

NHMFL User Committee Report 2021

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

NMR/MRI/ICR/EMR Vice-Chair: Aaron Rossini (Iowa State University)

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PFF Committee: Adam Aczel (Oak Ridge National Laboratory), Nicholas P. Butch (Executive Committee Member, NIST Center for Neutron Research), Paul Goddard (University of Warwick, UK), Lu Li (University of Michigan), Brad Ramshaw (Cornell University), Priscila Rosa (Los Alamos National Laboratory)

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ICR Committee: Jack Beauchamp (Caltech), Rene Boiteau (Oregon State University), Franklin Leach (Executive Committee Member, University of Georgia), Paul Thomas (Northwestern University), Patricia Medeiros (University of Georgia), Nathalie Agar (Harvard)

(1) Executive summary

This year's user meeting was still dominated by the impact of the COVID-pandemic, with limited user operation and physical access to the facility. The entire user community stands united in applauding the magnet lab for its management of this crisis. With user travel suspended, the staff scientists volunteer to take the burden of running experiments remotely - sacrificing their free time and their own scientific programs to prepare experiments and take data for the users. With the long hours of magnet time, and the even longer hours of preparation, this goes well beyond any reasonable expectations. It reached a level that users voice concerns about overworked staff, risking burn-out by stretching too far in this ongoing state of crisis. **The user committee urges the NSF and the partner institutions to do anything within their power to relieve this burden in an immediate and unbureaucratic fashion.** This should include the hire of temporary scientific and technical personnel to support them.

Infrastructure Maintenance. We saw a series of unfortunate electrical failures this year, which is ultimately linked to the aging electrical backbone infrastructure supporting magnet operations. The maglab has an effective maintenance and proactive servicing schedule that will ensure that the maglabs leading technology can be operated safely in the coming years.

We strongly appreciate the substantial support by the NSF and the partner institutions in upkeep, replacement and maintenance. Yet for reliable replacement strategies the maglab needs to secure funding for their ambitious maintenance plan. **The user committee would strongly welcome an invitation by the NSF for the maglab to provide a Conditional Assessment Report and an Asset Management Plan.** It is of critical importance to valorize the significant investments in magnet technology. We also suggest stronger communications and coordination at the highest levels between the maglab operations and the technical services at the partner institutions. This would be a no-cost measure to preempt loss of magnet time that occurred in this year (eg. network services, transformer ratings).

Diversity, Equity and Inclusion. We appreciate the ongoing efforts of the maglab to engage underrepresented minorities in natural sciences. The “Camp TESLA” is a summer program focused on students of color while SciGirls targets female high school students. We believe these efforts finally gain some traction reflected in the relative growth of the user base from underrepresented minorities. **We support these efforts, and would like to see more of them on all maglab sites.**

Human resources. The enhanced mobility during COVID and the growing demand for engineers and technical staff in the quantum technology sector causes a retention issue. The current pay scale for technical staff and lack of career development opportunities led to loss of talent. **We encourage the maglab and the institutions to find new solutions to adapt their conditions and salaries to the new market conditions.**

Housing. The user base looks forward to conducting experiments on site again, bringing back the issue of housing. Numerous complaints have reached the UC on two fronts: a) *frequent* price surges not covered by any funding agency due to special events (football weekend, balloon fiesta, Santa Fe arts market,...). b) The nature of science in the high B/T facility requires long stays up to 6 month. Hotel stays for this time are unsustainable, yet rent cannot be charged to grants. We agree the maglab should not enter the hotel business. **Hence 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.**

Renewal proposal. We enthusiastically support the renewal proposal by the magnet lab. The UC was often asked for input and our voices were heard in its creation.

FAIR Data. The UC acknowledges the need for transformation. We are worried that one global solution may not fit the different types of data of the various disciplines present at the maglab. We support the proactive yet cautious approach by the maglab and welcome the recent organization of workshops on this important topic.

(2) 2020 Report of the DC Field Facility User Advisory Committee

Overview: The DC Field-High B/T user advisory subcommittee is very pleased with the continued progress being made at the DC Field and High B/T facilities of the NHMFL.

