UKRI 1.2 GHz NMR Project

SUMMARY OF Town Hall Meetings 29 November and 07 December 2021

Tony Chapman, EPSRC, January 2022

Introduction

As part of the Government Spending Review settlement in June 2021 it was announced that early-stage work would commence to identify a preferred host for a 1.2 GHz NMR spectrometer within the UK, with funding for the spectrometer itself subject to the outcome of the Government Spending Review settlement for UKRI, to be announced in 2022. Two meetings were held virtually with the NMR community to inform them of the current situation, provide some key information about the spectrometer itself and review early results from spectrometers already installed elsewhere in Europe. Delegates were also given an opportunity to give their views on what the system should offer and what UKRI should account for when developing the call.

Summary of meeting discussions

At each meeting the delegates were sent to breakout groups to discuss two questions:

1. What should a 1.2 GHz NMR system be able to deliver for the community?
2. What should be taken into account to allow this to be delivered?

A summary of the key points identified in both meetings in response to these questions is summarised below. The output from the MIRO boards for each group at the meetings is shown in Appendix 1.

Probe strategy –

- the number and type of probes,
- phasing of probe purchase and interchange of probes … don't buy everything at the start or have a plan for ongoing investment as user base develops.
- as well as the user community served through each probe,
- Value of the unique capability of a probe
- Sensitivity and resolution
- Should seek to lead developments and advances in NMR rather than follow
- Resolution (at this stage) appears to be the big advantage of 1.2 GHz NMR probes

(Financial) sustainability

- Retention of key RTP staff
- Institutional vs UKRI support
- Charging models, Operating models and access models – aim to minimise cost at point of use

- A sharp ramp up of cost recovery (20%-50%) may not be feasible. NB there seems to be a difference of views on charging models and cost recovery from different communities.
- Some running costs will be important to allow the facility to establish itself; it will be important not to set up the system to be a failure.
- Differing views over FOPOU access. UKRI would not accept a 100% FOPOU model
- Long term plan is required.
- Means of cost recovery… need to make clear as UKRI that equipment on grants is a legitimate cost to include on grants – seems to be more of an issue with perception in BBSRC and MRC thank EPSRC.
- A lot of commitment will be required from the host institution

(environmental and scientific) sustainability

- Expertise in liquid and solid-state NMR will be needed.
- Sustainability of He & N use and recycling will need to be demonstrated.
- Being part of a wider ecosystem is very important. This need not necessarily mean facilities in the same building or site.
- Need to offer a high-quality user experience.
- How can this system capitalise on the UKs inherent strengths in NMR?
- Need a strategy for developing new communities.
- Access management
    - Ease of access
    - Accessibility for new users and new communities
    - Diversity of users
    - Engagement with business
    - Balance: the proportion of time allocated to the host institution vs time to the user community needs to be right.
    - Planning experiments takes time and some experiments take time. Access should reflect experimental need rather than hours.
    - Who decides on the access model? UKRI sets core expectations, but the applicants themselves must develop a model that meets these expectations and works for them as hosts and the community as users.
    - Protocols to ensure divers and inclusive access should be in place.
- Joint hosting
- Technical support
    - Good quality technical support (RTP) is essential
    - Expertise should be readily available to users, for advice, service provision and training of users
- Call
    - The timescale of the call will be very short – more time to negotiate internally to generate a realistic proposal would be beneficial.
    - A lot of discussion in the session is about logistics – this comes across as similar to an NRF process (EPSRC)
    - The timescale is too short. If a significant capital and resource investment is required by the applicants this will take time to negotiate with the host institution.

