# NHMFL User Committee Report 2024

**Chair:** Franklin E. Leach III (University of Georgia)

**DC/Pulsed/High B/T Vice-Chair:** Brad Ramshaw (Cornell University)

**NMR/MRI/ICR/EMR Vice-Chair:** Galia Debelouchina (University of California San Diego)



## (1) Executive summary and general comments

Overall, the User Committee (UC) continues to be pleased with the National High Magnetic Field Laboratory (MagLab)'s performance and exciting future ahead under the new leadership of Dr. Kathleen Amm. The MagLab retains its leading position as the provider of high magnetic fields to a broad research community that impacts a diverse swath of scientific disciplines from basic to applied science. We thank the NSF and institutional partners for their continued support and commitment to maintaining the excellence of the MagLab. Here we provide a summary of important points that affect the MagLab community as a whole. Facility-specific discussions are in the following sections.

**Meeting:** The UC held its annual meeting from November 19-21, 2024 in Gainesville, FL, where we were hosted by the University of Florida site. We appreciate the hospitality of our institutional partner, personnel at the UF MagLab campus, and overall support from the MagLab User Program staff that enabled a productive gathering. Our annual meeting was preceded by a day of concurrent workshops that focused on the frontiers of high magnetic field science. These were titled "One magnet to rule them all: is there an optimal superconducting magnet design that can meet the needs of physicists, biologists, and materials scientists?" and "Quantum Information Science and Devices". We gratefully acknowledge the efforts of the UF hosts to develop a program that provided insights from contributors in these conceptual areas and led to fruitful discussions about future directions.

**Director Search:** The UC is appreciative of our inclusion in the search and interview process for the new MagLab director. It cannot be overstated that the voice of the user community should be heard as the facilities evolve so that our interests can be properly represented to successfully carry forward the core mission of the MagLab – to serve users around the globe. We look forward to future constructive conversations and transparency related to the future of facility leadership.

The UC was pleased with the selection of Dr. Kathleen Amm to serve as the new MagLab director. Based on our in-person interactions at the UC meeting, we were impressed with her future vision for "MagLab 3.0" as she seeks to continue and elevate the tradition of global leadership held by the MagLab. We particularly wish to convey our appreciation for her expressed intent to bringing back online critical flagship magnet systems and infrastructure needing repair and/or replacement. These efforts will be supported by her prior efforts in high field science and wealth of experience building partnerships. Additionally, we welcome a new era of increased interaction and open dialogue with Director Amm as the laboratory culture evolves based on the implementation of a formal set of core values.

**Condition Assessment:** The UC welcomed the news that the Facilities Condition Assessment (FCA) site reviews were conducted after our 2023 meeting and that a report was delivered in early 2024 by Aerospace Corp. The initial outcome is an Asset Management Plan (AMP) that will provide a roadmap for equipment and infrastructure preventative maintenance and replacement of capital assets necessary to maintain the lab's position at the forefront of high magnetic field science. An important component of these efforts are activities to increase resilience to climate change. The UC gratefully acknowledges continued, significant financial support from the National Science Foundation and the MagLab's institutional partners (State of Florida, Florida State University, University of Florida, and Los Alamos National Laboratory) to support these facility needs. These include replacement of the DC facility switchgear, cooling tower, and power supply. Additional items of note include the repair of the rotor and replacement generator drive/exciter at the LANL PFF generator and replacement of the AMRIS 11 T magnet for MRI/S. All of these assets are key to enabling sustainable, high-quality science for the user community.

We are also encouraged with the recent update that there is broad support for funding of the power delivery controllers (PSRs) at the LANL site. The PSRs present a major weak link for the PFF after the generator is brought back online. This outdated system has been maintained through the creative and industrious efforts of the facility staff. Based on our awareness, failure would lead to another delay of approximately 1-2 years for this user community. This scenario would be disastrous after the extended downtime experienced during the rotor repair.

Additionally, we remain concerned about the lack of clean, uninterruptible power for the UF High B/T facility. The procurement of funds for this need should be of the highest priority. The lack of this modern infrastructure presents a substantial risk for experimental failure as these measurements often require weeks (and sometimes months) to achieve and a loss of power during data acquisition negates significant effort on the part of users and scientific staff. This aging equipment also prevents our users achieving the lowest temperature regimes where novel, emergent phenomena are observed and lead to high impact science.

While we are aware of a tiered approach to the FCA dependent upgrades and replacements, we encourage diligent planning to avoid any delays in the Tier 2 category items which represent key needs for the resonance user community to maintain a reliable user infrastructure. The timeline for enhancement of these assets is not clear to the user committee and should be communicated as these plans are finalized.

**Limitations of Lab Access and Foreign Countries of Concern:** The MagLab UC community is a diverse group of scientists that includes US citizens, foreign visitors, and foreign nationals. The implementation of increased scrutiny for members of the user community by the State of Florida presents an elevated concern for the UC. We acknowledge that these requirements have not originated from within MagLab nor NSF and based on the location of the FSU and UF sites, adherence to this statute is required. Although at present it applies only to facilities at UF and FSU, such a policy could potentially push many users away from NHMFL including PFF, as experiments carried out at PFF are often based on prior results obtained from FSU and/or UF site(s).

