NHMFL User Committee Report 2020

Chair: Nathanael Fortune (Smith College)
DC/Pulsed/High B/T Vice-Chair: Philip Moll (EPFL, Switzerland)
NMR/MRI/ICR/EMR Vice-Chair: Aaron Rossini (Iowa State University)

DC/High B/T Committee: Joseph Checkelsky (Massachusetts Institute of Technology), Nathanael Fortune (Executive Committee Member, Smith College), Ben Hunt (Carnegie Mellon), Philip Moll (Executive Committee Member, EPFL, Switzerland), Janice Musfeldt (University of Tennessee), Raivo Stern (National Institute of Chemical Physics and Biophysics, Estonia), Jairo Velasco (University of California, Santa Cruz), Matt Yankowitz (University of Washington), Andrea Young (University of California, Santa Barbara)
PFF Committee: Adam Aczel (Oak Ridge National Laboratory), Nicholas P. Butch (Executive Committee Member, NIST Center for Neutron Research), Krzysztof Gofryk (Idaho National Lab), Zhiqiang Mao (Pennsylvania State University), Brad Ramshaw (Cornell University), Priscila Rosa (Los Alamos National Laboratory)
NMR/MRI Committee: Brian Hansen (University of Aarhus), Len Mueller (Executive Committee Member, UC Riverside), Aaron Rossini (Executive Committee Member, Iowa State University), Christian Bonhomme (Laboratoire de Chimie de la Matière Condensée de Paris), Vladimir Michaelis (University of Alberta), Doug Morris (National Institute of Health), Dylan Murray (University of California, Davis), Thoralf Niendorf (Max Delbruck Center for Molecular Medicine), Anant Paravastu (GeorgiaTech)
EMR Committee: Troy Stich (Executive Committee Member, Wake Forest University), Joseph Zadrozny (Colorado State University), Joshua Telser (Roosevelt University), Stergios Piligkos (University of Copenhagen), Rodolphe Clérac (Centre de Recherche Paul Pascal)
ICR Committee: Ying Ge (University of Wisconsin), Kristina Hakansson (Executive Committee Member, University of Michigan), Jack Beauchamp (Caltech), Rene Boiteau (Oregon State University), Franklin Leach (University of Georgia), Paul Thomas (Northwestern University)

This User Committee meeting took place during the COVID-19 period, and due to the resulting health restrictions was held in an unusual format. The meeting took place over 3 days through videoconferencing, for about 3 hours each day. The outbriefs by the MagLab representatives were provided to the User Committee as prerecorded talks prior to the meeting, in order to focus the reduced time budget on effective discussions of the key issues. To accommodate the revised schedule of the NSF site visit, the Committee was asked to prepare the brief accelerated report you now have before you. While this meeting was quite distinct compared to the previous years, the User Committee explicitly commends the flexibility of the MagLab leadership in adjusting to this unusual mode and to create a welcoming and productive atmosphere as much as possible under these circumstances.

(1) Executive summary

COVID-19: The pandemic has naturally had a strong impact on the MagLab operation. The user committee strongly supports the measures taken by the MagLab management to keep the laboratory running at a reduced level, to explore new routes of remote user participation and to utilize the unexpected downtime for maintenance and repairs as much as feasible.

Due to the compressed format of the remote meeting, the UC was unable to discuss all issues of importance to the user community but rather focused onto the urgent matters in this period of crisis detailed in this report. Other topics from last year's report not touched upon this year remain a high priority for the UC and will be reviewed again at the next meeting. These include (1) housing for visiting users, (2) the FAIR data initiative, (3) real-time communication channels, and (4) maintaining safe operations for visitors and staff.

Infrastructure: All main projects are on track. The 32T all-superconducting magnet is operating and the user committee is excited that it will soon become available to the regular user program. This magnet is a true quantum leap in magnet technology, providing static fields of superb quality for indefinite time to users. We expect a series of advances mostly in NMR, low-temperature science, and thermal experiments. The progress of the pulsed duplex magnet, the ongoing repair of the PFF generator, and the evolving convergence lab in the HBT facility promise to bring exciting magnet technology online soon.

Outreach and diversity: The user committee welcomes the addition of lower-field magnets for preliminary measurements into the user program. These systems will allow many users, particularly from under-represented institutions with limited capabilities, to perform a diverse set of measurements which in some cases can be used as prior results, helping them to submit stronger proposals and conduct more efficient experiments. The success of the outreach activities, before their end due to COVID-19, continues to impress the committee. The MagLab increased the number of visitors to their ever popular public open house event to more than 10 thousand this year. It also operates successful web- and YouTube outlets.

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

Progress Report: The DC Field-High B/T user advisory subcommittee was briefed on the current status of the facilities at Florida State University and the University of Florida, as well as on the ongoing efforts aimed to address prior recommendations made by the subcommittee. Progress reports regarding the development projects aiming to expand the capabilities were also presented by the lead representatives of DC Field and High B/T facilities.

New Magnet Developments: The 2020 review period encompasses an exciting time for high field science in which major magnet projects came online and the preparations and plannings of the past came to fruition. The User Committee at large is excited to see the 32T all superconducting magnet (SCM4) to become operational and included in the user program soon. This unique magnet will allow new science at unprecedented field stability with low operational cost, in particular condensed matter NMR will benefit from this magnet. This is not an incremental improvement but marks a true quantum leap in high field technology with global visibility. We support proposals to limit initial general user operations to a slightly lower threshold field as the lab monitors the response of the magnet under real-world conditions and then to raise that threshold in stages to the maximum 32 T field as experience is gained.

COVID-19: Undoubtedly COVID-19 posed a major setback for society and the scientific community worldwide. The subcommittee in unison is impressed by the quick changes of the DC-field facility to adapt to a new normal by enhancing opportunities for remote collaboration on experiments. These efforts include: (i) building a “virtual presence rig” equipped with webcams and computers to allow remote users to stay connected with their experiment; (ii) revising a new experimental shift plan to perform those experiments in which user presence is not essential; (iii) adjusting the daily operations to ensure the equipment does not suffer from degradation due to extended downtimes; (iv) diverting the reduced staff towards keeping the user program operational as much as possible. It is an excellent example of leadership and staff pulling together to overcome this crisis. It is not without cost — magnet time was already in short supply compared to demand and is now even more so! — but we applaud the MagLab’s efforts to maximize experimental throughput while maintaining safety.