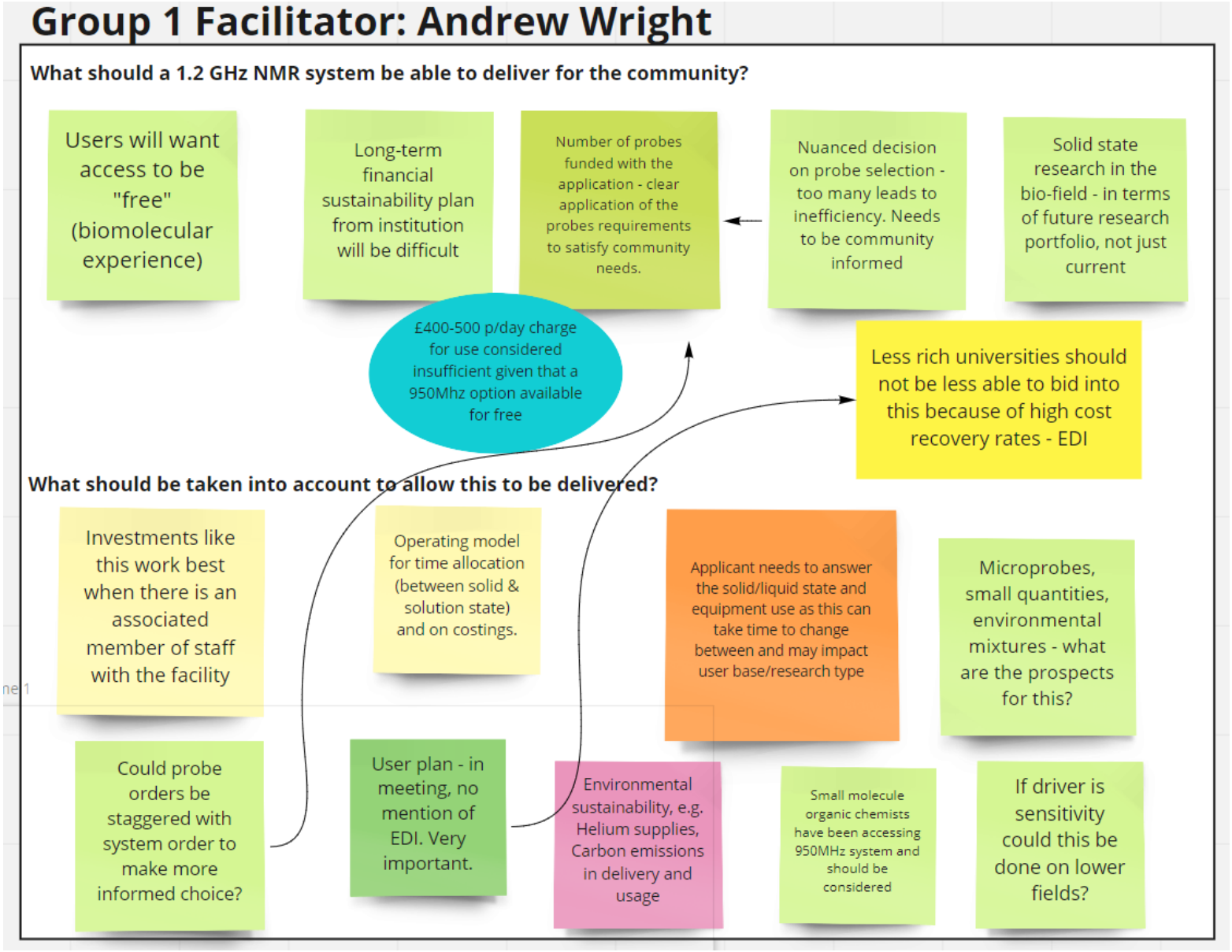
- Requirements
    - Available space needs to be a bare minimum 9m x 9m with a minimum height of 5.3m. Either suitable space needs to made available within an existing site or a new building is needed that meets these minimum requirements.
    - The system weighs 8.4t in total. Most standard laboratory floors should be able to support such weight, but the issue may be the ability to move the system into place.
    - The largest component measures 220x240x300 cm… it must be possible to move an object of this size into the laboratory space.
    - What is the possibility of a 1.4 GHz system in the intervening time? No plans from Bruker to increase field strength for now.
- Risks
    - Staff recruitment and retention
    - Risk of under use (…on what basis? Access costs? Sub-optimal management?)
    - Consideration and management of risks will be important

Notes from Plenary session

Key points raised in breakout groups and plenary discussion

- Reduce barriers for potential hosts to host the facility; at present this represents a major capital and resource commitment.
- Staff are key to the successful operation of the facility at all levels.
- Sustainability Plan
    - Expertise in liquid and solid-state NMR will be needed.
    - Sustainability of He & N use will need to be demonstrated.
    - Being part of a wider ecosystem is very important. This need not necessarily mean facilities in the same building or site.
    - Need to offer a high-quality user experience.
    - Future plans for additional probes… don't buy everything at the start or have a plan for ongoing investment as user base develops.
    - How can this system capitalise on the UKs inherent strengths in NMR?
- Access models and operating costs
    - Differing views over FOPOU access
    - Long term plan
    - Means of cost recovery
- Risks
    - Staff recruitment and retention
    - Risk of under use (…on what basis? Access costs? Sub-optimal management?)
    - Consideration and management of risks will be important

Town Hall Meeting #1 (29 November 2021)



Group 2 Facilitator: Kay Yeung

What should a 1.2 GHz NMR system be able to deliver for the community?

