NMR Infrastructure for The Physical Sciences and Engineering

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UK NMR Managers Meeting

Edinburgh 19 June 2013

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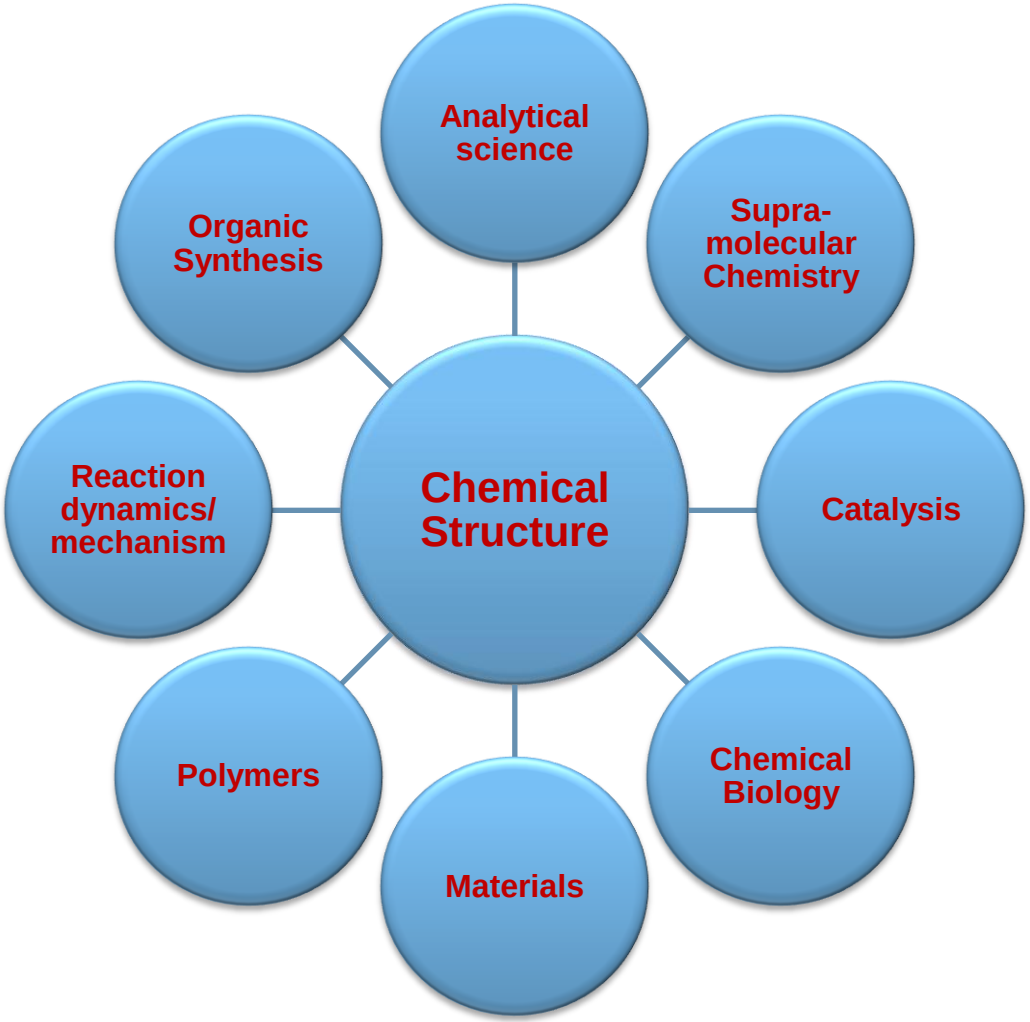
NMR: An Underpinning Technology



