

NMR Infrastructure for The Physical Sciences and Engineering



Daniel Emmerson

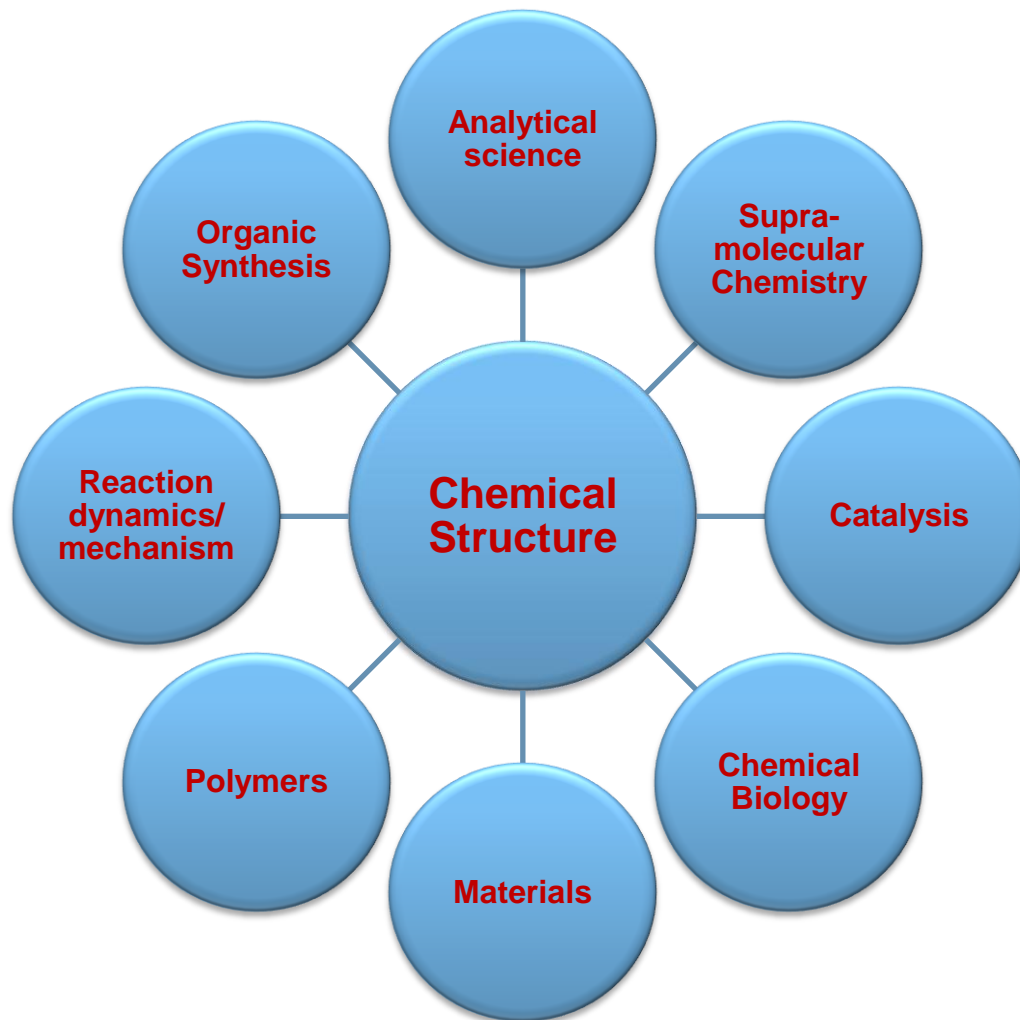
UK NMR Managers Meeting

Edinburgh 19 June 2013

EPSRC

Engineering and Physical Sciences
Research Council

NMR: An Underpinning Technology