Sensitivity and resolution

in cell NMR

Analysing complex systems (applications e.g. biomolecular systems)

Significant benefits over existing 1.0GHz systems?

Unique probes underpinning unique experiments, technology permitting

What should be taken into account to allow this to be delivered?

Financial sustainability of this system over longer period (running costs, inc He costs)

Access management
- fair access
- prioritisation plan

Who would prioritise access?

Accessibility to all users

Having dedicated team to run 1.2GHz NMR owing to technical complications

Helium recovery systems to minimise running costs

Possibility of creating joint facility between different Universities

Group 3 Facilitator: David Bryce

What should a 1.2 GHz NMR system be able to deliver for the community?

- Cannot burden the host institution
- Do not use 1.2 GHz to replace an older instrument
- solids/liquids capabilities
- standard probes ok for now
- technical expertise on site
- Institutional support? Staffing? Long-term support?
- Cost-recovery must be realistic
- logistics of bookings, prioritization of user access
- "internal" vs "external" users?
- opportunities for collaboration with UK for new technology?

What should be taken into account to allow this to be delivered?

- Be sure that the infrastructure and personnel is supported long-term
- UKRI needs to be creative about long-term support for operations/staffing
- What does the host institution get out of this
- Need commitment of full-time staff
- clarify institutional responsibilities /commitments
- enable/encourage diversity of users (background, geography, etc.)

Group 4

Facilitator - Colin Miles

What should a 1.2 GHz NMR system be able to deliver for the community?

1.4GHz! Include potential for higher field if tech exists. Lead the world, don't follow.

Industrial engagement from the outset. Pharma, energy, materials, biotech, polymers.

What should be taken into account to allow this to be delivered?

Expertise. And retaining that expertise.

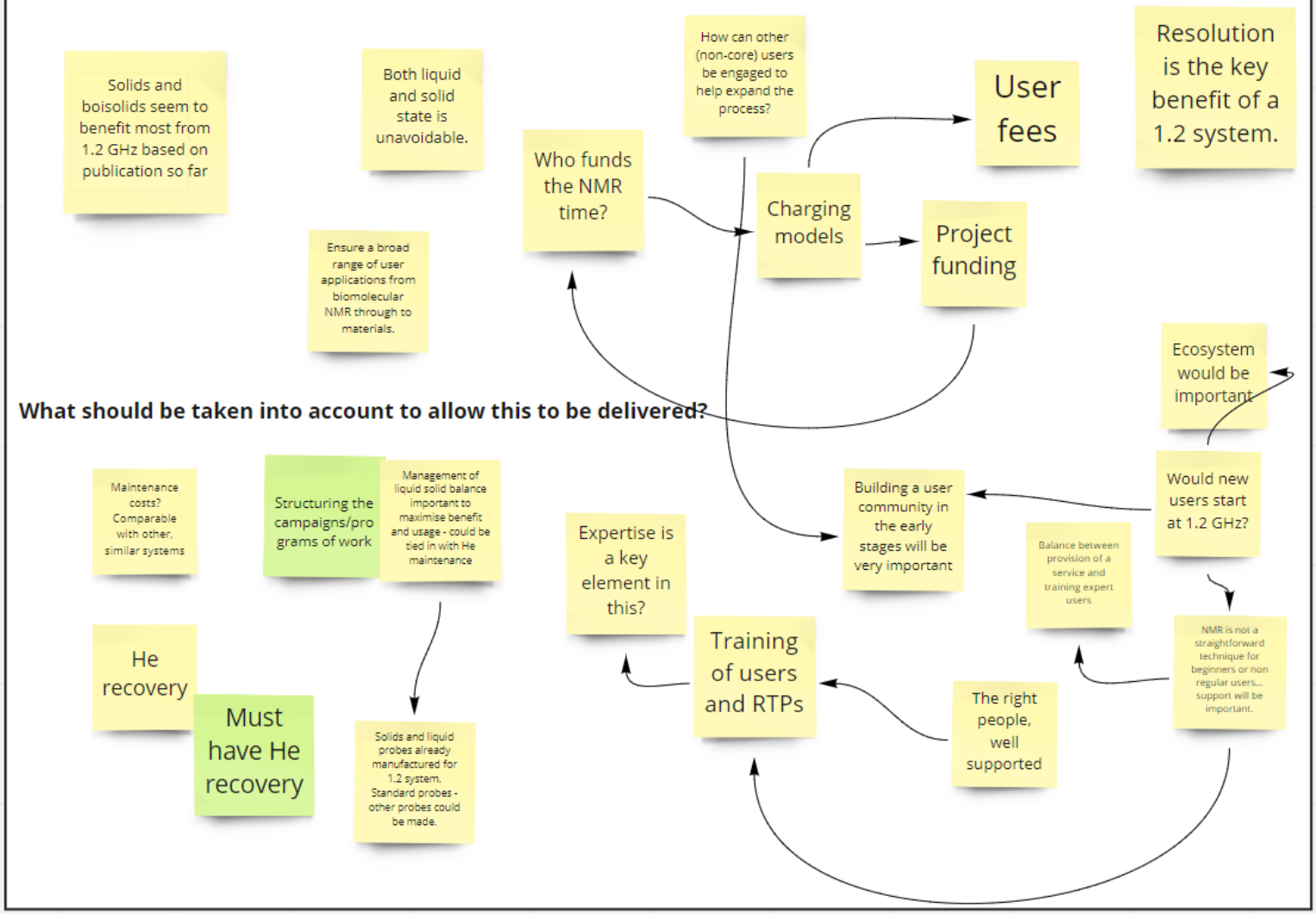
Running costs. Base level support to maintain operational sustainability. Tapering down of underpinning funds.