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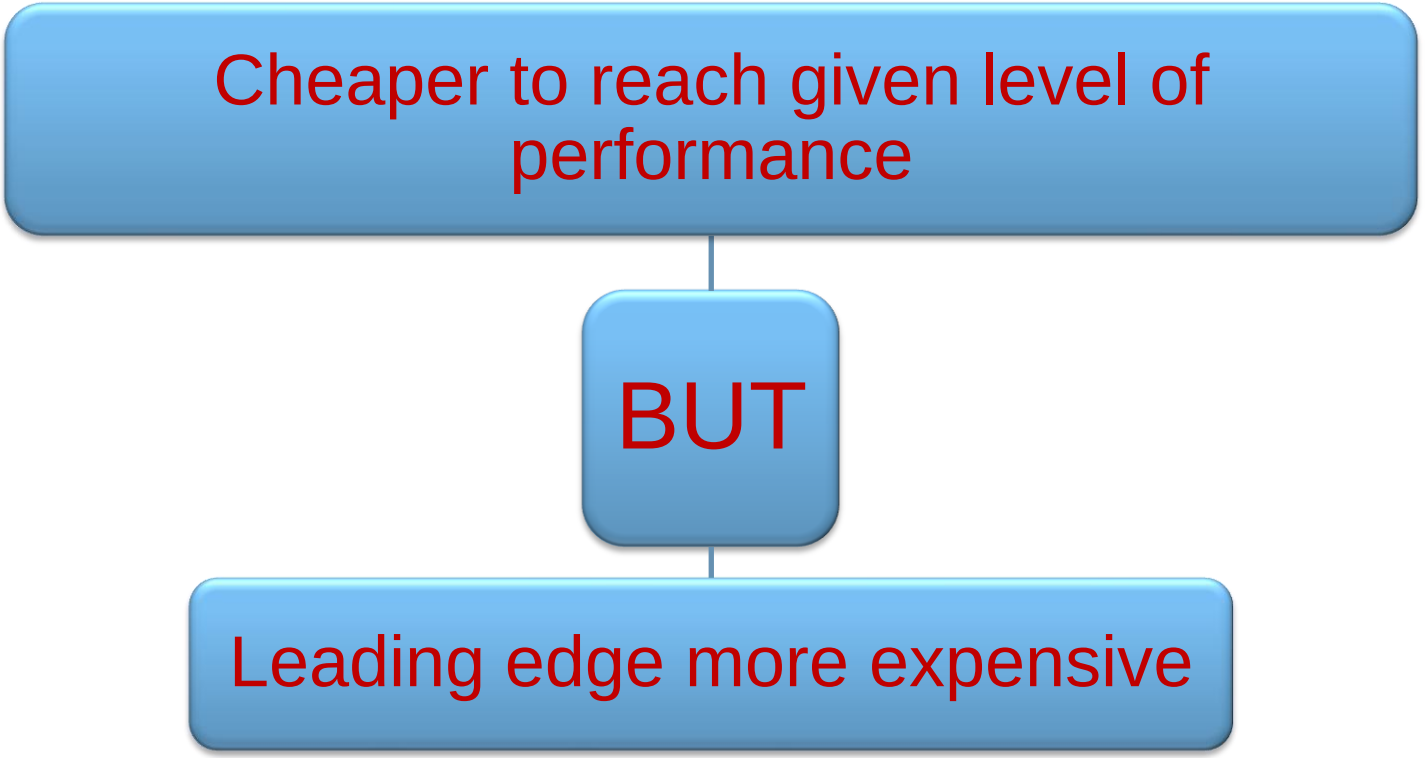
Background



