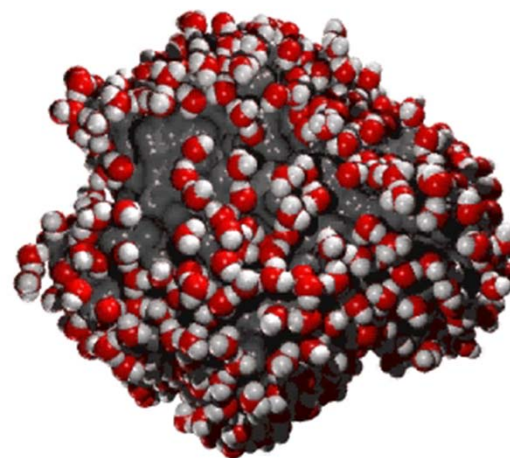
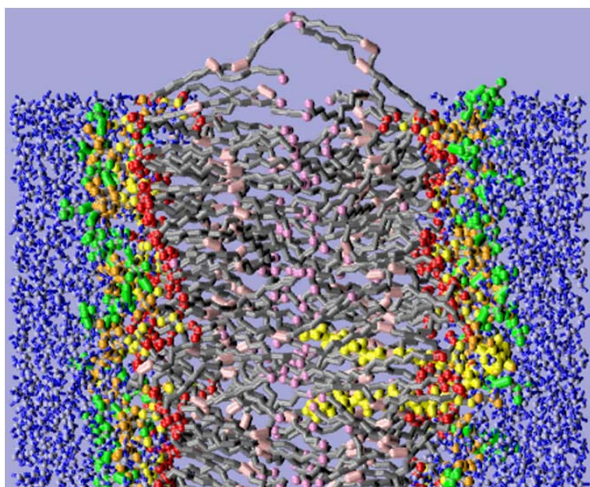
Structure and stress distribution in single nano-particles; fs diffraction
But sometimes you need to look at more than one ...



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Computers



Simulation and modeling cover a very similar (r,t) range to neutrons
Neutron data can be calculated directly and easily from simulations



Conclusions

- Neutron scattering is (always going to be) an expensive technique
 - We must provide a quality product
- Neutron instruments must exploit neutron strengths, not amplify neutron weaknesses
 - e.g. absolute accuracy, signal to noise
- Neutron instruments must exploit complementarity
 - e.g. molecular spectroscopy, computer simulation
- Do not design or build a neutron instrument just because it's better than another neutron instrument ...
 - ... which is usually the first thing people do ...



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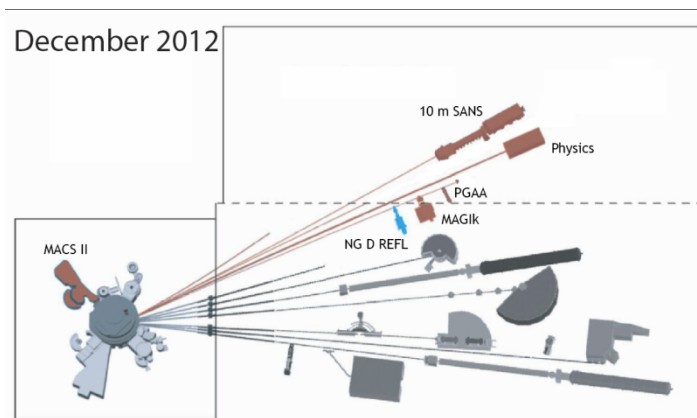
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Non-scattering Neutron techniques

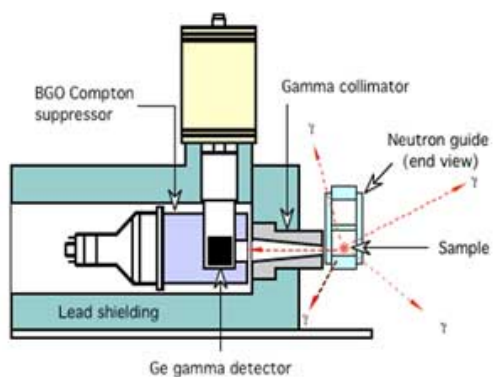


Activation analysis

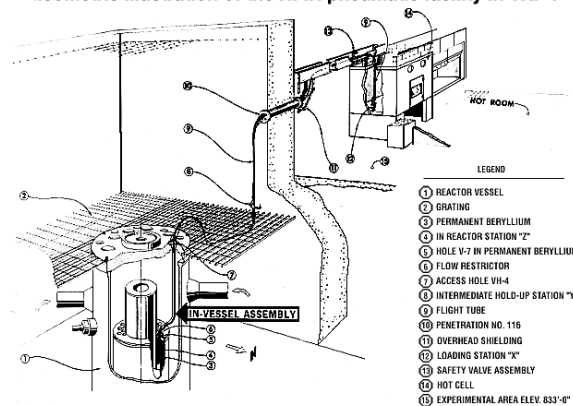
Prompt gamma



Delayed gamma



Isometric illustration of the HFIR pneumatic facility in VXF-7

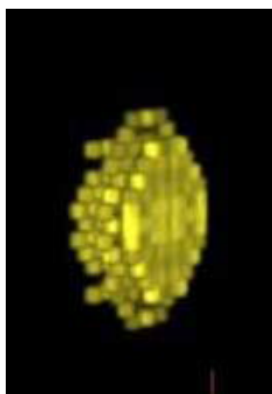




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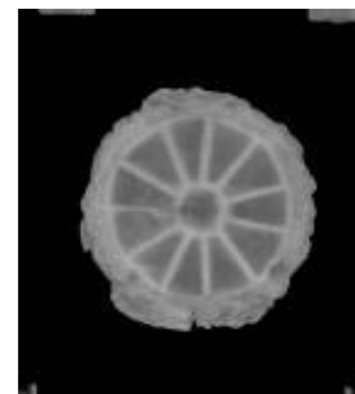
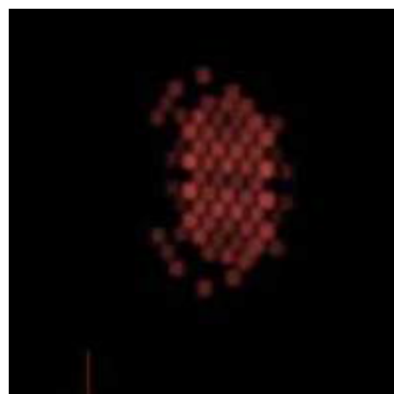
Prompt Gamma Activation Imaging



Gold



Copper



Neutron radiography



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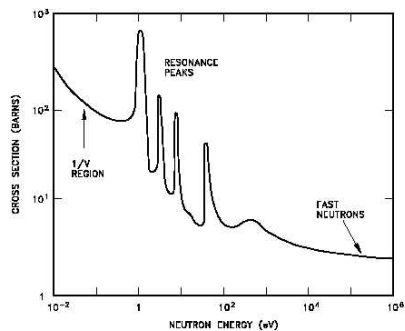
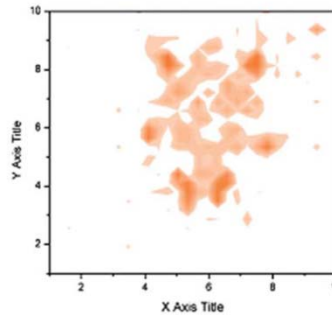
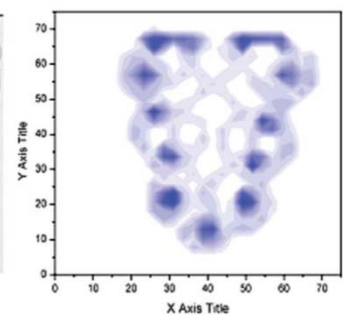
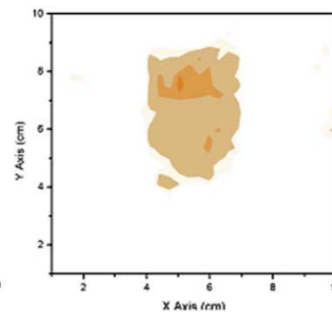
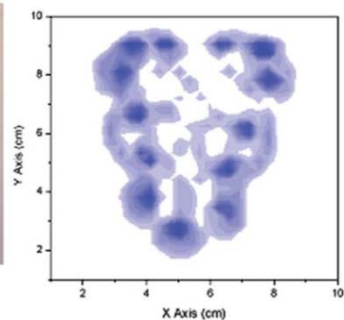
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Neutron autoradiography