Part of a network with other instruments, so people can apply for the most appropriate

More lead time to negotiate costs/support within institutions. Several £M building and long-term personnel costs to get negotiated.

Group 5

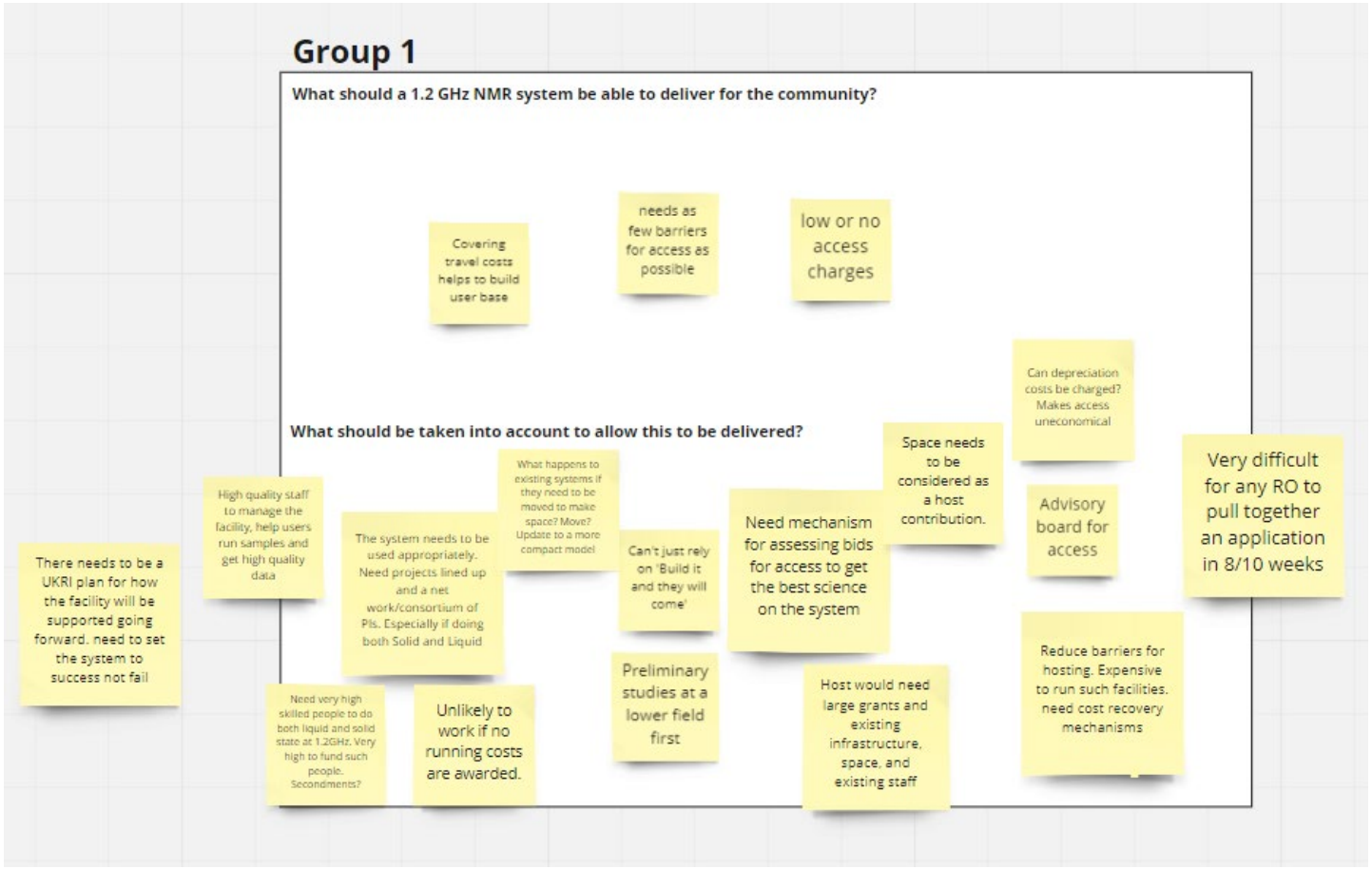
What should a 1.2 GHz NMR system be able to deliver for the community?