Our primary concern lies in the core fact that this regulatory process stands in direct contrast with the mission of the MagLab and spirit of science as whole. Not only does this program induce additional administrative burden to process approvals and extended delays (~6-12 months) for the ability to perform science, it implies a discriminatory attitude towards our non-US users and colleagues. We fear the unforeseen consequences of this statute including diversion of potential users to other non-MagLab facilities and in the worst-case scenario, broaching the topic of whether or not the MagLab should remain at sites where the apolitical nature of science is not respected.

**National Academies Report:** Due to the proximity of the formal release of the 2024 NAS report, "The Current Status and Future Direction of High-Magnetic-Field Science and Technology in the United States", to our annual meeting, our user community has not fully processed this material. Facility committees have been tasked with evaluation of this information as relevant to their programs in latter sections herein and for future discussion. A key NAS recommendation that we fully support is the collaborative advancement of high field science via jointly-funded support from the appropriate federal agencies including NSF, DOE, NIH and DOD. Substantial investments continue in Europe and Asia and will lead to a loss of technology leadership and status at MagLab if a concerted effort is not made domestically.

**Future Magnet Development:** We continue to recognize the importance of sustained funding for the development of new magnet materials and designs to support future technology development for high field science. The historical division of and lack of continued funding streams has posed some limitations. Recent reductions in staff for the MagLab Magnet Science and Technology (MS&T) Program based on completion of capital projects and lack of ongoing funding have hampered support capability. The proposal of a risk

tolerant environment akin to 'Skunk Works' was a welcome notion along with new partnerships such as one with FermiLab to advance magnet technology. The need for continued domestic development and production of high temperature superconducting (HTS) materials was also buoyed by recent APRA-E funding.

The UC is excited to hear about a recent NSF MRI application to support a Large-Bore Resistive Magnet (LBRM) which will provide nearly two times the magnetic field over what is presently available in the US with bore sizes of 160 mm or greater. In the future, the UC would welcome some interaction with developmental magnets to facilitate both advancement towards a production magnet and as a means for exploratory basic science but not at the expense of progress towards reliable production of magnet systems. At the end of such a period and for all magnets, we strongly encourage well planned and documented hand-offs to the operations staff so that these transitions proceed smoothly without incident and to ensure robust and safe operation over time. Building on the "One Magnet" workshop, we encourage the MagLab to utilize this discussion to energize efforts to advance high field technologies required for the resonance facilities. Unfortunately, these disciplines are approaching a sole-source scenario where a single vendor will dictate the design and availability for these systems with accountability to shareholders potentially taking priority over scientific advancement.

**Workplace Enhancement***:* The UC applauds the development of a workplace values system that was launched in July 2024. Both the MagLab organization and user community will benefit from the establishment of norms for expectations that will be based on respect and clear communication. Moving forward, these activities will promote staff retention while also providing an attractive environment to recruit new talent for user support and technology development.

**Helium**: The UC is pleased with and encourages the MagLab to continue their efforts at helium recovery due to the nonrenewable nature of this required resource for high magnetic field science and inherent ability to decouple need from the volatility of market supply and demand. The inclusion of helium infrastructure upgrades as a Tier 2 component of the FCA is indicative of this progressive approach*.*

**Data**: The MagLab continues to serve as a leader in developing and implementing an open data framework. We anticipate future updates once the NSF has released their new Public Access Plan, and we continue to encourage engagement between the NSF and the MagLab FAIR data team. The effort to implement ORCiD will greatly facilitate the ability to track and monitor user output. We also acknowledge the future intent to expand the advisory capacity of the MagLab with community experts.

**Housing:** The limited availability and elevated expense of housing near all MagLab campuses is an ongoing concern for the user community. Given the spirit of an NSF user facility is to enable and democratize science, we again suggest that the NSF make a concerted effort to support travel and housing for MagLab experiments to ensure access to all. We also provide a reminder that other global high-field experimental sites routinely provide travel reimbursement and may start to present a more viable option to some users who have historically been affiliated with MagLab.

We are encouraged by the news that Director Amm has already worked to establish a relationship with the City of Tallahassee and that economic developments are planned that will likely provide additional housing and food options in closer proximity to the MagLab campus at FSU. We hope to see similar progress at the

LANL and UF campus dependent upon user needs. However, once new lodging is made available at the FSU site, we still anticipate the need for fixed-rate block housing agreements and/or needs based travel subsidies during periods of surge-based pricing at the DC facility (such as home football games and State legislative sessions). There also remains an important need for non-rent based affordable long-term dorm/visitor housing at the B/T site, as 6-month hotel stays are impossible, and rent cannot be charged to grants.

A creative solution to housing at the FSU site was realized by a member of the UC. To alleviate some of the supply and surge pricing issues during the collegiate football season, it was recommended that extended periods of facility downtime for maintenance be shifted from early summer to the latter part of the calendar year in fall. The football schedules are typically released at the end of the year prior which should provide ample time to strategically position downtimes. This transition also conveniently shifts downtime to overlap with hurricane season which can also hamper both facility uptime and user access due to storm activity. These cancellations necessitate complex rescheduling efforts on the part of the user program staff and such a shift would reduce the impact to both users and MagLab staff.

**Outreach and Access**: The MagLab maintains several excellent and popular outreach programs including an RF coil building workshop, several winter/summer schools, and community outreach days that occur annually. The committee recognizes those efforts and continues to encourage the MagLab to consider additional funding avenues for training new PI and young scientist users. These opportunities are required to sustain a thriving high field science community, especially in light of the emerging impact due to the largest workforce turnover in history as the 'baby boomer' generation heads to retirement. Prior discussions resulted in multiple approaches, some of which already exist and might be expanded upon: travel assistance or fellowships at the MagLab specifically for underserved scientific communities; summer-long internships for graduate students focused on building and developing instrumentation; and a MagLab small training grant for learning new techniques. The forthcoming loss of institutional knowledge in all high field science disciplines should not be underestimated.