COVID-19 has also provided us with an opportunity to newly appreciate the often unheralded informal training in advanced measurement techniques, signal/noise reduction, and general technology transfer between magnet lab staff and new users — particularly grad students and postdocs — during the users visits to the lab for experiments. This day to day in-person training (which goes beyond the justly acclaimed summer school sessions) makes a tremendous difference to the success of user experiments and the future success of these students and postdocs. We encourage the lab to find new ways to resume and expand summer school offerings by adding remote video training options and live consultations.

General Infrastructure Upgrade: The subcommittee is impressed by the continued efforts to improve the existing infrastructure. This effort addresses directly a key concern of the User Committee regarding the reliability of the aging equipment. While the MagLab aims to bring more and more record magnet systems online, it is important that robustness, reliability and failure safety are addressed at the same pace. We appreciate seeing the new cooling water treatment system, new electrical switchgear and the new chillers coming online, and look forward to the completion of the ongoing projects including the upgrades of switchgear II, the power supply units and the magnet cooling water pumps. These upgrades will ensure the reliable operation of the MagLab into the future.

Outreach activities: The User Committee recognizes the strong outreach culture of the MagLab leadership and facility, in particular towards underrepresented minorities. We jointly hope to soon reengage in these critical efforts once the current health crisis has passed.

Personnel: The subcommittee is particularly thrilled about the positive developments with the recent hires, filling critical voids in the existing user support structure. We welcome Shalinee Chikara, Elizabeth Green, Lin Jiao, Kaya Wei and Dylan Kolb-Bond into the MagLab. Their expertise will allow continued user operations in the millikelvin-lab, boost the condensed matter NMR research, reinforce the workhorse techniques of transport and magnetization, X-Ray diffraction, and high-field magnet design.

Recommendations:

The MagLab support is increasingly understaffed: This was the main issue discussed in the subcommittee. It is obvious that the exponential growth in users over the past decade has not been matched by a corresponding increase in support staff. This growth was possible by stretching the existing personnel and diverting scientists and staff from the key development projects sustaining the user program. The MagLab is in danger of becoming a victim of its own success, and we urge the responsible leadership to mitigate this imbalance immediately. The MagLab is clearly at risk to lose its global pole position if the developments of future flagship systems are halted at the expense of maintaining the status quo. We recommend an increase of the DC-field technician headcount by 3 FTE, the electronics shop by 2 FTE and the optics team by 2 FTE (see below). We also note a bottleneck in the machine shop for CNC milling projects. The subcommittee recommends to implement all positions, yet prioritizes those associated with the reduction of noise and implementation of probe improvement, as well as reinstating support of the electronics workshop. We also prioritize a second research FTE on the Split-Helix to relieve the burden of Steve McGill.

Electronics shop: The electronics shop serves three roles: It supports the user program through specialized electronics and equipment repair; it performs critical facility maintenance; and drives the development of new systems. The subcommittee notes the understaffing has already led to severe project delays. For example, the power supply upgrade has drawn resources from the 32T magnet project, resulting in delays of this important project. The extent of upcoming work packages exceeds the current staffing by far, such as the 45T modernization, resistive magnet protection system; and controllers for superconducting magnet power supplies. We recommend an increase by 2 FTE to allow one person to focus directly on the user program needs such as instrumentation updates and reduction of electronic noise; and one person to support the new magnet development. This would free up the existing personnel to work on the major upgrade projects.

Noise reduction: The user base experiences inefficiencies in conducting their experiments due to the omnipresent electrical noise in the facility. We recommend a second building-wide initiative to expand upon the activities carried out in 2005-2006 to find and reduce/eliminate these noise sources. Experimental noise is also a major cost factor to the experiments, as more noise implies longer averaging time at high fields to obtain the same quality of data. As part of this initiative, the existing probes should be rewired according to the current state-of-the-art, temperature control should be optimized (and field-calibrated), and new means to isolate vibrational noise should be explored. *This critical effort requires one additional technician FTE.*

Probe development: We recognize that a complete physical picture requires to investigate a sample with a diverse set of techniques. We recommend the MagLab strengthen its efforts to capitalize on the user base expertise to turn experimental setups into the regular user operation. We particularly applaud the recent efforts by staff scientists Arneil Reyes and Elizabeth Green in developing cond-mat NMR probes for the SCH and 32 T magnets and Ali Bengura in developing new ac-microcalorimeters and field-calibrated thermometers. The calorimetry and thermometry work — done in collaboration with current magnet lab users from outside institutions — serves as an example of the benefits derived from such collaborations. *Expanding and sustaining these efforts requires an additional technician FTE.*

Instrumentation improvement: Users have encountered situations in which small instrumentation improvements would have enabled or greatly improved an experiment resolution and/or efficiency, yet their implementation was not possible due to the understaffing situation. Examples include low-temperature preamplifiers, “in-probe” preamplifiers with low input capacitance, multi-channel probes and rotators of improved precision. Implementing such improvements in a robust way to be rolled out into the user program is a challenging task. *We recommend an additional technician FTE for this effort*.

Additional Research Faculty in optics: The subcommittee recognizes that a world-unique magnet system, the Florida Helix, is at the moment severely underused. Currently staff scientist Steve McGill is running this operation single handedly. This being only part of his responsibilities, the committee expresses concern both about the risk of burnout from extended operation under such stretched conditions, as well as the unused potential of the magnet. A second scientist is urgently required. In addition, we see the enormous scientific potential of micro-magneto optical spectroscopy that has been developed by Dmitry Smirnov. We would strongly welcome rolling this technique out into the user program, and would require a dedicated person due to the complexity of the technique.

Additional Research Faculty in Cond-Mat NMR: The subcommittee encourages further collaboration with Florida State University with a goal to hire a new faculty member who would take advantage of the considerable resources at the MagLab and eventually, hopefully, become a new leader of the cond-mat NMR team. Currently, only one senior staff scientist, Arneil Reyes, is responsible for all the low-temperatures probes construction and maintenance for DC magnets (including the 45T Hybrid, SCH and 32T system) with some help from newly hired Elizabeth Green.