Despite substantial ongoing challenges related to the pandemic and localized critical infrastructure failures and upgrades, the DC Field facility was able to offer a substantial amount of user magnet time in a remote format, while simultaneously making available to users a revolutionary new 32T superconducting magnet. All of this was achieved while maintaining the typically excellent standard of user satisfaction.

Core Operations: We commend the DC Field facility for its continued operation through the ongoing COVID pandemic. The facility rapidly developed remote measurement capabilities in response to the pandemic. Users sent samples to the scientific research staff and collaborated to perform the measurements using a “virtual presence rig.” As users increasingly return to the lab for on-site measurements, the virtual presence rig can be used by PIs or other project participants to become involved in the measurements without needing to travel to the lab. This improved communication should help better foster student training by PIs who would otherwise have limited ability to interact with them in real time. The committee strongly encourages a full return to in-person experiments as soon as conditions safely allow. Although it may be possible to continue to perform fully-remote experiments in exceptional cases, we believe these should be done sparingly since they are a significant strain on the time and energy of scientific research staff, and hold less value for student training.

New Magnet Developments: The 2021 review period encompasses a unique time for high field science, in which the development of major magnet projects progressed in spite of the COVID-19 pandemic. We are extremely pleased that the 32 T all-superconducting magnet (SCM4) has been successfully installed and is now open to external users. Bringing the system online has not been without some technical challenges. However, we view these as expected and necessary components of developing a new magnet system, and we believe the Magnet Lab is taking impressive steps to test the system quickly and carefully. We view the development of future superconducting magnets wound from high-temperature superconducting materials as a flagship effort of the Magnet Lab. In particular, we strongly support the development plans for a 40 T all-superconducting magnet and an associated 60 T hybrid magnet. These ambitious endeavors will continue to maintain the Maglab’s position as the unambiguous world-leading high field facility.

General Infrastructure Maintenance: Infrastructure failures have resulted in down time for a number of magnets in the DC Field facility, most notably due to power system failures. Such issues are often predictable, and could therefore possibly be prevented. Doing so, however, requires an adequate, reliable, and timely stream of funding for routine maintenance of infrastructure approaching the end of its known useful life. Current funding for maintenance is too low in amount and, when new problems are identified, too slow in arrival to reliably avoid otherwise preventable failures. We are strongly supportive of the DC Field facility’s ongoing efforts to upgrade its magnet power supply units, since efforts like these increase magnet performance in addition to the reliability of the facility overall. We stress the importance of taking a proactive approach towards the repair and updating of critical major equipment. We recommend building open dialog between the Maglab, NSF, and FSU to identify and address these issues prior to critical equipment failures. Towards this end, we hope that NSF will begin requesting formal *Condition Assessment Reports* and

Asset Management Plans from the Magnet Lab as a way of starting a much-needed conversation regarding anticipated maintenance and replacement expenses prior to the renewal proposal.

Personnel: Staffing turnover, although now commonplace as a result of the pandemic, can threaten the operation of the lab and its future development efforts. Key personnel from staff scientists to technicians have left the lab recently to take external positions. In many cases, retention offers were uncompetitive. We greatly appreciate the recent commitment from FSU to address this issue, and stress the importance of attracting and maintaining world-class talent for maintaining the Magnet Lab's world-leading efforts.

High B/T Facility: We are excited that the High B/T facility has expanded its laboratory space by over 50% in the past year, including the opening of the new High Bay Convergence Lab (HBCL). The research staff has also developed impressive new capabilities for state-of-the-art user experiments, including new methods of ultra-low temperature thermometry and sample mounting. However, we believe that there is a critical need to hire an additional scientific researcher to support the facility, as there is currently no dedicated staff for the HBCL. An engineering position is also needed to support the facility.