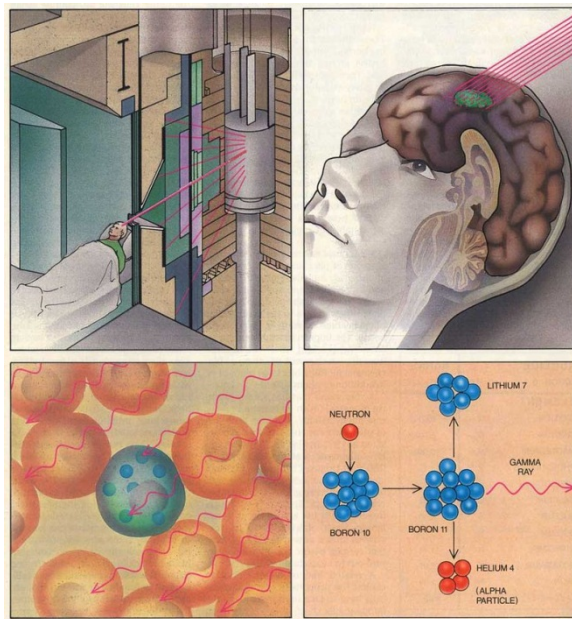


Neutron Resonant Capture Imaging

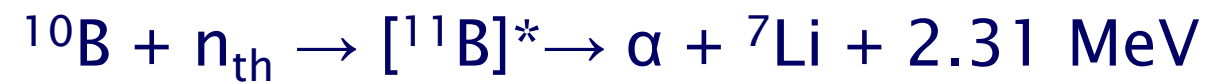




Boron Neutron Capture Therapy (BNCT)

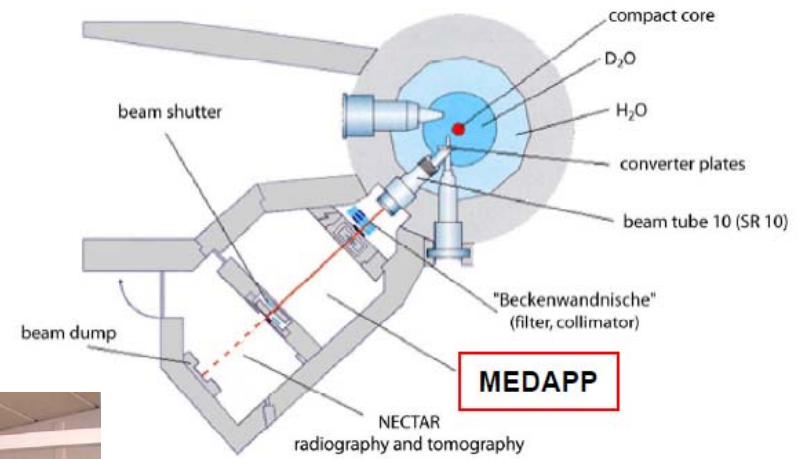
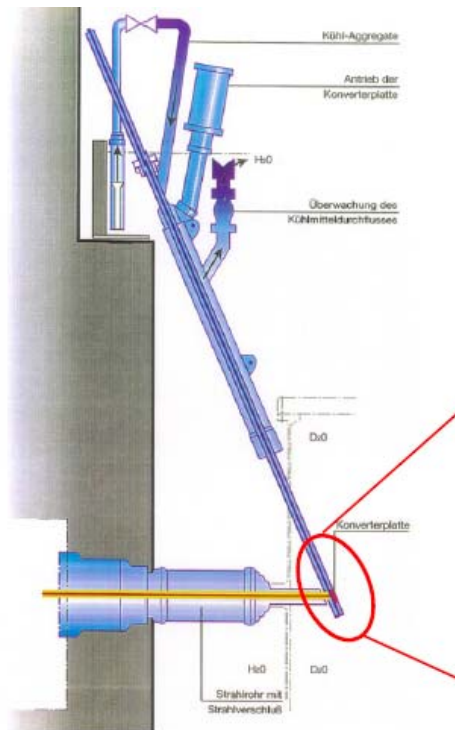


BNCT treatment at the Studsvik R2-0 reactor





Fast Neutron Therapy

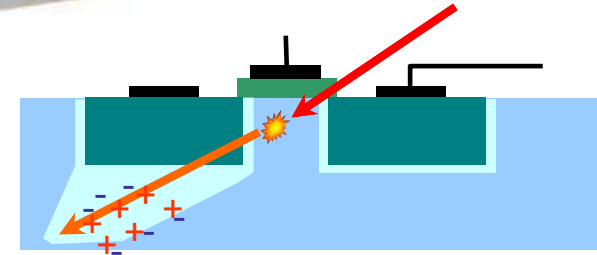


MEDAPP facility at the FRM-II reactor

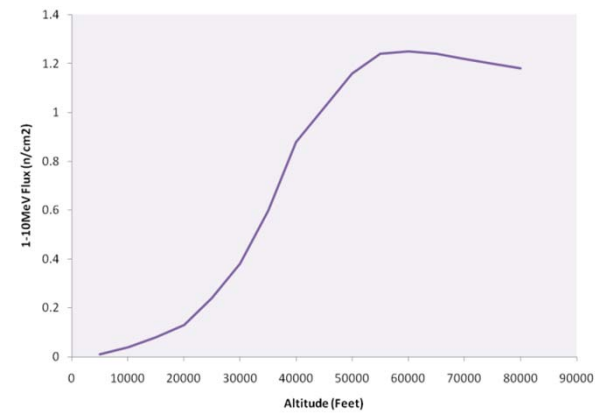
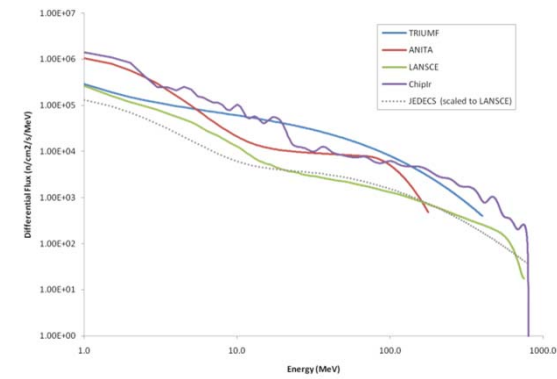
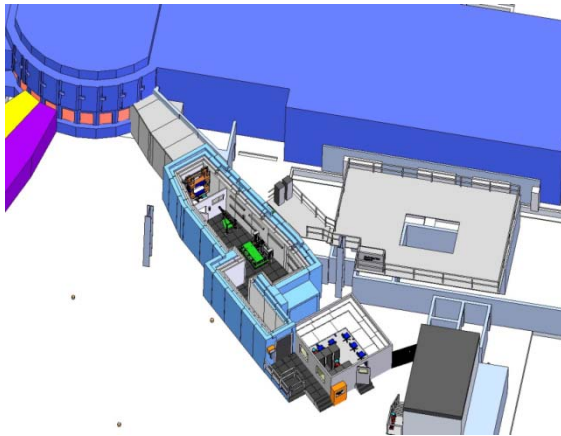