COVID-19 continuity: We ask the MagLab to explore how to improve further the remote user operations (e.g. standardized interfaces; pucks to ship to users; etc). The subcommittee is particularly concerned regarding the lack of hands-on teaching of graduate students when the experiments are performed by expert scientists alone and the users receive only the data. Especially if the COVID-19 situation were to continue for a longer period of time, we recommend to explore new ways of training. This could include a “live-setup” of the experiment, a virtual summer school, or providing detailed schematics of the experimental setup. Although we fervently hope the current pandemic is overcome soon, we suggest it is nonetheless prudent for the lab to develop a contingency plan for the next renewal period. We also expect that even users with substantial experience will require expanded safety and operations retraining once they do return to the magnet lab.

User satisfaction survey: The user base is more than satisfied with the conditions at the MagLab. In the survey, 91% were satisfied with the equipment and facilities; 91% satisfied with the proposal process; and an astonishing 97% satisfied with the assistance by the MagLab staff. This is well reflected in the direct feedback the executive committee receives from those users choosing to do so.

High B/T Facility: We commend the MagLab for its outstanding recent hires for this facility: Lucia Steinke and Chao Huan. The new members of staff come with a wealth of ideas, a quest for nimbleness, and a demonstrably ebullient attitude regarding B/T prospects. They are already putting into place plans to expand the range of available measurements and increase the throughput of the lab with respect to existing facilities. The possibilities described for the Physics Building High Bay Research Lab are also strongly encouraging. This new shared space is an exciting opportunity meriting continued investment. Emergency power backup (generator and switches) are also a high priority for the renewal. There are still critical unfilled needs on the UF campus however, and more staff need training in the operation and maintenance of the helium liquefaction system the campus and MagLab facilities are increasingly reliant upon.

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

Overview: The Pulsed Field Facility (PFF) subcommittee is pleased to commend the NHMFL PFF at Los Alamos National Laboratory (LANL) for continuing to provide world-leading instrumentation and excellent user support across a broad swath of pulsed high-field science. The mixture of outstanding expertise and involvement of exceptional staff creates a unique and very successful research environment. During the meeting, the PF user committee was presented with the current status of the facility and its existing and planned research capabilities. A significant part of the review has also been devoted to the generator's rotor repair and ideas for the future advancement of magnet technology and measurement techniques. The pulsed facility at Los Alamos National Laboratory is the world leader in generating the highest (non-destructive) magnetic fields up to 100 T. Therefore we are thrilled with the current support from LANL regarding the rotor repair, especially that the generator is a crucial part of the future "beyond 100 T" magnet development initiative. The PFF subcommittee is very pleased with the way PPF handled the current COVID-19 pandemic and the travel restrictions related to that situation. In particular, we recognize the possibility of conducting online experiments that are fully supported by the local PFF staff. Below, we elaborate in more detail on several points raised during the meeting.

Core operations: We applaud the PFF's focus on infrastructure and strengthening the core of its user program. The PFF articulates a clear priority on providing reliable magnetic fields and measurement capabilities to the user community. We feel that this is a particularly important commitment as near-term research plans have been disrupted by the coronavirus pandemic. The ability to confidently plan future pulsed field measurements is fundamentally important to the individual research programs of the user community.

The PFF identified several sets of magnet coils that must be manufactured for different magnets. Work continues on the 60T long pulse magnet, which is important for relatively slow measurements such as calorimetry. The magnet coils for the 60T magnet are scheduled for completion in summer of 2021 and we look forward to the magnet coming online in autumn of 2021. We agree with the PFF regarding the need for spare coils, as the manufacturing time is long, and having replacements on hand will dramatically reduce downtime following an inevitable coil failure. This is particularly important because most of these experiments cannot be performed using the other magnets. Upgrades were also identified for magnetic fields of 100T and greater. Coils 3 and 4 of the outsert for the 100T magnet need to be upgraded, as does the duplex insert. These improvements should lead to longer magnet lifetimes and higher magnetic fields. We encourage the PFF to continue with plans to make 100T shots as regularly and reliably available to the user community as possible, as we also recognize excellent work put into parallel efforts like Duplex operations.

The PFF described critical hires necessary for smooth operation of the user program. The PFF operates a mature program that requires thoughtful upkeep. For example, we recognize the long-term need to replace racks of aging electronics and applaud the PFF's efforts to mitigate the failure risk. We support hiring a programmer-designer for critical control systems and a technician for generator operations and maintenance. We also recognize the need for more scientific staff to support the user program. This is a continuing concern - temporary staff, such as postdoctoral associates, develop a new experimental technique that cannot be fully supported in the user program in the long term because of staffing limitations. We particularly emphasize our support for the development of a career path in the LANL promotion system that is focused on, assessed, and rewarded on the basis of reliable, high quality user support. We particularly emphasize our support for the development of a career path focused on user support, which would be essential to attracting new staff. We believe that this career path needs to be categorized as a staff scientist that fully engages in the science, specifically not a technician or engineering position, whose focus is driving the users' science rather than their own. The incentive structure needs to be put in place for such a position to be attractive and rewarding as a career for research scientists.

The coronavirus pandemic presents a new set of challenges to the current operation of user facilities. We believe that flexibility is of paramount importance and find that the PFF has done a good job of outreach to the community. We encourage the PFF to more precisely convey to users the measurement limitations with respect to measurement time, probe availability, and remote experiment operation. We support a survey of the user community in mid-November 2021 to acquire an understanding of individual travel limitations and likewise suggest that the MagLab provide a clear outline of travel rules and restrictions at each of its facilities. Most importantly, we believe that the PFF should not plan to accept external users onsite unless it finds that it is absolutely safe to do so. We encourage continued support of remote user experiments. as staffing limitations and local health safety regulations allow.