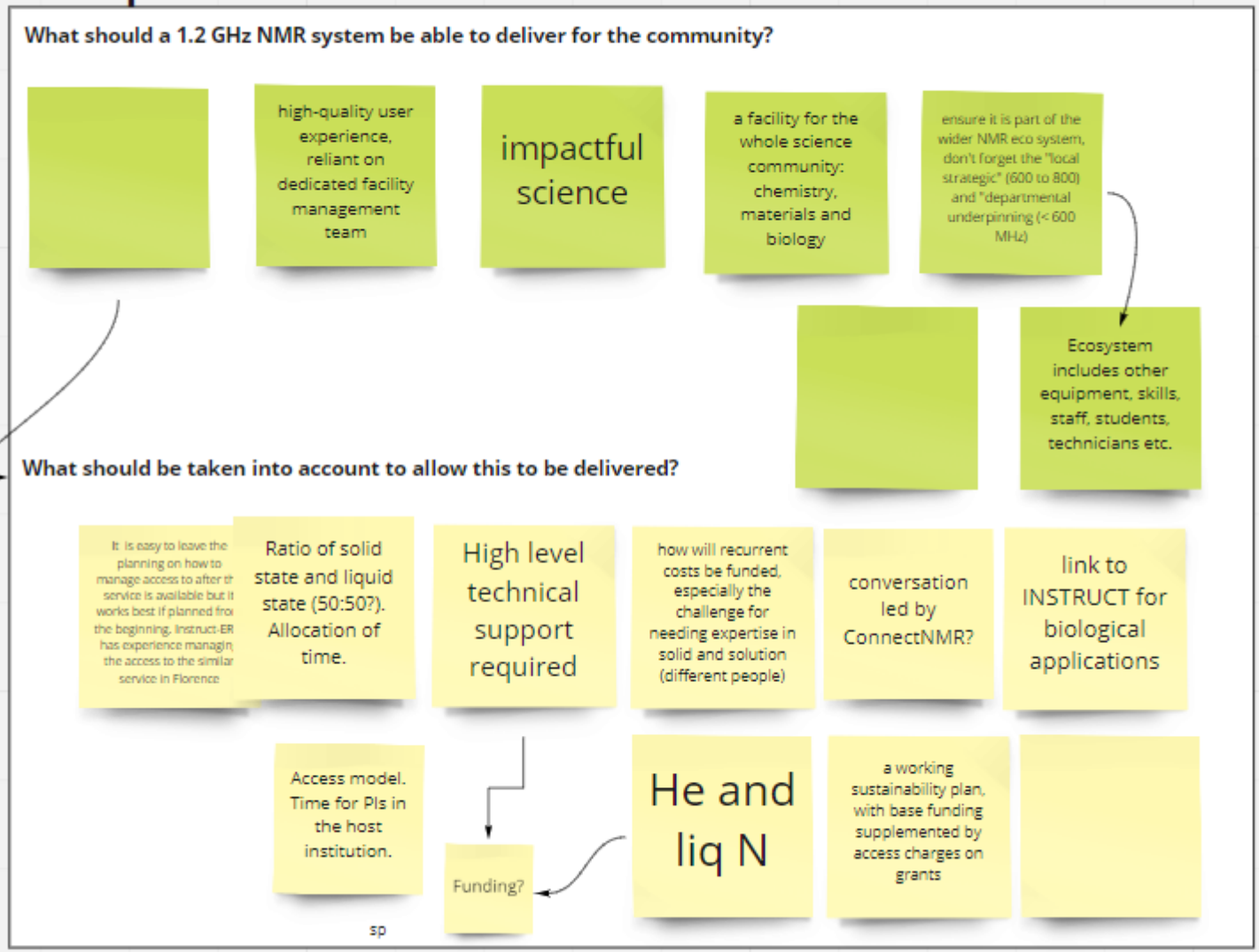
What should be taken into account to allow this to be delivered?