Background

Cheaper to reach given level of performance

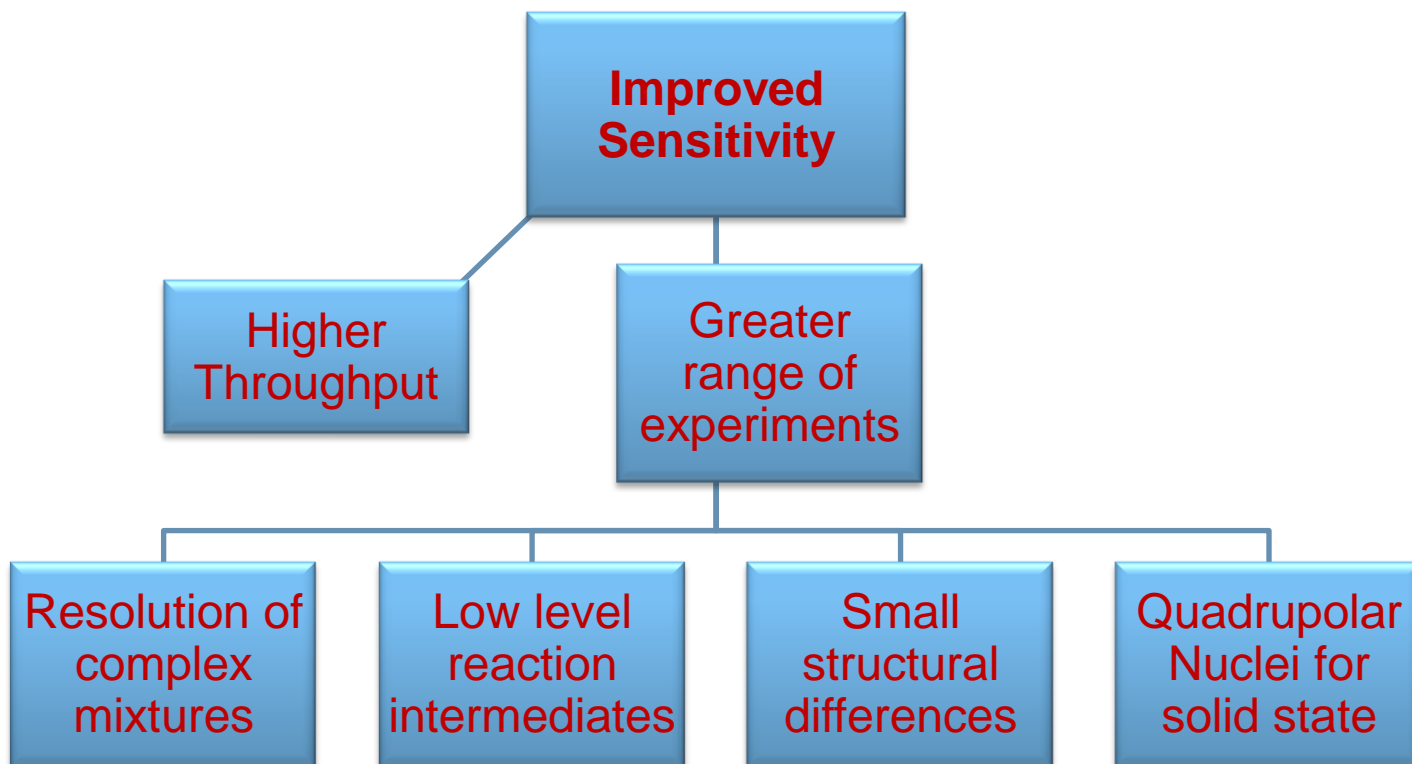
BUT

Leading edge more expensive

Recent Technical Innovations

- ❑ Gradient Shimming
- ❑ Shaped Adiabatic Pulses
- ❑ Multi-channel Operation
- ❑ Fast MAS
- ❑ Cryoprobes