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Chip Irradiation





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Constructability

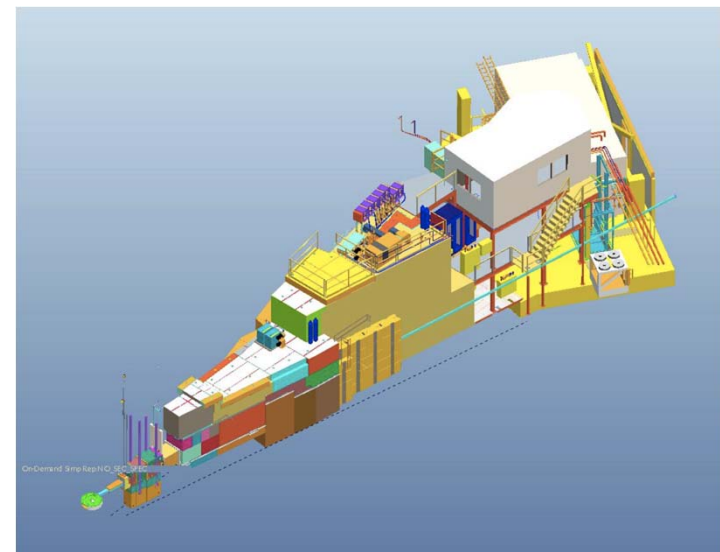
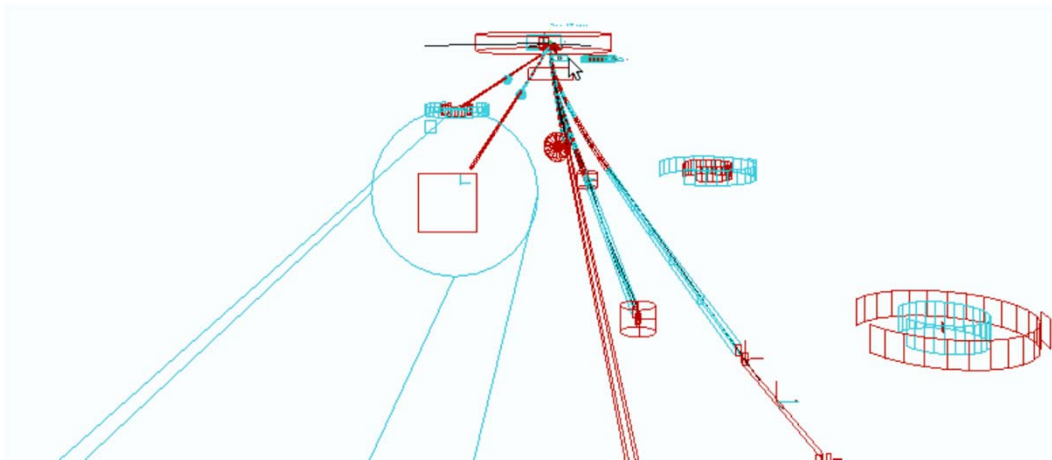
Getting real ...

Robert McGreevy

ISIS, STFC Rutherford Appleton Laboratory, UK



These are the easy bits ...





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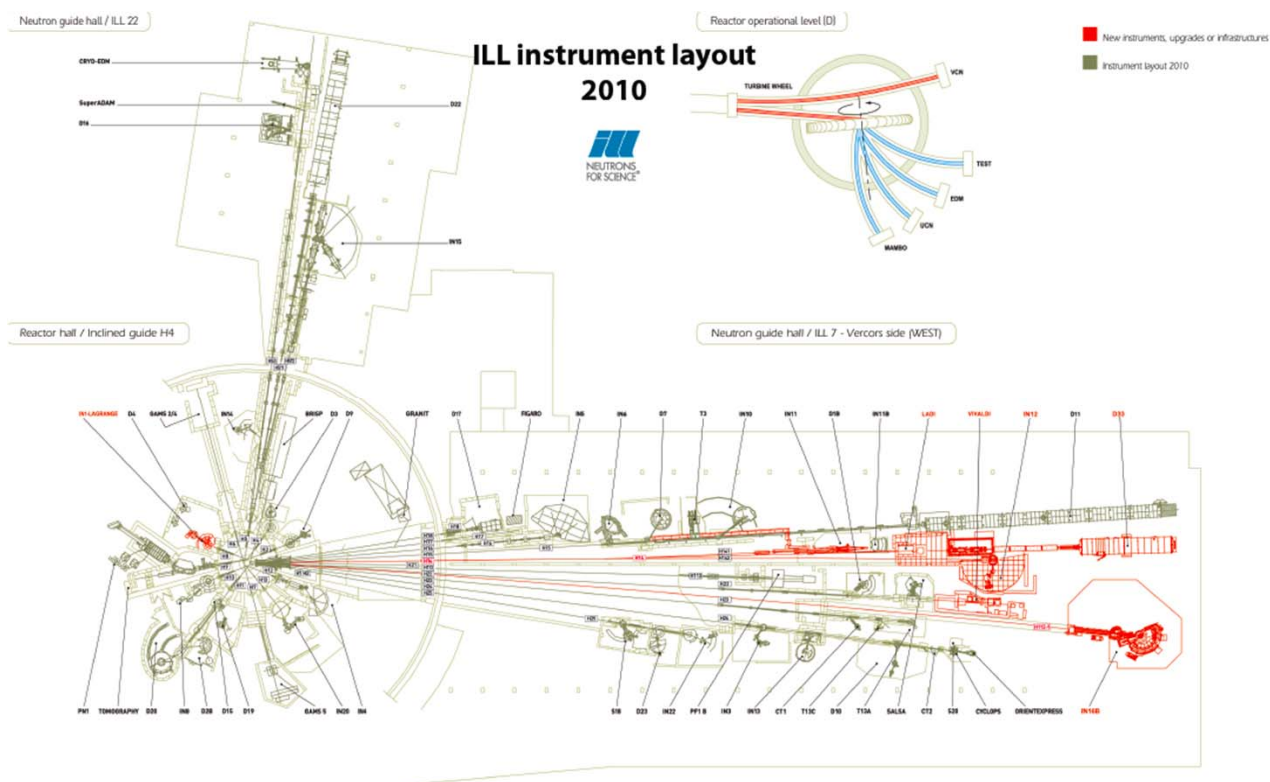
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A real instrument will have a budget and it will never be big enough