## (2) Report of the DC Field and High B/T Facility User Advisory Committee

We begin by applauding the hiring of Dr. Kathleen Amm as the new director of the National High Magnetic Field Laboratory (NHMFL).

**Magnet technology and infrastructure:**

The highest technical priorities of this subcommittee are

1. Rebuilding the DC facility 32 T superconducting magnet and returning it to service
2. Installing uninterruptible clean power supplies for the high B/T laboratory

**Rebuilding of the 32 T SC magnet system**: The 32 T provided unique, highly productive experimental space, as evidenced by the series of publications from experiments in that system that are and continue to be cited as science highlights by NHMFL. The absence of the 32 T has been sorely felt by users and the slow pace of reconstruction efforts prior to Dr. Amm's appointment has been a matter of concern. We therefore applaud Dr. Amm's decisions to reinvigorate the system rebuild through two recent actions: (1) devoting at least 50% of one of the lab's senior magnet designer's (Dr. Mark Bird) time to the redesign of

the 32 T starting in the summer of 2024 and (2) establishing a collaboration with Fermilab to accelerate the magnet's rebuilding (beginning April 2025).

It is our understanding that the rebuild provides an opportunity to take advantage of both the lessons learned during the 32 T magnet's initial period of service and those from the 40 T magnet project and use these lessons to make design changes that would improve performance and reliability. We also understand that decisions regarding target field, availability of materials, and timetable for completion will affect what changes are possible to implement. We hope that as those decisions are made, the desire of users for a speedy return to service is clearly heard. Specifically, we ask that the lab adopt our recommendation that any redesigned and rebuilt system (1) be compatible with the current dilution refrigerator insert and probes, (2) reach a field of no less than 30 T, and (3) be returned to service no later than April 2027 and be made available to regular outside users as soon as possible thereafter.

We also endorse a design put forward during a workshop for user committee members prior to the start of our official meeting for a possible Quantum Limit Lab that would provide an electronically and vibrationally quieter facility for experiments in the extreme quantum limit. We encourage the lab to make this facility — and the development and availability of 25T + Bi-based superconducting magnets featured as part of the proposal — to further explore what would be required to construct this facility and to make the advancement of its design and construction part of the lab's next renewal proposal.

Towards that end, we encourage the DC lab to accelerate the reconstruction of probes for existing systems to allow for removable/insertable filtering and thermalization modules as well as magnetic-field compatible cryogenic amplifiers. We also note and applaud the continued work of the lab to upgrade the power supplies and associated magnet infrastructure (such as magnet cooling systems) to improve capabilities and replace obsolete components.

Finally, there is a need to extend the capability of the DC facility to allow users to carry out THz spectroscopy in the 0.3 ~ 3 THz range of magnon excitations. This is an area of high user demand. This would require an upgrade of available instrumentation, as the existing FT-FIR (THz) setup for the 35 T currently does not allow measurements below < 100 cm-1 (3 THz).

**Installation of a clean, uninterruptible power system for the High B/T facility**: In the years since the failure of the original system providing clean power for the High B/T facility, a number of worldleading experiments that used to be possible to perform at this flagship facility have no longer been possible due to increased parasitic heating and higher levels of electronic noise. Further, the experiments that are able to take place and the apparatus used to accomplish them are seriously endangered by the loss of uninterruptible backup power. There are critical periods during the typically month-long cooling process where the demagnetization refrigeration systems are particularly vulnerable to a sudden loss of electrical power. During these periods, the loss of power could lead to catastrophic failure of costly, custom-designed instrumentation and a loss of capabilities for years to come.

It is our understanding that a redesign is complete, that the cost of the redesign is now known, and that work can proceed immediately once funding is approved. We recognize that part of that approval process depends on passage of a federal budget for science institutions; we hope that the magnet lab's partner institutions will be ready to act to expedite the restoration of clean uninterruptible power for the high B/T facility as soon as possible. This is our highest priority for the B/T facility.

**Personnel:** We applaud the persistent efforts of magnet lab and the agreement of its partner institutions to secure opportunities for career advancement and promotion for some of the lab's technical staff, and look forward, almost as eagerly as the staff themselves, to the addition of similar opportunities for programmers and administrative staff. **The importance of this to us as users cannot be overstated.** Low noise facilities, resilient infrastructure, and superior magnets make great measurements possible. The staff make them happen.

With that in mind, we ask the lab to survey its DC magnet support staff and the full DC field user community as to the following proposal to make magnet-time less grueling on users by ending the evening shift earlier than 2:30 am. We propose a change for hours of operation of the DC facility from 6:30 AM – 2 :30 AM OPERATION to run instead either from 4 AM to midnight or from 5 AM to 1 AM. As a committee we are unanimous that this would greatly reduce late night experimental errors and lead to a favorable shift for both us and our data. Before pursuing this further, however, we would like to hear the opinion of the lab staff and full DC user base as to the desirability and feasibility of this proposal.

We also encourage the lab to look not just at the regular day to day work load for administrative staff but also to develop plans to better accommodate (1) the surges in staff workload that occur when there are unscheduled weather disasters or system failures requiring rescheduling of experiments and users and (2) the surge in workload associated with the introduction of new users at the beginning of each scheduling period requiring additional state and federal clearance before they can be granted access to the lab .

