NHMFL User Committee Report 2022

Chair: Nicholas Butch (NIST & University of Maryland)
DC/Pulsed/High B/T Vice-Chair: Brad Ramshaw (Cornell University)
NMR/MRI/ICR/EMR Vice-Chair: Aaron Rossini (Iowa State University)

(1) Executive summary

The user committee is pleased overall with the MagLab's performance and progress toward a return to pre-pandemic operations. The MagLab continues as the premier provider of high magnetic fields for a broad research community representing a spectrum of scientific disciplines. We commend the NSF and institutional partners for their continued financial and logistical support. Here we provide a summary of important points that affect the whole MagLab. Facility-specific discussions are in the following sections.

Capability Improvement: The users largely continue to be impressed by the quality and number of magnet systems available at the MagLab. We support the ongoing development of planned hybrid systems and HTS superconducting magnets. We fully encourage collaborations between industrial magnet manufacturers and the MagLab magnet development teams.

Infrastructure Maintenance: The user committee looks forward to a Conditional Assessment, although we are concerned about uncertainty related to the process and scope. Maintenance of existing infrastructure is of fundamental importance. LANL's support for the generator repair is a wonderful example of the necessary efforts, but aging equipment exists MagLab-wide. We encourage the NSF and host institutions to work with the MagLab to address these issues now, before they become existential problems.

Staffing: MagLab management has been proactive in filling many requested positions across the lab. However, the NSF, institutional partners, and NHMFL management should continue to address issues related to retention and hiring of staff. Excessive workload for permanent staff can be partly alleviated by providing the requested funding for post-doctoral fellows and technical staff. MagLab management has discussed a number of concrete steps to ensure that staff are retained and we encourage them to follow through on these initiatives.

Helium: We were pleased to learn about efforts to improve helium recycling across MagLab sites. It is crucial for MagLab and partner institutions to support upgrading and installation of helium recapture, recycling, and liquefaction facilities. Increasing costs of electricity are also impacting the MagLab operations.

Data: The majority of users agree with the principles of FAIR data initiatives. However, FAIR data protocols need to be carefully implemented and devised so that they do not become an excessive financial or time burden on MagLab users and staff.

Housing: Limited and expensive housing availability in the vicinity of the MagLab sites continues to be a concern for many users, and the situation has only worsened recently. It is a particular financial strain for users with limited funding. While we recognize that there are no easy solutions, we ask that the NSF and partner institutions find ways to reduce or mitigate the cost of housing for onsite users.

Future 30 T Magnets: NSF and the National Academies have advocated for commercialization of 30 T superconducting magnets and for creation of user facilities across the country. We are supportive of installation of 30 T magnet systems that will be open to users. However, we caution that these magnets need to be installed at sites that will fully support and maintain these magnets going forwards. We also recommend that the deployment of magnets at other sites does not occur at the expense of existing MagLab facilities and operations, which are already strained.

(2) 2022 Report of the DC Field Facility User Advisory Committee

Overview: Our advisory subcommittee is very pleased with the continued progress being made at the DC Field and High B/T facilities. The user base is back in person near pre-pandemic levels and several critical infrastructure upgrades are in progress. Excellent progress has been made on the 32T superconducting magnet system. Additionally, impressive advancements with measurements in extreme conditions have been made by research personnel.

DC Field: We are very pleased to see the progress made in the past year for running user experiments in the 32 T superconducting magnet system. Further improvement of the performance of this system, including both the magnet and the sample electronic temperature, is important for users and for generating scientific output. It would be very helpful for users if the magnet lab were to install electronic filtering and thermalization circuitry on each of the probes provided for this system (as has been done for a prototype specific heat probe). We also encourage efforts to more accurately measure the value of the magnetic field as the field is being ramped.

We are also strongly supportive of the DC Field facility's ongoing efforts to upgrade its magnet power supply system and are appreciative of the State of Florida stepping in to provide funding for essential switchgear and power conditioning circuitry. These efforts will increase magnet performance in addition to the reliability of the facility overall as they will mitigate voltage fluctuations in the incoming 12.5 kV feeders. These fluctuations have led to repeated trips of the 36 T series connected hybrid (SCH) during magnet runs and also affect other magnets with high inductance. The trips lead to a significant loss of magnet time. These are highly sought-after magnets and issues with fluctuations in the incoming power are demonstrably reducing research productivity. For these same reasons of stability and reliability we also call for urgent implementation of an infrastructure upgrade identified in the renewal proposal (for which funds have not been allocated) to replace and modernize the current power supply thyristor control units before they reach the end of their service life.