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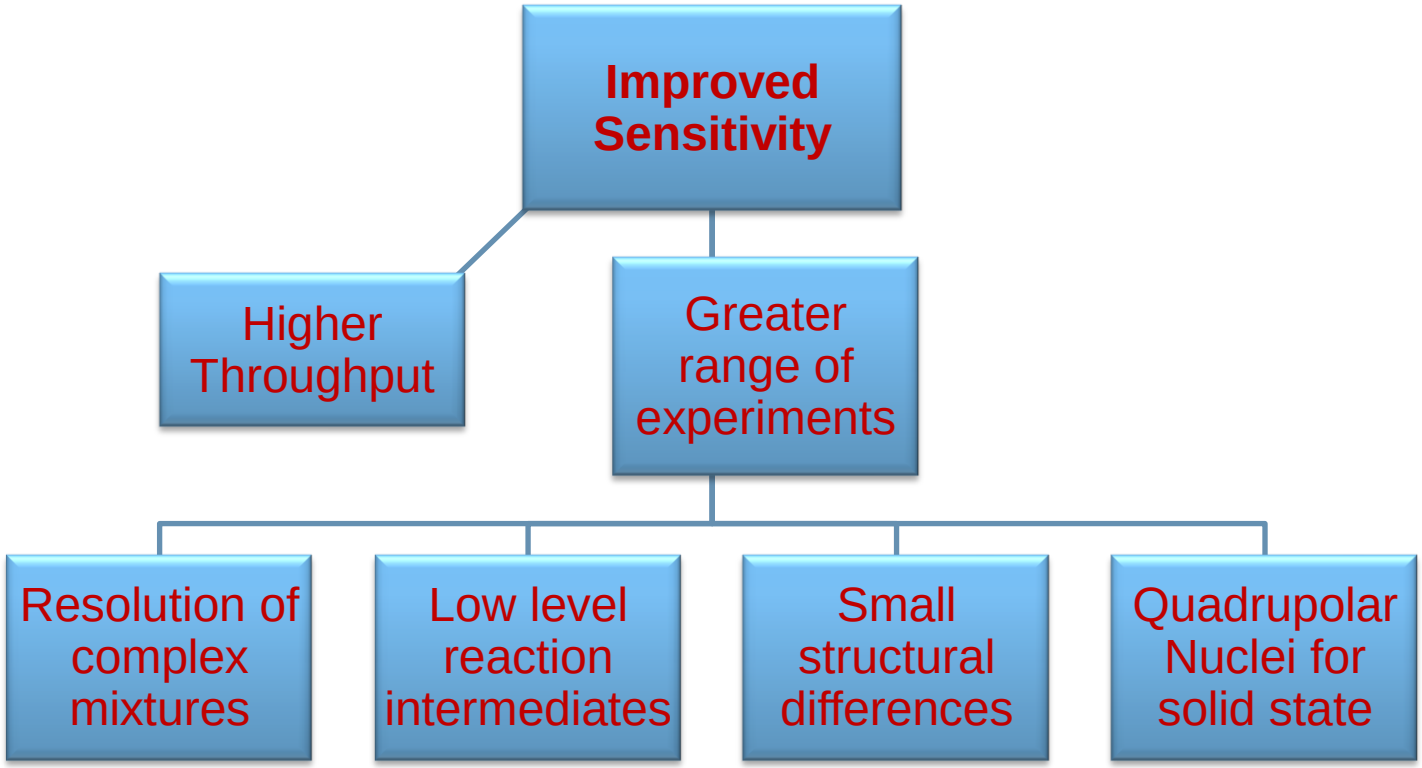
Recent Technical Innovations