Generator repair and 100 tesla magnet development: We fully support the MagLab's commitment to returning the generator to full operation. The generator supplies power to both the 100 tesla and 60 tesla long-pulse magnets, which are unique capabilities that are highly attractive to the user base. From a user standpoint, the generator brings a level of reliability to high-field operations that is absolutely unmatched by any other power-delivery system, anywhere else in the world. We note that other magnet labs, particularly in Dresden and Toulouse, have intermittently offered magnetic fields above 90 tesla, but that these capacitor-bank driven magnets always fail (catastrophically) after a short period of operation. These competing magnets bring far too much uncertainty for the user - we never know when they will be available, when they might fail during an experiment, whether they will destroy the capacitor bank along with the magnet (which happened recently in Toulouse), or when they will return to operation. The generator-driven 100 T, in contrast, consistently and regularly delivers fields above 90 tesla for periods long enough to perform multiple experiments. This is the type of system that enables external users to write grants where fields above 90 tesla play a central role, or to dedicate a PhD student's entire 5-year career.

We are heartened by LANL's large financial commitment to returning the generator to full operation. This shows a level of support from LANL to the MagLab that, again, brings certainty to the user base that the PFF will continue to be supported by their host institution. We note that both LANL and the NHMFL are committing to upgrade other parts of the power delivery system for the generator, including the power output controllers. We also note that the PFF is putting in place a plan to upgrade and service several other parts of the generator over the coming years, and to build scheduled maintenance shutdowns into the generator operations. We do not view scheduled shutdowns as negative - rather, they reduce uncertainty for the user base by reducing the likelihood of unplanned shutdowns due to equipment failure. We fully support LANL and the NHMFL's efforts in this regard.

Science at and above 100 tesla continues to be important to the user base, with quantum-limit physics in topological semimetals, quantum oscillations in high-temperature superconductors, and nematic and density-wave states in heavy fermions as just a few examples of the many active areas of research. We hope that future technical developments in high-field measurement techniques will enable transport in 2D materials in pulsed magnetic fields. The physics of 2D materials has rapidly grown to be one of the most productive areas of research for users at the DC field facility. Should the technical challenges associated with pulsed fields and 2D materials be overcome, it would open up research areas like large-gap fractional quantum Hall states, Wigner crystallization of electrons, and the creation of parafermions (Majorana-like quasiparticles that would enable universal quantum computation).

Extreme environments in pulsed fields: The subcommittee is particularly excited by the recent advances in high applied pressure capabilities at the PFF, which have been supported by the User Collaboration Grants Program (UCGP). Applied pressure provides a powerful tuning parameter that compliments magnetic fields and allows fundamental new science to be uncovered—including the effect of quantum critical fluctuations and the discovery of new phases of matter—that can feed back into the design and growth of new functional materials. Thanks to the development of pressure-tunable materials and the discovery of near room temperature superconductivity at ultra-high pressures, there is a growing interest in these kinds of measurements that goes beyond the specialist groups that traditionally dominated the field. An opportunity now exists for a user-driven, high-impact science output, provided the necessary support is provided.

The NHMFL DC Field facility has long been an internationally leading center for research in this area. However, because of the additional technical challenges, a reliable high-pressure user program in fields above 45 T has so far been lacking. Thanks to the UCGP funding, many of the technical issues have been overcome. The committee strongly supports maximizing on this investment and rolling out this capability to the user program. Due to the technical nature of the experiments this will necessitate a new, dedicated PFF staff member (1 FTE) to finalize 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 new 'extreme conditions' capability at the PFF.

Terahertz measurements in pulsed fields: The PFF subcommittee commends the development of time-domain THz spectroscopy measurements in pulsed fields to 31 T and their successful demonstration in the study of a high-temperature superconducting cuprate (LSCO) [Post et al, arXiv:2006.09131 (2020)]. These measurements not only enabled the first direct detection of cyclotron resonance in LSCO but also represent an exciting new avenue to probe the role of electron-electron interactions in quantum materials. The current tabletop magnet for free-space THz and far-infrared spectroscopy (100 GHz- 2 THz) is a powerful tool for the user community that enables direct measurement of both real and complex parts of a material's conductivity. In addition, the low energy scales probed by this technique enable the investigation of a breadth of phenomena relevant to the MagLab's upcoming science drivers. The investigation of quantum, correlated, and topological phenomena in atomically thin materials is of particularly importance as these measurements are most powerful in transmission mode. The timing for this development is excellent precisely because of recent improvements in the quality of thin film samples. The user community is thrilled by this sought-after capability that can be applied to non-collinear magnets, excitonic systems, van der Waals heterostructures, and strongly correlated materials. The implementation of concurrent transport measurements also would be very beneficial to the user community.

The PFF subcommittee strongly supports the continuation of this project towards incorporation into the user program with a dedicated cell for optical measurements. Further, the subcommittee encourages not only the continuation of collaborations with external users who are experts in THz spectroscopy but also the start of a broader network of collaborations including users who may not be as familiar with this type of spectroscopy. The formation of a strong user base with expanded training for beginning users is needed for the success of this endeavor. To this end, we recommend the hire of a dedicated staff member (1 FTE).

Single-turn magnet system: The future of the single-turn magnet system was discussed. Currently, the single-turn coil setup is able to provide 150 T pulses without damaging the sample. The system can be successfully integrated with fiber Bragg dilatometry and some preliminary results have been obtained. The single-turn setup has the potential to be introduced to the user program in the future, especially if measurements can be performed beyond 200 T in a way that reliably allows for survival of the sample during a long series of pulses . We acknowledge the PFF's concerns regarding the high operating costs and limited use of this equipment. We request that the PFF provide to the user community a summary of the scientific impact and development and operating costs of this instrument.