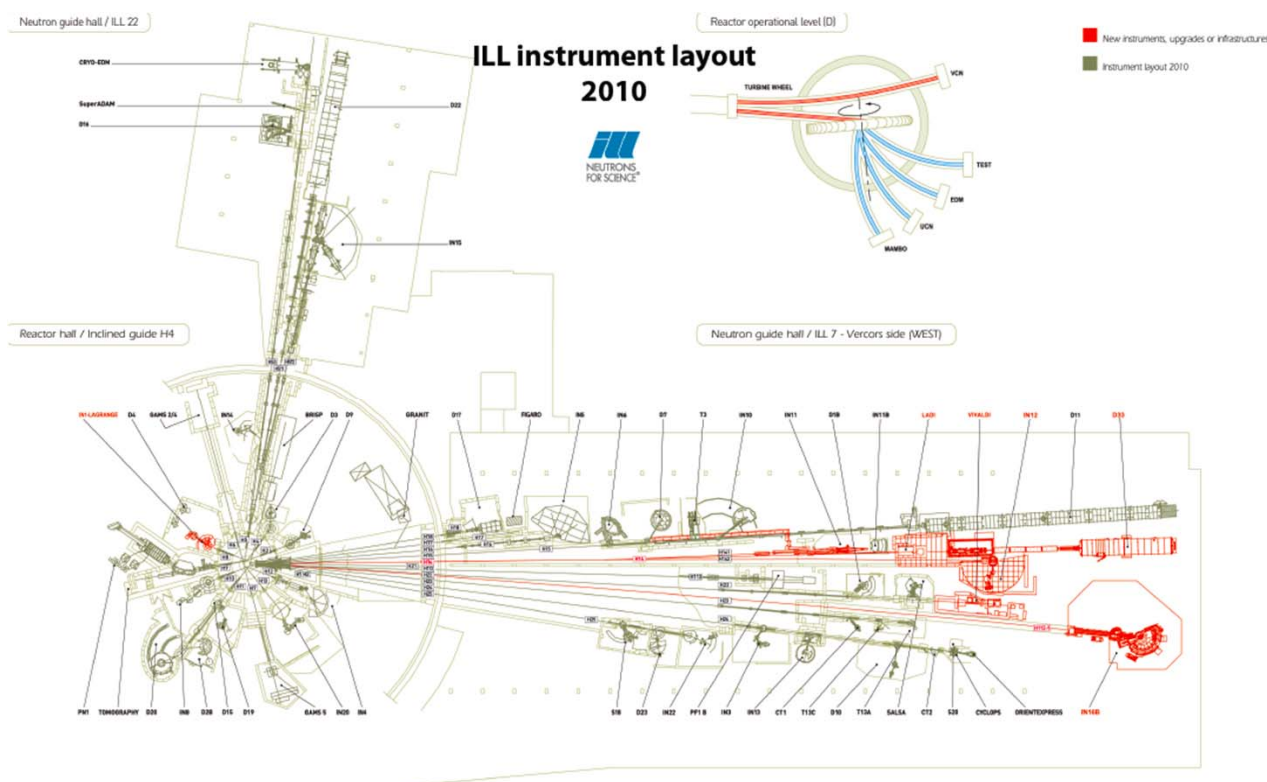


Guides transformed neutron scattering





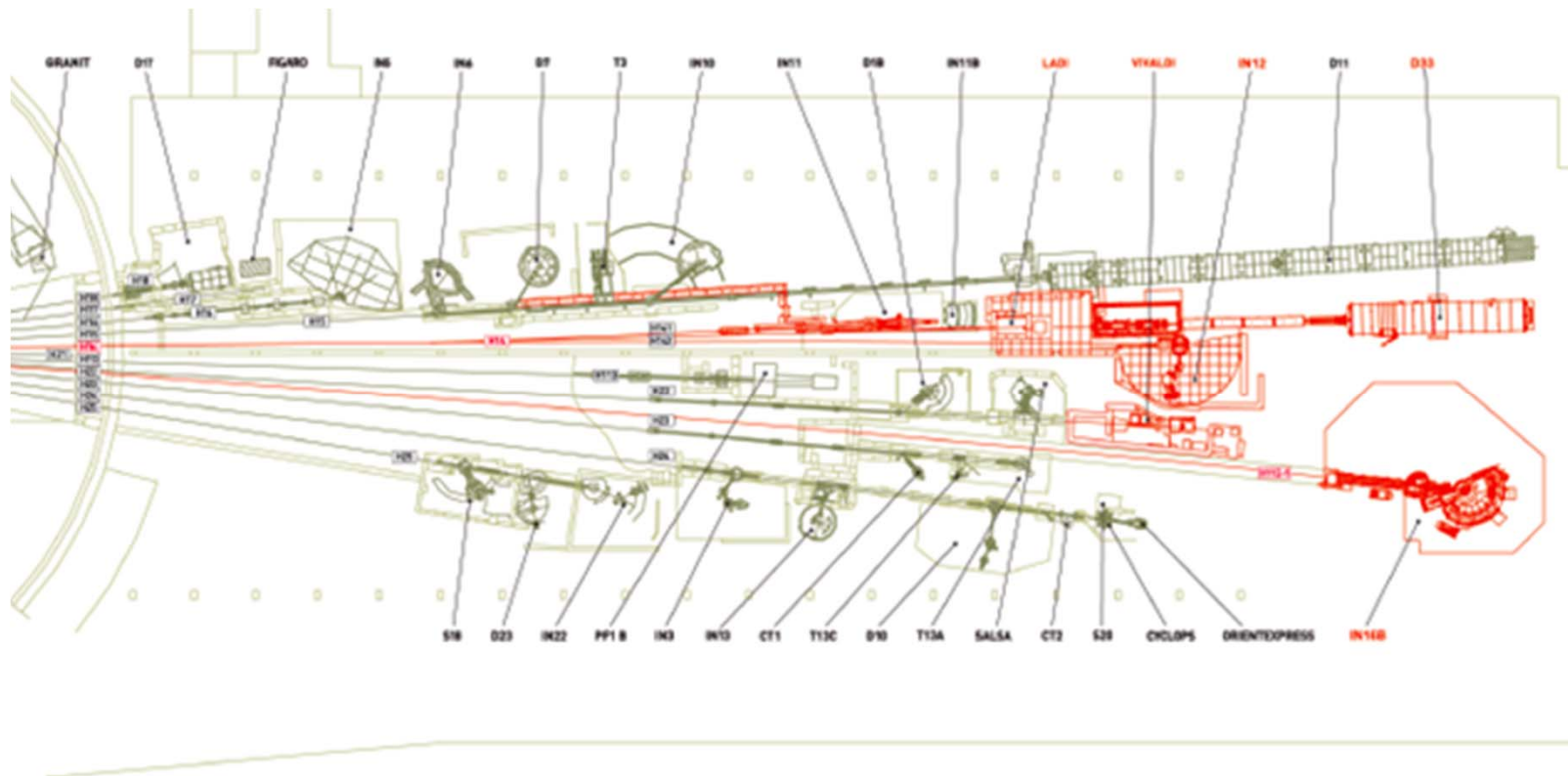
A real instrument will have to fit into a real space,
and it will never be big enough ...



For many continuous source instruments, the length is not a parameter;
for all pulsed source instruments it is.