New capability

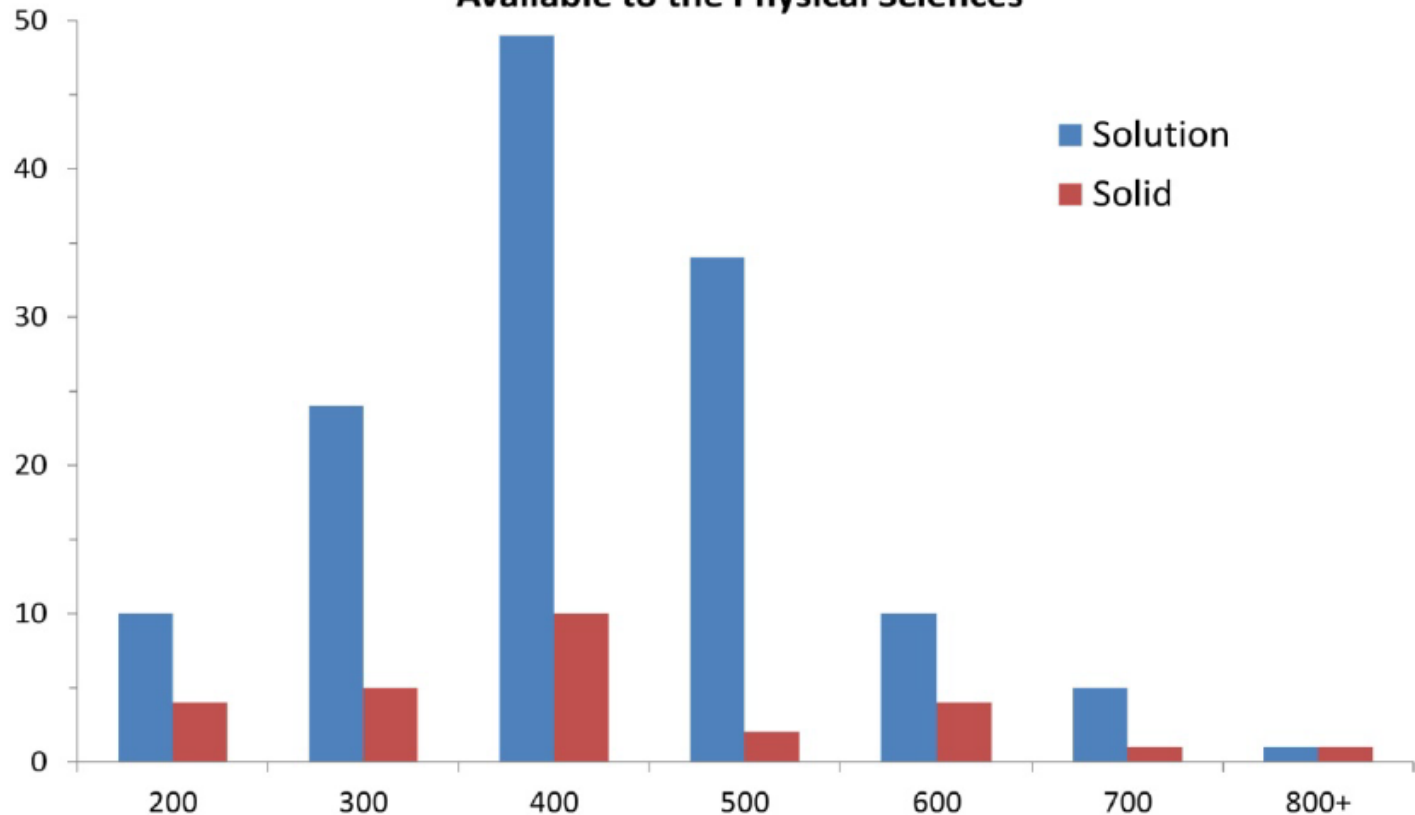


Aims of Roadmap

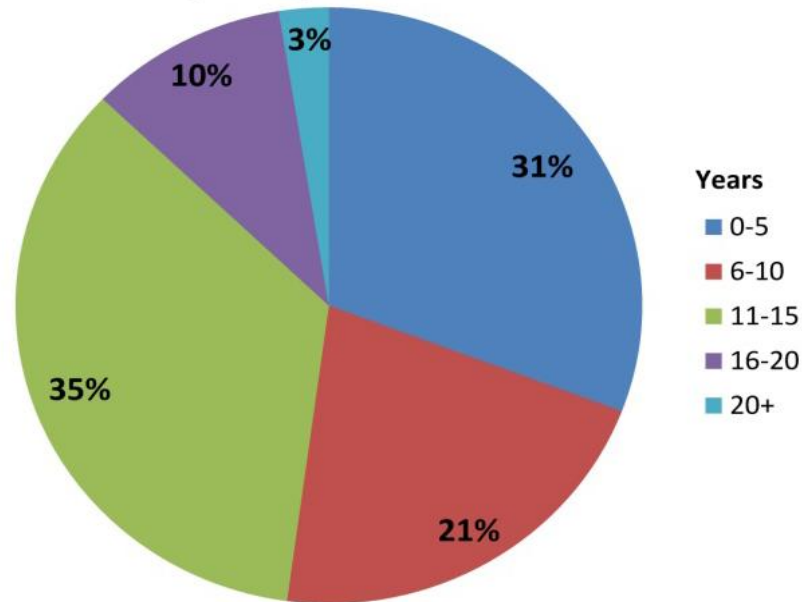
- ❑ Overview of **current** NMR infrastructure and **requirements** to inform strategic approach for UK
- ❑ Short and longer term requirements
- ❑ Challenges for **funding** the NMR equipment base and advice to Strategic Equipment Panel
- ❑ How can equipment be managed **sustainably**?
- ❑ Scope limited to Physical Sciences and Engineering
- ❑ Need to understand overlap with requirements of life sciences

Availability of different field strengths for Physical Sciences

Distribution of Magnetic Fields in Proton Resonance Frequency Available to the Physical Sciences



Age of Spectrometers



- ❑ 50% of instruments “last generation”
- ❑ Support of older equipment can be expensive

Findings

- ❑ 5:1 Solution : Solid
- ❑ Stock is aging
- ❑ 400 MHz is still dominant in spite of ready availability of 500 MHz machines
- ❑ Only 2 machines for solid state NMR above **600 MHz**
- ❑ Lower than expected uptake of **cryoprobe** technology
- ❑ High **utilisation** rate (80%)