**Recruitment and support of new users:** The focus of NHMFL facilities has been advertising from unique capabilities and providing preferential access to first time users. We would like the lab to add tools that focus on "How to get started" as a NHMFL user. These could include

1. Pamphlets, procedures, and personnel
2. "On ramp" and stepping stone magnets, instrumentation, and support personnel
3. Internships for industrial partners, extended schooling/ apprenticeships for students
4. Delineated starter proposals for stepping stone systems requiring a 1 – 2 experiment proposal in lieu of standalone proposal + experimental supplements
5. Routine scheduling of two week sequences in which users would use a lower field magnet (such as SCM1 or SCM7) the first week followed by a higher field flagship the second week or, when appropriate, two weeks in the same magnet, so as to allow time to get on the air and gain experience with measurements, increasing the fraction of magnet time associated with productive data

Our goals are for people to be prepared and motivated to use the flagship systems, to have better initial data for full proposals to lab and individual investigator grants, and to improve the odds for successful experiments.

**Increased communication and collaboration**: Finally, we write to support Dr. Amm's proposal for more frequent communication and collaboration between the NHMFL User Advisory Committee and the NHMFL during the year.

For the DC and High B/T facilities, we suggest short quarterly meetings with the facility directors and corresponding user subcommittees over Zoom when we would receive updates on ongoing projects — i.e., general infrastructure upgrades, repairs, and/or failures, plus regular updates on progress in the

rebuilds of the DC facility 32 T system and high B/T facility clean uninterruptible power supply — and provide immediate feedback as needed on proposals requiring input prior to the next annual meeting (such as scheduling of the summer school).

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

**Overview:** The PFF UC acknowledges the hard work of the MagLab staff that has kept the PFF world-leading in terms of available fields and measurement techniques, experimental throughput, and scientific output over the last year. The committee is pleased to note that the number of users, and particularly the number of pulses per day, in 2024 has surpassed those in 2023. Additionally, the UC is very pleased with the implementation of the 75 T duplex and the 60 T mid-pulse magnets.

**Maintaining world-leading position:** attention is needed from the NSF and the MagLab if the NHMFL-PFF is to remain the world-leader in the future. We note that the 1.4 GW LANL generator remains the only demonstrated platform for repeatedly accessing 100 T-scale fields and will play a key role in the future position of the PFF in the world standing. Every effort should be made to prioritize its return to service and future-proof the ancillary equipment and associated magnet design and development. The UC is pleased to hear that the replacement process of the rotor for the LANL generator is on track. We appreciate that this is a complex, multifaceted project. We are actively looking forward to user operations in fields up to 100 T scheduled for the fourth quarter of 2025. We ask the PFF to contact the user community in advance of this to allow time for high-quality 100 T magnet time proposals to be developed. The UC is very pleased to hear the plan for designing and developing a 120 T magnet system. This will be an important step forward in maintaining our leading role in magnet development and design. We note that other institutes worldwide, including those with significantly higher funding levels than the PFF, are currently working on magnets with specifications that match or surpass those currently at PFF.

The UC is very happy with the 75 T duplex and the 60 T mid-pulse magnets put in place to fill the gap left while generator-driven magnets are down. Also appreciated is the imminent addition of the 85 T duplex magnet and the new magnet cell to accommodate it.

The UC encourages continued development of boundary-pushing experimental techniques and sample environments, including spectroscopy, current-controlled electronic transport, and applied pressures. We are also pleased about the refurbishment and standardization of the 65 T short-pulse magnet cells. The new short-pulse magnets appear to be a step-change in the design, providing unprecedented shot repetition rates for fields above 60 T. We note that the PFF leads the world in this regard and should be commended for both this development and for retaining and cultivating the talent needed to do so.

The UC also appreciates efforts made to balance funding from NSF and other sources to maintain sufficient technical and scientific staff on the user program. The UC greatly appreciates the very high level of support that the PFF receives from LANL, particularly in regard to the generator.

We remain significantly concerned about the replacement of the aging magnet-power delivery controllers (known as PSRs). The UC sees this as an existential issue for the PFF user program. This issue is intimately tied to the NSF Conditional Assessment, which is a process the UC welcomes in order to identify and

replace critical equipment, including the PSRs. However, we remain confused about exactly how the process is expected to evolve after the assessment has taken place and are worried that the timescale–over a year, by our understanding—of this process will endanger the prompt and safe return of the generator-driven magnets to the user program.

**Magnet Materials**: 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. At present, the sole source of Cu:Nb with adequate performance is in the Russian Federation. We understand that the current stock of Cu:Nb at the PFF is enough to produce around 5 insert coils for the 100 T magnet (for example). This situation provides a direct risk to NHMFL users' access to the world's highest fields. Moreover, several of the MagLab's competitor institutes retain access to this conductor, which endangers the MagLab's position as a world-leader in pulsed-field delivery. We appreciate that the PFF is aware of this situation and is taking steps to prioritize the remaining stock. However, the UC strongly believes that NSF should work with the MagLab and take urgent action to address this issue, such as directly funding the production of this wire.

**Data:** We are happy that the FAIR data guiding principles are taken seriously by the PFF and their implementation is on the right track.

**User Access:** We appreciate that some of the LANL badging issues identified by users have been mitigated with the introduction of a badge office in Los Alamos town center but would like to see greater transparency and for users to have the ability to check on the status of their badge application. We emphasize that it needs to be clearer whether students from particular countries will have their badges eventually approved.