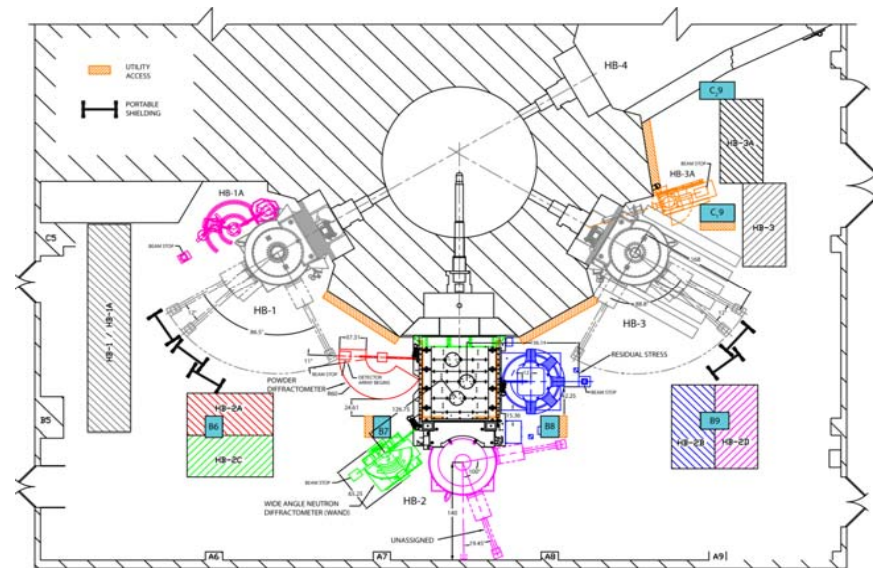
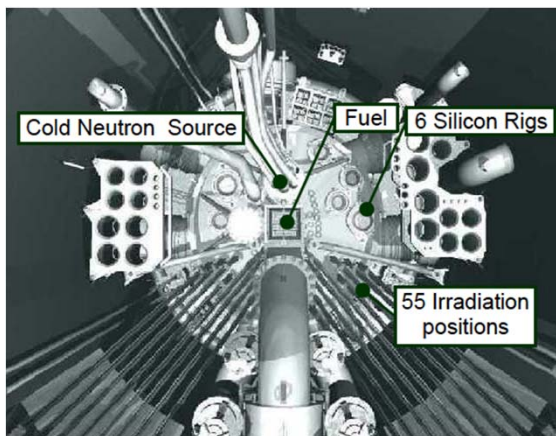
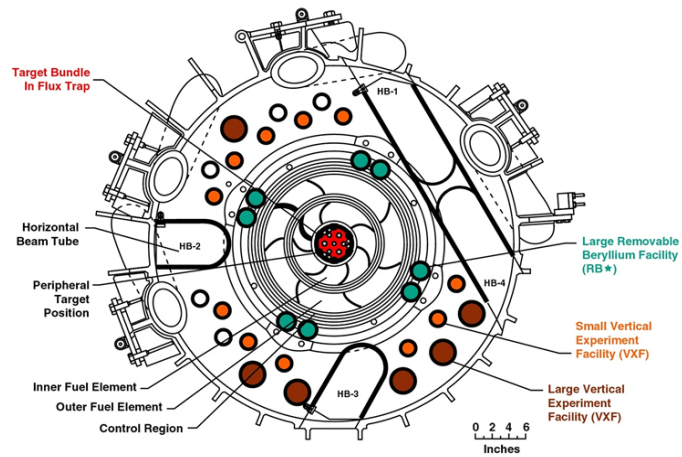
A real instrument will have to fit into a real space,
and it will never be big enough ...



Continuous sources can build multiple (narrow bandwidth) instruments
on a single beamline, for pulsed sources you (generally) cannot



A real instrument will have to fit into a real space,
and it will never be big enough ...





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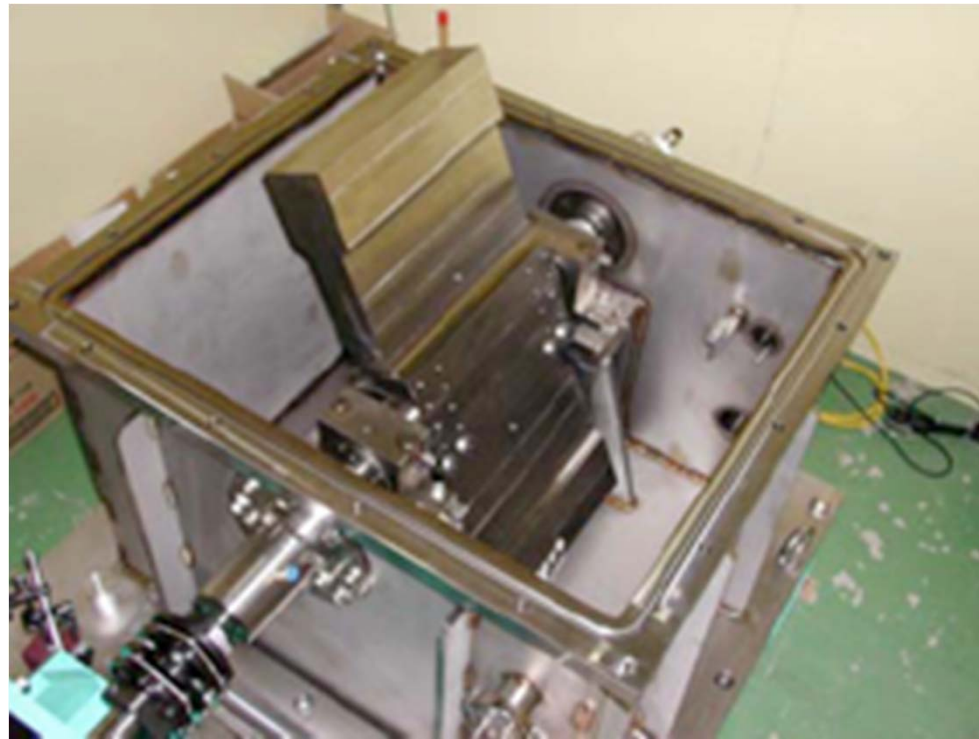
A real instrument will have to fit into a real space,
and it will never be big enough ...



Unless yours is the first instrument ...



A real instrument will have to fit into a real space,
and it will never be big enough ...



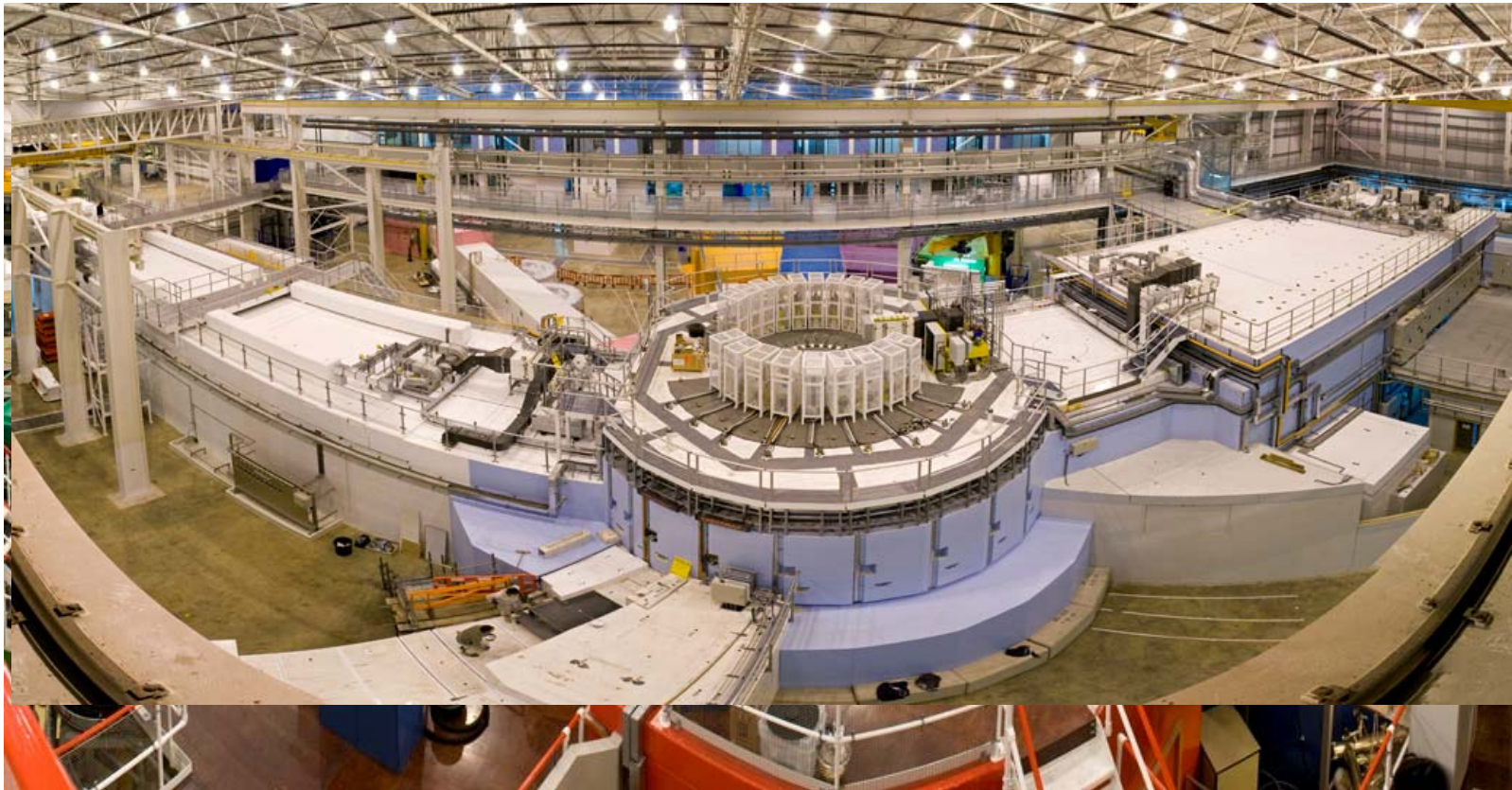
T0 chopper 0.7m diameter + 2*0.6m shielding @ 11m = 18°