Sustainability

Small Research Facility

- <300k replacement value
- Direct costs only

Major research facility

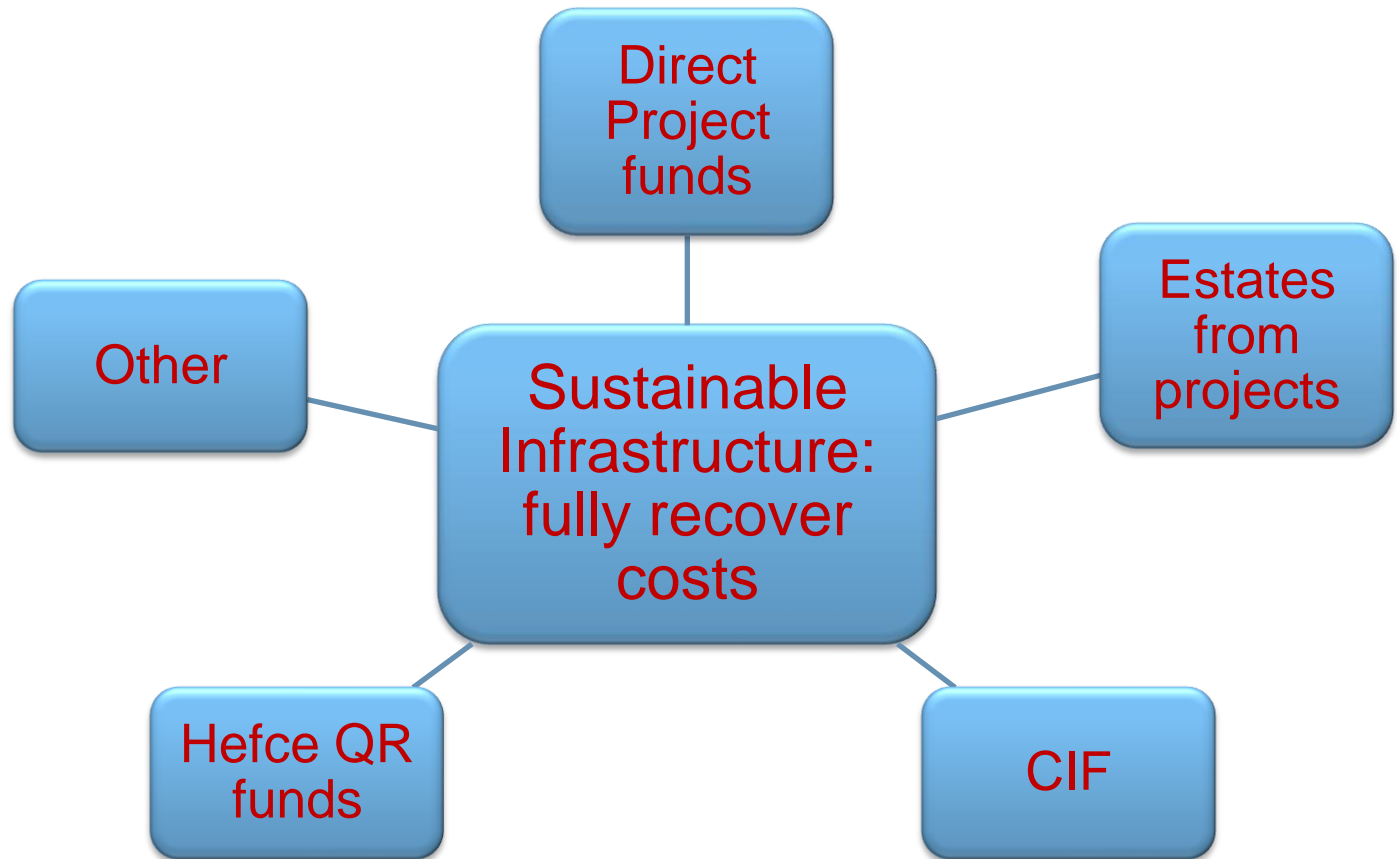
- >300k replacement value
- All costs including depreciation

Costs of PhD students using equipment

Upgrading Instrumentation

- Shielded magnets
- Helium recycling
- Cryoprobes

Other Funding sources



EPSRC Funding Opportunities

❑ Strategic Equipment

- ❑ Since Autumn 2011
- ❑ To underpin leading research

❑ Core Chemistry call Autumn 2012

- ❑ 40% of funds on NMR
- ❑ 8 new machines
 - ❑ 600 MHz
 - ❑ 3 x 500 MHz
 - ❑ 4 x 400 MHz
- ❑ 10+ upgrades
 - ❑ Probes
 - ❑ Consoles

❑ 8 Great Technologies call

Equipment Sharing

- ❑ Searchable databases
- ❑ Regional Consortia
 - ❑ N8
 - ❑ M5
 - ❑ SES
 - ❑ WestChem
 - ❑ EastChem
 - ❑ SES
 - ❑ Southwest
- ❑ Sharing of human resources/ skills
- ❑ Sharing between life and physical sciences
- ❑ What is the cost threshold at which sharing becomes likely?
- ❑ How is access managed?