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

**Overview:** The Committee is excited to see the cutting-edge science that the NMR/MRI and AMRIS facilities continue to produce and is impressed with the continued development of NMR probes and MRI coils for various applications, with performance that is significantly better compared to commercially available instruments. Despite necessary maintenance and repairs to several systems in Tallahassee and restructuring at AMRIS due to the core funds budget cuts, the user program has remained very strong and the number of new users has continued to grow. As a testament to this, all spectrometers and imaging systems not under repair continue to be utilized at maximum capacity, and the productivity as measured by the number of high impact publications, has continued to increase.

The NHMFL continues to support several unique instruments and capabilities, including the 36 T SCH spectrometer, the highest field NMR magnet in the world; the ultra-wide bore 21.1 T, the highest field MRI/MRS system in the world; a highly productive 600 MHz DNP spectrometer; several NMR/MRI/MRS systems with hyperpolarization capabilities; and advanced NMR probes and MRI coils that support unique applications. The Committee is also grateful for the outstanding support by the NHMFL partner institutions (FSU, UF, and LANL) who continue to invest in infrastructure, staff support, and instrument repairs and replacements. We also commend the facility directors for finding creative solutions to compensate for some of the budget cuts from the core funds (e.g., applying for other funding sources, working with commercial users, reshuffling positions), but we also recognize the stress that this has caused, and the additional responsibilities taken on by the current staff. We hope that together with the NHMFL leadership and

funding agencies, more long-term solutions can be found to this challenging issue. Several new hires are also needed to maintain competitiveness in research and cutting-edge probe designs and take off some of the load from the current staff. The Committee also supports potential partnerships with industry for the construction and acquisition of new equipment, as well as coordinated apprenticeship programs to exchange expertise.

**Condition Assessment:** The Committee commends the ongoing condition assessment efforts by the NHMFL leadership and NSF, however, there are several critical outstanding issues related to the NMR/MRI and AMRIS facilities that cause concern. This includes the replacement of the aging equipment in the control room for the 900 MHz (21 T) MRI/NMR system at Tallahassee, which includes instrument control and quench protection equipment that is more than twenty years old. This instrument is unique in the world with its extra-wide bore size which enables valuable MRI studies of small animals at ultrahigh fields. If the magnet were to quench due to a lack of support, it is unclear whether the system could be brought back up to field again, and even if it could, the associated costs would be prohibitive. Given the comparatively modest $310k cost required for the control room upgrade, this should be funded at the earliest possible time.

The Committee is also highly concerned that the 11 T MRI system installed at UF is nearing its end of life. Safety concerns have also been brought up regarding the instrument's large stray fields that have already led to minor injuries. The system supports unique capabilities from molecular studies to *in vivo* imaging, and is heavily used, especially for cutting edge X nuclei studies that require the greater sensitivity that comes from high fields. If the magnet were to quench due to ageing seals, it is unclear whether the system could be brought back up to field again, and even if it could, the associated costs would be prohibitive. The Laboratory views the replacement of this instrument with a more powerful and safer, shielded 15 T MRI system as a Tier 2 priority; a point that is supported by the User Committee.

**Staffing:** Budgetary cuts in core funding for the NHMFL have contributed to an increased level of strain for the permanent staff of the Lab. The NMR group has already lost two research faculty and the hiring of a new research faculty member to join the DNP effort would greatly help alleviate strain in this highly productive and world-leading user program. Administrative support for the large NMR, MRI, and ICR programs is currently handled through a single manager and two professional assistants, which has proven to be insufficient for handling the ca. 100+ person program (this includes staff, affiliates, graduate students, and postdocs). There is furthermore an increased need for more admin support to help with the increased barriers required for users outside of the U.S. to access the facilities at the Florida sites.

**NMR and MRI at high fields:** The Committee is excited to hear that the 36 T SCH magnet will be available to users again soon. When operational, this system is the highest magnetic field NMR spectrometer in the world (1.5 GHz); it is highly productive and in very high demand. The restricted availability (7 hrs a day), however, limits the type of NMR experiments that can be performed (e.g., biological samples often require several days of uninterrupted time). The impressive productivity and high utilization of the 36 T SCH magnet demonstrates a clear need for the installation of a superconducting high field instrument that could be run continuously. Therefore, the Committee strongly supports the ongoing efforts by the facility directors to secure funding for a commercial superconducting magnet operating at 1.2 GHz (and possibly beyond). While several 1.0 - 1.2 GHz systems have recently been installed at several sites in the US, they are typically run on a cost-recovery basis and as a result can never achieve the level of reach that the NHMFL would with

such instruments. In addition, the NHMFL uniquely has the expertise to build advanced NMR probes and support new MRI applications at such high magnetic fields.

The Committee also supports the acquisition and installation of a 1.0 GHz DNP and cryoMAS instrument. This instrument would enable enhanced-sensitivity experiments at high fields for samples where DNP cannot be applied owing to the loss of dynamics at low temperatures, or the chemical sensitivity of the samples. The proposed 1.0 GHz instrument would further introduce ultrahigh-field DNP capabilities to the United States and the broader scientific community, providing unrivaled sensitivity and resolution. The plan to make this a shared DNP and cryoMAS instrument is also commendable as it would ensure nearly 100% utilization of the instrument even during the early stages of the high-field DNP development.