Data Management: We are impressed by the substantial efforts already taken by the Magnet Lab to comply with the FAIR Data protocol. These include setting up a system for users to easily publish FAIR-compliant data acquired at the NHMFL, and the hosting of a one-day workshop discussion on the topic immediately preceding this User Committee Meeting. The committee notes that additional supporting personnel will be required to adequately address FAIR Data compliance and database development going forward.

(3) 2020 Report of the Pulsed Field Facility User Advisory Committee

Overview: The Pulsed Field Facility (PFF) subcommittee commends the NHMFL PFF at Los Alamos National Laboratory (LANL) for its continued world-leading pulsed-field magnet science and excellence in user support across a breadth of disciplines. We highlight the successful continuation and expansion of core operations, the restart of the user program after COVID shutdowns, and the many important new hires. We are pleased that the user program has opened to onsite users, which is expected to increase available magnet time. The PFF subcommittee applauds LANL for its commitment to the PFF as evidenced by the \$24M support for the purchase of a new rotor. We support ongoing development and hiring efforts, and the initiative to develop magnet technology for fields exceeding 100 T.

Core operations: The effects of the COVID pandemic have had a large impact on the PFF, and the staff have done an admirable job operating the user program in a remote mode over the past year. User demand for magnet time has remained healthy over the course of the pandemic, with requests exceeding availability. Although a reduced number of magnet-hours has been available, we recognize that operating fully remotely has placed a large burden on the staff, who are to be commended. The PFF has recently opened to visiting users, which will increase user access and productivity, and provide valuable experience for students and

early career scientists. The number of concurrently operating magnet cells is expected to return to normal in the near future.

A critical recent development is the introduction of the capacitor-bank powered 77 T duplex magnet. This system provides an important experimental capability for users while the generator is out of commission. The subcommittee particularly commends the PFF facility for the swift development of the 77 T magnet to fill this gap. There is now significant user demand for this system and several high-impact publications have already resulted from experiments in this magnet. In the absence of generator-driven magnetic fields, the users also appreciate the availability of the 55 T mid-pulse magnet, whose long pulse allows for a number of otherwise inaccessible experimental techniques. The PFF has continued to deliver its proposed milestones, but sustained world-leading pulsed field science will only be possible with the strategic replacement of aging equipment. The cost of replacing the generator rotor is being met by LANL, whose continued support is lauded. The estimated delivery date is spring 2024, and first user experiments are expected in early 2025. The PFF subcommittee is in full support of the request in the 2023–27 Renewal Proposal for new magnet-power delivery controllers. If these controllers are not replaced, both existing and future programs will likely experience lengthy and avoidable delays that will severely impact user science. The PFF subcommittee emphasizes that the continued scientific output from the PFF also depends on the expansion of its user program operation budget, and we are in full support of this expansion.

The PFF subcommittee encourages the PFF staff to seriously consider hosting a summer school to advertise the science enabled by pulsed fields and train future users. Such outreach will grow the user base and attract a diverse pool of junior scientists to the workforce pipeline.

Hires & staffing: The PFF subcommittee is pleased with the recent hiring of three new staff scientists, Arkady Shekhter, Johanna Palmstron, and Minseong Lee, to address needs in high-field science, user support, and LANL-related programs. PFF management and more senior staff are strongly encouraged to identify and implement retention strategies not only to enable new staff to thrive in Los Alamos but also to foster an environment that will retain new and existing staff as well as sustain the PFF's recent growth.

The PFF subcommittee strongly supports an additional four hires for positions to support new magnets and recently-developed capabilities: 1) Magnet designer/engineer; 2) Designer/programmer for critical control systems; 3) Optical/THz spectroscopy scientist; 4) Extreme environments scientist. In particular, the first two hires bolster the 120 T project.

Initiatives

The PFF subcommittee commends three key PFF initiatives.

- Duplex: The next larger duplex magnet will offer magnetic fields of approximately 85 T, and the PFF subcommittee is pleased with the NSF “surge” funding for the associated 30kV capacitor bank, which will also enable testing required for the 120 T program. The PFF has admirably devised alternative strategies in the face of a delay

in the delivery of the 30kV capacitor bank. We support the upgrade and recognize the central importance of this effort to develop fields greater than 100 T.