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

Overview: The NMR/MRI user subcommittee (USC) is pleased with the continued progress being made at the NMR and AMRIS facilities of the NHMFL: they are pushing the boundaries of sensitivity and resolution and advancing science that simply cannot be done anywhere else. The 36 T Series-Connected Hybrid (SCH) magnet continues to provide incredible insights into chemical structure and dynamics and is opening up the Periodic Table of the Elements for NMR spectroscopy. The SCH remains a revolutionary and unique instrument for NMR. The USC recognizes the importance of the novel studies that have been carried out on the SCH, exemplified by recent publications in *Science* and *PNAS*. The USC was also pleased to learn that the SCH Research Faculty position should be filled soon, which will help to further support this instrument. However, MagLab management needs to address short-term challenges related to COVID and longer-term challenges related to staffing; these challenges have limited SCH access. Furthermore, all modern high-field, superconducting magnets are running near 100% capacity, a testament to the success of the facility, but also demonstrating the strong need for additional high-field systems. Therefore, the USC also strongly recommends investing in all-superconducting NMR magnets with fields of 28 T (1.2 GHz) or higher to retain the NHMFL's position as a world-leader in high-field NMR spectroscopy. There are 13 1.2 GHz NMR magnet sites presently in the world, of these only 2 are in the US (Ohio State University and a proposed system in GA/WI/CT). Clearly the USA is falling behind the rest of the world in this area. In comparison to the other 1.2 GHz spectrometer sites in the USA, NHMFL is the only true users' facility. The MagLab can also bring their vast experience with high-field probe construction to support this instrument, further differentiating them from other sites in the world. The USC also notes the success of the 14.1 T MAS DNP user program and fully encourages development of helium magic-angle spinning (MAS). The USC is very supportive of longer term plans for development of a high-resolution 35 T/1.5 GHz superconducting magnet. Finally, the USC was enthusiastic about the proposed Science Drivers that will be used in the renewal of the NSF operating grant.

The USC acknowledges that the staffing recommendations made in previous USC reports were in part fulfilled. Wenping Mao was hired to help with RF probe construction. The USC is also pleased with the continued progress on fast MAS probe development; a variety of fast MAS probes are now available for users. The NHMFL has made significant advances in RF probe development and has a solid roadmap for near-term projects to expand NMR probe offerings for superconducting magnets, the SCH and MAS DNP systems. Finally, we commend all members of the MagLab team and their institutional partners for their handling of difficulties related to COVID. Staff have been very effective in running remote operations for users. Institutional partners have also provided critical salary support to make up for shortfalls from user fees.

Priority Recommendations:
- Ensure continued and sustainable access to the SCH for NMR users.
- Pursue a 1.2 GHz high-resolution NMR system as soon as possible.
- Pursue helium magic-angle spinning DNP at 600 MHz.
- New console & gradients for 600/750 MHz NMR/MRI systems to improve microimaging
- Continue long-term plans to develop a high-resolution 1.5 GHz superconducting NMR system.

Series-Connected Hybrid (SCH) Access: The USC continues to be impressed with results from the SCH. The NMR community used 23 weeks of SCH in 2018, while 22 weeks were used in 2019. The NMR usage of the SCH in 2020 will likely be much worse, partly due to COVID. Therefore, the USC strongly supports all actions to increase the availability of SCH time. The USC understands that the safety of MagLab staff is the number one priority and this will limit operating time of the SCH. However, we ask that MagLab leadership make every effort to distribute hybrid magnet time equitably across all areas. In the longer term, staffing continues to be a bottleneck to further SCH access. While the hiring of an SCH Research Faculty will partly help to alleviate SCH access issues, the research faculty hiring comes at the expense of post-doctoral staff. The USC encourages MagLab faculty/staff and users to pursue external funding to open up additional SCH magnet time.

Personnel: The USC commends Prof. Robert Schurko for his role as the new director of magnetic resonance; there has been continuity in the operation in Tallahassee. The USC notes the addition of Dr. Wenping Mao to the RF probe development staff. Dr. Mao is helping to develop fast MAS capabilities across the MagLab. Dr. Faith Scott has been a great addition to the DNP program. She will be an invaluable contributor to developing fast MAS and helium MAS DNP systems. The USC was pleased to learn that previous personnel recommendations have largely been addressed. It is critical that the 3 approved and open positions for a SCH Research Faculty, MRI/S Research Faculty, and MRI RF Engineer be filled as soon as possible. As was noted above, there is a strong need for additional post-docs to support future SCH Research Faculty. The USC recommends that 2 post-docs be added to support the SCH. With the progress on fast MAS probes, one of these post-docs (or a potential lab technician) should have expertise in packing biological samples into small diameter fast MAS rotors and performing fast MAS biosolids experiments.

Ultrahigh-Field Superconducting Magnets for NMR: The USC recognizes the world-leading status of the ultrahigh-field SCH magnet. While significant research breakthroughs have been achieved with this system, the residual temporal inhomogeneity on the order of 0.3 ppm in the magnetic field limits some applications, particularly in biomolecular solid-state NMR. There are three 800 MHz and one 830 MHz solids spectrometers, all of which are running at 100% capacity and currently turning away about half of user requests. Therefore, there is a clear need for more high-field instrumentation. The USC supports the conversion of the solution 800 MHz NMR spectrometer at FSU to a solids instrument and the partnership with FSU to add a 700 MHz solutions NMR instrument for the Users' Program. Given the high demand on high-field instruments and the limited time on the SCH, there is a critical and immediate need for a commercial superconducting 1.2 GHz spectrometer with high spatial and temporal field stability that would complement the capabilities of the SCH magnet and cement the MagLab's status as a leader in ultrahigh-field NMR access. We note that eleven such instruments have already been ordered at various institutions in Europe and it is critical that the US obtain similar instrumentation to remain competitive. In-house built probes will guarantee that a 1.2 GHz magnet sited at NHMFL will outperform similar instruments hosted in Europe or elsewhere. A 1.2 GHz spectrometer equipped with a 0.75 mm fast MAS MagLab probe would be a game changer for the US biosolids community. The 1.2 GHz system would also help to alleviate demand on existing high field instrumentation. Simultaneously, the USC strongly supports long-term plans to develop a superconducting 1.5 GHz narrow-bore magnet, with field homogeneity suitable for high-resolution solid-state NMR spectroscopy. This five-to-ten-year plan will ensure the NHMFL remains as the international leader in high-field NMR/MRI and will fully realize the potential gains offered by high fields for metabolomics, imaging, materials and biomolecular NMR applications.

Upgrading aged consoles of existing NMR spectrometers: The USC stresses that upgrading of ageing consoles is a critical issue for all facility users. High priority should be given to upgrading 750 MHz and 600 MHz #2 systems, the latter of which is equipped with a console from 2004. We were also pleased to learn of support from partner institutions for console upgrades. Upgraded consoles are critical for performing cutting-edge experiments by the NMR/MRI users. The USC encourages NHMFL administration to ensure that there are definitive plans for a sustained and continuous re-investment in console infrastructure.