The acquisition and installation of these high field superconducting instruments is viewed by the Committee as a high priority for the United States to remain competitive in high magnetic field NMR and MRI research for materials, chemical, biological, and imaging applications. Lastly, a key component of the success of the NMR programs at the NHMFL has been the probe development team. This team is facing disruptions in access to global probe components. It is likely that there will be a more than a doubled increase on the cost of sourced components in the near future, impacting the group competitiveness on the global stage.

**Outreach**: The NMR/MRI program is actively involved in dispensing knowledge and technical know-how through workshops. In 2024, the first edition of the solid-state NMR school and a specialized school for rf coil design were organized and well received by the magnetic resonance community. These are commendable initiatives and should continue to be pursued. The committee is also excited about potential apprenticeship programs (e.g., TAships or summer internships) where students can acquire in depth knowledge of RF probe design, DNP, NMR and MRI instrumentation. Considering the extensive expertise of the staff at the NHMFL in these areas, such initiatives will be tremendously valuable for the magnetic resonance community.

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

**Overview:** The user committee (UC) recognizes the EMR group's continued progress on sourcing of critical support and replacement equipment and efforts on maintaining its role as a leader in the EMR community. We note user numbers continue their return to 2019/pre-pandemic levels with even a slight increase from last year.

The UC is excited by the addition of new postdoc and student group members over the last year. However, there is still no highly qualified permanent (i.e. staff) personnel dedicated to operating and maintaining the high-power pulsed W-band spectrometer (HiPER), which we suggested last year following the unexpected retirement of Dr. Likai Song. HiPER is one of two main workhorse instruments responsible for a large number of publications in the EMR group, and in which a substantial investment ($750k) has recently been made. To assure the continued success of the EMR group and in support of efforts to grow the biological user base, we again strongly advocate for the addition of a staff member with a background appropriate for the highly specialized instrument and expertise in the methodology (i.e., deep understanding of EPR pulse sequences, and the applications) which preferably includes biophysical/biomedical EPR. The UC also shares the concern of the EMR group regarding the transfer of knowledge surrounding multiple upcoming

generational turnovers within the group. We recognize this is a concern across the lab and is especially crucial as many of the NHMFL-constructed spectrometers are unique in the world. We strongly encourage the Maglab and EMR group to take a proactive approach in identifying and hiring personnel to be trained by outgoing staff prior to their retirement.

The UC is extremely grateful to the Maglab and new director, Kathleen Amm, for enabling the last-minute purchase of a 1 kW EIK amplifier from CPI, the sole manufacturer of this product who unexpectedly disclosed their plans to discontinue production. The EIK provides the high-power capabilities unique to HiPER and the UC encourages the EMR group to begin now to identify solutions for another high-power amplifier source.

Echoing our report last year, the UC thanks the Maglab for prioritizing end-of-cycle funds for replacing aging superconducting magnets on HiPER and the transmission spectrometer, vital instruments in the EMR group. However, the UC is concerned about installation delays on these magnets due to manufacturing issues on Oxford's end (not a fault of the EMR group) which have led to significant downtime on both spectrometers. We applaud the group for continuing a high level of productivity and publishing despite this, and, given current troubleshooting progress, are happy it appears HiPER will return to service soon. The timeline on the other magnet is less certain and we encourage the Maglab to support the EMR group however possible in their dealings with Oxford on this issue.

**Personnel:** The UC would like to express our gratitude for the continued hard work of EMR staff and director in their dedication to advancing the role of the Maglab EMR group as a leader in the greater EMR community, eg, organization of an EPR symposium at the 2024 International Conference on Coordination Chemistry by EMR director Steve Hill and former EMR member Sam Greer, plans for EMR workshop associated with regional magnetic resonance conferences and for development of a national EMR User School at the Maglab. These efforts are despite the high existing time and admin burden within the group, which is only increasing due to loss of dedicated admin support staff and state of Florida mandated user screening.

The UC recognizes a strong need for the dedicated allocation of EMR staff on the most complex and specialized instruments in the group, specifically the high-powered pulsed W-band spectrometer (HiPER). The transition of Thierry Debroca from the EMR group - who had been helping with HiPER operation as a facet of his DNP research, although not his main responsibility - only amplifies this need. Given the substantial investment in HiPER, in line with its huge user demand and world unique status, the UC continues to recognize the need for a dedicated EMR staff to ensure smooth operation of and user support on HiPER.

The UC is concerned over preparations for imminent generational turnover in the EMR group. The upcoming retirement of Jurek Krzystek and Andrew Ozarowski necessitates hiring of replacement staff to allow for smooth transition of knowledge. Additionally, the UC is also concerned that administrative responsibilities are spread out across many MagLab-wide positions. The EMR program needs a dedicated admin support who can wear multiple hats (familiarity with user program, grants/budgets). In the last year Andrew Sapronetti's support for the EMR program was effectively cut completely and he currently only conducts student appointments. This was a concern of the UC last year and now even more so as the loss of his knowledge of the user program has furthered complications for operation of the EMR program. For future

hires, the committee recommends that the EMR team be encouraged to advertise widely, with a focus on attracting candidates from underrepresented groups, in alignment with FSU's non-discriminatory hiring policy.