Strategic Priorities Identified

- ❑ **700 MHz provision for solid and solution phase NMR**
 - ❑ Regional Facilities?
- ❑ **DNP capability**
 - ❑ National facility
- ❑ **RCUK-wide discussion about ≥ 1 GHz provision**
- ❑ **Other considerations:**
 - ❑ Extreme diffusion
 - ❑ Novel Engineering applications
 - ❑ Wider temperature capability
- ❑ **Strategic Equipment Scheme is appropriate route for funding**
 - ❑ ≥ 600 MHz solution phase
 - ❑ ≥ 500 MHz solid phase

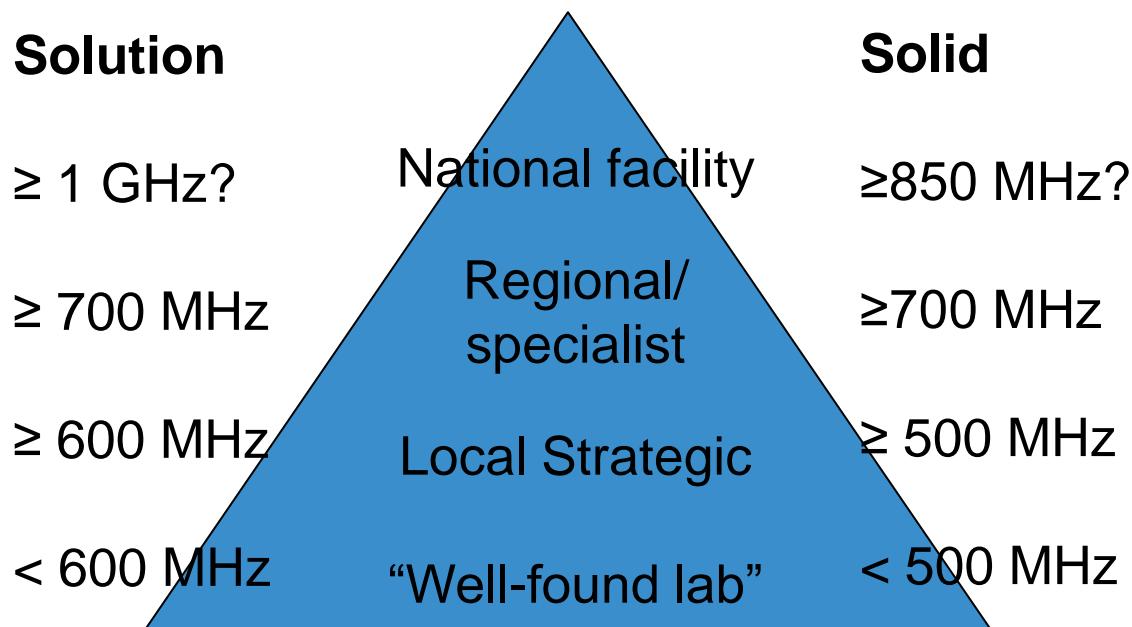


Strategic Equipment Scheme

- ❑ **Quality** of Science underpinned
 - ❑ **Added value of instrument**
- ❑ Fit to EPSRC **Strategic priorities**
- ❑ **Sharing** if appropriate
- ❑ **Sustainability**
- ❑ Institutional Backing
 - ❑ **Strategy** for capital investment
 - ❑ What **institutional contribution** is appropriate?
- ❑ Management of **access**

An Integrated NMR Infrastructure

Are these the right numbers **now**? For **future** planning?



NMR Landscape

	Lower range machines (<400 MHz?)	Mid-range machines (500-700 MHz?)	Top end machines (> 700 MHz?)
• Requirement for new machines			
• Requirement for replacement /upgrade of existing machines (eg cryoprobes)			
• Model for networking eg regional hubs?			
• Scope for resource sharing with life sciences?			



Monitoring

- Reporting from National service
- Institutional Equipment account annual reports
- Impact studies
 - Underpinning for impact from science
 - Direct impact
 - Trained people
 - UK competitiveness
 - Industrial users