High B/T Facility: We are excited that the High B/T facility has continued to expand its laboratory capabilities including the addition of a cryogen-free dilution refrigerator equipped with a 14 T magnet. The research staff is to be commended for their development of impressive new capabilities for state-of-the-art user experiments, including new methods of ultra-low temperature thermometry, sample mounting and filtering, as well as developing new experiments to achieve ultra-low electron temperatures. Nevertheless, issues with keeping the magnet cold between users due to inefficient helium recovery remain. Based on our discussions with research staff these issues could be resolved with some additional funding. Given the increasing cost and shortage of liquid helium, we strongly encourage this to be done.

We also feel that the expertise, knowledge-base, and resources at the High B/T facility strongly position it to host a second generation 30 - 32 T superconducting magnet facility. Lessons learned from this effort would be an essential step towards the standardization and commercialization of this technology needed for 30 T class satellite magnet labs.

Measurement equipment update/development: We are delighted to see that improvements to equipment and measurement capabilities have picked up in the last two years of operation. We would like to encourage the DC Field facility to continue to make improvements and, furthermore, explore new techniques for measurements and reducing electrical noise and thermometry at high fields.

Recommendations:

- Improved rotators (better knowledge of angle, better angle control).
- Better setups for filtering noise and switching filters in and out for probes.

- Write up and share technical guidelines for troubleshooting noise in well-known experimental setups (SdH, dHvA, Fan diagrams, TDO).
- Dedicated and thoroughly tested NMR probe for 32 T.
- Make trampolometer magnetometer and tuning fork thermometry measurements available to users of DC field facility in all appropriate magnets and cryostats.

Personnel: Key personnel such as staff scientists and technicians have left the lab recently to take external positions or retirements, severely reducing staff scientist support in condensed matter NMR and the mK facility. Salaries and benefits provided to staff appear to no longer be market competitive. Additionally, 30% of users reported some level of disruption to their experiment caused by staff turnover due to COVID. We greatly appreciate the commitment from FSU to address staff turnovers and look forward to developments on this front. Attracting and retaining world-class talent is essential to preserving the MagLab's world-leading status.

Data Management: We are impressed by the substantial efforts being taken by the MagLab to comply with the FAIR Data protocols. However, these efforts continue to pull financial and human resources. Having users work on FAIR data protocols would severely reduce scientific productivity. Therefore, we strongly recommend that sufficient support be allocated for hiring additional magnet lab staff for the development of software and domain specialists needed to meet the requirements of the FAIR Data protocols. We also recommend removing the existing maglabusers.org site because of its limited use. Instead, we suggest it is replaced with the "Comment Card" plan, which is a more effective method to receive user feedback.

Housing: We ask the partner institutions who already offer housing solutions (e.g. dorm rooms, on-site campus hotels) to find creative solutions to help us do the work at your sites, especially when stays overlap with home football games. One committee member suggested the use of RVs.

(3) 2022 Report of the Pulsed Field Facility User Advisory Committee

Overview: The UC is grateful that MagLab staff have worked extremely hard to keep the PFF world-leading in terms of available fields and measurement techniques, experimental throughput, and scientific output over the last year despite numerous difficulties. Efforts in technique development, such as high pressures, applied strains, new optical and THz capabilities, and current control in transport measurements are greatly appreciated.

Generator: We are extremely pleased to hear about the repairs of the 1.4 GW generator, and are very happy about the progress regarding the creation of the new rotor and grateful to LANL for funding and support. We are actively looking forward to user operations on generator-driven 100 T and 60T Long-Pulse magnets scheduled for 2025. However, as mentioned in our last report, we remain deeply concerned that these advances are endangered by lack of core funding for replacement of the aging magnet-power delivery controllers (*i.e.* PSRs). We anticipate that failure of these modules could take

down user operations on generator-driven magnets for extended periods. The UC sees this as a major problem that needs to be addressed.