**Personnel Recommendations:** The high-power pulsed W-band spectrometer (HiPER) is one of the two major instruments that contributes to 75% of all publications of the EMR division. However, as emphasized last year, there is no dedicated staff scientist to operate the system. Dr. Dubroca has helped to keep the instrument operational but has departed from the EMR division. This amplifies the need to hire a core-grant funded, long-term staff scientist that stabilizes the user support on the HiPER instrument and ensures vital, instrument-specific technical knowledge is retained in the group and not subject to turnover. In this context, the UC would like to reiterate that the majority of users are not EMR specialists, and thus, the user's success heavily depends on the intellectual and hand-on contribution by the EMR group. The new staff scientist would ideally also be responsible for maintenance and operation of the pulse X-/Q-band EPR spectrometer which was acquired via NSF MRI funding.

The UC is concerned that the distribution of the administrative operation of the EMR division is fragmented and potentially suboptimal. The UC recommends a more streamlined and focused allocation of administrative tasks to enhance the operational efficiency of the team. Ideally, the NHMFL administrative workload is assigned to staff with expertise in grant submissions, rapid onboarding of new hires, and management for PIs in the EMR division.

**User Program:** The UC applauds the ability of the EMR Facility to continue producing impactful science (19 publications in 2023, 24 so far in 2024) despite extensive downtime on both the transmission spectrometer and HiPER due to faulty magnets from Oxford. These two instruments alone were responsible for 75% of the EMR group's publications in 2023.

The UC notes apparent changes in the demographics of the EMR group user base (more senior and fewer PD/students) and in the type of user (fewer onsite). Although the share of first-time users has remained constant the latter development is worrying because when users send their samples for analysis it is a much higher burden on EMR support staff and resources.

**User Program Recommendations:** With the acquisition of a new X- and Q-instrument, the EMR group needs to advertise to the user base. One possibility to make users aware of the new spectrometer is the EMR school that is planned for the near future. Providing hands-on training on such commercial instrumentation during the school will significantly benefit students and postdoctoral fellows, enabling them to transition more seamlessly to utilizing advanced high-field instrumentation in their future research in EMR facilities.

**Capabilities:** The UC is disappointed to hear about the technical problems of the new superconducting magnets, one servicing the heterodyne transmission spectrometer and one for HiPER. These issues have led to significant downtime on these vital instruments which is still ongoing and are greatly impacting the ability of the EMR group to continue its work.

The UC is excited to know the pulse X-/Q-band EPR spectrometer and tunable OPO laser purchased through an NSF-MRI obtained last year by Steve Hill have very recently been delivered on-site. We hope that their

installation will proceed smoothly and quickly. This new ability for optical excitation can be integrated with existing W-band and high-field instrumentation, further expanding the NHMFL capabilities.

**Capability Recommendations:** The UC is very concerned about the inevitable upcoming failure of crucial, lower-cost (<$500k) components, for example, the investment in replacing the magnet of the workhorse heterodyne transmission system would be lost if the front-end frequency multiplier chain were to fail and not be replaced/repaired. We recognize this requires planning and highly recommend consideration of central funding or funding mechanism for de-risking total instrument failure due to failure of these components.

To improve the visibility and dissemination of research, the committee recommends that the EMR team leverages social media platforms as a strategic outreach tool. This approach will enable broader engagement with diverse audiences, including academic peers, industry professionals, and the general public, thereby amplifying the impact of their work.

The EIK provides the high-power capabilities unique to HiPER and while this purchase has alleviated any near-term issues, the UC is concerned about the inevitable need for another high-power amplifier source and encourages the EMR group to begin work now on identifying solutions for another high-power amplifier source.

## (6) Report of the ICR User Advisory Committee

**Overview:** The ICR program continues to lead globally in instrumental capabilities that span biological and environmental user research interests. This facility continues to build upon 30 years of investment by the NSF which has led to remarkable high-accuracy mass measurements that now enable the generation and analysis of datasets that reveal novel chemical insights unattainable by any other mass spectrometry platform. The program maintains a diverse user portfolio, demonstrating exceptional outreach efforts. Due to the time committed to upgrading the mass spectrometers attached to the 15 T and 21 T magnets, the number of users declined slightly this year. However, we anticipate that the number will return to, or even exceed, pre-pandemic levels in 2025 due to these enhanced capabilities which will lower the barrier to user access on these platforms. Additionally, the concurrent restoration of the passively shielded 9.4 T to prior performance levels and the coming addition of a new FT-ICR system on the actively-shielded 9.4 T system will result in the use of all magnets in the facility.

The ICR-UAC commends the institutional hiring committee for appointing Dr. Kathleen Amm as the new director of the NHMFL. Her leadership and vision are expected to drive the facility to new heights and ensure continued excellence in magnet science and technology. We also applaud the hiring of Prof. Kristina (Kicki) Håkansson as the new director of the ICR program after the retirement of Prof. Alan Marshall. Dr. Håkansson brings a wealth of experience and expertise that will drive the program forward and ensure that it continues to lead the ICR field. We believe that her leadership will attract new students, post docs, and staff to further enable the continued success of the ICR program. The ICR-UAC further supports continuous R&D to keep the NHMFL at the forefront of magnet science and technology, particularly concerning the development of higher field resonance magnets. The ICR-UAC also greatly appreciates the NSF Division of Chemistry's ongoing support of the ICR program.