MEETING 2 07 DECEMBER 2021

Facilitation boards



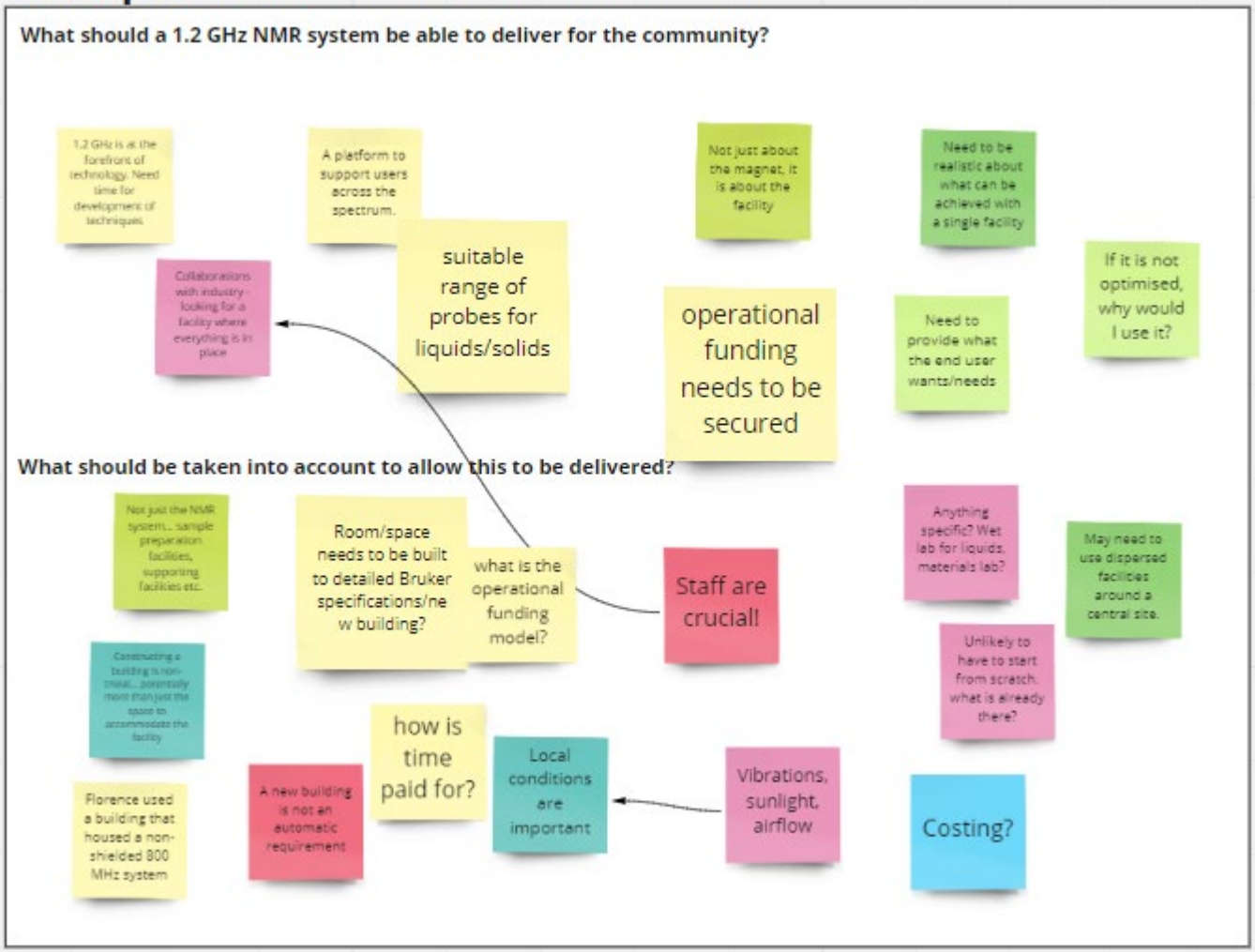
Group 2


What should a 1.2 GHz NMR system be able to deliver for the community?
high-quality user experience, reliant on dedicated facility management team
impactful science
a facility for the whole science community: chemistry, materials and biology
ensure it is part of the wider NMR eco system, don't forget the "local strategic" (600 to 800) and "departmental underpinning (< 600 MHz)
Ecosystem includes other equipment, skills, staff, students, technicians etc.
What should be taken into account to allow this to be delivered?
It is easy to leave the planning on how to manage access to after th service is available but it works best if planned fro the beginning. Instruct-ER has experience managin the access to the similar service in Florence
Ratio of solid state and liquid state (50:50?). Allocation of time.
High level technical support required
how will recurrent costs be funded, especially the challenge for needing expertise in solid and solution (different people)
conversation led by ConnectNMR?
link to INSTRUCT for biological applications
Access model. Time for PIs in the host institution.
Funding?
He and liq N
a working sustainability plan, with base funding supplemented by access charges on grants
sp

Group 3


What should a 1.2 GHz NMR system be able to deliver for the community?
Will probes be costed upfront or over time? 3-4 year period? Money set aside - concern
Distribution between use of solid and solution machines. Materials and bio requirements - hardware
New probe development to accompany the equipment - need for a broad range for the community. Timing issue.
Funding package - contingency funding for extra probes/ development.
Industrial applications - demands are quite different for complex mixtures. Need funds for probe development and future probe demands - at least 3 years. UK could be a leader in biotechnology applications and everyday materials and this should be a focus. (3)
Deadline for when money should be spent. Option to develop probes.
Currently a focus on solution probes
What
unt to allow this to be delivered?
What are the best probes to serve the community? How is that decided? How
Level of staffing and the right expertise - challenge. Mixed mode will demand high level of and varied expertise on one site. Now breadth in UK for the chosen site. Consortium bids welcome.