DNP: The USC is very impressed by the operation of the high-field 14.1 T MAS DNP system. The USC commends the work being performed by Dr. Frédéric Mentink-Vigier and collaborators on simulating DNP mechanisms and developing better biradicals; this work is extremely important to progress in the field. The USC fully supports immediate plans to develop helium MAS on the 14.1 T DNP system. Implementing helium MAS will provide immediate access to faster MAS frequencies that improve resolution and sensitivity. Helium MAS is also a key step for longer-term development of lower-temperature (20-40 K) and fast MAS probes for the 14.1 T DNP system. These short- and long-term MAS DNP developments should be given a high priority as they are critical for maximizing DNP sensitivity gains and improving resolution. The demand for the 14.1 T DNP instrument currently exceeds capacity, validating the importance of this technique to the user community. Given the high demand for MAS DNP there is clearly a strong need for additional instrumentation. The USC strongly supports the planned implementation of 400 MHz or 800 MHz DNP systems. DNP at 800 MHz could offer considerably improved resolution and sensitivity. A 400 MHz DNP system would offer significant sensitivity gains for many materials and help alleviate demand on higher field DNP systems. The USC was enthusiastic about the longer-term development of a 32 T static sample, helium temperature DNP system. Finally, the committee encourages the continued collaboration between EMR and NMR/MRI on the development of novel DNP instrumentation such as the 600 MHz Overhauser DNP system and time domain solid-state DNP.

Magnetic Resonance Imaging: The USC recognizes the need for a strong RF coil development program at AMRIS and the vertical bore MRI program at the MagLab NMR/MRI facility at FSU. The cryo-coil RF development initiative at AMRIS is a cutting-edge project and serves as a technology driver to build a program. The USC strongly supports the additional hires of engineers and RF technicians to support this program. Adapting solution NMR cryoprobe technology to MRI could provide a significant breakthrough in sensitivity and resolution for all nuclides, but especially for low-gamma nuclei. This capability would allow AMRIS to maximize sensitivity gains from dissolution DNP and allow previously inaccessible nuclei such as deuterium to be used in MRI experiments. The AMRIS and MagLab imaging programs should add parallel imaging and transmit facilities to increase sensitivity and reduce imaging times.

High Bay Convergence Lab: The USC was supportive of the new High Bay Convergence Lab at UF that will consolidate resources between the AMRIS and high B/T facilities.

Equipment for User Support: An ultracentrifuge, additional lab supplies, and dedicated space are required in Tallahassee to be used for packing biological samples into small diameter fast MAS rotors. The users committee believes that the addition of an ultracentrifuge would be of great benefit to biosolids users and help attract new users.

NSF Renewal: The USC was impressed by the proposed science drivers for the NSF renewal that incorporate magnetic resonance. The USC believes that these science drivers touch on all aspects of magnetic resonance spectroscopy/imaging research performed at the facility. The proposed instrumentation would provide breakthroughs in sensitivity and resolution that would have a broad and substantial impact on all areas of magnetic resonance.

Outreach: The USC acknowledges the outreach and educational activities by the NMR/MRI staff at the NHMFL. The RF coil development workshop especially continues to be innovative. MagLab staff presented contingency plans to move towards online outreach activities during COVID.

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

Present: Troy Stich (Wake Forest University, chair), Joshua Telser (Roosevelt University), Joseph Zadrozny (Colorado State University), Rodolphe Clérac (Université de Bordeaux - CNRS) Sandrine Heutz (Imperial London), Stergios Piligkos (University of Copenhagen), Carole Duboc (Université Grenoble Alpes)

Overview: The user committee (UC) recognizes the impressive scientific achievements by the EMR group over the past year, despite facing several major challenges outside of their control (construction-induced shutdown, COVID). In particular, we note the EMR program's engagement in cutting-edge quantum research. Quantum information science is at the forefront of not only the NSF, but many different funding agencies in the US: Department of Energy, Department of Defense, etc. Thus, the EMR user committee was surprised to see how little emphasis was placed on quantum information processing, sensing, imaging, etc. in the science drivers and future plans of the MagLab. The UC strongly supports different domains of investigation, and we note that major progress has been made in studies of other areas such as materials, energy, and life. Below are our comments and recommendations aimed at maximizing the use of equipment and expertise housed within the EMR group and growing these to meet the demands of the future.

Personnel

Comments

- 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 Marcus Giansiracusa from Manchester to a post-doctoral position despite the unfortunate delay in his arrival due to COVID. The UC praises the flexibility of the EMR group to temporarily fill this position with recent alumnus Jonathan Marbey.
- In general, we are pleased to note that the EMR group is able to recruit researchers of the highest caliber internationally (e.g. Daphne Lubert-Perquel), which is an indicator of its world-class reputation.
- The UC congratulates the EMR director for securing substantial external funding from NSF, NIH, DOE, and AFOSR for work in quantum technologies. Inevitably, these awards strongly benefit the EMR program.

Recommendations

- The UC *strongly* recommends that new leading early-career scientists be added to the permanent staff of the EMR Facility at the MagLab. We see them as an absolutely necessary addition to inject new ideas and drive the scientific missions of the EMR Facility and the MagLab into the future.This should be considered a priority for the MagLab as the recruitment and integration of such top scientists will take time and the current team needs to be strengthened quickly.

- Thierry Dubroca is a cornerstone of the DNP program. His presence is essential to the success of these efforts. The UC is concerned that he is still in a visiting scientist position and recommends establishing a clear path for him towards a permanent appointment.

- The UC encourages further collaboration with Florida State University. We further encourage FSU to hire a new faculty member who would take advantage of the considerable resources at the MagLab and eventually, hopefully, become part of the EMR team. We also encourage further collaboration with the University of Florida in common areas of interest such as DNP.

User Program

Comments

- The user committee (UC) is overall impressed by the ability of the EMR Facility to pursue impactful science (34 published or all-but-published papers in 2020) despite the lab being totally shut down from December 2019 to January 2020 for electrical systems overhaul, and then the coronavirus pandemic causing an unplanned shutdown from March 2020 to May 2020, with visiting user in-person access still essentially impossible at this time. These results are featured in the best possible journals (e.g. Science, Nature Chemistry, etc.).

- No major issues were brought forward from users to the UC in the past year.