- Pressure: The PFF continues to plan an applied pressure capability above 45 T for the user program. These specialized experiments will require a new, dedicated PFF staff member to finalize equipment and support the measurements, a post which the subcommittee firmly believes should be prioritized. We also recommend that the ability to make pulsed-field measurements on materials under applied strain should be included in this thrust.
- Terahertz: The PFF subcommittee supports the continuation of the terahertz project towards incorporation into the user program with a dedicated cell for optical measurements. This effort will require the hire of a new dedicated staff member. The formation of a strong user base with training for non-experts will be key to the continued success of this effort.

FAIR data: The PFF subcommittee is pleased that the FAIR data guiding principles are taken seriously by the PFF and their implementation is on the right track. The efforts led by Fedor Balakirev are in coordination with other NHMFL facilities as well as the internal LANL efforts. Data generated in the facility were categorized into user's data and the magnet operations and were subsequently given identifiers. Both sets are maintained such that they can be incorporated into the facility-wide FAIR data center eventually. This preliminary database has been working successfully.

(4) 2020 Report of the NMR/MRI User Advisory Committee

Overview: The NMR/MRI user committee was impressed with the ideas put forward in the NSF core renewal proposal. The addition of the instrumentation and staff described in the proposal is critical for the NHMFL to continue to address important challenges in materials science, catalysis, biochemistry and fundamental nuclear magnetic resonance spectroscopy/imaging. The proposed introduction of low-temperature closed-loop He spinning to the 14.1 T DNP system and construction of a static 30 T DNP system would push the boundaries of sensitivity and resolution and guarantee that the NHMFL continues to be a world class facility, with unique capabilities that attracts a broad base of users. Moreover, given their international user group, NHMFL has the opportunity to play a leadership role in the FAIR data initiative, as the NMR/MRI community has little experience with open data sharing. Traditional outreach activities for school-aged children have been difficult during the pandemic. These valuable efforts should be ramped back up as the pandemic subsides.

Recognizing that there are constraints on the core NSF budget, we commend staff for seeking other external funding opportunities to bring additional state-of-the-art DNP and ultra high-field instrumentation to NHMFL, including high-resolution NMR systems operating at frequencies above 1 GHz. Such systems are attractive to users as evidenced by results from the 36 T SCH system. European and Asian institutions will add more than 10 1.2 GHz NMR instruments in the next 3 years. Hence, high-resolution GHz NMR systems are desperately needed to maintain US competitiveness. The future development of > 35 T high-resolution magnet systems by NHMFL staff will provide a path to maintain competitive advantages over

other international NMR facilities. Solid plans are in place to expand the capabilities of existing instrumentation by implementing new fast MAS solids/solution NMR/MRI probes and converting existing magnet systems to better serve solids and MRI needs. It is crucial that NSF and NHMFL provide funding for routine console upgrades as these are the backbone of the entire NMR user program.

We commend the outstanding efforts of NHMFL staff to provide remote access to the facility during the pandemic. Within the context of the pandemic, the use of the facility by users remained extremely high (>80% of spectrometer time) and publication output from NMR and AMRIS was excellent (>150 publications in 2020). We commend FSU and UF for their significant investments into NHMFL staffing and infrastructure, despite the challenging financial environment faced by state institutions. However, the NSF, institutional partners, and NHMFL management need to address issues related to retention and hiring of staff. Excessive workload for permanent staff can be partly alleviated by the requested funding for post-doctoral fellows to operate the SCH and run biosolids user experiments.

Priority Recommendations

Series-Connected Hybrid (SCH) Access: The 36 T SCH system remains the highest-field, high-resolution NMR system in the world and continues to deliver groundbreaking results. Every effort needs to be made by NSF and NHMFL to maintain access to this precious resource. It is critical that funding for infrastructure be provided to prevent a recurrence of the issues that caused a substantial loss of SCH access in 2021. It is crucial that post-docs and other staff be funded to maximize the use of available SCH time. New applications on this instrument will be opened up by the solid-state NMR probes constructed by NHMFL staff. The planned addition of imaging capabilities to the SCH is also an exciting development.