Development: The UC is very happy that during the current down time in the generator-driven magnets, the PFF have made strong efforts to keep peak fields, magnet-shot numbers, and scientific output at a very high level. Much of this is thanks to strong efforts from the staff and has been enabled by surge-funding. We particularly note the following items:

- We see as a great success the 75 T duplex magnet program and the reported 600 shots in excess of 70T.
- We relish the prospect of 85 T (and higher) user magnets powered by the new surge-funded 30 kJ capacitor bank.
- We appreciate efforts to bring online soon an interim 85 T magnet, powered by existing capacitor banks to mitigate COVID-related delays to the new capacitor bank.

Funding and Infrastructure: The committee is extremely concerned that shortfalls in the core NSF budget, amplified by inflation and global crises, are impacting directly on the user program. Lack of core funding for user-support staff as well as magnet design and operations staff, coupled with increased costs in consumables (*e.g.* helium, high strength conductors) will lead to a 20% reduction in magnet time available to users (close to 130 magnet-cell days will be lost), as well as a slowdown in magnet development which will profoundly impact future experiments. In addition to this, the magnet-power delivery controllers (*i.e.* PSRs) are seen as a significant potential danger to future user measurements.

We understand that an NSF Conditional Assessment process is imminent which in principle we welcome, but urgently request clarification from the NSF regarding what this process will involve and how it will help with the replacement of aging mission-critical equipment.

Another major concern of the UC is the future availability of Cu:Nb high-strength conductor, which is currently a vital component of the PFF's highest field magnets, specifically the inserts of the 75 T and 85 T duplex magnets, and the world-leading 100 T magnet. At present, the sole source of Cu:Nb is located in the Russian Federation. This situation provides a direct risk to NHMFL users' access to the world's highest fields. Moreover, with magnet laboratories in other countries retaining access to this conductor, this issue also impacts on US competitiveness in the area of high magnetic fields. The UC strongly believes that action should be taken now to invest in research/development and manufacturing of the highest strength conductor within the US, before local stocks are depleted.

Data: The UC is pleased that the FAIR data guiding principles are taken seriously by the PFF and their implementation is on the right track. However, we have the impression that there is significant confusion and ambiguity regarding implementation of the FAIR data and open-access practices, particularly in light of the recent OSTP August 2022 policy announcement, as well as an unrealistically low level of funding for this complex and far-reaching initiative provided by the NSF.

Other concerns: The UC has received several reports from users regarding LANL-badging problems post-covid, with users at times arriving on site and unexpectedly finding that they do not have access. While these issues appear to be in the minority of cases, they are still concerning and should be addressed. The

problems appear to be partly due to staffing issues at the PFF, but also due to changes in the LANL badge-office protocols and the need for appointments. We understand that in the future there will be a LANL badge office located in Los Alamos town which should improve access. However, more could be done to assist users with the frequently opaque badging process. It would be very helpful for users to have the ability to check on progress of their badge application, as we understand is the situation at other US national laboratories.

The UC would like to see the ability to access video conferencing on site, even in a limited capacity, for example in a dedicated quiet space at the magnet lab. This would better enable PIs to attend extended magnet time and still deal with commitments at their home institutes, with the overall goal of improving PI presence at LANL.

We also note again that availability and cost of lodging in the Los Alamos area remains a concern.

(4) 2022 Report of the NMR/MRI User Advisory Committee

Overview: We commend the outstanding efforts of NMR/MRI staff for running a world-class users program and also pushing the boundaries of magnetic resonance technologies. Work at the MagLab has enabled NMR experiments that provide important advances in the understanding of materials, chemical and biological systems. This is truly an exciting time to work in the field of magnetic resonance given the developments of high-field magnets for spectroscopy and MRI and the development of DNP techniques. However, the cost of these instruments usually far exceeds resources available to single PIs. Hence, the availability of these instruments at a shared user facility is crucial to many areas of research; without these facilities many research programs would become non-competitive or fail.