- The UC is impressed that the EMR Facility has been able to accommodate user demand during the coronavirus pandemic by running samples on its four main instruments and praises its resilience and dedication to the users.

Recommendations

- The UC emphasizes that we believe that the MagLab leadership should embrace Quantum Information Processing research programs.
- To further grow the user base, the UC recommends the group to again host the EMR School (possibly in a winter time slot, which has less competition than summer for such events).

Capabilities

Comments

- The viability of the EMR program must be assured by replacement of the ageing magnets for the 15T/17T and the HiPER systems. To the UC, these are viewed as basic infrastructure requirements that absolutely have to be secured.
- The UC recognizes that quantum information sciences are at the leading edge of interest from the NSF perspective and we see the EMR group as being ideally positioned to be at the forefront of such efforts—as demonstrated by EMR's recent publications and externally funded proposals.
- The UC is thankful for the EMR group having the foresight to contract with Boris Epel to implement SpecMan for total arbitrary waveform generator control of the HiPER system making it easier to operate for external users.
- The UC supports the EMR group's efforts to realize the development plan for EPR in conjunction with the 36 T series-connect hybrid (SCH) magnet.

Recommendations

- To maintain excellence, the superconducting magnets for both the 15T/17T and the HiPER systems *must be* replaced. These are workhorse instruments and to lose them would cost the EMR group 50%+ of their productivity. The HiPER system magnet exhibits significant hysteresis which limits its utility in certain applications and squanders the investment into HiPER capabilities over the previous years. We note that the proposed new HiPER magnet has a footprint and configuration that opens the instrument up to new experimental methods. If we had to prioritize a specific capability recommendation, replacing these two ageing magnet systems would be the first one.
- In the last report, the addition of optical excitation techniques was requested. We note that this year, 50% of the talks during the workshop that preceded the User Committee Meeting employed laser light excitation. Thus, current user demand for light excitation is already high, and a functioning laser system is prerequisite. This photoexcitation capability will continue to broaden the user base and enable new and exciting science to be performed in the EMR group.
- Given the importance of optical detection of coherent qubit manipulations relevant to Quantum Information Processing technologies, the UC recommends that optical detection capabilities are developed for pulse EPR qubit manipulation protocols.
- We recommend pursuing upgrades and replacements of components for the high-frequency heterodyne instrument. This instrument provides truly unique capabilities that cannot be found elsewhere in the world. Ensuring this instrument stays the state of the art is needed to continue this facility's world-leading status.

- The UC would welcome the ability to operate at higher magnetic fields and at frequencies of the order of 1-10 GHz. This would allow the study of coherent superposition of states at magnetic-field induced level anticrossings.

(6) 2020 Report of the ICR User Advisory Committee

Facility Overview:

The ICR program at the MagLab continues to provide measurements unattainable with other types of instrumentation. The unprecedented molecular composition analysis for highly complex mixtures, including environmental, petrochemical, and biofuel samples, continues to enable new science with the added capability of acquiring structural information on individual species in such mixtures, thus allowing next generation analysis in these areas. The capabilities of the high field ICR instruments are also leveraged for novel implementations of top-down protein analysis and record resolution mass spectrometry imaging. The ICR program continues to add new users from a range of disciplines and from geographical origins across the globe. 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.

In the past year, ICR program staff have successfully added both external and internal funding to the in-house research programs. Research Faculty Chen was awarded (as co-PI) a collaborative NSF grant with the Florida A&M School of Environment, adding to her two ongoing grants with Florida A&M College of Engineering, and with Morgan State University, Department of Biology as well as an ongoing collaborative DoD grant with Colorado State University (co-PI McKenna) and ongoing funding through the *International Complex Matrices Molecular Characterization* (co-PI Rodgers). Internal funding from the User Collaboration Grants Program (UCGP) was again awarded in 2020 to Research Faculty McKenna, adding to the successful UCGP grants to Research Faculty Anderson (2018) and Smith (2019). These grants have allowed the hiring of postdoctoral scholars and acquisition of new equipment critical to the mission of the ICR Program. However, particularly with the recent loss of one staff member in an emerging research area, the committee has mild concerns over the ability to sustain diverse capabilities without placing undue burden on existing staff.

The ICR program continues to excel in education, dissemination, and outreach. In-person visits to the ICR Facility by external students and postdocs are tremendous opportunities for hands-on training and advanced learning in the area of high-end analytical measurements. The ICR staff also continues to engage high school and undergraduate students in research, and even added middle school students in Fall, 2019. The biannual North American FTMS Conference, organized by the ICR program, continues to bring together top international scientists in the field.

Enabling New Technologies:

The committee is excited about the near term prioritization to upgrade the outdated Thermo-Fisher Scientific Velos Pro front end of the flagship 21 Tesla ICR instrument to a state-of-the-art Thermo-Fisher Scientific interface with improved sensitivity, mass & dynamic range. These characteristics will enhance acquisition speed and improve the analytical capabilities for all application areas described below. The ultrahigh resolution precursor ion isolation allowing tandem mass spectrometry (MS/MS) experiments for individual molecular compositions in highly complex mixtures (published this year) is considered transformative. Enabling this type of analysis on an LC time-scale in a data-dependent manner would further revolutionize complex mixture analysis. Likewise the described gas-phase depletion of sample contaminants is a significant contribution for improved dynamic range in complex mixture analysis.

The continued development of next generation ICR cells, including the newest version dynamically harmonized cell with further reduced capacitance and the 3Ω design for faster data acquisition at fixed resolving power, will increase sensitivity and throughput. Developments in proton transfer reactions/parallel ion parking (PTR/PIP), enabled by the linear ion trap front end, are also exciting for improved top-down protein analysis.

Sustainable Planet Earth:

The ICR program continues to be a leader in complex organic mixture analysis including petroleum, metal binding ligands, biomass-derived oils, natural organic matter, wastewater, and emerging contaminants. This leadership role is well reflected by the number of publications (>30 appearing Jan-Sep, 2020) and the number of returning and new users in 2020 seeking to benefit from advanced high magnetic field methods in studying the synthesis, structure, composition, degradation, & behavior of complex organic mixtures. The environmentally focused postdoc requested in the renewal proposal is much needed to keep up with this heavy user project load. As stated above, the committee was impressed with the recent advancements in high resolution SWIFT isolation methods combined with photofragmentation for distinguishing between related structural isomers in petrochemicals and asphaltenes that have very different environmental fates because they undergo distinct degradation pathways. This technology will benefit many user applications that need fragmentation to help identify structures.