Ultrahigh-Field Superconducting Magnets for NMR: NHMFL is an ideal site to host a 1.2 GHz high-resolution solution/solids NMR system. We urge the NMR/AMRIS leadership to coordinate with PIs from other US universities on instrumentation grants to implement a coordinated network of 1.2 GHz NMR instruments with broad geographical coverage. Proposals from these external PIs would be strengthened by support from the NHMFL's NMR Technology Group, which could supply unparalleled NMR probes to the network. In this scheme, the NHMFL would be providing leadership in high field NMR spectroscopy while enabling broad access to these instruments across the US.

NMR and MRI Infrastructure: We commend the NHMFL staff for successfully repurposing aging consoles; however, in the long run, the NSF must provide steady funding for upgrading outdated consoles. The committee considers the upgrade of the AMRIS 17.6 T console to be a high priority as it could alleviate demand on the 21.1 T MRI system. We strongly support core funding for the AMRIS High Bay Convergence Lab. Core funding for repurposing of the 18.8 T narrow-bore magnet at the Tallahassee facility will alleviate the ~200% oversubscription of the three 800/830 systems.

DNP: The committee fully supports continued collaborations on DNP between the NMR and EMR groups. A low temperature MAS DNP setup (~30 K) will provide much needed sensitivity for biological and material samples. Pushing DNP into the high field regime at 30 T would enable many potential applications in materials science. Both of these systems would be unique for the NHMFL and ensure that it remains a leader in DNP. Furthermore, the committee laud efforts at obtaining external funding to support 400 and 800 MHz DNP platforms dedicated to development of new DNP methodologies and studies of materials and biological systems.

(5) 2020 Report of the EMR Facility User Advisory Committee

Overview: The user committee (UC) recognizes the impressive scientific achievements in 6 of 8 Science Drivers (as defined by the NSF renewal proposal) by the EMR group over the past year, despite the ongoing challenges caused by COVID. We note that the EMR program's engagement in cutting-edge research within the quantum information sciences is in line with not only NSF's Quantum Leap Big Idea, but also with directives of other funding agencies in the US: Department of Energy, Department of Defense, etc. Additionally, we note EMR's collaborative role in developing Dynamic Nuclear Polarization (DNP), a key component of three Science Drivers. Part of these development efforts include the lab's recently advertised position for a Research Faculty member to build new instrumentation and develop new capabilities in high-field DNP. Such efforts imbue the EMR and NMR groups with new ideas and new functionality that ensure the long-term viability of the DNP program. The UC strongly recommends that the team hire a leading early-career EMR scientist (who would fulfill the "research faculty for high-pulsed EPR" specified in the renewal budget) and that the superconducting magnets for the HiPER and 15 T/17 T systems must be upgraded (consistent with the budget item to "replace aging superconducting magnets"). Doing so will arm the EMR group with the best tools and personnel to innovate in the immediate and far future. Further comments and recommendations follow.

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 glad that the EMR program was able to attract Elvin Salerno from Univ. Michigan to a post-doctoral position. Dr. Salerno brings expertise in time-resolved spectroscopy to initiate an effort to conduct proof-of-concept experiments in optically excited/detected EPR using the newly acquired laser.
- The UC is excited that the MagLab has advertised a position within the DNP group and that Thierry Dubroca is one of the applicants.
- The UC congratulates the EMR group for securing substantial external funding from NSF, NIH, DOE, and AFOSR for work in quantum technologies. Inevitably, these awards benefit the EMR program and guide development of the next generation of Science Drivers.

Recommendations

The UC repeats our *strong* recommendation from last year's meeting that new leading early-career scientists be added to the permanent staff of the EMR Facility at the MagLab. We see them as an absolute necessary addition in the short-term to inject new ideas and drive the scientific missions of the EMR Facility and the MagLab into the future. It is time *now* to have this search to be proactive about personnel replacement. We recognize the EMR Director's deep professional network that will provide access to a bevy of well-qualified candidates. And we would hope that one of these open positions would be considered for a faculty appointment in either the Physics or Chemistry Department at Florida State University.