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

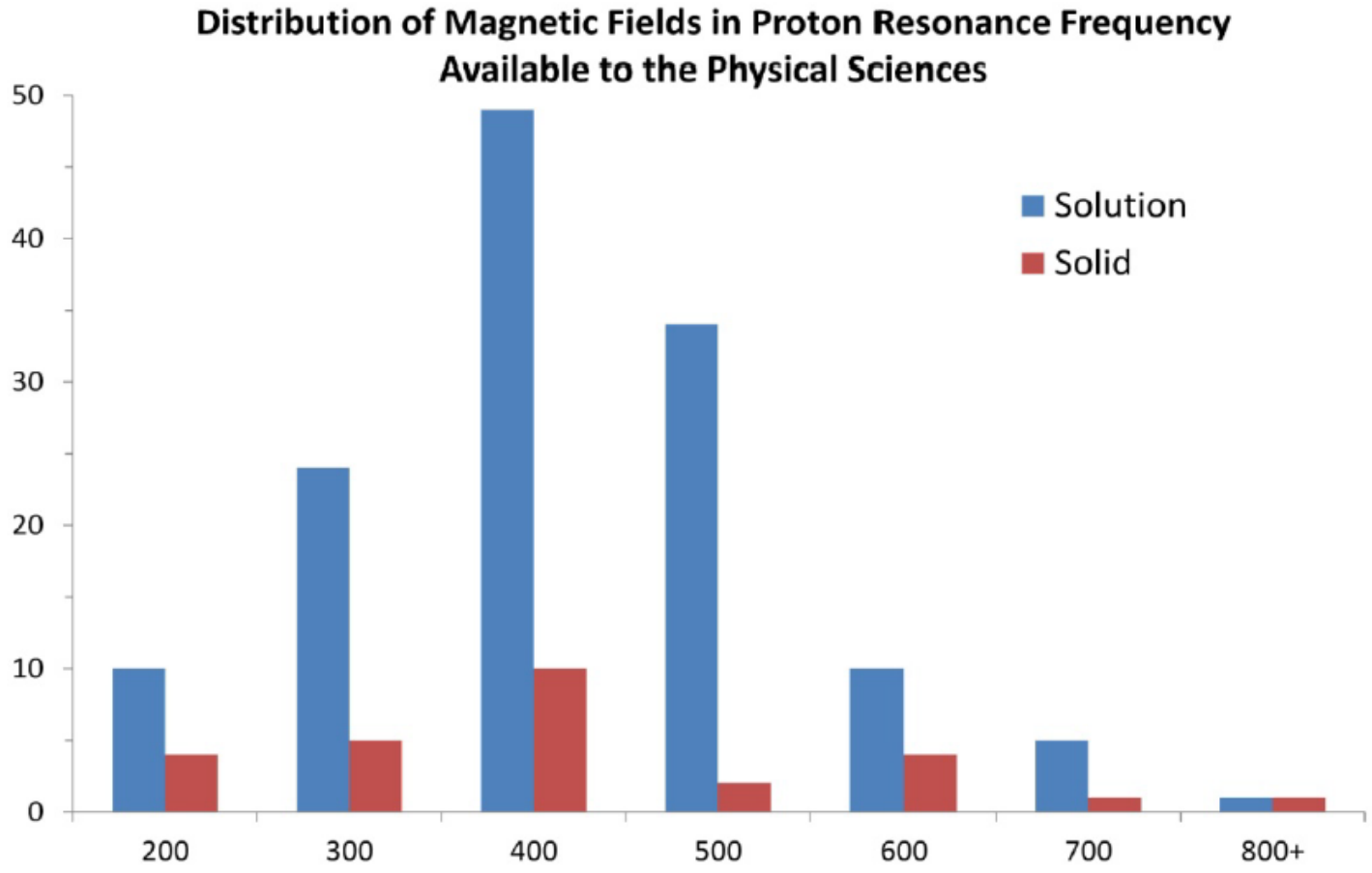
New capability



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



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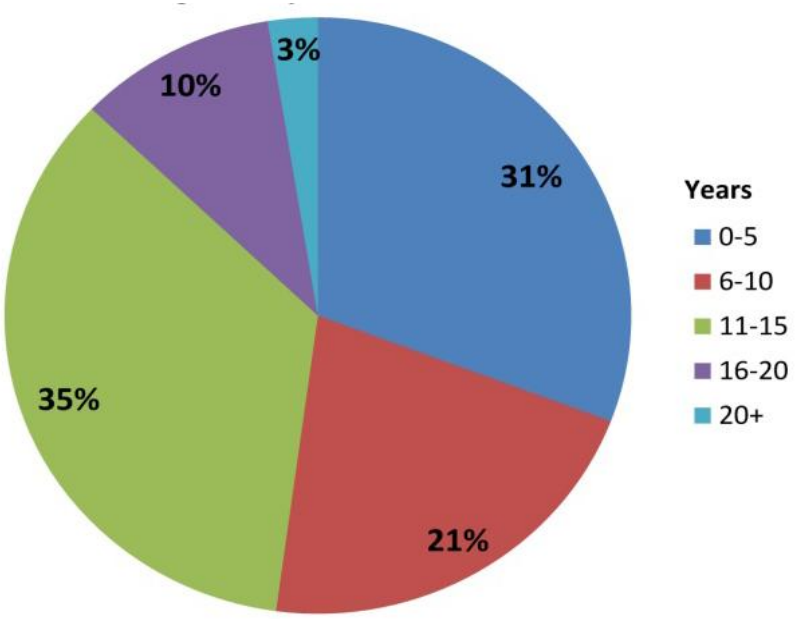
Age of Spectrometers



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

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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