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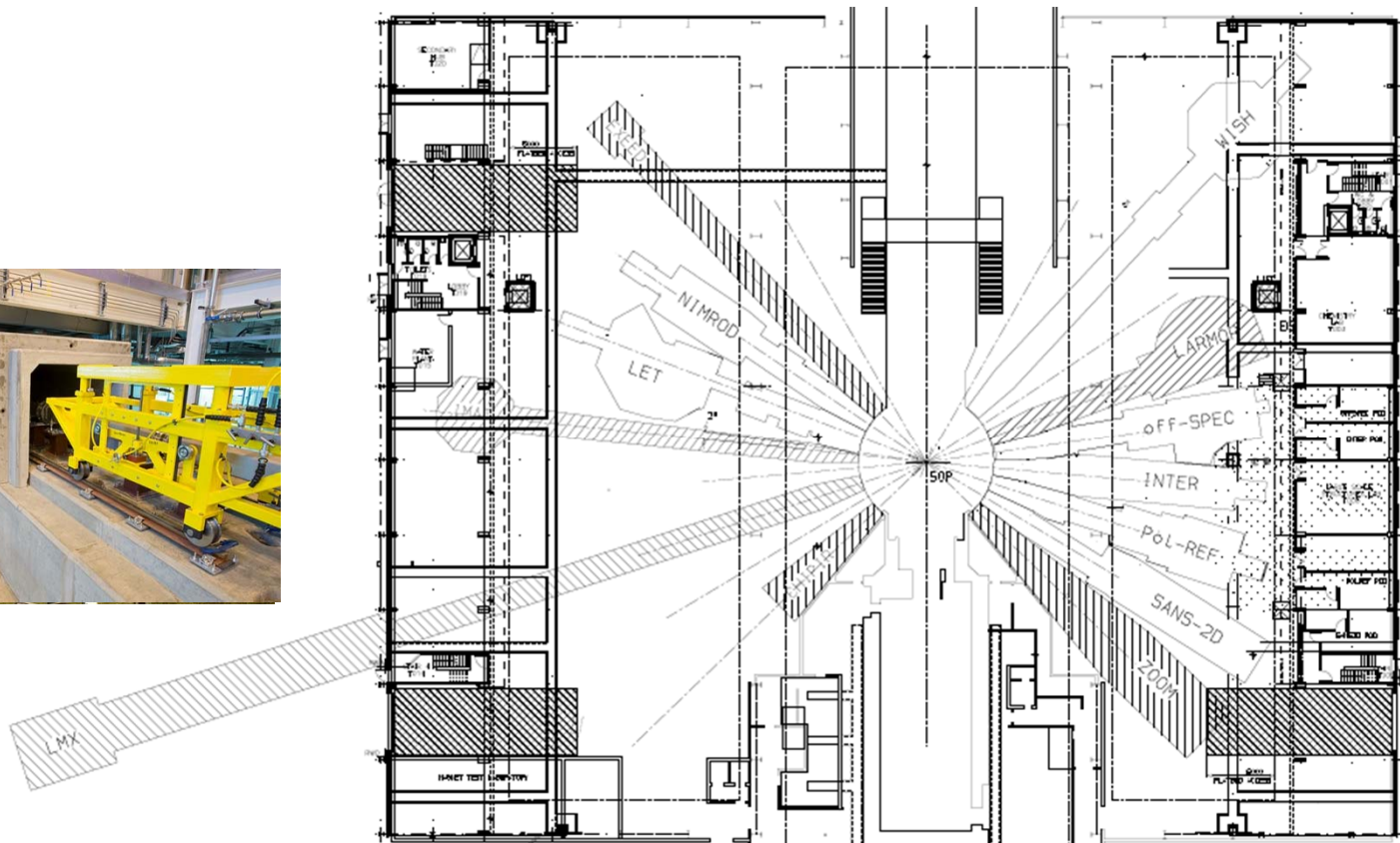
What is the most important piece of equipment in an instrument hall?



The crane!



A real instrument will have to fit in a real space, and it will never be in the right place ...

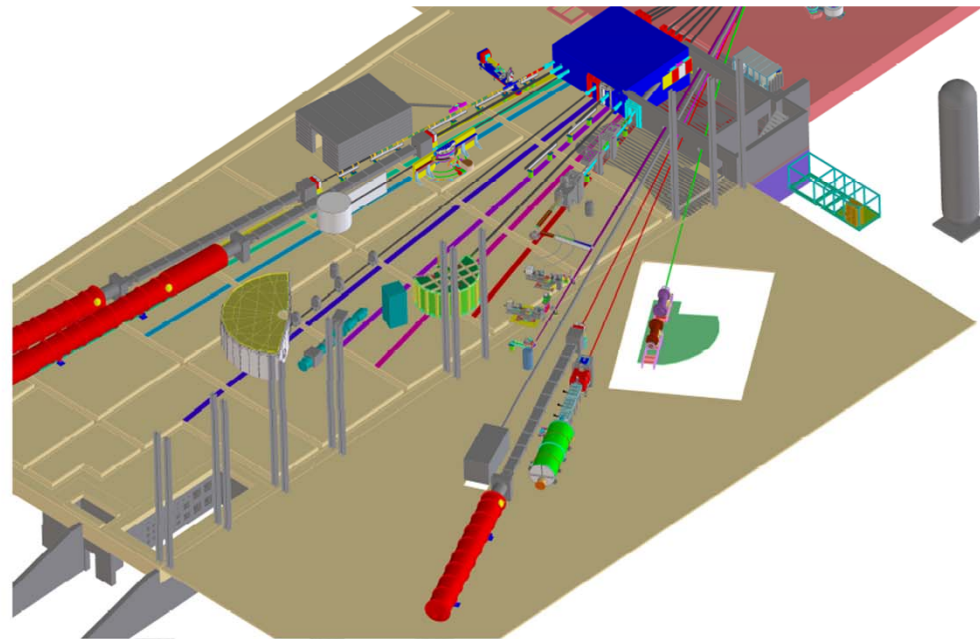




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Integrating and optimising multiple instrument designs