User Program

Comments

- The user committee (UC) is overall impressed by the ability of the EMR Facility to pursue impactful science (43 published papers). These results are featured in the best possible journals (e.g., *Science*, *J. Am. Chem. Soc.*, etc.). There were even three publications in *Nature* family journals in 2021, demonstrating that the group continued its stellar productivity even in the pandemic.
- No major issues were brought forward from users to the UC in the past year.

Recommendations

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 symposium may be an option.

Capabilities

- 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 happy to see the EMR group move ahead with implementing EPR 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 the effects of the pandemic.
- In the vein of "improvement and innovation" the UC reiterates its previous concern about two high-use spectrometers: the HiPER and the 15 T/17 T systems. These two systems are workhorse instruments and any interruption in their function would seriously hamper the EMR group's productivity. The HiPER system was originally built using a 20-year-old "borrowed" magnet. Upgrades to this magnet/cryostat would make the instrument more user-friendly, allowing for a greater variety of experiments (e.g., quantum science experiments at low temperatures) to be performed and expand the user base. The 15 T/17 T system is unique in its ability to determine zero-field splitting parameters of complexes (a key metric relevant for spin-based quantum information processing). An upgrade to the superconducting magnet and frequency generation arm of the instrument would raise the S/N ratio. Higher sample through-put would result, and the new types of samples (e.g., highly dilute spins in

solids) would be able to be explored. The proposed upgrade would result in substantially greater field impact for this device.

Recommendations

- To allow for further innovations building upon the bedrock HiPER and 15 T/17 T systems, their superconducting magnets *must* be upgraded.
- To take full advantage of Dr. Salerno's spectroscopy expertise, we encourage the addition of tunable and high-powered photoexcitation (along with necessary safety infrastructure) capabilities. These new technologies will continue to broaden the user base and enable new and exciting science to be performed in the EMR group.
- We recommend pursuing upgrades and replacement of components for the high-frequency heterodyne instrument. This instrument provides truly unique capabilities that cannot be found elsewhere in the world and ensuring this instrument stays as the state of the art will continue the world-leading nature of this facility. These improvements would make the instrument more user-friendly—offering greater opportunity for student/visitor training and freeing EMR group staff for other activities. This should have the effect of increasing the throughput of samples and again further broaden the user base.

(6) 2020 Report of the ICR User Advisory Committee

Facility Overview: The ICR program at the MagLab continues to advance what are already the best high-resolution mass spectrometers in the world, opening new doors to chemical discovery across biological and environmental fields. These instruments continue to push the boundaries forward for molecular composition analysis of highly complex mixtures and large proteins in a wide range of biological and environmental fields. The committee is very excited about the recent addition of new front-end capabilities such as MALDI and a dedicated UPLC for environmental work. These systems will enable new analyses that leverage the unprecedented resolving power of the 21T FTICR instrument. The ICR program continues to add new users from a range of disciplines across the globe, with emerging contaminants, “forever chemicals”, and soil organic matter forming the latest applications. This ongoing broadening of the scope of science enabled by the capabilities at the MagLab should continue to result in quality publications addressing high impact research questions.

We commend ICR Facility for making their data align with FAIR data principles, spearheaded by David Butcher. The new data management plan and Open Science Framework has been easy for users to adopt, making all of the data generated by the facility findable and widely available. Well done. We also commend the investment that the state of Florida has made in diversity in hiring Martha Chacón-Patiño and Huan Chen to lead new research programs in the ICR group. The partnerships that they have established between the MagLab and minority serving institutions like FAMU and Morgan State are prime examples of how the development of cutting edge technology at the Maglab can also promote diversity, equity and inclusion in STEM. We see opportunities for other MagLab facilities, such as NMR, to engage with and contribute to these research programs. We

encourage the continued support of staff leading these efforts and see them as a model for MagLab to follow.