There is clearly a high demand for the NMR and MRI facilities. Usage of the facilities has returned to pre-pandemic levels and we were very pleased to learn about the large influx of new users; in 2021 32% of the users were first-time users and more than half of all users were post-docs, students and young scientists. The productivity of the user program remains excellent as gauged by the number of peer-reviewed publications (100+) and the high impact factor of journals where they are published. Staff has also restored access to the 36 T SCH system back to peak levels and this system continues to deliver ground-breaking results in both materials and biological sciences. The planned developments of imaging capabilities for 21 and 35 T systems and extensions of NMR experiments to the 32 T DC magnet are all exciting developments fully supported by the NMR/MRI user committee. The NMR/MRI staff and leadership have gone above and beyond expectations to obtain external funding that helps to support the user program and provides novel equipment and capabilities to the MagLab. In-house probe development continues to be exemplary with a variety of MAS probes coming online for the 36 T SCH and 600 MHz DNP systems and X-nuclei probes for imaging.

Funding: The NMR/MRI user committee is extremely concerned about the budget cuts imposed by the NSF. These budget cuts are especially alarming because the USA is falling further behind European institutions, and will soon be outpaced by Asian institutions, in the installation of high-field NMR systems.

Access to high field NMR and MRI facilities is crucial for early career PIs and for training of graduate students and post-docs. In this regard, the committee strongly opposes the implementation of user fees to make up for NSF budget shortfalls as fees will create an insurmountable barrier to facility access for many users; we note that there are no user fees within European NMR facilities. The NMR/MRI committee strongly supports the idea that fee for service experiments for industrial users could help to partly offset budgetary cuts, although, there are obviously limits in the number of industrial clients and fee for service would mean less magnet time for users. MagLab management has been proactive in filling many requested positions in the NMR and MRI program. However, the NSF, institutional partners, and NHMFL management should continue to address issues related to retention and hiring of staff. Excessive workload for permanent staff can be partly alleviated by providing the requested funding for post-doctoral fellows and technical staff. MagLab management has discussed a number of concrete steps to ensure that staff are retained and we encourage them to follow through on these initiatives. We are generally supportive of the FAIR data initiative, however, we caution both the NSF and MagLab management to not make these initiatives into a time or financial burden. We encourage staff to find solutions to refurbish/replace aging high field NMR magnets and consoles that have served the user program well and are in high demand. Downtime of these systems will impose further demands on other NMR systems.

DNP: The committee is impressed with operations of the 600 MHz DNP (243 days of usage in 2021), which clearly continues to be a valuable resource for the materials and biological NMR communities. The MagLab continues to lead in technology development for DNP probes, polarization agents, helium cooling, and DNP theory development. This system, however, is getting old and the gyrotron, in particular, is getting close to the end of its projected lifetime. The committee is concerned about the consequences to the broader solids NMR community should this system fail. We urge the MagLab to develop a contingency plan in the event of DNP system failure. We also encourage program leaders to continue to seek funding (e.g. through the NSF MRI or NIH mechanisms) for additional DNP systems (e.g. 400 MHz and 800 MHz), which will alleviate the load on the 600 MHz system and continue to push the boundaries of DNP, probe development, helium cooling, and microwave technology development.

Imaging: The committee was excited about the plans to pursue high field MRI with relatively large bores that would allow cryoprobe detection for a wide range of nuclei. This would fill a gap in existing high field systems, which almost exclusively have smaller bores that limit access, and would take advantage of the MagLab staff's world-class expertise with X nuclei probes.

(5) 2022 Report of the EMR Facility User Advisory Committee

*The EMR committee met separately this year

Overview: The user committee (UC) recognizes the continued productivity, innovative development of new equipment, and pursuit of excellent science by the EMR group. We note a trending recovery of the user base after the initial drop induced by the global pandemic. One cannot expect an immediate recovery of these user bases; many labs of the users, across the world, were set back in various different ways.

Despite this point, the group continues to publish high-tier science, with manuscripts in prestigious journals such as *Nature Chemistry*, *Nature Communications*, *Journal of American Chemical Society*, and *Chemical Science*. With new capabilities and newly retrofitted equipment coming on-line, the UC hence expects the user base of the EMR group to return to pre-pandemic levels quickly.