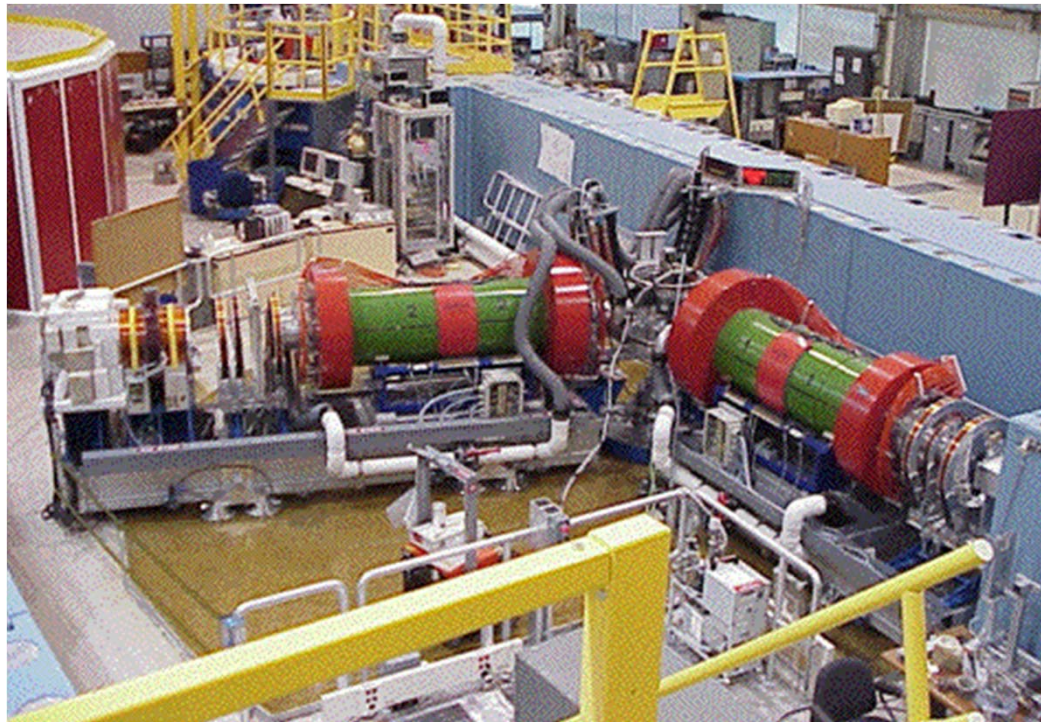
NCNR new guide hall



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Many neutron instruments use
(and are sensitive to) magnetic fields



Magnetic field policies are a nuisance for some, but life and death for others ...

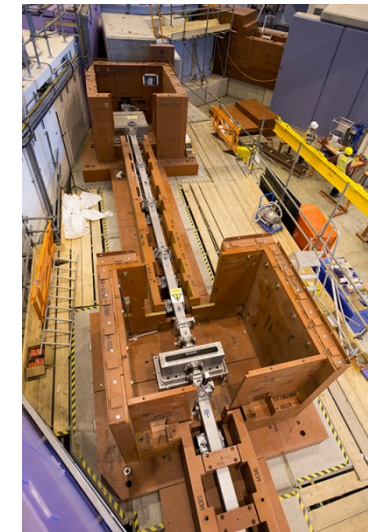
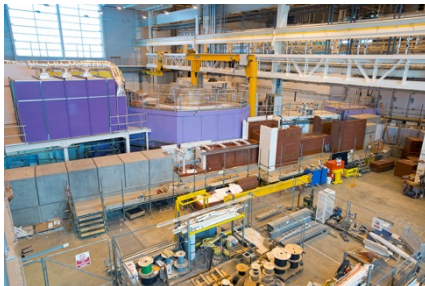


Shielding stops radiation from getting out, and from getting in ...

Shield against fast neutrons, thermal neutrons, gammas

- Hydrogeneous (concrete, wax, polyethylene, water)
- Iron (steel), lead
- Boron (B_4C , BN, $AlMgB_{14}$, ^{10}B)
- 6Li
- Cd
- Gd/GdO

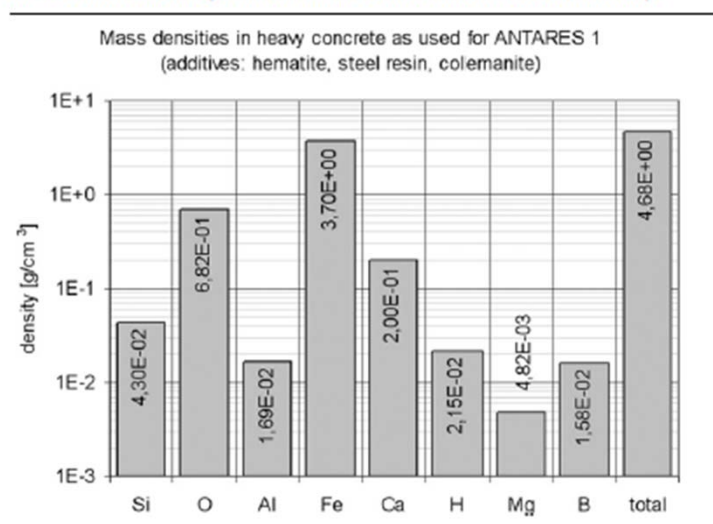
Need to consider neutron thermalisation
and gamma production





Shielding stops radiation from getting out, and from getting in ...

Table 1
Mass densities in heavy concrete as used for the former ANTARES facility.



Shield against fast neutrons,
thermal neutrons, gammas

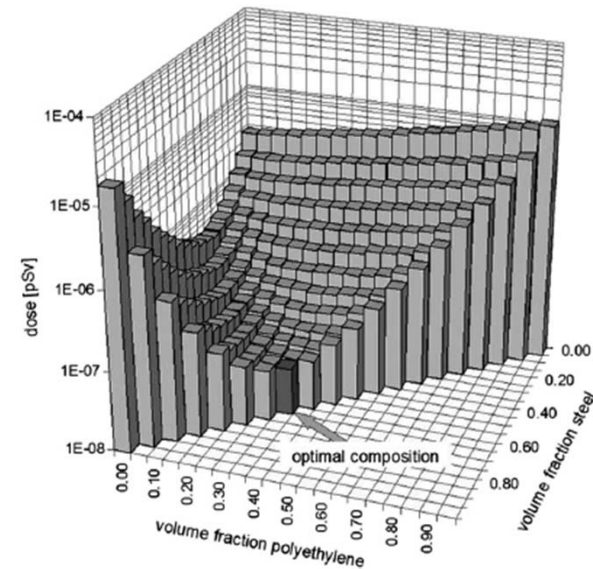


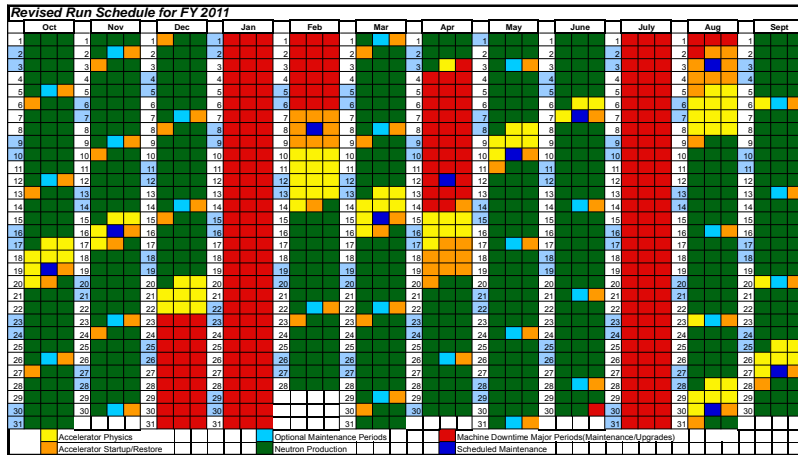
Fig. 4. Total dose on the outer surface of the sphere.