**Core Operations:** The ICR-UAC is pleased with the progress made during 2024 to enhance the performance of the instrumentation, while simultaneously easing the challenges of data acquisition and processing. The major instrumentation upgrade initiative for the 15 T and 21 T front ends in collaboration with Thermo Fisher has now completed phase 2 (of 3), which enables instrument control, method execution, and data viewing using programs which are already familiar to many mass spectrometrists. This effort yielded two instrument platforms with markedly higher performance and a more modern interface that will flatten the learning curve for new users. Replicating the front end across the two systems allows overflow experiments to be conducted with similar methods on the 15 T, along with providing a technology development platform for future implementation on the 21 T system.

Additional hardware upgrades of note in 2024 further enhance the biological user capabilities and include the conversion of the Spectroglyph MALDI imaging system for compatibility with the Eclipse front end of the 15 T and 21 T platforms, along with the acquisition of a Vanquish Neo UHPLC system which will improve online separation capabilities across multiple modalities, allow the use of commercial columns for method development or user projects, and dramatically increase experimental throughput for both mass spectrometers.

Numerous experimental bottlenecks have also been addressed to unburden ICR staff of routine tasks and improve overall productivity. This includes development of automated methods for flow injection analysis for complex mixtures, which will allow the instruments to operate in an unattended fashion and significantly increase sample throughput. Impressive progress has also been made in automating the critical post-acquisition recalibration and elemental assignment software to further simplify the user experience when converting complex mixture data to knowledge and allow the mining of existing datasets to gain new insights into sample composition. The concurrent development of a software platform capable of *de novo* protein sequencing from top-down MS2 fragment data will greatly enhance the ability of both the 15 T and 21 T ICR platforms to identify novel proteoforms within biological samples and provide an immensely valuable resource to the field of top-down proteomics.

In addition, the development of selective gas-phase ion depletion will increase the compositional coverage of complex environmental mixtures like dissolved organic matter and PFAS-containing foams, through the removal of chemical noise and dominant, well characterized components [CR Weisbrod, *et al.*, *J. Am. Soc. Mass Spectrom.*, 2024]. All of these advances have occurred alongside a range of notable publications, including an investigation of the impacts of wildfires on the soil metabolome [JP VanderRoest *et al., Environ. Sci. Technol.*, 2024], an examination of the thermal stability of bio-oils [DC Palacio Lozano *et al., Energy Fuels*, 2024], and a determination of whether internal fragment ions are observed with electron-based top-down MS2 methods [NN Mikawy *et al., MCP,* 2024].

Beyond productivity improvements, the instrumentation development capabilities that are critical to the success of the program have been enhanced through the hiring of experienced staff including Dr. Nathan Kaiser and the aforementioned addition of Dr. Håkansson. The ICR-UAC believes that this group will continue to ensure technical growth and maintain the world-leading performance available only with the ICR Facility at NHMFL.

**Priority Recommendations**

***Instrumentation:*** With the improved capabilities noted above, we expect the staff to face some challenges created by the availability of the new hardware. Although the Eclipse front ends are ready for

routine use, a challenging list of Phase 3 development goals has now been assembled to implement several advanced data acquisition and signal processing strategies. The ICR-UAC encourages the staff to prioritize and primarily focus on goals that will best demonstrate new instrument capabilities while providing influential supporting data in time for the upcoming renewal.

***Imaging:*** The imaging capabilities in the ICR program are poised to rapidly expand in the coming year. The ICR program has purchased both an HTX M3+ sprayer enabling sample preparation capabilities as well as a commercial Bruker FT-ICR system which can be configured to multiple magnets within the facility, which doubles the number of instruments that can perform MS imaging. This system will also enable access to ion mobility that will provide an additional degree of gas-phase separation for both imaging and proteomics experiments. These acquisitions are critical in establishing imaging at the MagLab. The next key step towards successfully establishing a functional imaging program will be to hire an experienced post-doc to expand and support this user capability.

***Data acquisition and handling:*** The improved automation of these flagship systems will also mean larger data volumes going forward. The upgraded 15 T and 21 T systems can generate in excess of 1TB of data/day when all raw data is maintained. The ICR program will benefit from additional assistance provided by the MagLab and FSU IT staff to deal with the storage and processing of these larger data volumes. The pace of in-house technology developments would benefit from more flexible administrative control of ICR program computers. Currently there is a time-consuming process for installation of new software, and administrative access to ICR computers by one or more of the ICR program staff would be beneficial.

***Automated data processing:*** The ICR-UAC encourages the further development of robust, automated processing software that helps to extract the most information from the high-quality data that is routinely generated by the ICR systems. Previously, this effort required time from experienced staff with application and instrumentation domain knowledge. This software development might benefit from the addition of more experienced software developers and could be achieved by expanding on collaborations with outside laboratories, or perhaps adding shared informatics expertise that could be supported by all the resonance programs.

***Electronics support****:* For the first 25 years of operation at the NHMFL, a fully staffed electronics shop supported various scientific programs. This shop provided numerous benefits for the ICR program, given that gas phase ion control requires sophisticated electronics to generate necessary electric and magnetic fields. Currently, any necessary electronics work is either provided by external vendors (such as GAA Custom Electronics) or is done by existing staff whose expertise would be best applied elsewhere. The ICR-UAC recommends that the ICR program consider working with the other resonance programs to fund an electronics FTE to support future instrumentation developments.

***Future resonance magnet development:*** We encourage the active engagement of the ICR program with the MagLab Magnet Science and Technology group along with other resonance programs to conceptually plan for the next achievable target for high field FT-ICR MS beyond 21 T. Fruitful discussions were held during the pre-meeting workshop entitled “One Magnet to Rule Them All” and this momentum should be leveraged to plan for future high field ICR science.