Personnel: The UC continues to be highly impressed by the expertise and the dedication of the EMR staff and its director. They are critical for the success of the EMR program. The UC is ecstatic that Thierry Dubroca has been brought on as a permanent member of the EMR staff. His hiring will provide long-term stability to the DNP program. The UC is glad that the EMR program was able to attract Tomas Orlando from Marina Bennati's group to a permanent position. His addition is expected to spark further growth in the biophysics/biochemistry user base.

The UC appreciates Likai Song's past service to the community. With Dr. Song's unexpected retirement, the UC recognizes that a replacement will be needed in the near-term. A particular focus should be placed on finding personnel who can maintain the sophisticated HiPER system and manage the heavy subscription of this instrument by the user base. In particular, the UC is concerned that some administrative aspects of HiPER operation are being delegated to FSU graduate students.

The UC recommends that the NHMFL hire administrative support for grant submission and management for PIs in the EMR division. Forcing PIs to handle a lot of the minutiae limits efficiency and successful smaller grants are integral to the success of the division. That Andrew Sarponetti has expanded duties within the MagLab necessarily has complications for operation of the EMR program.

The committee recommends that the selection committee for future hires continues to pay particular attention to EDI considerations in the selection process.

User Program: The UC is overall impressed by the ability of the EMR Facility to pursue impactful science (27 published papers in 2021 and 20 already in 2022). These results are featured in the best possible journals (e.g., *Science*, *J. Am. Chem. Soc.*, etc.). There have already been two publications in Nature family journals in 2022, demonstrating that the group continues its stellar productivity even in the pandemic. No major issues were brought forward from users to the UC in the past year.

To further grow the user base, the UC recommends the group to again host the EMR School once pandemic conditions allow. In-person is preferred, but a virtual or hybrid symposium may be a useful option. The UC commends EMR for hosting the Southeastern Magnetic Resonance Conference (SEMRC) in Tallahassee in November 2022. If the EMR school in Tallahassee is not an option, the UC suggests possible integration with the EPR school operated through the Rocky Mountain Magnetic Resonance Conference, or other conferences where EMR spectroscopy is applicable, e.g. those related to bioinorganic chemistry, or the SEMRC.

Capabilities: It is to the great relief of the UC, that the aging magnets for both the HiPER and homodyne spectrometers—two workhorse instruments—are being replaced. The UC thanks the MagLab for finally acting on this looming need before a crisis occurred. We expect these acquisitions to have an immediate

benefit in a variety of sub-fields, quantum science work in particular. The installation of these new magnets provides an opportunity to minimize helium consumption and make the facility more efficient and sustainable.

The UC recognizes the unique capabilities present at the EMR facility and is impressed with their approach of constant improvement and innovation. For example, the UC is excited to see EPR spectra acquired in conjunction with the 36 T series-connect hybrid (SCH) magnet! We further appreciate that the EMR group was resourceful and pursued these developments despite this being a need that continues to be unfunded. The UC is pleased that development of photoexcitation capabilities with proper safety standards has been achieved with the aid of recent hire, Dr. Elvin Salerno. The new technology implemented for the heterodyne instrument resulted in a 10x gain in S/N that will inevitably increase the throughput of samples and again further broaden the user base.

The UC supports an initiative to design lower frequency (10-20 GHz) equipment to function at higher fields. These capabilities could enable the MagLab to be a "one stop shop" for EPR, which the committee anticipates would dramatically expand the user base. Furthermore, the low-frequency/high-field space is almost completely unexplored with respect to spin dynamics.

We encourage the continued development of the photoexcitation capabilities to include a wide spectrum of tunable excitation wavelengths and ultrafast/pulsed laser-triggered optical detection.

FAIR Data/Open Access: The UC has reviewed the EMR group's website on FAIR Data use (https://nationalmaglab.org/images/user_resources/searchable_docs/request_magnet_time/data_management_plan_emr.pdf) and find it acceptable.

(6) 2022 Report of the ICR User Advisory Committee

Overview: Overall, the ICR program maintains a diverse user portfolio and is on track to recover from pandemic-related disruptions in user experiments (In fact, ICR publications increased during the pandemic.). Many users are opting to run remotely but some are starting to return to Tallahassee this fall. The program continues to be a world leader in instrumental capabilities across emphasis areas including biological and environmental applications. However, the sub-committee has significant concerns about sustaining growth and scientific diversification in this facility and has made appropriate recommendations to this end.