Steel, ferroboron, paraffin composite
Calzada et al. (Munich) NIMA 2011

We need to develop better (and cheaper) shielding ...

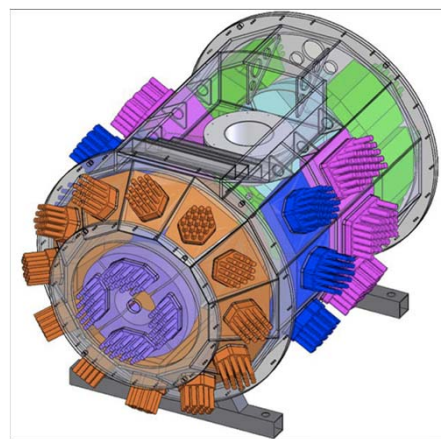
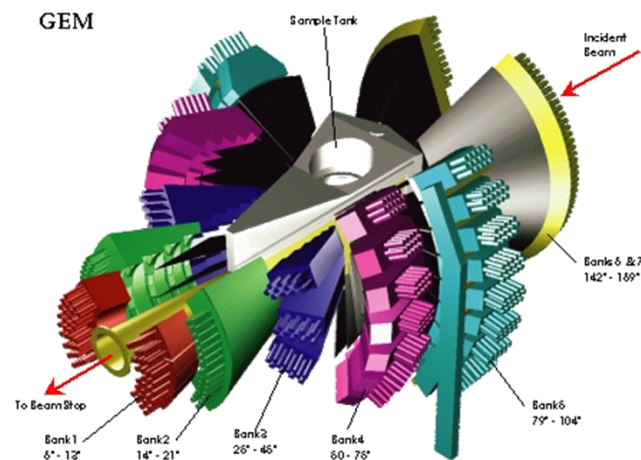


Building new instruments at a new facility is much easier (of course ...)





Instruments must be accessible for people ...



GEM and POLARIS instruments (ISIS powder diffraction)



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Instruments must be inaccessible for people ...





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Instruments must be accessible for samples and sample environment ...



VULCAN instrument (SNS materials/engineering diffraction) with multi-axial load frame



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Back to money ...

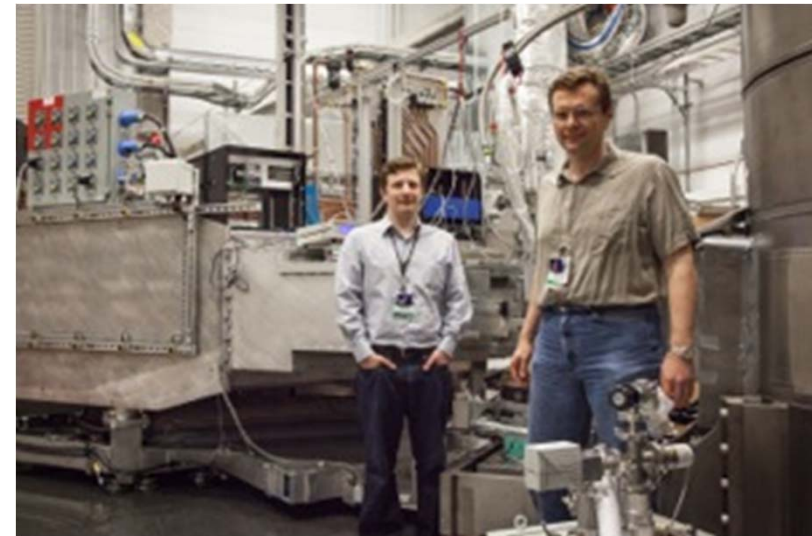
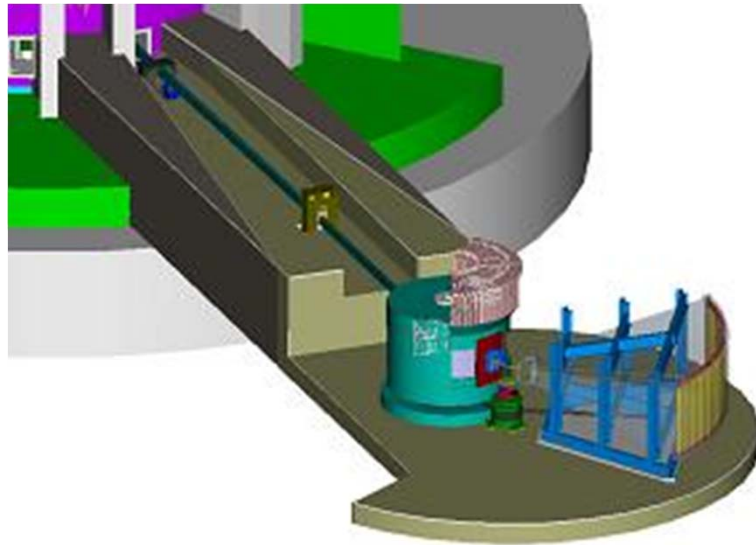




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What does it cost to build an instrument?





What does it cost to build an instrument?

- SNS SING-II: 4 instruments \$60M
 - ISIS TS2 Phase II: 4 instruments £30M
- ... and these are 'incomplete' instruments ...
(usually detectors are descoped)

75% Materials 25% Labour

Front end: shielding (concrete, steel, wax) \geq guide

and what was missing from the list?



Sample environment, software



The screenshot shows the MANTID website homepage. At the top is the MANTID logo and navigation links: Home, Downloads, Documentation, Develop, Contact Us, and Search. Below the navigation are three main sections: 'About MANTID', 'Quick Start Guide', and 'News'. The 'About MANTID' section describes the project as a framework for high-performance computing and visualization of scientific data, mentioning its support for Neutron and Muon scattering data. The 'Quick Start Guide' section offers a collection of training courses, including 'Mantid Introduction', 'Introduction To Python', 'Python in Mantid', 'Extending Mantid With Python', and 'Examples'. The 'News' section features two announcements from July 8th, 2014: 'Version 3.2 preparing for release' and 'September 2014 Training Courses'. A 'News Archive' link is visible at the bottom right of the page.

The screenshot displays the MANTID software interface. The main window shows two data plots: 'd0x_ph2' and 'TFC1393B-croconic acid at 10 K Run 3'. The 'd0x_ph2' plot shows intensity versus energy transfer (meV) with a peak at approximately 10 meV. The 'TFC1393B-croconic acid at 10 K Run 3' plot shows intensity versus energy transfer (meV) with a peak at approximately 10 meV. A 'DensityOfStates input dialog' is open, showing a 'Function' dropdown set to 'Lorentzian', a 'PeakWidth' of 10, and a 'Scale' of 1000. The 'DensityOfStates' section is expanded in the right-hand panel, showing a list of algorithms including 'Lorentzian', 'Gaussian', 'Crystal', 'DebyeWaller', 'Dynamics', 'Elastic', 'Filtering', 'Histograms', 'MantidTools', 'Optimization', 'PythonAlgorithms', 'Quantification', 'Radiationless', 'Scale', and 'SRO'.



A 'simple' example – optimising the cost of a guide



The higher the m value, the higher the cost



HRPD, ISIS: double elliptical focusing guide



Conclusions

- Neutron scattering is (always going to be) an expensive technique
so you must optimise the cost/benefit
and define the ‘benefit’
- Think about the engineering and operational practicalities in the design
or pay for it for the next 15 years
- The ‘clever’ bits of the instrument are equal in cost and equal in importance
to the ‘dumb’ bits, but both are much cheaper than the source
there is no point in putting effort into the source if you’re not
also going to put effort into the shielding
- Try not to be developing the technology at the same time as you’re building
the instrument ...