Support for RTPs. Should come together with funding for people (at least 2 or 3) - experimental officers who know the hardware but also the implementation for complicated experiments/ interpretation of results. Advanced techniques to bring NMR to the table. Role for partnership with Bruker?
Dedicated staff - skills and people exist but without the time allocated - right expertise - host institution and advisory board needs to make sure applicants dedicate appropriate staffing resource. Challenge!
Brucker application support - needs to be pinned down.
High sensitivity - area of focus as it might need probe design.
Bruker- what models used across Europe? Only every don as a collaboration with people site but no linked positions, bo would be fantastic. Not enoug people dedicated to the techni side. Co-technical officer. Negotiating contracts - this is something to bear in mind.
Building demands - sustainability
Risk of facilities being underused without the technical expertise. Need to explore capabilities. (1)
Government priorities and capitalise on growth areas e.g. materials (sustainable polymers, everyday substances). Potential hosts should address these capabilities as part of selection process. Enough people aligned in this area (2). Distinctiveness from other institutions - what can the UK do better?

Group 4


What should a 1.2 GHz NMR system be able to deliver for the community?
1.2 GHz is at the forefront of technology. Need time for development of techniques
A platform to support users across the spectrum.
Not just about the magnet, it is about the facility
Need to be realistic about what can be achieved with a single facility
If it is not optimised, why would I use it?
Collaborations with industry - looking for a facility where everything is in place
suitable range of probes for liquids/solids
operational funding needs to be secured
Need to provide what the end user wants/needs
What should be taken into account to allow this to be delivered?
Not just the NMR system... sample preparation facilities, supporting facilities etc.
Room/space needs to be built to detailed Bruker specifications/new building?
what is the operational funding model?
Staff are crucial!
Anything specific? Wet lab for liquids, materials lab?
May need to use dispersed facilities around a central site.
Unlikely to have to start from scratch, what is already there?
Constructing a building is non-trivial... potentially more than just the space to accommodate the facility
how is time paid for?
Local conditions are important
Vibrations, sunlight, airflow
Costing?
A new building is not an automatic requirement
Florence used a building that housed a non-shielded 800 MHz system