Instrumentation: We recognize that COVID restrictions have placed a heavy burden on the ICR staff to continue accommodating user projects. This has resulted in delays to some of the technological advancements, such as the development of an improved ICR cell for the 21T. We hope that this issue can be addressed in the coming year as the pandemic subsides. A new front end for 21T FTICR instrument, the Orbitrap Eclipse, replaces outdated technology and will be a boon to new investigations in the ICR group due to better sensitivity, faster analyses, greatly improved fragmentation capabilities, and extended mass range. We strongly suggest that the ICR group obtains another Eclipse MS to replace the Velos on the 14.5 T instrument. This would provide a platform for further technological advancements without interrupting operations on the 21T, which will likely experience an increase in user demand as these new capabilities come online.

We fully support the three requests made by the ICR group in the MagLab renewal proposal as top priorities. The 21T magnet service contract is necessary for continued operation of the world's highest resolution mass spectrometer. Additionally, users need 2D UHPLC and imaging MS support capabilities in order to use these state-of-the-art instruments for cutting-edge applications.

Biological Applications: Increasing efforts in the area of bacterial metabolomics are viewed as very innovative, and complementing existing efforts in top-down proteomics, petroleomics and environmental MS. These efforts should be further expanded to keep pace with developments in the field. It is recommended that additional training is provided in the data science aspects of metabolomics experiments and that collaborations are initiated in this front. Continued leadership has been shown for intact protein analysis. Work done on proton transfer with parallel ion parking has the ability to extend the mass range of top-down proteomics on a LC-timescale, especially with the introduction of the new Eclipse front end. To continue innovation in top-down proteomics, the user committee strongly supports the acquisition of a 2D-LC to enable multidimensional intact protein analysis, and we were happy to see this as part of the renewal proposal. Coupled with the Eclipse front end, this would enable truly best-in-class analyses for intact proteins.

Natural Organic Matter and Emerging Contaminants: The ICR program continues to be a leader in the analyses of complex organic mixtures including petroleum, asphaltenes, soil organic matter, biochar, and emerging contaminants such as microplastics and per- and polyfluoroalkyl substances (PFAS). The resolving power of the 21T FTICR instrument together with different ionization, polarity, and fragmentation modes give new insights into changes in contaminant polarity and different routes of entry, and ultimately, into the environmental fate of these persistent chemicals. By unraveling changes in composition of contaminants of concern to society after several processes (e.g., photochemistry, severe wildfires, etc.), science-based decisions can be made related to policies and management, especially now that a National MagLab chief scientist, Dr. Laura Greene, was appointed to serve on the President's Council of Advisors on Science and Technology. In addition, the unique capabilities and expertise of the ICR group support a growing user base by developing methods useful to the soil organic matter community. The new environmental

HPLC system is a very exciting addition that enables new analyses for examining molecular speciation of complex environmental and biological samples and increase in sample throughput. Developing a strategy for collecting automated LCMS data in adsorption mode w/ phase correction would further improve the performance of this system.

Recommendations: We encourage the ICR group to fill the open position for an imaging scientist as soon as possible. The lab is also encouraged to revisit staff salaries in order to retain top-tier scientists. The ICR staff is also encouraged to push forward with technical publications in the instrumentation area to more broadly advertise the unique capabilities of the ICR group. The expanding user base comes with new challenges to develop data processing routines (calibration, formula assignments, visualization) for new sample types, analyses, and end goals. Continuing to build/adapt resources to help users apply existing methods to their data sets is encouraged (including transitioning to latest data platforms, making recorded tutorials available).

(7) Conclusion

In conclusion, the Users Advisory Committee commends the MagLab scientists and staff for their achievements and commitment, applauds the renewed and expanded institutional support from NSF, DOE, FSU, UF, and LANL, eagerly awaits the reopening of the labs to normal operations once health and safety conditions at both the lab locations and the users host institutions allow this, and enthusiastically anticipates continuing to push beyond the current frontiers of science and technology during the next renewal cycle.