Core operations: A major instrumentation initiative for the upgrade of both the 21 T and 15 T system front ends has commenced under a collaborative agreement with Thermo Fisher Scientific. This effort will modernize and enhance the overall performance of these two platforms in key performance metrics such as acquisition speed and sensitivity. Concurrently, the advanced software architecture of this platform will enable the progression towards a more user-friendly GUI for experiments. The replication of the front end across the two systems will enable overflow experiments to be conducted with similar

methods on the 15 T and enable it to serve as a technology development platform for future implementation on the 21 T system.

The biological applications program continues to make significant contributions to the field of top-down proteomics. These achievements include core participation in the generation of the blood proteoform atlas, which is to date the largest top-down proteomics project ever published. This multi-institution effort resulted in a Science publication. Emerging user efforts include applications of top-down approaches to microbial systems.

The environmental/complex mixtures program continues to serve a large user base in the characterization of natural organic matter. An increasing number of users have focused on emerging and persistent pollutants such as PFAS ("forever chemicals"). Additional efforts have extended the institutional knowledge in petroleomics into the built environment.

Priority Recommendations: The number and diversity of user projects continues to increase each year and is not sustainable for the current staff number and organizational hierarchy. We encourage the ICR program to re-evaluate their current approach and consider alternatives such as increased experimental automation for sample introduction and data analysis pipelines as well as the recruitment of technical support staff to handle more routine tasks. These changes will allow the core staff to focus on research areas more suited to their high level of skill and training to further advance the user program. The upgrade of the two high field systems to a more user-friendly system is a key step in this direction.

The integration of the Eclipse system should be made a priority for the sole instrumentation staff member. To enable success and optimize the collaborative effort with Thermo Fisher Scientific personnel, a robust strategic plan and schedule of intermediate goals should be developed.

The ICR program should aggressively seek to hire a staff member to assume responsibility for the imaging user program. This position has been vacant for nearly 2 years. In tandem, this staff member should be engaged in a facility decision to update the ion source that had been previously purchased and is not compatible with the Eclipse front-end advancements. A recently commercialized imaging source that will be compatible with the Eclipse should be strongly considered as an upgrade path to further streamline instrumentation efforts and enable more facile user experiments. This upgrade should be considered in lieu of applying these funds toward the purchase of equipment for sample preparation. The most important utility of MS imaging in this facility is to provide extended MS performance beyond what users have at hand in their own labs or core facilities, not serve as an entry point for this technique. Users should provide demonstrable need for magnet time instead of relying on the ICR facility for exploratory experiments. Sample preparation for MS imaging is substrate dependent. The provision of such services is envisioned as an unnecessary burden. Sample preparation and data acquisition services on lower performance instrumentation can be achieved by the user at their home institution or in traditional core facilities where this capability is increasingly present.

A recurring recommendation in each recent review cycle has been the creation of a summer school type outreach event for complex mixture analysis. Such an effort does not have to be a condensed, in-person

week but could take the form of a virtual series of tutorial videos such as modules for MS fundamentals, instrumentation basics, and data analysis. This could be a collaborative project with key users to develop a repository of materials to lower the barrier to new ICR users and enhance onboarding.

Although the trend in mass spectrometry continues to be in applications and data analysis, we encourage the MagLab to renew the emphasis of the instrumentation program. This trend is also apparent in academic labs where student interest and funding for instrumental advancements has significantly declined, together with opportunities for workforce training. The ICR program has been the world leader for instrumentation developments in the field. Without continued efforts in this area, FT-ICR MS could become stagnant and the US lose its leadership.

It was brought to the committee's attention that Chief Scientist, Prof. Alan Marshall will be closing his research program in preparation for retirement. Prof. Marshall is co-inventor of the FT-ICR MS technique and has led the field during his career. His academic appointment at the Department of Chemistry in Florida State University, historically served as a trainee pipeline for the ICR program since its inception at the MagLab. We strongly recommend that the MagLab administration actively work with FSU to recruit an appropriate successor so they can establish their own training program to recruit top students. Without such collaboration between academic partners, the ICR program may lose its leadership in the FT-ICR MS community.