Last year we recommended acquisition of an LC front-end for the 21T instrument to automate sample analysis and enable online separations. Such an instrument has been purchased through the most recent UCGP grant. The committee is excited to see applications of this instrumentation that demonstrate new chemical characteristics of complex environmental samples by resolving isomers, reducing ion-suppression, elucidating isotopic fine structure patterns, and leveraging data analysis workflows that incorporate retention time and fragmentation spectra.

The major initiatives proposed for the next funding cycle will enable analyses that provide deeper information on the chemical composition of petroleum and organic matter. The proposed upgrade to a 3Ω cell on the 21T instrument will significantly improve the characterization of natural organic matter and halogenated/metal-organic species by enabling detection of minor components and isotopomers. In addition, the replacement of the front-end of the 21T ICR instrument will significantly extend the achievable mass range to allow for greater coverage of molecular species. Efforts over the past year to adapt SWIFT isolation methods to reduce chemical noise and suppress contaminants will also drastically improve the detection of species from environmental samples collected in contaminated systems such as wastewaters. Looking forward, we expect that environmental research will continue to serve a strong and growing user base that leverages the unique capabilities and expertise of the ICR group for complex mixture analysis.

Biological Applications:

Top Down Protein Analysis

The ICR team continues to provide world-leading resolving power for intact protein analysis, unmatched by commercially available instrumentation. This capability gap, once quite large, is shrinking as the Velos Pro front end (currently operating on ~10 year old technology) ages and competing Orbitrap instrumentation with more capable front-end optics emerges commercially. For this reason, the front end upgrade, proposed by the ICR group, will be critical to unleashing the full potential of the 21T ICR magnet. This upgraded instrument will be vastly superior to current Orbitrap technology owing to its resolving power, charge capacity, sensitivity and versatility for all types of intact protein analysis.

Analysis of large proteins remains a challenge in the field of intact protein characterization due to the nature of the electrospray ionization process for denatured proteins. The techniques of PTR-PIP demonstrated by the ICR group are extremely compelling as an approach to unlock the “high mass proteome” above 40 kDa, as demonstrated in a user project with Leslie Hicks from UNC-Chapel Hill. The challenge will come in its robust implementation for routine application by NHMFL users, but it is clear that the ICR team is up to the task. Even with the capabilities of the 21T instrument, the separation of intact proteins remains a challenge. The proposed purchase of a 2D LC system, coupled with the PEPPI-MS results published by the ICR group in collaboration with Nobu and Ayako Takemori from Ehime University, will unlock the ability to separate proteoforms in 3 dimensions; size, charge and hydrophobicity, allowing the intact proteome to be analyzed deeper than has been achieved in the past. Online LC analyses should be carefully evaluated prior to maximize instrument user time.

The user project on Tau proteoforms from the Rossol group at the Mayo clinic is exciting for multiple reasons. It shows the potential of PTR-PIP to be used for the analysis of a protein of great importance in neurodegenerative diseases. It additionally demonstrates potential for synergies between divisions of the MagLab. The same samples analyzed by the ICR group could also be measured by the NMR group to elevate the unified analysis. The new “3 omega cell” discussed above will also allow increased resolving power/speed for intact protein analysis. As these new technologies come online (the proposed upgraded front end and 2DLC acquisition), the ICR group will be able to generate incredibly large datasets, approaching terabytes in size from a single experiment.

MS Imaging

The ICR MALDI imaging program has made substantial progress in its first year and can be considered an operational capability. Primarily funded by the UCGP, a commercial ion source has been acquired and installed. To support this capability development, a post-doctoral scholar has joined the ICR group. Despite its infancy, the MALDI capability has recruited a small user base including leading scientists within the MS imaging community. It is recommended that efforts be placed on further establishing this user base with existing technologies. The user committee supports the proposed initiatives to acquire sample preparation equipment to further expand this capability. Future instrumentation efforts specific to imaging should be considered at a later time and currently the program should leverage its expertise in ICR technologies to solidify this effort.

Technology developments within the ICR instrumentation subgroup will further enhance the MALDI user program. Imaging experiments at high spatial resolution may require substantial allocations of magnet time. This burden will be alleviated by enhanced detection strategies (3Ω) that enable acquisition in 1/3 of the original time and absorption mode data processing that provides the option of a 2-fold reduction in acquisition time (or approximately 2-fold improvement in mass resolving power). Preliminary demonstrations of this approach have been made. Cumulatively, these advancements would make a 24 hr experiment achievable in 4 hrs. In combination with the baseline performance of the 21 T system, this platform would set the bar for mass analysis in MALDI imaging. To maximize 21 T user time, the imaging interface should be moveable for additional use at 14.5 and 9.4 Tesla.

The primary initiative of the next funding cycle, the acquisition of a state-of-the-art front end will also benefit the imaging capability on the 21 T instrument. This addition will enable more complex experimental sequences than current capabilities with the existing Velos and provide enhanced tandem mass spectrometry for structural determination of imaged ions as well as a broader mass range that will further enable protein imaging. The new front end will therefore leverage existing strengths for instrumentation and intact protein analysis to further advance imaging within the ICR program. Concurrently, the acquisition of a 2D-LC system for intact protein analysis would complement imaging efforts as an approach to validate tentative protein identifications.

Recommendations:

- Hire a bioinformatics specialist well-versed in “big data” to help manage user friendly data analysis and data sharing between users and MagLab scientists.
- Replace the departing staff member in the MALDI imaging area as soon as possible.
- Attempt to recruit additional post-doctoral scholars in each (or across) discipline.
- Encourage the staff to “dream big” with the instrumentation for transformative improvements, e.g., a vacuum system rebuild for lower pressure operation.
- Push on publications in the instrumentation area to more broadly advertise the unique capabilities.
- Organize summer school (course) for ICR, specifically for NOM analysis (PetroOrg, EnviroOrg) and/or top-down proteomics.
- Explore opportunities to better integrate with other Mag Lab facilities, particularly NMR.

(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.