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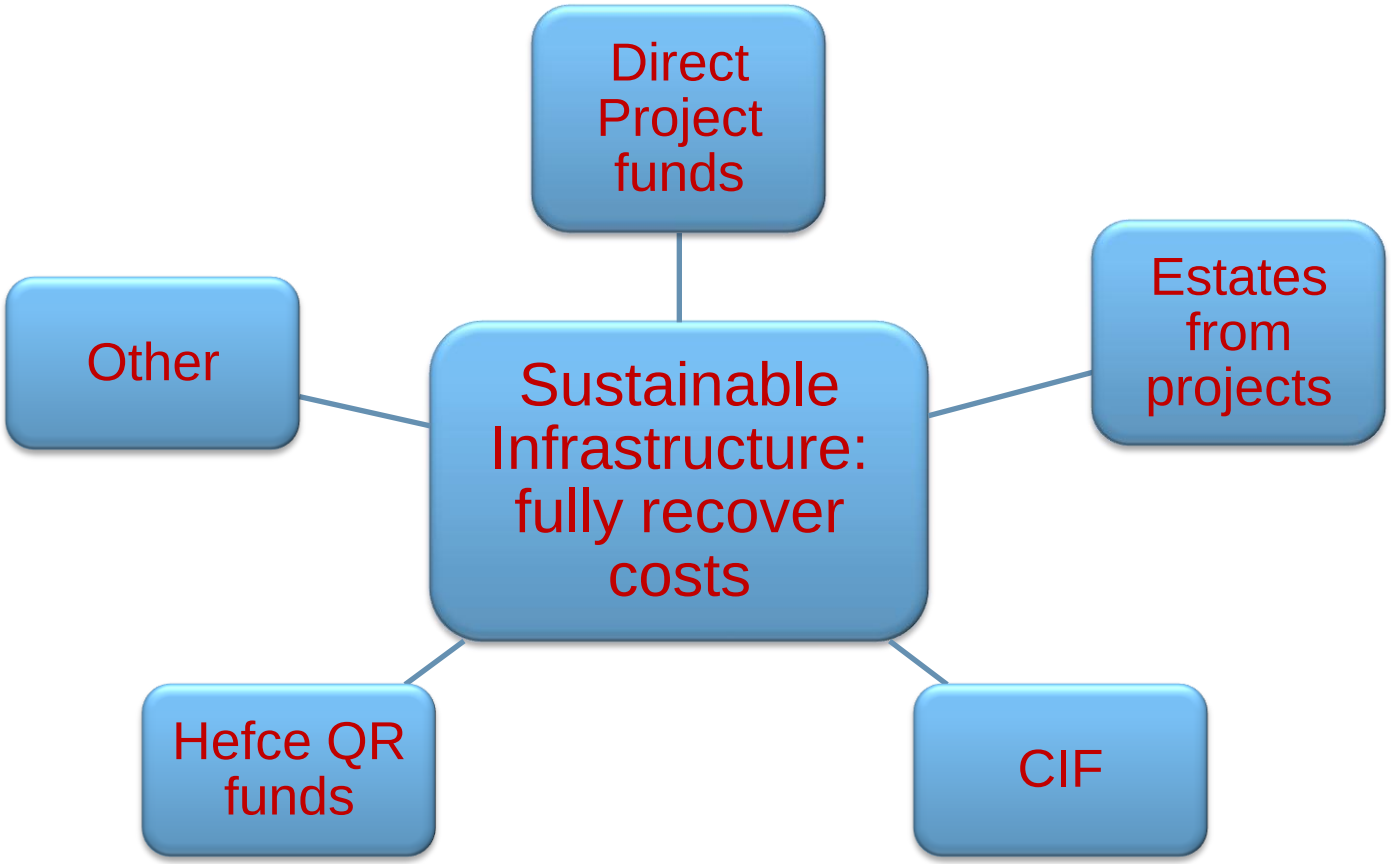
Other Funding sources



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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

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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?

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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

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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**

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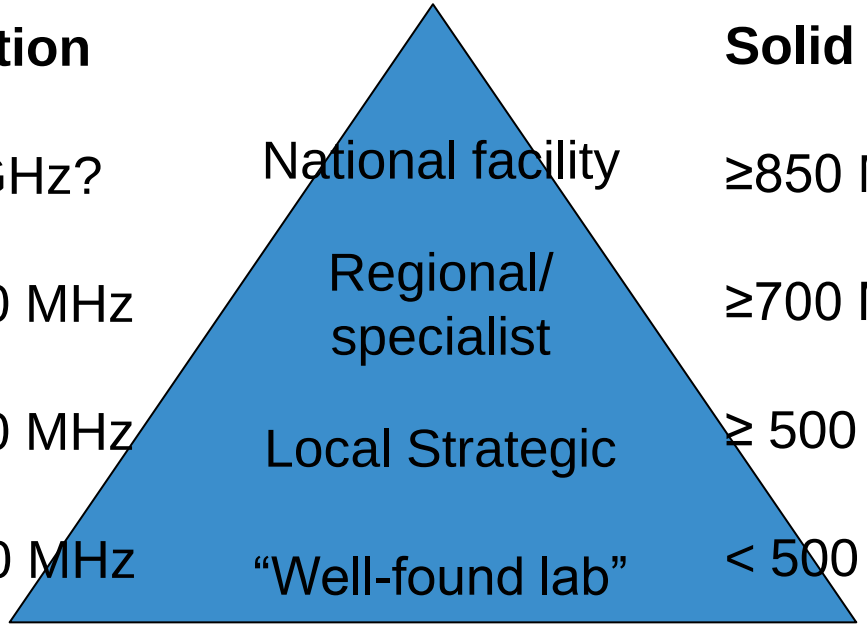
An Integrated NMR Infrastructure

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



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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?			

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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

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